



COMPSs Manual

Workflows and Distributed Computing Group



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Online version available at [COMPSs - ReadTheDocs](#)

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COMP Superscalar (COMPSs) is a **task-based programming model** which aims to ease the development of applications **for distributed infrastructures**, such as large High-Performance clusters (HPC), clouds and container managed clusters. COMPSs provides a **programming interface** for the development of the **applications** and a **runtime system** that **exploits the inherent parallelism** of applications **at execution time**.

To improve programming productivity, the **COMPSs programming model** has following **characteristics**:

- **Agnostic of the actual computing infrastructure:** COMPSs offers a model that abstracts the application from the underlying distributed infrastructure. Hence, COMPSs programs do not include any detail that could tie them to a particular platform, like deployment or resource management. This makes applications portable between infrastructures with diverse characteristics.
- **Single memory and storage space:** the memory and file system space is also abstracted in COMPSs, giving the illusion that a single memory space and single file system is available. The runtime takes care of all the necessary data transfers.
- **Standard programming languages:** COMPSs is based on the popular programming language Java, but also offers language bindings for Python (PyCOMPSs) and C/C++ applications. This makes it easier to learn the model since programmers can reuse most of their previous knowledge.
- **No APIs:** In the case of COMPSs applications in Java, the model does not require to use any special API call, pragma or construct in the application; everything is pure standard Java syntax and libraries. With regard the Python and C/C++ bindings, a small set of API calls should be used on the COMPSs applications.

This manual is divided in 9 sections:

Chapter 1

What is COMPSs?

COMP Superscalar (COMPSs) is a **task-based programming model** which aims to ease the development of applications **for distributed infrastructures**, such as large High-Performance clusters (HPC), clouds and container managed clusters. COMPSs provides a **programming interface** for the development of the **applications** and a **runtime system that exploits the inherent parallelism** of applications **at execution time**.

To improve programming productivity, the **COMPSs programming model** has following **characteristics**:

- **Sequential programming:** COMPSs programmers do not need to deal with the typical duties of parallelization and distribution, such as thread creation and synchronization, data distribution, messaging or fault tolerance. Instead, the model is based on sequential programming, which makes it appealing to users that either lack parallel programming expertise or are looking for better programmability.
- **Agnostic of the actual computing infrastructure:** COMPSs offers a model that abstracts the application from the underlying distributed infrastructure. Hence, COMPSs programs do not include any detail that could tie them to a particular platform, like deployment or resource management. This makes applications portable between infrastructures with diverse characteristics.
- **Single memory and storage space:** the memory and file system space is also abstracted in COMPSs, giving the illusion that a single memory space and single file system is available. The runtime takes care of all the necessary data transfers.
- **Standard programming languages:** COMPSs is based on the popular programming language Java, but also offers language bindings for Python (PyCOMPSs) and C/C++ applications. This makes it easier to learn the model since programmers can reuse most of their previous knowledge.
- **No APIs:** In the case of COMPSs applications in Java, the model does not require to use any special API call, pragma or construct in the application; everything is pure standard Java syntax and libraries. With regard the Python and C/C++ bindings, a small set of API calls should be used on the COMPSs applications.

PyCOMPSs/COMPSs can be seen as a **programming environment for the development of complex workflows**. For example, in the case of PyCOMPSs, while the task-orchestration code needs to be written in Python, it supports different types of tasks, such as Python methods, external binaries, multi-threaded (internally parallelised with alternative programming models such as OpenMP or pthreads), or multi-node (MPI applications). Thanks to the use of Python as programming language, PyCOMPSs naturally integrates well with data analytics and machine learning libraries, most of them offering a Python interface. PyCOMPSs also supports reading/writing streamed data.

At a lower level, the COMPSs runtime manages the execution of the workflow components implemented with the PyCOMPSs programming model. At runtime, it generates a **task-dependency graph** by analysing the existing data dependencies between the tasks defined in the Python code. The task-graph **encodes the existing parallelism of the workflow**, which is then scheduled and executed by the COMPSs runtime in the computing resources.

The COMPSs runtime is also able to **react to tasks failures and to exceptions** in order to adapt the behaviour accordingly. These functionalities, offer the possibility of designing a **new category of workflows with very dynamic behaviour**, that can change their configuration at execution time upon the occurrence of given events.

1.1 More information:

- Project website: <http://compss.bsc.es>
- Project repository: <https://github.com/bsc-wdc/compss>

Chapter 2

Quickstart

2.1 Install COMPSs

- Choose the installation method:

Pip - Local to the user

Requirements:

- Ensure that the required system [Dependencies](#) are installed.
- Check that your `JAVA_HOME` environment variable points to the Java JDK folder, that the `GRADLE_HOME` environment variable points to the GRADLE folder, and the `gradle` binary is in the `PATH` environment variable.
- Enable SSH passwordless to localhost. See [Configure SSH passwordless](#).

COMPSs will be installed within the `$HOME/.local/` folder (or alternatively within the active virtual environment).

```
$ pip install pycompss -v
```

Important: Please, update the environment after installing COMPSs:

```
$ source ~/.bashrc # or alternatively reboot the machine
```

If installed within a virtual environment, deactivate and activate it to ensure that the environment is properly updated.

Warning: If using Ubuntu 18.04 or higher, you will need to comment some lines of your `.bashrc` and do a complete logout. Please, check the [Post installation](#) Section for detailed instructions.

See [Installation and Administration](#) section for more information

Pip - Systemwide

Requirements:

- Ensure that the required system [Dependencies](#) are installed.
- Check that your `JAVA_HOME` environment variable points to the Java JDK folder, that the `GRADLE_HOME` environment variable points to the GRADLE folder, and the `gradle` binary is in the `PATH` environment variable.
- Enable SSH passwordless to localhost. See [Configure SSH passwordless](#).

COMPSs will be installed within the `/usr/lib64/pythonX.Y/site-packages/pycompss/` folder.

```
$ sudo -E pip install pycompss -v
```

Important: Please, update the environment after installing COMPSs:

```
$ source /etc/profile.d/compss.sh # or alternatively reboot the machine
```

Warning: If using Ubuntu 18.04 or higher, you will need to comment some lines of your `.bashrc` and do a complete logout. Please, check the [Post installation](#) Section for detailed instructions.

See [Installation and Administration](#) section for more information

Build from sources - Local to the user

Requirements:

- Ensure that the required system [Dependencies](#) are installed.
- Check that your `JAVA_HOME` environment variable points to the Java JDK folder, that the `GRADLE_HOME` environment variable points to the GRADLE folder, and the `gradle` binary is in the `PATH` environment variable.
- Enable SSH passwordless to localhost. See [Configure SSH passwordless](#).

COMPSs will be installed within the `$HOME/COMPSs/` folder.

```
$ git clone https://github.com/bsc-wdc/compss.git
$ cd compss
$ ./submodules_get.sh
$ ./submodules_patch.sh
$ cd builders/
$ export INSTALL_DIR=$HOME/COMPSs/
$ ./buildlocal ${INSTALL_DIR}
```

The different installation options can be found in the command help.

```
$ ./buildlocal -h
```

Please, check the [Post installation](#) Section.

See [Installation and Administration](#) section for more information

Build from sources - Systemwide

Requirements:

- Ensure that the required system [Dependencies](#) are installed.
- Check that your `JAVA_HOME` environment variable points to the Java JDK folder, that the `GRADLE_HOME` environment variable points to the GRADLE folder, and the `gradle` binary is in the `PATH` environment variable.
- Enable SSH passwordless to localhost. See [Configure SSH passwordless](#).

COMPSs will be installed within the `/opt/COMPSs/` folder.

```
$ git clone https://github.com/bsc-wdc/compss.git
$ cd compss
$ ./submodules_get.sh
$ ./submodules_patch.sh
$ cd builders/
$ export INSTALL_DIR=/opt/COMPSs/
$ sudo -E ./buildlocal ${INSTALL_DIR}
```

The different installation options can be found in the command help.

```
$ ./buildlocal -h
```

Please, check the [Post installation](#) Section.

See [Installation and Administration](#) section for more information

Supercomputer

Please, check the [Supercomputers](#) section.

Docker - PyCOMPSs Player

Requirements:

- [docker](#) $\geq$ 17.12.0-ce
- Python 3
- pip
- [docker](#) for python

Since the PyCOMPSs player package is available in Pypi ([pycompss-player](#)), it can be easily installed with `pip` as follows:

```
$ python3 -m pip install pycompss-player
```

A complete guide about the PyCOMPSs Player installation and usage can be found in the [PyCOMPSs Player](#) Section.

Tip: Please, check the PyCOMPSs player [Installation](#) Section for the further information with regard to the requirements installation and troubleshooting.

2.2 Write your first app

Choose your flavour:

Java

Application Overview

A COMPSs application is composed of three parts:

- **Main application code:** the code that is executed sequentially and contains the calls to the user-selected methods that will be executed by the COMPSs runtime as asynchronous parallel tasks.
- **Remote methods code:** the implementation of the tasks.
- **Task definition interface:** It is a Java annotated interface which declares the methods to be run as remote tasks along with metadata information needed by the runtime to properly schedule the tasks.

The main application file name has to be the same of the main class and starts with capital letter, in this case it is **Simple.java**. The Java annotated interface filename is *application name + Itf.java*, in this case it is **SimpleItf.java**. And the code that implements the remote tasks is defined in the *application name + Impl.java* file, in this case it is **SimpleImpl.java**.

All code examples are in the `/home/compss/tutorial_apps/java/` folder of the development environment.

Main application code

In COMPSs, the user's application code is kept unchanged, no API calls need to be included in the main application code in order to run the selected tasks on the nodes.

The COMPSs runtime is in charge of replacing the invocations to the user-selected methods with the creation of remote tasks also taking care of the access to files where required. Let's consider the Simple application example that takes an integer as input parameter and increases it by one unit.

The main application code of Simple application is shown in the following code block. It is executed sequentially until the call to the **increment()** method. COMPSs, as mentioned above, replaces the call to this method with the generation of a remote task that will be executed on an available node.

Code 1: Simple in Java (Simple.java)

```
package simple;

import java.io.FileInputStream;
import java.io.FileOutputStream;
import java.io.IOException;
import simple.SimpleImpl;

public class Simple {

    public static void main(String[] args) {
        String counterName = "counter";
        int initialValue = args[0];

        //-----//
        // Creation of the file which will contain the counter variable //
        //-----//
        try {
            FileOutputStream fos = new FileOutputStream(counterName);
            fos.write(initialValue);
            System.out.println("Initial counter value is " + initialValue);
            fos.close();
        } catch (IOException ioe) {
            ioe.printStackTrace();
        }

        //-----//
        //           Execution of the program           //
        //-----//
        SimpleImpl.increment(counterName);

        //-----//
        //   Reading from an object stored in a File   //
        //-----//
        try {
            FileInputStream fis = new FileInputStream(counterName);
            System.out.println("Final counter value is " + fis.read());
            fis.close();
        } catch (IOException ioe) {
            ioe.printStackTrace();
        }
    }
}
```

Remote methods code

The following code contains the implementation of the remote method of the *Simple* application that will be executed remotely by COMPSs.

Code 2: Simple Implementation (SimpleImpl.java)

```
package simple;

import java.io.FileInputStream;
import java.io.FileOutputStream;
import java.io.IOException;
import java.io.FileNotFoundException;

public class SimpleImpl {
    public static void increment(String counterFile) {
        try{
            FileInputStream fis = new FileInputStream(counterFile);
            int count = fis.read();
            fis.close();
            FileOutputStream fos = new FileOutputStream(counterFile);
            fos.write(++count);
            fos.close();
        }catch(FileNotFoundException fnfe){
            fnfe.printStackTrace();
        }catch(IOException ioe){
            ioe.printStackTrace();
        }
    }
}
```

Task definition interface

This Java interface is used to declare the methods to be executed remotely along with Java annotations that specify the necessary metadata about the tasks. The metadata can be of three different types:

1. For each parameter of a method, the data type (currently *File* type, primitive types and the *String* type are supported) and its directions (IN, OUT, INOUT, COMMUTATIVE or CONCURRENT).
2. The Java class that contains the code of the method.
3. The constraints that a given resource must fulfill to execute the method, such as the number of processors or main memory size.

The task description interface of the Simple app example is shown in the following figure. It includes the description of the *Increment()* method metadata. The method interface contains a single input parameter, a string containing a path to the file counterFile. In this example there are constraints on the minimum number of processors and minimum memory size needed to run the method.

Code 3: Interface of the Simple application (SimpleItf.java)

```
package simple;

import es.bsc.compss.types.annotations.Constraints;
import es.bsc.compss.types.annotations.task.Method;
import es.bsc.compss.types.annotations.Parameter;
import es.bsc.compss.types.annotations.parameter.Direction;
import es.bsc.compss.types.annotations.parameter.Type;

public interface SimpleItf {
```

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```

@Constraints(computingUnits = "1", memorySize = "0.3")
@Method(declaringClass = "simple.SimpleImpl")
void increment(
    @Parameter(type = Type.FILE, direction = Direction.INOUT)
    String file
);
}

```

Application compilation

A COMPSs Java application needs to be packaged in a *jar* file containing the class files of the main code, of the methods implementations and of the *Itf* annotation. This jar package can be generated using the commands available in the Java SDK or creating your application as a Apache Maven project.

To integrate COMPSs in the maven compile process you just need to add the *compss-api* artifact as dependency in the application project.

```

<dependencies>
  <dependency>
    <groupId>es.bsc.compss</groupId>
    <artifactId>compss-api</artifactId>
    <version>${compss.version}</version>
  </dependency>
</dependencies>

```

To build the jar in the maven case use the following command

```
$ mvn package
```

Next we provide a set of commands to compile the Java Simple application (detailed at [Java Sample applications](#)).

```

$ cd tutorial_apps/java/simple/src/main/java/simple/
~/tutorial_apps/java/simple/src/main/java/simple$ javac *.java
~/tutorial_apps/java/simple/src/main/java/simple$ cd ..
~/tutorial_apps/java/simple/src/main/java$ jar cf simple.jar simple/
~/tutorial_apps/java/simple/src/main/java$ mv ./simple.jar ../../../jar/

```

In order to properly compile the code, the CLASSPATH variable has to contain the path of the *compss-engine.jar* package. The default COMPSs installation automatically add this package to the CLASSPATH; please check that your environment variable CLASSPATH contains the *compss-engine.jar* location by running the following command:

```
$ echo $CLASSPATH | grep compss-engine
```

If the result of the previous command is empty it means that you are missing the *compss-engine.jar* package in your classpath. We recommend to automatically load the variable by editing the *.bashrc* file:

```

$ echo "# COMPSs variables for Java compilation" >> ~/.bashrc
$ echo "export CLASSPATH=$CLASSPATH:/opt/COMPSs/Runtime/compss-engine.jar" >> ~/.bashrc

```

Application execution

A Java COMPSs application is executed through the *runcompss* script. An example of an invocation of the script is:

```
$ runcompss --classpath=/home/compss/tutorial_apps/java/simple/jar/simple.jar simple.Simple 1
```

A comprehensive description of the *runcompss* command is available in the [Executing COMPSs applications](#) section.

In addition to Java, COMPSs supports the execution of applications written in other languages by means of bindings. A binding manages the interaction of the no-Java application with the COMPSs Java runtime, providing the necessary language translation.

Python

Let's write your first Python application parallelized with PyCOMPSs. Consider the following code:

Code 4: `increment.py`

```
import time
from pycompss.api.api import compss_wait_on
from pycompss.api.task import task

@task(returns=1)
def increment(value):
    time.sleep(value * 2) # mimic some computational time
    return value + 1

def main():
    values = [1, 2, 3, 4]
    start = time.time()
    for pos in range(len(values)):
        values[pos] = increment(values[pos])
    values = compss_wait_on(values)
    assert values == [2, 3, 4, 5]
    print(values)
    print("Elapsed time: " + str(time.time() - start_time))

if __name__ == '__main__':
    main()
```

This code increments the elements of an array (`values`) by calling iteratively to the `increment` function. The `increment` function sleeps the number of seconds indicated by the `value` parameter to represent some computational time. On a normal python execution, each element of the array will be incremented after the other (sequentially), accumulating the computational time. PyCOMPSs is able to parallelize this loop thanks to its `@task` decorator, and synchronize the results with the `compss_wait_on` API call.

Note: If you are using the PyCOMPSs player ([pycompss-player](#)), it is time to deploy the COMPSs environment within your current folder:

```
$ pycompss init
```

Please, be aware that the first time needs to download the docker image from the repository, and it may take a while.

Copy and paste the increment code it into `increment.py`.

Execution

Now let's execute `increment.py`. To this end, we will use the `runcompss` script provided by COMPSs:

```
$ runcompss -g increment.py
[Output in next step]
```

Or alternatively, the `pycompss run` command if using the PyCOMPSs player (which wraps the `runcompss` command and launches it within the COMPSs' docker container):

```
$ pycompss run -g increment.py
[Output in next step]
```

Note: The `-g` flag enables the task dependency graph generation (*used later*).

The `runcompss` command has a lot of supported options that can be checked with the `-h` flag. They can also be used within the `pycompss run` command.

Tip: It is possible to run also with the `python` command using the `pycompss` module, which accepts the same flags as `runcompss`:

```
$ python -m pycompss -g increment.py # Parallel execution
[Output in next step]
```

Having PyCOMPSs installed also enables to run the same code sequentially without the need of removing the PyCOMPSs syntax.

```
$ python increment.py # Sequential execution
[2, 3, 4, 5]
Elapsed time: 20.0161030293
```

Output

```
$ runcompss -g increment.py
[ INFO] Inferred PYTHON language
[ INFO] Using default location for project file: /opt/COMPSs/Runtime/configuration/xml/
→projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSs/Runtime/configuration/xml/
→resources/default_resources.xml
[ INFO] Using default execution type: compss

----- Executing increment.py -----

WARNING: COMPSs Properties file is null. Setting default values
[(433)  API] - Starting COMPSs Runtime v2.7 (build 20200519-1005.
→r6093e5ac94d67250e097a6fad9d3ec00d676fe6c)
[2, 3, 4, 5]
Elapsed time: 11.5068922043
[(4389) API] - Execution Finished

-----
```

Nice! it run successfully in my 8 core laptop, we have the expected output, and PyCOMPSs has been able to run the `increment.py` application in almost half of the time required by the sequential execution. *What happened under the hood?*

COMPSs started a master and one worker (by default configured to execute up to four tasks at the same time) and executed the application (offloading the tasks execution to the worker).

Let's check the task dependency graph to see the parallelism that COMPSs has extracted and taken advantage of.

Task dependency graph

COMPSs stores the generated task dependency graph within the `$HOME/.COMPSs/<APP_NAME>_<00-99>/monitor` directory in dot format. The generated graph is `complete_graph.dot` file, which can be displayed with any dot viewer.

Tip: COMPSs provides the `compss_gengraph` script which converts the given dot file into pdf.

```
$ cd $HOME/.COMPSs/increment.py_01/monitor
$ compss_gengraph complete_graph.dot
$ evince complete_graph.pdf # or use any other pdf viewer you like
```

It is also available within the PyCOMPSs player:

```
$ cd $HOME/.COMPSs/increment.py_01/monitor
$ pycompss gengraph complete_graph.dot
$ evince complete_graph.pdf # or use any other pdf viewer you like
```

And you should see:

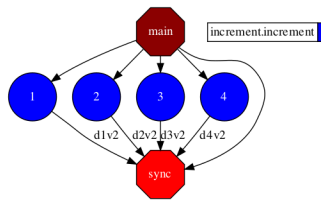


Figure 1: The dependency graph of the increment application

COMPSs has detected that the increment of each element is independent, and consequently, that all of them can be done in parallel. In this particular application, there are four `increment` tasks, and since the worker is able to run four tasks at the same time, all of them can be executed in parallel saving precious time.

Check the performance

Let's run it again with the tracing flag enabled:

```
$ runcompss -t increment.py
[ INFO] Inferred PYTHON language
[ INFO] Using default location for project file: /opt/COMPSs//Runtime/configuration/xml/
->projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSs//Runtime/configuration/xml/
->resources/default_resources.xml
[ INFO] Using default execution type: compss

----- Executing increment.py -----
```

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```

Welcome to Extrae 3.5.3

[... Extrae prolog ...]

WARNING: COMPSs Properties file is null. Setting default values
[(434)   API] - Starting COMPSs Runtime v2.7 (build 20200519-1005.
→r6093e5ac94d67250e097a6fad9d3ec00d676fe6c)
[2, 3, 4, 5]
Elapsed time: 13.1016821861

[... Extrae epililog ...]

mpi2prv: Congratulations! ./trace/increment.py_compss_trace_1587562240.prv has been
→generated.
[(24117)  API] - Execution Finished

-----

```

The execution has finished successfully and the trace has been generated in the `$HOME/.COMPSs/<APP_NAME>_<00-99>/trace` directory in prv format, which can be displayed and analysed with [PARAVER](#).

```

$ cd $HOME/.COMPSs/increment.py_02/trace
$ wxparaver increment.py_compss_trace_*.prv

```

Note: In the case of using the PyCOMPSs player, the trace will be generated in the `.COMPSs/<APP_NAME>_<00-99>/trace` directory:

```

$ cd .COMPSs/increment.py_02/trace
$ wxparaver increment.py_compss_trace_*.prv

```

Once Paraver has started, let's visualize the tasks:

- Click in **File** and then in **Load Configuration**
- Look for `/PATH/TO/COMPSs/Dependencies/paraver/cfgs/compss_tasks.cfg` and click **Open**.

Note: In the case of using the PyCOMPSs player, the configuration files can be obtained by downloading them from the [COMPSs repository](#).

And you should see:

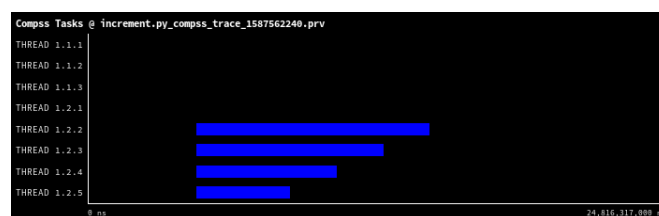


Figure 2: Trace of the increment application

The X axis represents the time, and the Y axis the deployed processes (the first three (1.1.1-1.1.3) belong to the master and the fourth belongs to the master process in the worker (1.2.1) whose events are shown with the `compss_runtime.cfg` configuration file).

The `increment` tasks are depicted in blue. We can quickly see that the four *increment* tasks have been executed in parallel (one per core), and that their lengths are different (depending on the computing time of the task represented by the `time.sleep(value * 2)` line).

Paraver is a very powerful tool for performance analysis. For more information, check the [Tracing](#) Section.

Note: If you are using the PyCOMPSs player, it is time to stop the COMPSs environment:

```
$ pycompss stop
```

C/C++

Application Overview

As in Java, the application code is divided in 3 parts: the Task definition interface, the main code and task implementations. These files must have the following notation: `<app_ame>.idl`, for the interface file, `<app_name>.cc` for the main code and `<app_name>-functions.cc` for task implementations. Next paragraphs provide an example of how to define this files for matrix multiplication parallelised by blocks.

Task Definition Interface

As in Java the user has to provide a task selection by means of an interface. In this case the interface file has the same name as the main application file plus the suffix “idl”, i.e. `Matmul.idl`, where the main file is called `Matmul.cc`.

Code 5: `Matmul.idl`

```
interface Matmul
{
    // C functions
    void initMatrix(inout Matrix matrix,
                   in int mSize,
                   in int nSize,
                   in double val);

    void multiplyBlocks(inout Block block1,
                      inout Block block2,
                      inout Block block3);
};
```

The syntax of the interface file is shown in the previous code. Tasks can be declared as classic C function prototypes, this allow to keep the compatibility with standard C applications. In the example, `initMatrix` and `multiplyBlocks` are functions declared using its prototype, like in a C header file, but this code is C++ as they have objects as parameters (objects of type `Matrix`, or `Block`).

The grammar for the interface file is:

```
[ "static" ] return-type task-name ( parameter { , parameter } * );

return-type = "void" | type

ask-name = <qualified name of the function or method>

parameter = direction type parameter-name

direction = "in" | "out" | "inout"
```

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```

type = "char" | "int" | "short" | "long" | "float" | "double" | "boolean" |
      "char[<size>]" | "int[<size>]" | "short[<size>]" | "long[<size>]" |
      "float[<size>]" | "double[<size>]" | "string" | "File" | class-name

class-name = <qualified name of the class>

```

Main Program

The following code shows an example of matrix multiplication written in C++.

Code 6: Matrix multiplication

```

#include "Matmul.h"
#include "Matrix.h"
#include "Block.h"
int N; //MSIZE
int M; //BSIZE
double val;
int main(int argc, char **argv)
{
    Matrix A;
    Matrix B;
    Matrix C;

    N = atoi(argv[1]);
    M = atoi(argv[2]);
    val = atof(argv[3]);

    compss_on();

    A = Matrix::init(N,M,val);

    initMatrix(&B,N,M,val);
    initMatrix(&C,N,M,0.0);

    cout << "Waiting for initialization...\n";

    compss_wait_on(B);
    compss_wait_on(C);

    cout << "Initialization ends...\n";

    C.multiply(A, B);

    compss_off();
    return 0;
}

```

The developer has to take into account the following rules:

1. A header file with the same name as the main file must be included, in this case **Matmul.h**. This header file is automatically generated by the binding and it contains other includes and type-definitions that are required.
2. A call to the **compss_on** binding function is required to turn on the COMPSs runtime.
3. As in C language, out or inout parameters should be passed by reference by means of the "&" operator before the parameter name.

4. Synchronization on a parameter can be done calling the **compss_wait_on** binding function. The argument of this function must be the variable or object we want to synchronize.
5. There is an **implicit synchronization** in the init method of Matrix. It is not possible to know the address of “A” before exiting the method call and due to this it is necessary to synchronize before for the copy of the returned value into “A” for it to be correct.
6. A call to the **compss_off** binding function is required to turn off the COMPSs runtime.

Functions file

The implementation of the tasks in a C or C++ program has to be provided in a functions file. Its name must be the same as the main file followed by the suffix “-functions”. In our case Matmul-functions.cc.

```
#include "Matmul.h"
#include "Matrix.h"
#include "Block.h"

void initMatrix(Matrix *matrix,int mSize,int nSize,double val){
    *matrix = Matrix::init(mSize, nSize, val);
}

void multiplyBlocks(Block *block1,Block *block2,Block *block3){
    block1->multiply(*block2, *block3);
}
```

In the previous code, class methods have been encapsulated inside a function. This is useful when the class method returns an object or a value and we want to avoid the explicit synchronization when returning from the method.

Additional source files

Other source files needed by the user application must be placed under the directory “src”. In this directory the programmer must provide a **Makefile** that compiles such source files in the proper way. When the binding compiles the whole application it will enter into the src directory and execute the Makefile.

It generates two libraries, one for the master application and another for the worker application. The directive COMPSS_MASTER or COMPSS_WORKER must be used in order to compile the source files for each type of library. Both libraries will be copied into the lib directory where the binding will look for them when generating the master and worker applications.

Application Compilation

The user command “**compss_build_app**” compiles both master and worker for a single architecture (e.g. x86-64, armhf, etc). Thus, whether you want to run your application in Intel based machine or ARM based machine, this command is the tool you need.

When the target is the native architecture, the command to execute is very simple;

```
$~/matmul_objects> compss_build_app Matmul
[ INFO ] Java libraries are searched in the directory: /usr/lib/jvm/java-1.8.0-openjdk-amd64//
→jre/lib/amd64/server
[ INFO ] Boost libraries are searched in the directory: /usr/lib/
...

[Info] The target host is: x86_64-linux-gnu

Building application for master...
g++ -g -O3 -I. -I/Bindings/c/share/c_build/worker/files/ -c Block.cc Matrix.cc
```

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```

ar rvs libmaster.a Block.o Matrix.o
ranlib libmaster.a

Building application for workers...
g++ -DCOMPSS_WORKER -g -O3 -I. -I/Bindings/c/share/c_build/worker/files/ -c Block.cc -o Block.
↪o
g++ -DCOMPSS_WORKER -g -O3 -I. -I/Bindings/c/share/c_build/worker/files/ -c Matrix.cc -o↪
↪Matrix.o
ar rvs libworker.a Block.o Matrix.o
ranlib libworker.a

...

Command successful.

```

Application Execution

The following environment variables must be defined before executing a COMPSs C/C++ application:

JAVA_HOME Java JDK installation directory (e.g. /usr/lib/jvm/java-8-openjdk/)

After compiling the application, two directories, master and worker, are generated. The master directory contains a binary called as the main file, which is the master application, in our example is called Matmul. The worker directory contains another binary called as the main file followed by the suffix “-worker”, which is the worker application, in our example is called Matmul-worker.

The `runcompss` script has to be used to run the application:

```
$ runcompss /home/compss/tutorial_apps/c/matmul_objects/master/Matmul 3 4 2.0
```

The complete list of options of the `runcompss` command is available in Section [Executing COMPSs applications](#).

Task Dependency Graph

COMPSs can generate a task dependency graph from an executed code. It is indicating by a

```
$ runcompss -g /home/compss/tutorial_apps/c/matmul_objects/master/Matmul 3 4 2.0
```

The generated task dependency graph is stored within the `$HOME/.COMPSs/<APP_NAME>_<00-99>/monitor` directory in dot format. The generated graph is `complete_graph.dot` file, which can be displayed with any dot viewer. COMPSs also provides the `compss_gengraph` script which converts the given dot file into pdf.

```

$ cd $HOME/.COMPSs/Matmul_02/monitor
$ compss_gengraph complete_graph.dot
$ evince complete_graph.pdf # or use any other pdf viewer you like

```

The following figure depicts the task dependency graph for the Matmul application in its object version with 3x3 blocks matrices, each one containing a 4x4 matrix of doubles. Each block in the result matrix accumulates three block multiplications, i.e. three multiplications of 4x4 matrices of doubles.

The light blue circle corresponds to the initialization of matrix “A” by means of a method-task and it has an implicit synchronization inside. The dark blue circles correspond to the other two initializations by means of function-tasks; in this case the synchronizations are explicit and must be provided by the developer after the task call. Both implicit and explicit synchronizations are represented as red circles.

Each green circle is a partial matrix multiplication of a set of 3. One block from matrix “A” and the correspondent one from matrix “B”. The result is written in the right block in “C” that accumulates the partial block multipli-

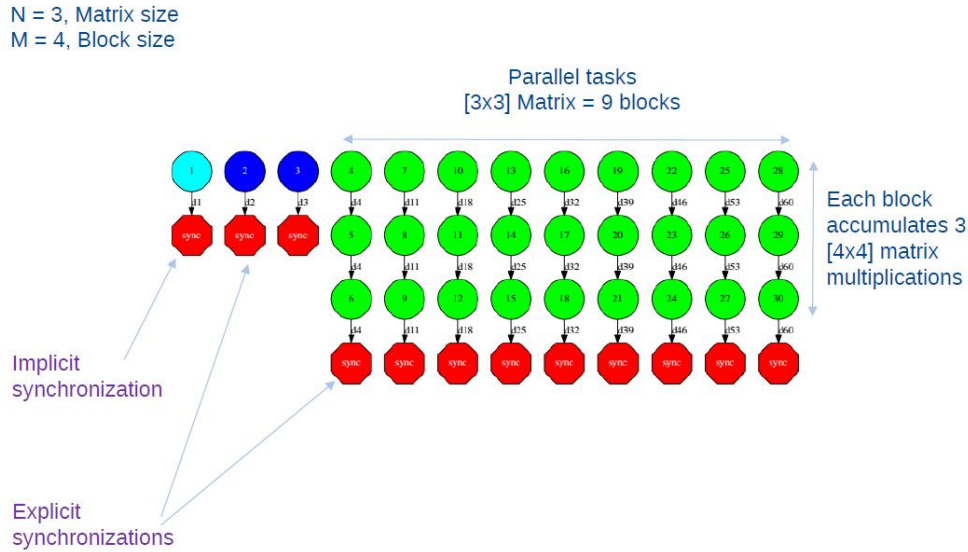


Figure 3: Matmul Execution Graph.

cations. Each multiplication set has an explicit synchronization. All green tasks are method-tasks and they are executed in parallel.

2.3 Useful information

Choose your flavour:

Java

- Syntax detailed information -> [Java](#)
- Constraint definition -> [Constraints](#)
- Execution details -> [Executing COMPSs applications](#)
- Graph, tracing and monitoring facilities -> [COMPSs Tools](#)
- Other execution environments (Supercomputers, Docker, etc.) -> [Supercomputers](#)
- Performance analysis -> [Tracing](#)
- Troubleshooting -> [Troubleshooting](#)
- Sample applications -> [Java Sample applications](#)
- Using COMPSs with persistent storage frameworks (e.g. dataClay, Hecuba) -> [Persistent Storage](#)

Python

- Syntax detailed information -> [Python Binding](#)
- Constraint definition -> [Constraints](#)
- Execution details -> [Executing COMPSs applications](#)
- Graph, tracing and monitoring facilities -> [COMPSs Tools](#)
- Other execution environments (Supercomputers, Docker, etc.) -> [Supercomputers](#)
- Performance analysis -> [Tracing](#)
- Troubleshooting -> [Troubleshooting](#)
- Sample applications -> [Python Sample applications](#)
- Using COMPSs with persistent storage frameworks (e.g. dataClay, Hecuba) -> [Persistent Storage](#)

C/C++

- Syntax detailed information -> [C/C++ Binding](#)
- Constraint definition -> [Constraints](#)
- Execution details -> [Executing COMPSs applications](#)
- Graph, tracing and monitoring facilities -> [COMPSs Tools](#)
- Other execution environments (Supercomputers, Docker, etc.) -> [Supercomputers](#)

- Performance analysis -> [*Tracing*](#)
- Troubleshooting -> [*Troubleshooting*](#)
- Sample applications -> [*C/C++ Sample applications*](#)

Chapter 3

Installation and Administration

This section is intended to walk you through the COMPSs installation.

3.1 Dependencies

Next we provide a list of dependencies for installing COMPSs package. The exact names may vary depending on the Linux distribution but this list provides a general overview of the COMPSs dependencies. For specific information about your distribution please check the *Depends* section at your package manager (apt, yum, zypper, etc.).

Table 1: COMPSs dependencies

Module	Dependencies
COMPSs Runtime	openjdk-8-jre, graphviz, xdg-utils, openssh-server
COMPSs Python Binding	libtool, automake, build-essential, python (>= 2.7 >=3.5), python-dev python3-dev, python-setuptools python3-setuptools, libpython2.7
COMPSs C/C++ Binding	libtool, automake, build-essential, libboost-all-dev, libxml2-dev
COMPSs Autoparallel	libgmp3-dev, flex, bison, libbison-dev, texinfo, libffi-dev, astor, sympy, enum34, islpy
COMPSs Tracing	libxml2 (>= 2.5), libxml2-dev (>= 2.5), gfortran, papi

As an example for some distributions:

Ubuntu 20.04

Ubuntu 20.04 dependencies installation commands:

```
$ sudo apt-get install -y openjdk-8-jdk graphviz xdg-utils libtool automake build-essential
python python-dev libpython2.7 python3 python3-dev libboost-serialization-dev libboost-
iostreams-dev libxml2 libxml2-dev csh gfortran libgmp3-dev flex bison texinfo python3-pip
libpapi-dev
$ sudo wget https://services.gradle.org/distributions/gradle-5.4.1-bin.zip -O /opt/gradle-5.4.
1-bin.zip
$ sudo unzip /opt/gradle-5.4.1-bin.zip -d /opt
```

Attention: Before installing it is important to have a proper `JAVA_HOME` environment variable definition. This variable must contain a valid path to a Java JDK (as a remark, it must point to a JDK, not JRE). So, please, export this variable and include it into your `.bashrc`:

```
$ echo 'export JAVA_HOME=/usr/lib/jvm/java-8-openjdk-amd64/' >> ~/.bashrc
$ export JAVA_HOME=/usr/lib/jvm/java-8-openjdk-amd64/
```

Ubuntu 18.04

Ubuntu 18.04 dependencies installation commands:

```
$ sudo apt-get install -y openjdk-8-jdk graphviz xdg-utils libtool automake build-essential
↳python python-dev libpython2.7 python3 python3-dev libboost-serialization-dev libboost-
↳iostreams-dev libxml2 libxml2-dev csh gfortran libgmp3-dev flex bison texinfo python3-pip
↳libpapi-dev
$ sudo wget https://services.gradle.org/distributions/gradle-5.4.1-bin.zip -O /opt/gradle-5.4.
↳1-bin.zip
$ sudo unzip /opt/gradle-5.4.1-bin.zip -d /opt
```

Attention: Before installing it is important to have a proper `JAVA_HOME` environment variable definition. This variable must contain a valid path to a Java JDK (as a remark, it must point to a JDK, not JRE). So, please, export this variable and include it into your `.bashrc`:

```
$ echo 'export JAVA_HOME=/usr/lib/jvm/java-8-openjdk-amd64/' >> ~/.bashrc
$ export JAVA_HOME=/usr/lib/jvm/java-8-openjdk-amd64/
```

Ubuntu 16.04

Ubuntu 16.04 dependencies installation commands:

```
$ sudo apt-get install -y openjdk-8-jdk graphviz xdg-utils libtool automake build-essential
↳python2.7 libpython2.7 libboost-serialization-dev libboost-iostreams-dev libxml2 libxml2-
↳dev csh gfortran python-pip libpapi-dev
$ sudo wget https://services.gradle.org/distributions/gradle-5.4.1-bin.zip -O /opt/gradle-5.4.
↳1-bin.zip
$ sudo unzip /opt/gradle-5.4.1-bin.zip -d /opt
```

Attention: Before installing it is important to have a proper `JAVA_HOME` environment variable definition. This variable must contain a valid path to a Java JDK (as a remark, it must point to a JDK, not JRE). So, please, export this variable and include it into your `.bashrc`:

```
$ echo 'export JAVA_HOME=/usr/lib/jvm/java-8-openjdk-amd64/' >> ~/.bashrc
$ export JAVA_HOME=/usr/lib/jvm/java-8-openjdk-amd64/
```

OpenSuse Tumbleweed

OpenSuse Tumbleweed dependencies installation commands:

```
$ sudo zypper install --type pattern -y devel_basis
$ sudo zypper install -y java-1_8_0-openjdk-headless java-1_8_0-openjdk java-1_8_0-openjdk-
↳devel graphviz xdg-utils python python-devel python3 python3-devel python3-decorator
↳libtool automake libboost_headers1_71_0-devel libboost_serialization1_71_0 libboost_
↳iostreams1_71_0 libxml2-2 libxml2-devel tcsh gcc-fortran papi libpapi gcc-c++ libpapi papi
↳papi-devel gmp-devel
$ sudo wget https://services.gradle.org/distributions/gradle-5.4.1-bin.zip -O /opt/gradle-5.4.
↳1-bin.zip
$ sudo unzip /opt/gradle-5.4.1-bin.zip -d /opt
```


Attention: Before installing it is important to have a proper `JAVA_HOME` environment variable definition. This variable must contain a valid path to a Java JDK (as a remark, it must point to a JDK, not JRE). So, please, export this variable and include it into your `.bashrc`:

```
$ echo 'export JAVA_HOME=/usr/lib64/jvm/java-1.8.0-openjdk/' >> ~/.bashrc
$ export JAVA_HOME=/usr/lib64/jvm/java-1.8.0-openjdk/
```

OpenSuse Leap 15.1

OpenSuse Leap 15.1 dependencies installation commands:

```
$ sudo zypper install --type pattern -y devel_basis
$ sudo zypper install -y java-1_8_0-openjdk-headless java-1_8_0-openjdk java-1_8_0-openjdk-
→devel graphviz xdg-utils python python-devel python-decorator python3 python3-devel python3-
→decorator libtool automake libboost_headers1_66_0-devel libboost_serialization1_66_0_
→libboost_iostreams1_66_0 libxml2-2 libxml2-devel tcsh gcc-fortran papi libpapi gcc-c++_
→libpapi papi papi-devel gmp-devel
$ sudo wget https://services.gradle.org/distributions/gradle-5.4.1-bin.zip -O /opt/gradle-5.4.
→1-bin.zip
$ sudo unzip /opt/gradle-5.4.1-bin.zip -d /opt
```

Attention: Before installing it is important to have a proper `JAVA_HOME` environment variable definition. This variable must contain a valid path to a Java JDK (as a remark, it must point to a JDK, not JRE). So, please, export this variable and include it into your `.bashrc`:

```
$ echo 'export JAVA_HOME=/usr/lib64/jvm/java-1.8.0-openjdk/' >> ~/.bashrc
$ export JAVA_HOME=/usr/lib64/jvm/java-1.8.0-openjdk/
```

OpenSuse 42.2

OpenSuse 42.2 dependencies installation commands:

```
$ sudo zypper install --type pattern -y devel_basis
$ sudo zypper install -y java-1_8_0-openjdk-headless java-1_8_0-openjdk java-1_8_0-openjdk-
→devel graphviz xdg-utils python python-devel libpython2_7-1_0 python-decorator libtool_
→automake boost-devel libboost_serialization1_54_0 libboost_iostreams1_54_0 libxml2-2_
→libxml2-devel tcsh gcc-fortran python-pip papi libpapi gcc-c++ libpapi papi papi-devel gmp-
→devel
$ sudo wget https://services.gradle.org/distributions/gradle-5.4.1-bin.zip -O /opt/gradle-5.4.
→1-bin.zip
$ sudo unzip /opt/gradle-5.4.1-bin.zip -d /opt
```

Warning: OpenSuse provides Python 3.4 from its repositories, which is not supported by the COMPSs python binding. Please, update Python 3 (`python` and `python-devel`) to a higher version if you expect to install COMPSs from sources.

Alternatively, you can use a virtual environment.

Attention: Before installing it is important to have a proper `JAVA_HOME` environment variable definition. This variable must contain a valid path to a Java JDK (as a remark, it must point to a JDK, not JRE). So, please, export this variable and include it into your `.bashrc`:

```
$ echo 'export JAVA_HOME=/usr/lib64/jvm/java-1.8.0-openjdk/' >> ~/.bashrc
$ export JAVA_HOME=/usr/lib64/jvm/java-1.8.0-openjdk/
```

Fedora 32

Fedora 32 dependencies installation commands:

```
$ sudo dnf install -y java-1.8.0-openjdk java-1.8.0-openjdk-devel graphviz xdg-utils libtool
↳ automake python27 python3 python3-devel boost-devel boost-serialization boost-iostreams
↳ libxml2 libxml2-devel gcc gcc-c++ gcc-gfortran tcsh @development-tools bison flex texinfo
↳ papi papi-devel gmp-devel
$ # If the libxml softlink is not created during the installation of libxml2, the COMPSs
↳ installation may fail.
$ # In this case, the softlink has to be created manually with the following command:
$ sudo ln -s /usr/include/libxml2/libxml/ /usr/include/libxml
$ sudo wget https://services.gradle.org/distributions/gradle-5.4.1-bin.zip -O /opt/gradle-5.4.
↳ 1-bin.zip
$ sudo unzip /opt/gradle-5.4.1-bin.zip -d /opt
```

Attention: Before installing it is important to have a proper `JAVA_HOME` environment variable definition. This variable must contain a valid path to a Java JDK (as a remark, it must point to a JDK, not JRE). So, please, export this variable and include it into your `.bashrc`:

```
$ echo 'export JAVA_HOME=/usr/lib/jvm/java-1.8.0-openjdk/' >> ~/.bashrc
$ export JAVA_HOME=/usr/lib/jvm/java-1.8.0-openjdk/
```

Fedora 25

Fedora 25 dependencies installation commands:

```
$ sudo dnf install -y java-1.8.0-openjdk java-1.8.0-openjdk-devel graphviz xdg-utils libtool
↳ automake python python-libs python-pip python-devel python2-decorator boost-devel boost-
↳ serialization boost-iostreams libxml2 libxml2-devel gcc gcc-c++ gcc-gfortran tcsh
↳ @development-tools redhat-rpm-config papi
$ # If the libxml softlink is not created during the installation of libxml2, the COMPSs
↳ installation may fail.
$ # In this case, the softlink has to be created manually with the following command:
$ sudo ln -s /usr/include/libxml2/libxml/ /usr/include/libxml
$ sudo wget https://services.gradle.org/distributions/gradle-5.4.1-bin.zip -O /opt/gradle-5.4.
↳ 1-bin.zip
$ sudo unzip /opt/gradle-5.4.1-bin.zip -d /opt
```

Attention: Before installing it is important to have a proper `JAVA_HOME` environment variable definition. This variable must contain a valid path to a Java JDK (as a remark, it must point to a JDK, not JRE). So, please, export this variable and include it into your `.bashrc`:

```
$ echo 'export JAVA_HOME=/usr/lib/jvm/java-1.8.0-openjdk/' >> ~/.bashrc
$ export JAVA_HOME=/usr/lib/jvm/java-1.8.0-openjdk/
```

Debian 8

Debian 8 dependencies installation commands:

```
$ su -
$ echo "deb http://ppa.launchpad.net/webupd8team/java/ubuntu xenial main" | tee /etc/apt/
↳ sources.list.d/webupd8team-java.list
```

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```
$ echo "deb-src http://ppa.launchpad.net/webupd8team/java/ubuntu xenial main" | tee -a /etc/
↳apt/sources.list.d/webupd8team-java.list
$ apt-key adv --keyserver hkp://keyserver.ubuntu.com:80 --recv-keys EEA14886
$ apt-get update
$ apt-get install oracle-java8-installer
$ apt-get install graphviz xdg-utils libtool automake build-essential python python-decorator
↳python-pip python-dev libboost-serialization1.55.0 libboost-iostreams1.55.0 libxml2 libxml2-
↳dev libboost-dev csh gfortran papi-tools
$ wget https://services.gradle.org/distributions/gradle-5.4.1-bin.zip -O /opt/gradle-5.4.1-
↳bin.zip
$ unzip /opt/gradle-5.4.1-bin.zip -d /opt
```

Attention: Before installing it is important to have a proper `JAVA_HOME` environment variable definition. This variable must contain a valid path to a Java JDK (as a remark, it must point to a JDK, not JRE). A possible value is the following:

```
$ echo $JAVA_HOME
/usr/lib64/jvm/java-openjdk/
```

So, please, check its location, export this variable and include it into your `.bashrc` if it is not already available with the previous command.

```
$ echo 'export JAVA_HOME=/usr/lib64/jvm/java-openjdk/' >> ~/.bashrc
$ export JAVA_HOME=/usr/lib64/jvm/java-openjdk/
```

CentOS 7

CentOS 7 dependencies installation commands:

```
$ sudo rpm -iUvh https://dl.fedoraproject.org/pub/epel/epel-release-latest-7.noarch.rpm
$ sudo yum -y update
$ sudo yum install java-1.8.0-openjdk java-1.8.0-openjdk-devel graphviz xdg-utils libtool
↳automake python python-libs python-pip python-devel python2-decorator boost-devel boost-
↳serialization boost-iostreams libxml2 libxml2-devel gcc gcc-c++ gcc-gfortran tcsh
↳@development-tools redhat-rpm-config papi
$ sudo pip install decorator
```

Attention: Before installing it is important to have a proper `JAVA_HOME` environment variable definition. This variable must contain a valid path to a Java JDK (as a remark, it must point to a JDK, not JRE). A possible value is the following:

```
$ echo $JAVA_HOME
/usr/lib64/jvm/java-openjdk/
```

So, please, check its location, export this variable and include it into your `.bashrc` if it is not already available with the previous command.

```
$ echo 'export JAVA_HOME=/usr/lib64/jvm/java-openjdk/' >> ~/.bashrc
$ export JAVA_HOME=/usr/lib64/jvm/java-openjdk/
```

Attention: Before installing it is also necessary to export the `GRADLE_HOME` environment variable and include its binaries path into the `PATH` environment variable:

```
$ echo 'export GRADLE_HOME=/opt/gradle-5.4.1' >> ~/.bashrc
$ export GRADLE_HOME=/opt/gradle-5.4.1
```

```
$ echo 'export PATH=/opt/gradle-5.4.1/bin:$PATH' >> ~/.bashrc
$ export PATH=/opt/gradle-5.4.1/bin:$PATH
```

3.1.1 Build Dependencies

To build COMPSs from sources you will also need `wget`, `git` and `maven` ([maven web](#)). To install with Pip, pip for the target Python version is required.

3.1.2 Optional Dependencies

For the Python binding it is recommended to have `dill` ([dill project](#)) and `guppy` ([guppy project](#))/`guppy3` ([guppy3 project](#)) installed. The `dill` package increases the variety of serializable objects by Python (for example: lambda functions), and the `guppy`/`guppy3` package is needed to use the `@local` decorator. Both packages can be found in `pyPI` and can be installed via `pip`.

Since it is possible to execute python applications using workers spawning MPI processes instead of multiprocessing, it is necessary to have `openmpi`, `openmpi-devel` and `openmpi-libs` system packages installed and `mpi4py` with `pip`.

3.2 Building from sources

This section describes the steps to install COMPSs from the sources.

The first step is downloading the source code from the Git repository.

```
$ git clone https://github.com/bsc-wdc/compss.git
$ cd compss
```

Then, you need to download the embedded dependencies from the git submodules.

```
$ compss> ./submodules_get.sh
$ compss> ./submodules_patch.sh
```

Finally you just need to run the installation script. You have two options:

For all users

For installing COMPSs for all users run the following command:

```
$ compss> cd builders/
$ builders> export INSTALL_DIR=/opt/COMPSs/
$ builders> sudo -E ./buildlocal ${INSTALL_DIR}
```

Attention: Root access is required.

For the current user

For installing COMPSs for the current user run the following commands:

```
$ compss> cd builders/
$ builders> INSTALL_DIR=$HOME/opt/COMPSs/
$ builders> ./buildlocal ${INSTALL_DIR}
```

Tip: The `buildlocal` script allows to disable the installation of components. The options can be found in the command help:

```
$ compss> cd builders/
$ builders> ./buildlocal -h

Usage: ./buildlocal [options] targetDir
* Options:
    --help, -h                Print this help message

    --opts                    Show available options

    --version, -v             Print COMPSs version

    --monitor, -m             Enable Monitor installation
    --no-monitor, -M          Disable Monitor installation
                                Default: true

    --bindings, -b           Enable bindings installation
    --no-bindings, -B         Disable bindings installation
                                Default: true

    --pycompss, -p            Enable PyCOMPSs installation
    --no-pycompss, -P         Disable PyCOMPSs installation
                                Default: true

    --tracing, -t             Enable tracing system installation
    --no-tracing, -T          Disable tracing system installation
                                Default: true

    --autoparallel, -a        Enable autoparallel module installation
    --no-autoparallel, -A     Disable autoparallel module installation
                                Default: true

    --kafka, -k               Enable Kafka module installation
    --no-kafka, -K            Disable Kafka module installation
                                Default: true

    --jacoco, -j              Enable Jacoco module installation
    --no-jacoco, -J           Disable Jacoco module installation
                                Default: true

    --nothing, -N             Disable all previous options
                                Default: unused

    --user-exec=<str>         Enables a specific user execution for maven compilation
                                When used the maven install is not cleaned.
                                Default: false

    --skip-tests              Disables MVN unit tests
                                Default:

* Parameters:
    targetDir                 COMPSs installation directory
                                Default: /opt/COMPSs
```

3.2.1 Post installation

Once your COMPSs package has been installed remember to log out and back in again to end the installation process.

Caution: Using Ubuntu version 18.04 or higher requires to comment the following lines in your `.bashrc` in order to have the appropriate environment after logging out and back again (which in these distributions it must be from the complete system (e.g. gnome) not only from the terminal, or restart the whole machine).

```
# If not running interactively, don't do anything
# case $- in
#     *) ;;
#     *) return;;
# esac
```

In addition, COMPSs requires **ssh passwordless access**. If you need to set up your machine for the first time please take a look at [Additional Configuration](#) Section for a detailed description of the additional configuration.

3.3 Pip

3.3.1 Pre-requisites

In order to be able to install COMPSs and PyCOMPSs with Pip, the dependencies (excluding the COMPSs packages) mentioned in the [Dependencies](#) Section must be satisfied (*do not forget* to have proper `JAVA_HOME` and `GRADLE_HOME` environment variables pointing to the java JDK folder and Gradle home respectively, as well as the `gradle` binary in the `PATH` environment variable) and Python `pip`.

3.3.2 Installation

Depending on the machine, the installation command may vary. Some of the possible scenarios and their proper installation command are:

Install systemwide

Install systemwide:

```
$ sudo -E pip install pycompss -v
```

Attention: Root access is required.

It is recommended to restart the user session once the installation process has finished. Alternatively, the following command sets all the COMPSs environment in the current session.

```
$ source /etc/profile.d/compss.sh
```

Install in user local folder

Install in user home folder (`.local`):

```
$ pip install pycompss -v
```

It is recommended to restart the user session once the installation process has finished. Alternatively, the following command sets all the COMPSs environment.

```
$ source ~/.bashrc
```

Within a virtual environment

Within a Python virtual environment:

```
(virtualenv) $ pip install pycompss -v
```

In this particular case, the installation includes the necessary variables in the activate script. So, restart the virtual environment in order to set all the COMPSs environment.

3.3.3 Post installation

If you need to set up your machine for the first time please take a look at [Additional Configuration](#) Section for a detailed description of the additional configuration.

3.4 Supercomputers

The COMPSs Framework can be installed in any Supercomputer by installing its packages as in a normal distribution. The packages are ready to be reallocated so the administrators can choose the right location for the COMPSs installation.

However, if the administrators are not willing to install COMPSs through the packaging system, we also provide a **COMPSs zipped file** containing a pre-build script to easily install COMPSs. Next subsections provide further information about this process.

3.4.1 Prerequisites

In order to successfully run the installation script some dependencies must be present on the target machine. Administrators must provide the correct installation and environment of the following software:

- Autotools
- BOOST
- Java 8 JRE

The following environment variables must be defined:

- JAVA_HOME
- BOOST_CPPFLAGS

The tracing system can be enhanced with:

- PAPI, which provides support for hardware counters
- MPI, which speeds up the tracing merge (and enables it for huge traces)

3.4.2 Installation

To perform the COMPSs Framework installation please execute the following commands:

```
$ # Check out the last COMPSs release
$ wget http://compss.bsc.es/repo/sc/stable/COMPSs_<version>.tar.gz

$ # Unpackage COMPSs
$ tar -xvzf COMPSs_<version>.tar.gz

$ # Install COMPSs at your preferred target location
```

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```
$ cd COMPSs
$ ./install [options] <targetDir> [<supercomputer.cfg>]

$ # Clean downloaded files
$ rm -r COMPSs
$ rm COMPSs_<version>.tar.gz
```

The installation script will install COMPSs inside the given `<targetDir>` folder and it will copy the `<supercomputer.cfg>` as default configuration. It also provides some options to skip the installation of optional features or bound the installation to an specific python version. You can see the available options with the following command.

```
$ ./install --help
```

Attention: If the `<targetDir>` folder already exists it will be **automatically erased**.

After completing the previous steps, administrators must ensure that the nodes have passwordless ssh access. If it is not the case, please contact the COMPSs team at support-compss@bsc.es.

The COMPSs package also provides a `compssenv` file that loads the required environment to allow users work more easily with COMPSs. Thus, after the installation process we recommend to source the `<targetDir>/compssenv` into the users `.bashrc`.

Once done, remember to log out and back in again to end the installation process.

3.4.3 Configuration

To maintain the portability between different environments, COMPSs has a pre-built structure of scripts to execute applications in Supercomputers. For this purpose, users must use the `enqueue_compss` script provided in the COMPSs installation and specify the supercomputer configuration with `--sc_cfg` flag.

When installing COMPSs for a supercomputer, system administrators must define a configuration file for the specific Supercomputer parameters. This document gives an overview about how to modify the configuration files in order to customize the `enqueue_compss` for a specific queue system and supercomputer. As overview, the easier way to proceed when creating a new configuration is to modify one of the configurations provided by COMPSs. System administrators can find configurations for **LSF**, **SLURM**, **PBS** and **SGE** as well as several examples for Supercomputer configurations in `<installation_dir>/Runtime/scripts/queues`. For instance, the configuration for the *MareNostrum IV* Supercomputer and the *Slurm* queue system, can be used as base file for new supercomputer and queue system cfs. Sysadmins can modify these files by changing the flags, parameters, paths and default values that corresponds to your supercomputer. Once, the files have been modified, they must be copied to the queues folder to make them available to the users. The following paragraph describe more in detail the scripts and configuration files. If you need help, contact support-compss@bsc.es.

3.4.3.1 COMPSs Queue structure overview

All the scripts and cfg files shown in [Figure 4](#) are located in the `<installation_dir>/Runtime/scripts/` folder. `enqueue_compss` and `launch_compss` (**launch.sh in the figure**) are in the user subfolder and `submit.sh` and the cfs are located in queues. There are two types of cfg files: the *queue system cfg* files, which are located in `queues/queue_systems`; and the *supercomputers.cfg* files, which are located in `queues/supercomputers`.

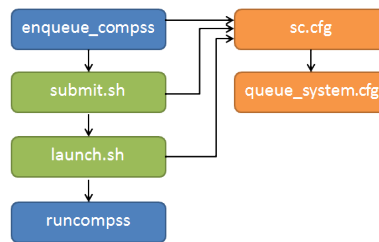


Figure 4: Structure of COMPSs queue scripts. In Blue user scripts, in Green queue scripts and in Orange system dependant scripts

3.4.3.2 Configuration Files

The cfg files contain a set of bash variables which are used by the other scripts. On the one hand, the queue system cfgs contain the variables to indicate the commands used by the system to submit and spawn processes, the commands or variables to get the allocated nodes and the directives to indicate the number of nodes, processes, etc. Below you can see an example of the most important variable definition for Slurm

```

# File: Runtime/scripts/queues/queue_systems/slurm.cfg

#####
## SUBMISSION VARIABLES
#####
# Variables to define the queue system directives.
# They are built as #${QUEUE_CMD} ${QARG_*}${QUEUE_SEPARATOR}value (submit.sh)
QUEUE_CMD="SBATCH"
SUBMISSION_CMD="sbatch"
SUBMISSION_PIPE="< "
SUBMISSION_HET_SEPARATOR=" : "
SUBMISSION_HET_PIPE=" "

# Variables to customize the commands know job id and allocated nodes (submit.sh)
ENV_VAR_JOB_ID="SLURM_JOB_ID"
ENV_VAR_NODE_LIST="SLURM_JOB_NODELIST"

QUEUE_SEPARATOR=""
EMPTY_WC_LIMIT=":00"

QARG_JOB_NAME="--job-name="
QARG_JOB_DEP_INLINE="false"
QARG_JOB_DEPENDENCY_OPEN="--dependency=afterany:"
QARG_JOB_DEPENDENCY_CLOSE=""

QARG_JOB_OUT="-o "
QARG_JOB_ERROR="-e "
QARG_WD="--workdir="
QARG_WALLCLOCK="-t"

QARG_NUM_NODES="-N"
QARG_NUM_PROCESSES="-n"
QNUM_PROCESSES_VALUE="\$(expr \${num_nodes} \/* \${req_cpus_per_node})"
QARG_EXCLUSIVE_NODES="--exclusive"
QARG_SPAN=""

QARG_MEMORY="--mem="
QARG_QUEUE_SELECTION="-p "

```

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```

QARG_NUM_SWITCHES="--gres="
QARG_GPUS_PER_NODE="--gres gpu:"
QARG_RESERVATION="--reservation="
QARG_CONSTRAINTS="--constraint="
QARG_QOS="--qos="
QARG_OVERCOMMIT="--overcommit"
QARG_CPUS_PER_TASK="-c"
QJOB_ID="%J"
QARG_PACKJOB="packjob"

#####
## LAUNCH VARIABLES
#####
# Variables to customize worker process spawn inside the job (launch_compss)
LAUNCH_CMD="srun"
LAUNCH_PARAMS="-n1 -N1 --odelist="
LAUNCH_SEPARATOR=""
CMD_SEPARATOR=""
HOSTLIST_CMD="scontrol show hostname"
HOSTLIST_TREATMENT="| awk {' print \$1 '}' | sed -e 's/\\.\\[\\^\\ ]*//g'"

#####
## QUEUE VARIABLES
## - Used in interactive
## - Substitute the %JOBID% keyword with the real job identifier dinamically
#####
QUEUE_JOB_STATUS_CMD="squeue -h -o %T --job %JOBID%"
QUEUE_JOB_RUNNING_TAG="RUNNING"
QUEUE_JOB_NODES_CMD="squeue -h -o %N --job %JOBID%"
QUEUE_JOB_CANCEL_CMD="scancel %JOBID%"
QUEUE_JOB_LIST_CMD="squeue -h -o %i"
QUEUE_JOB_NAME_CMD="squeue -h -o %j --job %JOBID%"

#####
## CONTACT VARIABLES
#####
CONTACT_CMD="ssh"

```

To adapt this script to your queue system, you just need to change the variable value to the command, argument or value required in your system. If you find that some of this variables are not available in your system, leave it empty.

On the other hand, the supercomputers cfg files contains a set of variables to indicate the queue system used by a supercomputer, paths where the shared disk is mounted, the default values that COMPSs will set in the project and resources files when they are not set by the user and flags to indicate if a functionality is available or not in a supercomputer. The following lines show examples of this variables for the *MareNostrum IV* supercomputer.

```

# File: Runtime/scripts/queues/supercomputers/mn.cfg

#####
## STRUCTURE VARIABLES
#####
QUEUE_SYSTEM="slurm"

#####
## ENQUEUE_COMPSS VARIABLES
#####

```

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```

DEFAULT_EXEC_TIME=10
DEFAULT_NUM_NODES=2
DEFAULT_NUM_SWITCHES=0
MAX_NODES_SWITCH=18
MIN_NODES_REQ_SWITCH=4
DEFAULT_QUEUE=default
DEFAULT_MAX_TASKS_PER_NODE=-1
DEFAULT_CPUS_PER_NODE=48
DEFAULT_IO_EXECUTORS=0
DEFAULT_GPUS_PER_NODE=0
DEFAULT_FPGAS_PER_NODE=0
DEFAULT_WORKER_IN_MASTER_CPUS=24
DEFAULT_WORKER_IN_MASTER_MEMORY=50000
DEFAULT_MASTER_WORKING_DIR=.
DEFAULT_WORKER_WORKING_DIR=local_disk
DEFAULT_NETWORK=infiniband
DEFAULT_DEPENDENCY_JOB=None
DEFAULT_RESERVATION=disabled
DEFAULT_NODE_MEMORY=disabled
DEFAULT_JVM_MASTER=""
DEFAULT_JVM_WORKERS="-Xms16000m,-Xmx92000m,-Xmn1600m"
DEFAULT_JVM_WORKER_IN_MASTER=""
DEFAULT_QOS=default
DEFAULT_CONSTRAINTS=disabled

#####
## Enabling/disabling passing
## requirements to queue system
#####
DISABLE_QARG_MEMORY=true
DISABLE_QARG_CONSTRAINTS=false
DISABLE_QARG_QOS=false
DISABLE_QARG_OVERCOMMIT=true
DISABLE_QARG_CPUS_PER_TASK=false
DISABLE_QARG_NVRAM=true
HETEROGENEOUS_MULTIJOB=false

#####
## SUBMISSION VARIABLES
#####
MINIMUM_NUM_NODES=1
MINIMUM_CPUS_PER_NODE=1
DEFAULT_STORAGE_HOME="null"
DISABLED_STORAGE_HOME="null"

#####
## LAUNCH VARIABLES
#####
LOCAL_DISK_PREFIX="/scratch/tmp"
REMOTE_EXECUTOR="none" # Disable the ssh spawn at runtime
NETWORK_INFINIBAND_SUFFIX="-ib0" # Hostname suffix to add in order to use infiniband network
NETWORK_DATA_SUFFIX="-data" # Hostname suffix to add in order to use data network
SHARED_DISK_PREFIX="/gpfs/"
SHARED_DISK_2_PREFIX="/.statelite/tmpfs/gpfs/"
DEFAULT_NODE_MEMORY_SIZE=92
DEFAULT_NODE_STORAGE_BANDWIDTH=450

```

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```
MASTER_NAME_CMD=hostname # Command to know the mastername
ELASTICITY_BATCH=true
```

To adapt this script to your supercomputer, you just need to change the variables to commands paths or values which are set in your system. If you find that some of this values are not available in your system, leave them empty or as they are in the MareNostrum IV.

3.4.3.3 How are cfg files used in scripts?

The `submit.sh` is in charge of getting some of the arguments from `enqueue_compss`, generating the a temporal job submission script for the `queue_system` (function `create_normal_tmp_submit`) and performing the submission in the scheduler (function `submit`). The functions used in `submit.sh` are implemented in `common.sh`. If you look at the code of this script, you will see that most of the code is customized by a set of bash vars which are mainly defined in the `cfg` files.

For instance the `submit` command is customized in the following way:

```
eval ${SUBMISSION_CMD} ${SUBMISSION_PIPE}${TMP_SUBMIT_SCRIPT}
```

Where `${SUBMISSION_CMD}` and `${SUBMISSION_PIPE}` are defined in the `queue_system.cfg`. So, for the case of Slurm, at execution time it is translated to something like `sbatch < /tmp/tmp_submit_script`

The same approach is used for the queue system directives defined in the submission script or in the command to get the assigned host list.

The following lines show the examples in these cases.

```
##${QUEUE_CMD} ${QARG_JOB_NAME}${QUEUE_SEPARATOR}${job_name}
```

In the case of Slurm in MN, it generates something like `#SBATCH --job-name=COMPSs`

```
host_list=\${HOSTLIST_CMD} \${ENV_VAR_NODE_LIST}${env_var_suffix} ${HOSTLIST_TREATMENT}
```

The same approach is used in the `launch_compss` script where it is using the defined vars to customize the `project.xml` and `resources.xml` file generation and spawning the master and worker processes in the assigned resources.

At first, you should not need to modify any script. The goal of the `cfg` files is that sysadmins just require to modify the supercomputers `cfg`, and in the case that the used queue system is not in the `queue_systems`, folder it should create a new one for the new one.

If you think that some of the features of your system are not supported in the current implementation, please contact us at support-compss@bsc.es. We will discuss how it should be incorporated in the scripts.

3.4.4 Post installation

To check that COMPSs Framework has been successfully installed you may run:

```
$ # Check the COMPSs version
$ runcompss -v
COMPSs version <version>
```

For queue system executions, COMPSs provides several prebuild queue scripts than can be accessible through the `enqueue_compss` command. Users can check the available options by running:

```
$ enqueue_compss -h

Usage: /apps/COMPSs/2.9/Runtime/scripts/user/enqueue_compss [queue_system_options] [COMPSs_
...options] application_name application_arguments
```

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```

* Options:
  General:
    --help, -h                Print this help message
    --heterogeneous           Indicates submission is going to be heterogeneous
                                Default: Disabled

  Queue system configuration:
    --sc_cfg=<name>           SuperComputer configuration file to use. Must
    ↪ exist inside queues/cfgs/
                                Default: default

  Submission configuration:
  General submission arguments:
    --exec_time=<minutes>     Expected execution time of the application (in
    ↪ minutes)
                                Default: 10
    --job_name=<name>         Job name
                                Default: COMPSs
    --queue=<name>            Queue name to submit the job. Depends on the
    ↪ queue system.
                                For example (MN3): bsc_cs | bsc_debug | debug |
    ↪ interactive
                                Default: default
    --reservation=<name>      Reservation to use when submitting the job.
                                Default: disabled
    --constraints=<constraints> Constraints to pass to queue system.
                                Default: disabled
    --qos=<qos>               Quality of Service to pass to the queue system.
                                Default: default
    --cpus_per_task           Number of cpus per task the queue system must
    ↪ allocate per task.
                                Note that this will be equal to the cpus_per_node
    ↪ in a worker node and
                                equal to the worker_in_master_cpus in a master
    ↪ node respectively.
                                Default: false
    --job_dependency=<jobID>   Postpone job execution until the job dependency
    ↪ has ended.
                                Default: None
    --storage_home=<string>    Root installation dir of the storage
    ↪ implementation
                                Default: null
    --storage_props=<string>   Absolute path of the storage properties file
                                Mandatory if storage_home is defined

  Normal submission arguments:
    --num_nodes=<int>         Number of nodes to use
                                Default: 2
    --num_switches=<int>      Maximum number of different switches. Select 0
    ↪ for no restrictions.
                                Maximum nodes per switch: 18
                                Only available for at least 4 nodes.
                                Default: 0
    --agents=<string>         Hierarchy of agents for the deployment. Accepted
    ↪ values: plain|tree
                                Default: tree
    --agents                  Deploys the runtime as agents instead of the
    ↪ classic Master-Worker deployment.

```

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Heterogeneous submission arguments:	Default: disabled
--type_cfg=<file_location>	Location of the file with the descriptions of U
→node type requests	File should follow the following format:
	type_X(){
	cpus_per_node=24
	node_memory=96
	...
	}
	type_Y(){
	...
	}
--master=<master_node_type>	Node type for the master
→type_cfg flag)	(Node type descriptions are provided in the --
--workers=type_X:nodes,type_Y:nodes	Node type and number of nodes per type for the U
→workers	(Node type descriptions are provided in the --
→type_cfg flag)	
Launch configuration:	
--cpus_per_node=<int>	Available CPU computing units on each node
	Default: 48
--gpus_per_node=<int>	Available GPU computing units on each node
	Default: 0
--fpgas_per_node=<int>	Available FPGA computing units on each node
	Default: 0
--io_executors=<int>	Number of IO executors on each node
	Default: 0
--fpga_reprogram=<string>	Specify the full command that needs to be U
→executed to reprogram the FPGA with	
→absolute path.	the desired bitstream. The location must be an U
	Default:
--max_tasks_per_node=<int>	Maximum number of simultaneous tasks running on a U
→node	
	Default: -1
--node_memory=<MB>	Maximum node memory: disabled <int> (MB)
	Default: disabled
--node_storage_bandwidth=<MB>	Maximum node storage bandwidth: <int> (MB)
	Default: 450
--network=<name>	Communication network for transfers: default U
→ethernet infiniband data.	
	Default: infiniband
--prolog=<string>	Task to execute before launching COMPSs (Notice U
→the quotes)	
→rather than spaces.	If the task has arguments split them by ", " U
→than one prolog action	This argument can appear multiple times for more U
--epilog=<string>	Default: Empty
→application (Notice the quotes)	Task to execute after executing the COMPSs U
→rather than spaces.	If the task has arguments split them by ", " U

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→than one epilog action	This argument can appear multiple times for more
	Default: Empty
--master_working_dir=<path>	Working directory of the application
--worker_working_dir=<name path>	Worker directory. Use: local_disk shared_disk
→<path>	Default: local_disk
--worker_in_master_cpus=<int>	Maximum number of CPU computing units that the
→master node can run as worker. Cannot exceed cpus_per_node.	Default: 24
--worker_in_master_memory=<int> MB	Maximum memory in master node assigned to the
→worker. Cannot exceed the node_memory.	Mandatory if worker_in_master_cpus is specified.
--worker_port_range=<min>,<max>	Default: 50000
→side	Port range used by the NIO adaptor at the worker
	Default: 43001,43005
--jvm_worker_in_master_opts="<string>"	Extra options for the JVM of the COMPSs Worker in
→the Master Node.	Each option separated by "," and without blank
→spaces (Notice the quotes)	Default:
--container_image=<path>	Runs the application by means of a container
→engine image	Default: Empty
--container_compss_path=<path>	Path where compss is installed in the container
→image	Default: /opt/COMPSs
--container_opts="<string>"	Options to pass to the container engine
--elasticity=<max_extra_nodes>	Default: empty
→nodes (ONLY AVAILABLE FORM SLURM CLUSTERS WITH NIO ADAPTOR)	Activate elasticity specifying the maximum extra
--automatic_scaling=<bool>	Default: 0
→(for elasticity)	Enable or disable the runtime automatic scaling
--jupyter_notebook=<path>,	Default: true
→jupyter notebook from the specified path.	Swap the COMPSs master initialization with
--jupyter_notebook	Default: false
--ipython	Swap the COMPSs master initialization with
→ipython.	Default: empty
Runcompss configuration:	
Tools enablers:	
--graph=<bool>, --graph, -g	Generation of the complete graph (true/false)
	When no value is provided it is set to true
	Default: false
--tracing=<level>, --tracing, -t	Set generation of traces and/or tracing level ([
→true basic] advanced scorep arm-map arm-ddt false)	

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<code>→traces.</code>	True and basic levels will produce the same
<code>--monitoring=<int>, --monitoring, -m</code>	When no value is provided it is set to 1 Default: 0 Period between monitoring samples (milliseconds) When no value is provided it is set to 2000 Default: 0
<code>--external_debugger=<int>, --external_debugger →specified port (or 9999 if empty)</code>	Enables external debugger connection on the
<code>--jmx_port=<int></code>	Default: false Enable JVM profiling on specified port
Runtime configuration options:	
<code>--task_execution=<compss storage></code>	Task execution under COMPSs or Storage. Default: compss
<code>--storage_impl=<string></code>	Path to an storage implementation. Shortcut to
<code>→setting pypath and classpath. See Runtime/storage in your installation folder.</code>	
<code>--storage_conf=<path></code>	Path to the storage configuration file Default: null
<code>--project=<path></code>	Path to the project XML file Default: /apps/COMPSs/2.9//Runtime/configuration/
<code>→xml/projects/default_project.xml</code>	
<code>--resources=<path></code>	Path to the resources XML file Default: /apps/COMPSs/2.9//Runtime/configuration/
<code>→xml/resources/default_resources.xml</code>	
<code>--lang=<name></code>	Language of the application (java/c/python) Default: Inferred is possible. Otherwise: java
<code>--summary →the application execution</code>	Displays a task execution summary at the end of
<code>--log_level=<level>, --debug, -d →trace</code>	Default: false Set the debug level: off info api debug
<code>→disabling asserts and __debug__</code>	Warning: Off level compiles with -O2 option Default: off
Advanced options:	
<code>--extrae_config_file=<path></code>	Sets a custom extrae config file. Must be in a
<code>→shared disk between all COMPSs workers.</code>	
<code>--trace_label=<string></code>	Default: null Add a label in the generated trace file. Only
<code>→used in the case of tracing is activated.</code>	
<code>--comm=<ClassName></code>	Default: None Class that implements the adaptor for
<code>→communications</code>	
	Supported adaptors:
	└ es.bsc.compss.nio.master.NIOAdaptor
	└ es.bsc.compss.gat.master.GATAdaptor
	Default: es.bsc.compss.nio.master.NIOAdaptor
<code>--conn=<className></code>	Class that implements the runtime connector for
<code>→the cloud</code>	
	Supported connectors:
	└ es.bsc.compss.connectors.
<code>→DefaultSSHConnector</code>	
	└ es.bsc.compss.connectors.
<code>→DefaultNoSSHConnector</code>	

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↪DefaultSSHConnector	Default: es.bsc.compss.connectors.
--streaming=<type>	Enable the streaming mode for the given type. Supported types: FILES, OBJECTS, PSCOS, ALL, NONE Default: NONE
--streaming_master_name=<str>	Use an specific streaming master node name. Default: null
--streaming_master_port=<int>	Use an specific port for the streaming master. Default: null
--scheduler=<className>	Class that implements the Scheduler for COMPSs Supported schedulers:
↪fifodatalocation.FIFODataLoctionScheduler	— es.bsc.compss.scheduler.
↪FIFOScheduler	— es.bsc.compss.scheduler.fifonew.
↪FIFODataScheduler	— es.bsc.compss.scheduler.fifodatanew.
↪LIFOScheduler	— es.bsc.compss.scheduler.lifonew.
↪TaskScheduler	— es.bsc.compss.components.impl.
↪LoadBalancingScheduler	— es.bsc.compss.scheduler.loadbalancing.
↪LoadBalancingScheduler	Default: es.bsc.compss.scheduler.loadbalancing.
--scheduler_config_file=<path>	Path to the file which contains the scheduler ↪
↪configuration.	
--library_path=<path>	Default: Empty Non-standard directories to search for libraries ↪
↪(e.g. Java JVM library, Python library, C binding library)	Default: Working Directory
--classpath=<path>	Path for the application classes / modules Default: Working Directory
--appdir=<path>	Path for the application class folder. Default: /home/group/user
--pythonpath=<path>	Additional folders or paths to add to the ↪
↪PYTHONPATH	Default: /home/group/user
--base_log_dir=<path>	Base directory to store COMPSs log files (a .
↪COMPSs/ folder will be created inside this location)	Default: User home
--specific_log_dir=<path>	Use a specific directory to store COMPSs log ↪
↪files (no sandbox is created)	Warning: Overwrites --base_log_dir option Default: Disabled
--uuid=<int>	Preset an application UUID Default: Automatic random generation
--master_name=<string>	Hostname of the node to run the COMPSs master Default:
--master_port=<int>	Port to run the COMPSs master communications. Only for NIO adaptor Default: [43000,44000]
--jvm_master_opts="<string>"	Extra options for the COMPSs Master JVM. Each ↪
↪option separated by "," and without blank spaces (Notice the quotes)	Default:
--jvm_workers_opts="<string>"	Extra options for the COMPSs Workers JVMs. Each ↪
↪option separated by "," and without blank spaces (Notice the quotes)	

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```

--cpu_affinity="<string>"           Default: -Xms1024m,-Xmx1024m,-Xmn400m
                                     Sets the CPU affinity for the workers
                                     Supported options: disabled, automatic, user_
→defined map of the form "0-8/9,10,11/12-14,15,16"
                                     Default: automatic
--gpu_affinity="<string>"           Sets the GPU affinity for the workers
                                     Supported options: disabled, automatic, user_
→defined map of the form "0-8/9,10,11/12-14,15,16"
                                     Default: automatic
--fpga_affinity="<string>"          Sets the FPGA affinity for the workers
                                     Supported options: disabled, automatic, user_
→defined map of the form "0-8/9,10,11/12-14,15,16"
                                     Default: automatic
--fpga_reprogram="<string>"         Specify the full command that needs to be_
→executed to reprogram the FPGA with the desired bitstream. The location must be an absolute_
→path.
                                     Default:
--io_executors=<int>                 IO Executors per worker
                                     Default: 0
--task_count=<int>                   Only for C/Python Bindings. Maximum number of_
→different functions/methods, invoked from the application, that have been selected as tasks
                                     Default: 50
--input_profile=<path>               Path to the file which stores the input_
→application profile
                                     Default: Empty
--output_profile=<path>              Path to the file to store the application profile_
→at the end of the execution
                                     Default: Empty
--PyObject_serialize=<bool>          Only for Python Binding. Enable the object_
→serialization to string when possible (true/false).
                                     Default: false
--persistent_worker_c=<bool>         Only for C Binding. Enable the persistent worker_
→in c (true/false).
                                     Default: false
--enable_external_adaptation=<bool> Enable external adaptation. This option will_
→disable the Resource Optimizer.
                                     Default: false
--gen_coredump                       Enable master coredump generation
                                     Default: false
--python_interpreter=<string>        Python interpreter to use (python/python2/_
→python3).
                                     Default: python Version: 2
--python_propagate_virtual_environment=<true> Propagate the master virtual environment_
→to the workers (true/false).
                                     Default: true
--python_mpi_worker=<false>          Use MPI to run the python worker instead of_
→multiprocessing. (true/false).
                                     Default: false
--python_memory_profile              Generate a memory profile of the master.
                                     Default: false

* Application name:
  For Java applications: Fully qualified name of the application
  For C applications: Path to the master binary
  For Python applications: Path to the .py file containing the main program

```

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```
* Application arguments:
  Command line arguments to pass to the application. Can be empty.
```

If none of the pre-build queue configurations adapts to your infrastructure (lsf, pbs, slurm, etc.) please contact the COMPSs team at support-compss@bsc.es to find out a solution.

If you are willing to test the COMPSs Framework installation you can run any of the applications available at our application repository <https://github.com/bsc-wdc/apps>. We suggest to run the java simple application following the steps listed inside its *README* file.

For further information about either the installation or the usage please check the *README* file inside the COMPSs package.

3.5 Additional Configuration

3.5.1 Configure SSH passwordless

By default, COMPSs uses SSH libraries for communication between nodes. Consequently, after COMPSs is installed on a set of machines, the SSH keys must be configured on those machines so that COMPSs can establish passwordless connections between them. This requires to install the OpenSSH package (if not present already) and follow these steps **on each machine**:

1. Generate an SSH key pair

```
$ ssh-keygen -t rsa
```

2. Distribute the public key to all the other machines and configure it as authorized

```
$ # For every other available machine (MACHINE):
$ scp ~/.ssh/id_rsa.pub MACHINE:./myRSA.pub
$ ssh MACHINE "cat ./myRSA.pub >> ~/.ssh/authorized_keys; rm ./myRSA.pub"
```

3. Check that passwordless SSH connections are working fine

```
$ # For every other available machine (MACHINE):
$ ssh MACHINE
```

For example, considering the cluster shown in [Figure 5](#), users will have to execute the following commands to grant free ssh access between any pair of machines:

```
me@localhost:~$ ssh-keygen -t id_rsa
# Granting access localhost -> m1.bsc.es
me@localhost:~$ scp ~/.ssh/id_rsa.pub user_m1@m1.bsc.es:./me_localhost.pub
me@localhost:~$ ssh user_m1@m1.bsc.es "cat ./me_localhost.pub >> ~/.ssh/authorized_keys; rm ./
↪me_localhost.pub"
# Granting access localhost -> m2.bsc.es
me@localhost:~$ scp ~/.ssh/id_rsa.pub user_m2@m2.bsc.es:./me_localhost.pub
me@localhost:~$ ssh user_m2@m2.bsc.es "cat ./me_localhost.pub >> ~/.ssh/authorized_keys; rm ./
↪me_localhost.pub"

me@localhost:~$ ssh user_m1@m1.bsc.es
user_m1@m1.bsc.es:~> ssh-keygen -t id_rsa
user_m1@m1.bsc.es:~> exit
# Granting access m1.bsc.es -> localhost
me@localhost:~$ scp user_m1@m1.bsc.es:~/.ssh/id_rsa.pub ~/userm1_m1.pub
me@localhost:~$ cat ~/userm1_m1.pub >> ~/.ssh/authorized_keys
# Granting access m1.bsc.es -> m2.bsc.es
```

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```

me@localhost:~$ scp ~/userm1_m1.pub user_m2@m2.bsc.es:~/userm1_m1.pub
me@localhost:~$ ssh user_m2@m2.bsc.es "cat ./userm1_m1.pub >> ~/.ssh/authorized_keys; rm ./
↪userm1_m1.pub"
me@localhost:~$ rm ~/userm1_m1.pub

me@localhost:~$ ssh user_m2@m2.bsc.es
user_m2@m2.bsc.es:~> ssh-keygen -t id_rsa
user_m2@m2.bsc.es:~> exit
# Granting access m2.bsc.es -> localhost
me@localhost:~$ scp user_m2@m1.bsc.es:~/.ssh/id_rsa.pub ~/userm2_m2.pub
me@localhost:~$ cat ~/userm2_m2.pub >> ~/.ssh/authorized_keys
# Granting access m2.bsc.es -> m1.bsc.es
me@localhost:~$ scp ~/userm2_m2.pub user_m1@m1.bsc.es:~/userm2_m2.pub
me@localhost:~$ ssh user_m1@m1.bsc.es "cat ./userm2_m2.pub >> ~/.ssh/authorized_keys; rm ./
↪userm2_m2.pub"
me@localhost:~$ rm ~/userm2_m2.pub

```

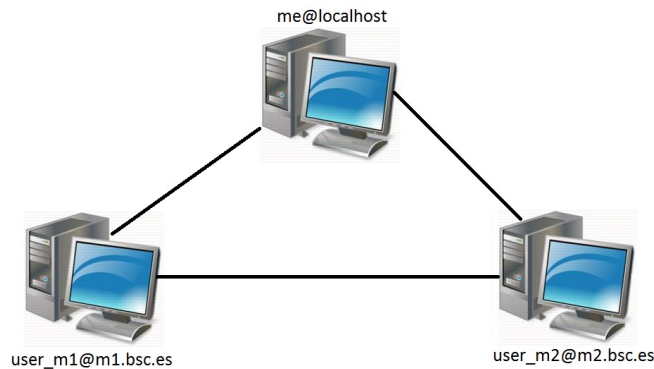


Figure 5: Cluster example

3.5.2 Configure the COMPSs Cloud Connectors

This section provides information about the additional configuration needed for some Cloud Connectors.

3.5.2.1 OCCI (Open Cloud Computing Interface) connector

In order to execute a COMPSs application using cloud resources, the rOCCI (Ruby OCCI) connector¹ has to be configured properly. The connector uses the rOCCI CLI client (upper versions from 4.2.5) which has to be installed in the node where the COMPSs main application runs. The client can be installed following the instructions detailed at <http://appdb.egi.eu/store/software/rocci.cli>

¹ <https://appdb.egi.eu/store/software/rocci.cli>

3.6 Configuration Files

The COMPSs runtime has two configuration files: `resources.xml` and `project.xml`. These files contain information about the execution environment and are completely independent from the application.

For each execution users can load the default configuration files or specify their custom configurations by using, respectively, the `--resources=<absolute_path_to_resources.xml>` and the `--project=<absolute_path_to_project.xml>` in the `runcompss` command. The default files are located in the `/opt/COMPSs/Runtime/configuration/xml/` path.

Next sections describe in detail the `resources.xml` and the `project.xml` files, explaining the available options.

3.6.1 Resources file

The `resources` file provides information about all the available resources that can be used for an execution. This file should normally be managed by the system administrators. Its full definition schema can be found at `/opt/COMPSs/Runtime/configuration/xml/resources/resource_schema.xsd`.

For the sake of clarity, users can also check the SVG schema located at `/opt/COMPSs/Runtime/configuration/xml/resources/resource_schema.svg`.

This file contains one entry per available resource defining its name and its capabilities. Administrators can define several resource capabilities (see example in the next listing) but we would like to underline the importance of **ComputingUnits**. This capability represents the number of available cores in the described resource and it is used to schedule the correct number of tasks. Thus, it becomes essential to define it accordingly to the number of cores in the physical resource.

```
compss@bsc:~$ cat /opt/COMPSs/Runtime/configuration/xml/resources/default_resources.xml
<?xml version="1.0" encoding="UTF-8" standalone="yes"?>
<ResourcesList>
  <ComputeNode Name="localhost">
    <Processor Name="P1">
      <ComputingUnits>4</ComputingUnits>
      <Architecture>amd64</Architecture>
      <Speed>3.0</Speed>
    </Processor>
    <Processor Name="P2">
      <ComputingUnits>2</ComputingUnits>
    </Processor>
    <Adaptors>
      <Adaptor Name="es.bsc.compss.nio.master.NIOAdaptor">
        <SubmissionSystem>
          <Interactive/>
        </SubmissionSystem>
        <Ports>
          <MinPort>43001</MinPort>
          <MaxPort>43002</MaxPort>
        </Ports>
      </Adaptor>
    </Adaptors>
    <Memory>
      <Size>16</Size>
    </Memory>
    <Storage>
      <Size>200.0</Size>
    </Storage>
    <OperatingSystem>
      <Type>Linux</Type>
    </OperatingSystem>
  </ComputeNode>
</ResourcesList>
```

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```

        <Distribution>OpenSUSE</Distribution>
    </OperatingSystem>
    <Software>
        <Application>Java</Application>
        <Application>Python</Application>
    </Software>
</ComputeNode>
</ResourcesList>

```

3.6.2 Project file

The project file provides information about the resources used in a specific execution. Consequently, the resources that appear in this file are a subset of the resources described in the `resources.xml` file. This file, that contains one entry per worker, is usually edited by the users and changes from execution to execution. Its full definition schema can be found at `/opt/COMPSs/Runtime/configuration/xml/projects/project_schema.xsd`.

For the sake of clarity, users can also check the SVG schema located at `/opt/COMPSs/Runtime/configuration/xml/projects/project_schema.xsd`.

We emphasize the importance of correctly defining the following entries:

installDir Indicates the path of the COMPSs installation **inside the resource** (not necessarily the same than in the local machine).

User Indicates the username used to connect via ssh to the resource. This user **must** have passwordless access to the resource (see [Configure SSH passwordless](#) Section). If left empty COMPSs will automatically try to access the resource with the **same username as the one that launches the COMPSs main application**.

LimitOfTasks The maximum number of tasks that can be simultaneously scheduled to a resource. Considering that a task can use more than one core of a node, this value must be lower or equal to the number of available cores in the resource.

```

compss@bsc:~$ cat /opt/COMPSs/Runtime/configuration/xml/projects/default_project.xml
<?xml version="1.0" encoding="UTF-8" standalone="yes"?>
<Project>
    <!-- Description for Master Node -->
    <MasterNode></MasterNode>

    <!-- Description for a physical node -->
    <ComputeNode Name="localhost">
        <InstallDir>/opt/COMPSs/</InstallDir>
        <WorkingDir>/tmp/Worker/</WorkingDir>
        <Application>
            <AppDir>/home/user/apps/</AppDir>
            <LibraryPath>/usr/lib/</LibraryPath>
            <Classpath>/home/user/apps/jar/example.jar</Classpath>
            <Pythonpath>/home/user/apps/</Pythonpath>
        </Application>
        <LimitOfTasks>4</LimitOfTasks>
        <Adaptors>
            <Adaptor Name="es.bsc.compss.nio.master.NIOAdaptor">
                <SubmissionSystem>
                    <Interactive/>
                </SubmissionSystem>
                <Ports>
                    <MinPort>43001</MinPort>
                    <MaxPort>43002</MaxPort>
                </Ports>
            </Adaptor>
        </Adaptors>
    </ComputeNode>
</Project>

```

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```

        <User>user</User>
    </Adaptor>
</Adaptors>
</ComputeNode>
</Project>

```

3.6.3 Configuration examples

In the next subsections we provide specific information about the services, shared disks, cluster and cloud configurations and several `project.xml` and `resources.xml` examples.

3.6.3.1 Parallel execution on one single process configuration

The most basic execution that COMPSs supports is using no remote workers and running all the tasks internally within the same process that hosts the application execution. To enable the parallel execution of the application, the user needs to set up the runtime and provide a description of the resources available on the node. For that purpose, the user describes within the `<MasterNode>` tag of the `project.xml` file the resources in the same way it describes other nodes' resources on the using the `resources.xml` file. Since there is no inter-process communication, adaptors description is not allowed. In the following example, the master will manage the execution of tasks on the MainProcessor CPU of the local node - a quad-core amd64 processor at 3.0GHz - and use up to 16 GB of RAM memory and 200 GB of storage.

```

<?xml version="1.0" encoding="UTF-8" standalone="yes"?>
<Project>
  <MasterNode>
    <Processor Name="MainProcessor">
      <ComputingUnits>4</ComputingUnits>
      <Architecture>amd64</Architecture>
      <Speed>3.0</Speed>
    </Processor>
    <Memory>
      <Size>16</Size>
    </Memory>
    <Storage>
      <Size>200.0</Size>
    </Storage>
  </MasterNode>
</Project>

```

If no other nodes are available, the list of resources on the `resources.xml` file is empty as shown in the following file sample. Otherwise, the user can define other nodes besides the master node as described in the following section, and the runtime system will orchestrate the task execution on both the local process and on the configured remote nodes.

```

<?xml version="1.0" encoding="UTF-8" standalone="yes"?>
<ResourcesList>
</ResourcesList>

```

3.6.3.2 Cluster and grid configuration (static resources)

In order to use external resources to execute the applications, the following steps have to be followed:

1. Install the *COMPSs Worker* package (or the full *COMPSs Framework* package) on all the new resources.
2. Set SSH passwordless access to the rest of the remote resources.
3. Create the *WorkingDir* directory in the resource (remember this path because it is needed for the `project.xml` configuration).
4. Manually deploy the application on each node.

The `resources.xml` and the `project.xml` files must be configured accordingly. Here we provide examples about configuration files for Grid and Cluster environments.

```
<?xml version="1.0" encoding="UTF-8" standalone="yes"?>
<ResourcesList>
  <ComputeNode Name="hostname1.domain.es">
    <Processor Name="MainProcessor">
      <ComputingUnits>4</ComputingUnits>
    </Processor>
    <Adaptors>
      <Adaptor Name="es.bsc.compss.nio.master.NIOAdaptor">
        <SubmissionSystem>
          <Interactive/>
        </SubmissionSystem>
        <Ports>
          <MinPort>43001</MinPort>
          <MaxPort>43002</MaxPort>
        </Ports>
      </Adaptor>
      <Adaptor Name="es.bsc.compss.gat.master.GATAdaptor">
        <SubmissionSystem>
          <Batch>
            <Queue>sequential</Queue>
          </Batch>
          <Interactive/>
        </SubmissionSystem>
        <BrokerAdaptor>sshtrilead</BrokerAdaptor>
      </Adaptor>
    </Adaptors>
  </ComputeNode>

  <ComputeNode Name="hostname2.domain.es">
    ...
  </ComputeNode>
</ResourcesList>
```

```
<?xml version="1.0" encoding="UTF-8" standalone="yes"?>
<Project>
  <MasterNode/>
  <ComputeNode Name="hostname1.domain.es">
    <InstallDir>/opt/COMPSs</InstallDir>
    <WorkingDir>/tmp/COMPSsWorker1</WorkingDir>
    <User>user</User>
    <LimitOfTasks>2</LimitOfTasks>
  </ComputeNode>
  <ComputeNode Name="hostname2.domain.es">
    ...
  </ComputeNode>
</Project>
```


3.6.3.3 Shared Disks configuration example

Configuring shared disks might reduce the amount of data transfers improving the application performance. To configure a shared disk the users must:

1. Define the shared disk and its capabilities
2. Add the shared disk and its mountpoint to each worker
3. Add the shared disk and its mountpoint to the master node

Next example illustrates steps 1 and 2. The `<SharedDisk>` tag adds a new shared disk named `sharedDisk0` and the `<AttachedDisk>` tag adds the mountpoint of a named shared disk to a specific worker.

```
<?xml version="1.0" encoding="UTF-8" standalone="yes"?>
<ResourcesList>
  <SharedDisk Name="sharedDisk0">
    <Storage>
      <Size>100.0</Size>
      <Type>Persistent</Type>
    </Storage>
  </SharedDisk>

  <ComputeNode Name="localhost">
    ...
    <SharedDisks>
      <AttachedDisk Name="sharedDisk0">
        <MountPoint>/tmp/SharedDisk</MountPoint>
      </AttachedDisk>
    </SharedDisks>
  </ComputeNode>
</ResourcesList>
```

On the other side, to add the shared disk to the **master node**, the users must edit the `project.xml` file. Next example shows how to attach the previous `sharedDisk0` to the master node:

```
<?xml version="1.0" encoding="UTF-8" standalone="yes"?>
<Project>
  <MasterNode>
    <SharedDisks>
      <AttachedDisk Name="sharedDisk0">
        <MountPoint>/home/sharedDisk</MountPoint>
      </AttachedDisk>
    </SharedDisks>
  </MasterNode>

  <ComputeNode Name="localhost">
    ...
  </ComputeNode>
</Project>
```

Notice that the `resources.xml` file can have multiple `SharedDisk` definitions and that the `SharedDisks` tag (either in the `resources.xml` or in the `project.xml` files) can have multiple `AttachedDisk` childrens to mount several shared disks on the same worker or master.

3.6.3.4 Cloud configuration (dynamic resources)

In order to use cloud resources to execute the applications, the following steps have to be followed:

1. Prepare cloud images with the *COMPSs Worker* package or the full *COMPSs Framework* package installed.
2. The application will be deployed automatically during execution but the users need to set up the configuration files to specify the application files that must be deployed.

The COMPSs runtime communicates with a cloud manager by means of connectors. Each connector implements the interaction of the runtime with a given provider's API, supporting four basic operations: ask for the price of a certain VM in the provider, get the time needed to create a VM, create a new VM and terminate a VM. This design allows connectors to abstract the runtime from the particular API of each provider and facilitates the addition of new connectors for other providers.

The `resources.xml` file must contain one or more `<CloudProvider>` tags that include the information about a particular provider, associated to a given connector. The tag **must** have an attribute **Name** to uniquely identify the provider. Next example summarizes the information to be specified by the user inside this tag.

```
<?xml version="1.0" encoding="UTF-8" standalone="yes"?>
<ResourcesList>
  <CloudProvider Name="PROVIDER_NAME">
    <Endpoint>
      <Server>https://PROVIDER_URL</Server>
      <ConnectorJar>CONNECTOR_JAR</ConnectorJar>
      <ConnectorClass>CONNECTOR_CLASS</ConnectorClass>
    </Endpoint>
    <Images>
      <Image Name="Image1">
        <Adaptors>
          <Adaptor Name="es.bsc.compss.nio.master.NIOAdaptor">
            <SubmissionSystem>
              <Interactive/>
            </SubmissionSystem>
            <Ports>
              <MinPort>43001</MinPort>
              <MaxPort>43010</MaxPort>
            </Ports>
          </Adaptor>
        </Adaptors>
        <OperatingSystem>
          <Type>Linux</Type>
        </OperatingSystem>
        <Software>
          <Application>Java</Application>
        </Software>
        <Price>
          <TimeUnit>100</TimeUnit>
          <PricePerUnit>36.0</PricePerUnit>
        </Price>
      </Image>
      <Image Name="Image2">
        <Adaptors>
          <Adaptor Name="es.bsc.compss.nio.master.NIOAdaptor">
            <SubmissionSystem>
              <Interactive/>
            </SubmissionSystem>
            <Ports>
              <MinPort>43001</MinPort>
              <MaxPort>43010</MaxPort>
            </Ports>
          </Adaptor>
        </Adaptors>
        <OperatingSystem>
          <Type>Linux</Type>
        </OperatingSystem>
        <Software>
          <Application>Java</Application>
        </Software>
        <Price>
          <TimeUnit>100</TimeUnit>
          <PricePerUnit>36.0</PricePerUnit>
        </Price>
      </Image>
    </Images>
  </CloudProvider>
</ResourcesList>
```

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```

        </Ports>
      </Adaptor>
    </Adaptors>
  </Image>
</Images>

<InstanceTypes>
  <InstanceType Name="Instance1">
    <Processor Name="P1">
      <ComputingUnits>4</ComputingUnits>
      <Architecture>amd64</Architecture>
      <Speed>3.0</Speed>
    </Processor>
    <Processor Name="P2">
      <ComputingUnits>4</ComputingUnits>
    </Processor>
    <Memory>
      <Size>1000.0</Size>
    </Memory>
    <Storage>
      <Size>2000.0</Size>
    </Storage>
  </InstanceType>
  <InstanceType Name="Instance2">
    <Processor Name="P1">
      <ComputingUnits>4</ComputingUnits>
    </Processor>
  </InstanceType>
</InstanceTypes>
</CloudProvider>
</ResourcesList>

```

The `project.xml` complements the information about a provider listed in the `resources.xml` file. This file can contain a `<Cloud>` tag where to specify a list of providers, each with a `<CloudProvider>` tag, whose **name** attribute must match one of the providers in the `resources.xml` file. Thus, the `project.xml` file **must** contain a subset of the providers specified in the `resources.xml` file. Next example summarizes the information to be specified by the user inside this `<Cloud>` tag.

```

<?xml version="1.0" encoding="UTF-8" standalone="yes"?>
<Project>
  <Cloud>
    <InitialVMs>1</InitialVMs>
    <MinimumVMs>1</MinimumVMs>
    <MaximumVMs>4</MaximumVMs>
    <CloudProvider Name="PROVIDER_NAME">
      <LimitOfVMs>4</LimitOfVMs>
      <Properties>
        <Property Context="C1">
          <Name>P1</Name>
          <Value>V1</Value>
        </Property>
        <Property>
          <Name>P2</Name>
          <Value>V2</Value>
        </Property>
      </Properties>
    </CloudProvider>
  </Cloud>
</Project>

```

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```

<Images>
  <Image Name="Image1">
    <InstallDir>/opt/COMPSs/</InstallDir>
    <WorkingDir>/tmp/Worker/</WorkingDir>
    <User>user</User>
    <Application>
      <Pythonpath>/home/user/apps/</Pythonpath>
    </Application>
    <LimitOfTasks>2</LimitOfTasks>
    <Package>
      <Source>/home/user/apps/</Source>
      <Target>/tmp/Worker/</Target>
      <IncludedSoftware>
        <Application>Java</Application>
        <Application>Python</Application>
      </IncludedSoftware>
    </Package>
    <Package>
      <Source>/home/user/apps/</Source>
      <Target>/tmp/Worker/</Target>
    </Package>
    <Adaptors>
      <Adaptor Name="es.bsc.compss.nio.master.NIOAdaptor">
        <SubmissionSystem>
          <Interactive/>
        </SubmissionSystem>
        <Ports>
          <MinPort>43001</MinPort>
          <MaxPort>43010</MaxPort>
        </Ports>
      </Adaptor>
    </Adaptors>
  </Image>
  <Image Name="Image2">
    <InstallDir>/opt/COMPSs/</InstallDir>
    <WorkingDir>/tmp/Worker/</WorkingDir>
  </Image>
</Images>
<InstanceTypes>
  <InstanceType Name="Instance1"/>
  <InstanceType Name="Instance2"/>
</InstanceTypes>
</CloudProvider>

<CloudProvider Name="PROVIDER_NAME2">
  ...
</CloudProvider>
</Cloud>
</Project>

```

For any connector the Runtime is capable to handle the next list of properties:

Table 2: Connector supported properties in the `project.xml` file

Name	Description
provider-user	Username to login in the provider
provider-user-credential	Credential to login in the provider
time-slot	Time slot
estimated-creation-time	Estimated VM creation time
max-vm-creation-time	Maximum VM creation time

Additionally, for any connector based on SSH, the Runtime automatically handles the next list of properties:

Table 3: Properties supported by any SSH based connector in the `project.xml` file

Name	Description
vm-user	User to login in the VM
vm-password	Password to login in the VM
vm-keypair-name	Name of the Keypair to login in the VM
vm-keypair-location	Location (in the master) of the Keypair to login in the VM

Finally, the next sections provide a more accurate description of each of the currently available connector and its specific properties.

Cloud connectors: rOCCI

The connector uses the rOCCI binary client¹ (version newer or equal than 4.2.5) which has to be installed in the node where the COMPSs main application is executed.

This connector needs additional files providing details about the resource templates available on each provider. This file is located under `<COMPSs_INSTALL_DIR>/configuration/xml/templates` path. Additionally, the user must define the virtual images flavors and instance types offered by each provider; thus, when the runtime decides the creation of a VM, the connector selects the appropriate image and resource template according to the requirements (in terms of CPU, memory, disk, etc) by invoking the rOCCI client through Mixins (heritable classes that override and extend the base templates).

Table 4 contains the rOCCI specific properties that must be defined under the `Provider` tag in the `project.xml` file and Table 5 contains the specific properties that must be defined under the `Instance` tag.

¹ <https://appdb.egi.eu/store/software/rocci.cli>

Table 4: rOCCI extensions in the `project.xml` file

Name	Description
auth	Authentication method, x509 only supported
user-cred	Path of the VOMS proxy
ca-path	Path to CA certificates directory
ca-file	Specific CA filename
owner	Optional. Used by the PMES Job-Manager
jobname	Optional. Used by the PMES Job-Manager
timeout	Maximum command time
username	Username to connect to the back-end cloud provider
password	Password to connect to the back-end cloud provider
voms	Enable VOMS authentication
media-type	Media type
resource	Resource type
attributes	Extra resource attributes for the back-end cloud provider
context	Extra context for the back-end cloud provider
action	Extra actions for the back-end cloud provider
mixin	Mixin definition
link	Link
trigger-action	Adds a trigger
log-to	Redirect command logs
skip-ca-check	Skips CA checks
filter	Filters command output
dump-model	Dumps the internal model
debug	Enables the debug mode on the connector commands
verbose	Enables the verbose mode on the connector commands

Table 5: Configuration of the `<resources>.xml` templates file

Instance	Multiple entries of resource templates.
Type	Name of the resource template. It has to be the same name than in the previous files
CPU	Number of cores
Memory	Size in GB of the available RAM
Disk	Size in GB of the storage
Price	Cost per hour of the instance

Cloud connectors: JClouds

The JClouds connector is based on the JClouds API version *1.9.1*. Table [Table 6](#) shows the extra available options under the *Properties* tag that are used by this connector.

Table 6: JClouds extensions in the `<project>.xml` file

Instance	Description
provider	Back-end provider to use with JClouds (i.e. aws-ec2)

Cloud connectors: Docker

This connector uses a Java API client from <https://github.com/docker-java/docker-java>, version 3.0.3. It has not additional options. Make sure that the image/s you want to load are pulled before running COMPSs with `docker pull IMAGE`. Otherwise, the connector will throw an exception.

Cloud connectors: Mesos

The connector uses the v0 Java API for Mesos which has to be installed in the node where the COMPSs main application is executed. This connector creates a Mesos framework and it uses Docker images to deploy workers, each one with an own IP address.

By default it does not use authentication and the timeout timers are set to 3 minutes (180.000 milliseconds). The list of **optional** properties available from connector is shown in Table 7.

Table 7: Mesos connector options in the <project>.xml file

Instance	Description
mesos-framework-name	Framework name to show in Mesos.
mesos-woker-name	Worker names to show in Mesos.
mesos-framework-hostname	Framework hostname to show in Mesos.
mesos-checkpoint	Checkpoint for the framework.
mesos-authenticate	Uses authentication? (true/false)
mesos-principal	Principal for authentication.
mesos-secret	Secret for authentication.
mesos-framework-register-timeout	Timeout to wait for Framework to register.
mesos-framework-register-timeout-units	Time units to wait for register.
mesos-worker-wait-timeout	Timeout to wait for worker to be created.
mesos-worker-wait-timeout-units	Time units for waiting creation.
mesos-worker-kill-timeout	Number of units to wait for killing a worker.
mesos-worker-kill-timeout-units	Time units to wait for killing.
mesos-docker-command	Command to use at start for each worker.
mesos-containerizer	Containers to use: (MESOS/DOCKER)
mesos-docker-network-type	Network type to use: (BRIDGE/HOST/USER)
mesos-docker-network-name	Network name to use for workers.
mesos-docker-mount-volume	Mount volume on workers? (true/false)
mesos-docker-volume-host-path	Host path for mounting volume.
mesos-docker-volume-container-path	Container path to mount volume.

TimeUnit avialable values: DAYS, HOURS, MICROSECONDS, MILLISECONDS, MINUTES, NANOSECONDS, SECONDS.

3.6.3.5 Services configuration

To allow COMPSs applications to use WebServices as tasks, the `resources.xml` can include a special type of resource called *Service*. For each WebService it is necessary to specify its wsdl, its name, its namespace and its port.

```
<?xml version="1.0" encoding="UTF-8" standalone="yes"?>
<ResourcesList>
  <ComputeNode Name="localhost">
    ...
  </ComputeNode>

  <Service wsdl="http://bscgrid05.bsc.es:20390/hmmerobj/hmmerobj?wsdl">
    <Name>HmmerObjects</Name>
    <Namespace>http://hmmerobj.worker</Namespace>
```

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```
        <Port>HmmerObjectsPort</Port>
    </Service>
</ResourcesList>
```

When configuring the `project.xml` file it is necessary to include the service as a worker by adding an special entry indicating only the name and the limit of tasks as shown in the following example:

```
<?xml version="1.0" encoding="UTF-8" standalone="yes"?>
<Project>
    <MasterNode/>
    <ComputeNode Name="localhost">
        ...
    </ComputeNode>

    <Service wsdl="http://bscgrid05.bsc.es:20390/hmmerobj/hmmerobj?wsdl">
        <LimitOfTasks>2</LimitOfTasks>
    </Service>
</Project>
```


Chapter 4

Application development

This section is intended to walk you through the development of COMPSs applications.

4.1 Java

This section illustrates the steps to develop a Java COMPSs application, to compile and to execute it. The *Simple* application will be used as reference code. The user is required to select a set of methods, invoked in the sequential application, that will be run as remote tasks on the available resources.

4.1.1 Programming Model

This section shows how the COMPSs programming model is used to develop a Java task-based parallel application for distributed computing. First, We introduce the structure of a COMPSs Java application and with a simple example. Then, we will provide a complete guide about how to define the application tasks. Finally, we will show special API calls and other optimization hints.

4.1.1.1 Application Overview

A COMPSs application is composed of three parts:

- **Main application code:** the code that is executed sequentially and contains the calls to the user-selected methods that will be executed by the COMPSs runtime as asynchronous parallel tasks.
- **Remote methods code:** the implementation of the tasks.
- **Task definition interface:** It is a Java annotated interface which declares the methods to be run as remote tasks along with metadata information needed by the runtime to properly schedule the tasks.

The main application file name has to be the same of the main class and starts with capital letter, in this case it is **Simple.java**. The Java annotated interface filename is *application name + Itf.java*, in this case it is **SimpleItf.java**. And the code that implements the remote tasks is defined in the *application name + Impl.java* file, in this case it is **SimpleImpl.java**.

All code examples are in the `/home/compss/tutorial_apps/java/` folder of the development environment.

Main application code

In COMPSs, the user's application code is kept unchanged, no API calls need to be included in the main application code in order to run the selected tasks on the nodes.

The COMPSs runtime is in charge of replacing the invocations to the user-selected methods with the creation of remote tasks also taking care of the access to files where required. Let's consider the Simple application example that takes an integer as input parameter and increases it by one unit.

The main application code of Simple application is shown in the following code block. It is executed sequentially until the call to the **increment()** method. COMPSs, as mentioned above, replaces the call to this method with the generation of a remote task that will be executed on an available node.

Code 7: Simple in Java (Simple.java)

```
package simple;

import java.io.FileInputStream;
import java.io.FileOutputStream;
import java.io.IOException;
import simple.SimpleImpl;

public class Simple {

    public static void main(String[] args) {
        String counterName = "counter";
        int initialValue = args[0];

        //-----//
        // Creation of the file which will contain the counter variable //
        //-----//
        try {
            FileOutputStream fos = new FileOutputStream(counterName);
            fos.write(initialValue);
            System.out.println("Initial counter value is " + initialValue);
            fos.close();
        } catch (IOException ioe) {
            ioe.printStackTrace();
        }

        //-----//
        //           Execution of the program           //
        //-----//
        SimpleImpl.increment(counterName);

        //-----//
        //   Reading from an object stored in a File   //
        //-----//
        try {
            FileInputStream fis = new FileInputStream(counterName);
            System.out.println("Final counter value is " + fis.read());
            fis.close();
        } catch (IOException ioe) {
            ioe.printStackTrace();
        }
    }
}
```

Remote methods code

The following code contains the implementation of the remote method of the *Simple* application that will be executed remotely by COMPSs.

Code 8: Simple Implementation (SimpleImpl.java)

```
package simple;

import java.io.FileInputStream;
import java.io.FileOutputStream;
import java.io.IOException;
import java.io.FileNotFoundException;

public class SimpleImpl {
    public static void increment(String counterFile) {
        try{
            FileInputStream fis = new FileInputStream(counterFile);
            int count = fis.read();
            fis.close();
            FileOutputStream fos = new FileOutputStream(counterFile);
            fos.write(++count);
            fos.close();
        }catch(FileNotFoundException fnfe){
            fnfe.printStackTrace();
        }catch(IOException ioe){
            ioe.printStackTrace();
        }
    }
}
```

Task definition interface

This Java interface is used to declare the methods to be executed remotely along with Java annotations that specify the necessary metadata about the tasks. The metadata can be of three different types:

1. For each parameter of a method, the data type (currently *File* type, primitive types and the *String* type are supported) and its directions (IN, OUT, INOUT, COMMUTATIVE or CONCURRENT).
2. The Java class that contains the code of the method.
3. The constraints that a given resource must fulfill to execute the method, such as the number of processors or main memory size.

The task description interface of the Simple app example is shown in the following figure. It includes the description of the *Increment()* method metadata. The method interface contains a single input parameter, a string containing a path to the file counterFile. In this example there are constraints on the minimum number of processors and minimum memory size needed to run the method.

Code 9: Interface of the Simple application (SimpleItf.java)

```
package simple;

import es.bsc.compss.types.annotations.Constraints;
import es.bsc.compss.types.annotations.task.Method;
import es.bsc.compss.types.annotations.Parameter;
import es.bsc.compss.types.annotations.parameter.Direction;
import es.bsc.compss.types.annotations.parameter.Type;

public interface SimpleItf {
```

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```
@Constraints(computingUnits = "1", memorySize = "0.3")
@Method(declaringClass = "simple.SimpleImpl")
void increment(
    @Parameter(type = Type.FILE, direction = Direction.INOUT)
    String file
);
}
```

The following sections show a detailed guide of how to implement complex applications.

4.1.1.2 Task definition reference guide

The task definition interface is a Java annotated interface where developers define tasks as annotated methods in the interfaces. Annotations can be of three different types:

1. Task-definition annotations are method annotations to indicate which type of task is a method declared in the interface.
2. The Parameter annotation provides metadata about the task parameters, such as data type, direction and other property for runtime optimization.
3. The Constraints annotation describes the minimum capabilities that a given resource must fulfill to execute the task, such as the number of processors or main memory size.
4. Scheduler hint annotation provides information about how to deal with tasks of this type at scheduling and execution

A complete and detailed explanation of the usage of the metadata includes:

Task-definition Annotations

For each declared methods, developers has to define a task type. The following list enumerates the possible task types:

- **@Method:** Defines the Java method as a task
 - **declaringClass** (Mandatory) String specifying the class that implements the Java method.
 - **targetDirection** This field specifies the direction of the target object of an object method. It can be defined as: INOUT” (default value) if the method modifies the target object, “CONCURRENT” if this object modification can be done concurrently, or “IN” if the method does not modify the target object. ()
 - **priority** “true” if the task takes priority and “false” otherwise. This parameter is used by the COMPSs scheduler (it is a String not a Java boolean).
 - **onFailure** Expected behaviour if the task fails. *OnFailure.RETRY* (default value) makes the task be executed again, *OnFailure.CANCEL_SUCCESSORS* ignores the failure and cancels the successor tasks, *OnFailure.FAIL* stops the whole application in a save mode once a task fails or *OnFailure.IGNORE* ignores the failure and continues with normal runtime execution.
- **@Binary:** Defines the Java method as a binary invocation
 - **binary** (Mandatory) String defining the full path of the binary that must be executed.
 - **workingDir** Full path of the binary working directory inside the COMPSs Worker.
 - **priority** “true” if the task takes priority and “false” otherwise. This parameter is used by the COMPSs scheduler (it is a String not a Java boolean).
- **@MPI:** Defines the Java method as a MPI invocation
 - **mpiRunner** (Mandatory) String defining the mpi runner command.
 - **binary** (Mandatory) String defining the full path of the binary that must be executed.
 - **processes** String defining the number of MPI processes spawn in the task execution. This can be combined with the constraints annotation to create define a MPI+OpenMP task. (Default is 1)
 - **scaleByCU** It indicates that the defined *processes* will be scaled by the defined *computingUnits* in the constraints. So, the total MPI processes will be *processes* multiplied by *computingUnits*. This

- functionality is used to groups MPI processes per node. Number of groups will be set in processes and the number of processes per node will be indicated by *computingUnits*
- **workingDir** Full path of the binary working directory inside the COMPSs Worker.
 - **priority** “true” if the task takes priority and “false” otherwise. This parameter is used by the COMPSs scheduler (it is a String not a Java boolean).
 - **@OmpSs**: Defines the Java method as a OmpSs invocation
 - **binary** (Mandatory) String defining the full path of the binary that must be executed.
 - **workingDir** Full path of the binary working directory inside the COMPSs Worker.
 - **priority** “true” if the task takes priority and “false” otherwise. This parameter is used by the COMPSs scheduler (it is a String not a Java boolean).
 - **@Service**: It specifies the service properties.
 - **namespace** Mandatory. Service namespace.
 - **name** Mandatory. Service name.
 - **port** Mandatory. Service port.
 - **operation** Operation type.
 - **priority** “true” if the service takes priority, “false” otherwise. This parameter is used by the COMPSs scheduler (it is a String not a Java boolean).

Parameter-level annotations

For each parameter of task (method declared in the interface), the user must include a **@Parameter** annotation. The properties

- **Direction**: Describes how a task uses the parameter (Default is IN).
 - **Direction.IN**: Task only reads the data.
 - **Direction.INOUT**: Task reads and modifies
 - **Direction.OUT**: Task completely modify the data, or previous content or not modified data is not important.
 - **Direction.COMMUTATIVE**: An INOUT usage of the data which can be re-ordered with other executions of the defined task.
 - **Direction.CONCURRENT**: The task allow concurrent modifications of this data. It requires a storage backend that manages concurrent modifications.
- **Type**: Describes the data type of the task parameter. By default, the runtime infers the type according to the Java datatype. However, it is mandatory to define it for files, directories and Streams. COMPSs supports the following types for task parameters:
 - **Basic types**: To indicate a parameter is a Java primitive type use the following types: *Type.BOOLEAN*, *Type.CHAR*, *Type.BYTE*, *Type.SHORT*, *Type.INT*, *Type.LONG*, *Type.FLOAT*, *Type.DOUBLE*. They can only have **IN** direction, since primitive types in Java are always passed by value.
 - **String**: To indicate a parameter is a Java String use *Type.STRING*. It can only have **IN** direction, since Java Strings are immutable.
 - **File**: The real Java type associated with a file parameter is a String that contains the path to the file. However, if the user specifies a parameter as *Type.FILE*, COMPSs will treat it as such. It can have any direction (IN, OUT, INOUT, COMMUTATIVE or CONCURRENT).
 - **Directory**: The real Java type associated with a directory parameter is a String that contains the path to the directory. However, if the user specifies a parameter as *Type.DIRECTORY*, COMPSs will treat it as such. It can have any direction (IN, OUT, INOUT, COMMUTATIVE or CONCURRENT).
 - **Object**: An object parameter is defined with *Type.Object*. It can have any direction (IN, INOUT, COMMUTATIVE or CONCURRENT).
 - **Streams**: A Task parameters can be defined as stream with *Type.STREAM*. It can have direction IN, if the task pull data from the stream, or OUT if the task pushes data to the stream.
- **Return type**: Any object or a generic class object. In this case the direction is always OUT. Basic types are also supported as return types. However, we do not recommend to use them because they cause an implicit synchronization
- **StdIOStream**: For non-native tasks (binaries, MPI, and OmpSs) COMPSs supports the automatic redirection of the Linux streams by specifying *StdIOStream.STDIN*, *StdIOStream.STDOUT* or *StdIOStream.STDERR*. Notice that any parameter annotated with the stream annotation must be of type *Type.FILE*, and with direction *Direction.IN* for *StdIOStream.STDIN* or *Direction.OUT/Direction.INOUT*

for *StdIOStream.STDOUT* and *StdIOStream.STDERR*.

- **Prefix:** For non-native tasks (binaries, MPI, and OmpSs) COMPSs allows to prepend a constant String to the parameter value to use the Linux joint-prefixes as parameters of the binary execution.
- **Weight:** Provides a hint of the size of this parameter compared to a default one. For instance, if a parameters is 3 times larger than the others, set the weigh property of this parameter to 3.0. (Default is 1.0).
- **keepRename:** Runtime rename files to avoid some data dependencies. It is transparent to the final user because we rename back the filename when invoking the task at worker. This management creates an overhead, if developers know that the task is not name nor extension sensitive (i.e can work with rename), they can set this property to true to reduce the overhead.

Constraints annotations

- **@Constraints:** The user can specify the capabilities that a resource must have in order to run a method. For example, in a cloud execution the COMPSs runtime creates a VM that fulfils the specified requirements in order to perform the execution. A full description of the supported constraints can be found in [Table 14](#).

Scheduler annotations

- **@SchedulerHints:** It specifies hints for the scheduler about how to treat the task.
 - **isReplicated** “true” if the method must be executed in all the worker nodes when invoked from the main application (it is a String not a Java boolean).
 - **isDistributed** “true” if the method must be scheduled in a forced round robin among the available resources (it is a String not a Java boolean).

4.1.1.3 Alternative method implementations

Since version 1.2, the COMPSs programming model allows developers to define sets of alternative implementations of the same method in the Java annotated interface. [Code 10](#) depicts an example where the developer sorts an integer array using two different methods: merge sort and quick sort that are respectively hosted in the *packagepath.Mergesort* and *packagepath.Quicksort* classes.

Code 10: Alternative sorting method definition example

```
@Method(declaringClass = "packagepath.Mergesort")
@Method(declaringClass = "packagepath.Quicksort")
void sort(
    @Parameter(type = Type.OBJECT, direction = Direction.INOUT)
    int[] array
);
```

As depicted in the example, the name and parameters of all the implementations must coincide; the only difference is the class where the method is implemented. This is reflected in the attribute *declaringClass* of the *@Method* annotation. Instead of stating that the method is implemented in a single class, the programmer can define several instances of the *@Method* annotation with different declaring classes.

As independent remote methods, the sets of equivalent methods might have common restrictions to be fulfilled by the resource hosting the execution. Or even, each implementation can have specific constraints. Through the *@Constraints* annotation, developers can specify the common constraints for a whole set of methods. In the following example ([Code 11](#)) only one core is required to run the method of both sorting algorithms.

Code 11: Alternative sorting method definition with constraint example

```
@Constraints(computingUnits = "1")
@Method(declaringClass = "packagepath.Mergesort")
@Method(declaringClass = "packagepath.Quicksort")
```

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```
void sort(
    @Parameter(type = Type.OBJECT, direction = Direction.INOUT)
    int[] array
);
```

However, these sorting algorithms have different memory consumption, thus each algorithm might require a specific amount of memory and that should be stated in the implementation constraints. For this purpose, the developer can add a `@Constraints` annotation inside each `@Method` annotation containing the specific constraints for that implementation. Since the Mergesort has a higher memory consumption than the quicksort, the [Code 12](#) sets a requirement of 1 core and 2GB of memory for the mergesort implementation and 1 core and 500MB of memory for the quicksort.

Code 12: Alternative sorting method definition with specific constraints example

```
@Constraints(computingUnits = "1")
@Method(declaringClass = "packagepath.Mergesort", constraints = @Constraints(memorySize = "2.0
↪"))
@Method(declaringClass = "packagepath.Quicksort", constraints = @Constraints(memorySize = "0.5
↪"))
void sort(
    @Parameter(type = Type.OBJECT, direction = Direction.INOUT)
    int[] array
);
```

4.1.1.4 Java API calls

COMPSs also provides a explicit synchronization call, namely *barrier*, which can be used through the COMPSs Java API. The use of *barrier* forces to wait for all tasks that have been submitted before the barrier is called. When all tasks submitted before the *barrier* have finished, the execution continues ([Code 13](#)).

Code 13: COMPSs.barrier() example

```
import es.bsc.compss.api.COMPSs;

public class Main {
    public static void main(String[] args) {
        // Setup counterName1 and counterName2 files
        // Execute task increment 1
        SimpleImpl.increment(counterName1);
        // API Call to wait for all tasks
        COMPSs.barrier();
        // Execute task increment 2
        SimpleImpl.increment(counterName2);
    }
}
```

When an object is used in a task, COMPSs runtime store the references of these object in the runtime data structures and generate replicas and versions in remote workers. COMPSs is automatically removing these replicas for obsolete versions. However, the reference of the last version of these objects could be stored in the runtime data-structures preventing the garbage collector to remove it when there are no references in the main code. To avoid this situation, developers can indicate the runtime that an object is not going to use any more by calling the `deregisterObject` API call. [Code 14](#) shows a usage example of this API call.

Code 14: COMPSs.deregisterObject() example

```
import es.bsc.compss.api.COMPSs;

public class Main {
    public static void main(String[] args) {
        final int ITERATIONS = 10;
        for (int i = 0; i < ITERATIONS; ++i) {
            Dummy d = new Dummy(d);
            TaskImpl.task(d);
            /*Allows garbage collector to delete the
            object from memory when the task is finished */
            COMPSs.deregisterObject((Object) d);
        }
    }
}
```

To synchronize files, the `getFile` API call synchronizes a file, returning the last version of file with its original name. Code 15 contains an example of its usage.

Code 15: COMPSs.getFile() example

```
import es.bsc.compss.api.COMPSs;

public class Main {
    public static void main(String[] args) {
        for (int i=0; i<1; i++) {
            TaskImpl.task(FILE_NAME, i);
        }
        /*Waits until all tasks have finished and
        synchronizes the file with its last version*/
        COMPSs.getFile(FILE_NAME);
    }
}
```

4.1.1.5 Managing Failures in Tasks

COMPSs provide mechanism to manage failures in tasks. Developers can specify two properties in the task definition what the runtime should do when a task is blocked or failed.

The `timeOut` property indicates the runtime that a task of this type is considered failed when its duration is larger than the value specified in the property (in seconds)

The `onFailure` property indicates what to do when a task of this type is failed. The possible values are:

- `OnFailure.RETRY` (Default): The task is executed twice in the same worker and a different worker.
- `OnFailure.CANCEL_SUCCESSORS`: All successors of this task are canceled.
- `OnFailure.FAIL`: The task failure produces a failure of the whole application.
- `OnFailure.IGNORE`: The task failure is ignored and the output parameters are set with empty values.

Usage examples of these properties are shown in Code 16

Code 16: Failure example

```
public interface FailuresItf{
    @Method(declaringClass = "example.Example", timeOut = "3000", onFailure = OnFailure.IGNORE)
    void task_example(@Parameter(type = Type.FILE, direction = Direction.OUT) String fileName);
}
```


4.1.1.6 Tasks Groups and COMPSs exceptions

COMPSs allows users to define task groups which can be combined with an special exception (`COMPSsException`) that the user can use to achieve parallel distributed try/catch blocks; [Code 17](#) shows an example of *COMPSsException* raising. In this case, the group definition is blocking, and waits for all task groups to finish. If a task of the group raises a *COMPSsException*, it will be captured by the runtime which reacts to it by canceling the running and pending tasks of the group and forwarding the *COMPSsException* to enable the execution except clause. Consequently, the *COMPSsException* must be combined with task groups.

Code 17: COMPSs Exception example

```
...
    try (COMPSsGroup a = new COMPSsGroup("GroupA")) {
        for (int j = 0; j < N; j++) {
            Test.taskWithCOMPSsException(FILE_NAME);
        }
    } catch (COMPSsException e) {
        Test.otherTask(FILE_NAME);
    }
...

```

It is possible to use a non-blocking task group for asynchronous behaviour (see [Code 18](#)). In this case, the try/catch can be defined later in the code surrounding the *COMPSs.barrierGroup*, enabling to check exception from the defined groups without retrieving data while other tasks are being executed.

Code 18: COMPSs Exception example

```
...
for (int i=0; i<10; i++){
    try (COMPSsGroup a = new COMPSsGroup("Group" + i, false)) {
        for (int j = 0; j < N; j++) {
            Test.taskWithCOMPSsException(FILE_NAME);
        }
    } catch (Exception e) {
        //This is just for compilation. Exception not catch here!
    }
}
for (int i=0; i<10; i++){
    // The group exception will be thrown from the barrier
    try {
        COMPSs.barrierGroup("FailedGroup2");
    } catch (COMPSsException e) {
        System.out.println("Exception caught in barrier!!");
        Test.otherTask(FILE_NAME);
    }
}
}

```

4.1.2 Application Compilation

A COMPSs Java application needs to be packaged in a *jar* file containing the class files of the main code, of the methods implementations and of the *Itf* annotation. This jar package can be generated using the commands available in the Java SDK or creating your application as a Apache Maven project.

To integrate COMPSs in the maven compile process you just need to add the *comps-api* artifact as dependency in the application project.

```
<dependencies>
  <dependency>
    <groupId>es.bsc.compss</groupId>
    <artifactId>compss-api</artifactId>
    <version>${compss.version}</version>
  </dependency>
</dependencies>
```

To build the jar in the maven case use the following command

```
$ mvn package
```

Next we provide a set of commands to compile the Java Simple application (detailed at [Java Sample applications](#)).

```
$ cd tutorial_apps/java/simple/src/main/java/simple/
~/tutorial_apps/java/simple/src/main/java/simple$ javac *.java
~/tutorial_apps/java/simple/src/main/java/simple$ cd ..
~/tutorial_apps/java/simple/src/main/java$ jar cf simple.jar simple/
~/tutorial_apps/java/simple/src/main/java$ mv ./simple.jar ../../../jar/
```

In order to properly compile the code, the CLASSPATH variable has to contain the path of the *compss-engine.jar* package. The default COMPSs installation automatically add this package to the CLASSPATH; please check that your environment variable CLASSPATH contains the *compss-engine.jar* location by running the following command:

```
$ echo $CLASSPATH | grep compss-engine
```

If the result of the previous command is empty it means that you are missing the *compss-engine.jar* package in your classpath. We recommend to automatically load the variable by editing the *.bashrc* file:

```
$ echo "# COMPSs variables for Java compilation" >> ~/.bashrc
$ echo "export CLASSPATH=$CLASSPATH:/opt/COMPSs/Runtime/compss-engine.jar" >> ~/.bashrc
```

If you are using an IDE (such as Eclipse or NetBeans) we recommend you to add the *compss-engine.jar* file as an external file to the project. The *compss-engine.jar* file is available at your current COMPSs installation under the following path: */opt/COMPSs/Runtime/compss-engine.jar*

Please notice that if you have performed a custom installation, the location of the package can be different.

4.1.3 Application Execution

A Java COMPSs application is executed through the *runcompss* script. An example of an invocation of the script is:

```
$ runcompss --classpath=/home/compss/tutorial_apps/java/simple/jar/simple.jar simple.Simple 1
```

A comprehensive description of the *runcompss* command is available in the [Executing COMPSs applications](#) section.

In addition to Java, COMPSs supports the execution of applications written in other languages by means of bindings. A binding manages the interaction of the no-Java application with the COMPSs Java runtime, providing the necessary language translation.

4.2 Python Binding

COMPSs features a binding for Python 2 and 3 applications. The next subsections explain how to program a Python application for COMPSs and a brief overview on how to execute it.

4.2.1 Programming Model

The programming model for Python is structured in the following sections:

4.2.1.1 Task Selection

As in the case of Java, a COMPSs Python application is a Python sequential program that contains calls to tasks. In particular, the user can select as a task:

- Functions
- Instance methods: methods invoked on objects.
- Class methods: static methods belonging to a class.

The task definition in Python is done by means of Python decorators instead of an annotated interface. In particular, the user needs to add a `@task` decorator that describes the task before the definition of the function/method.

As an example (Code 19), let us assume that the application calls a function *func*, which receives a file path (string parameter) and an integer parameter. The code of *func* updates the file.

Code 19: Python application example

```
def func(file_path, value):
    # update the file 'file_path'

def main():
    my_file = '/tmp/sample_file.txt'
    func(my_file, 1)

if __name__ == '__main__':
    main()
```

In order to select *func* as a task, the corresponding `@task` decorator needs to be placed right before the definition of the function, providing some metadata about the parameters of that function. The `@task` decorator has to be imported from the *pycompss* library (Code 20).

Code 20: Python task import

```
from pycompss.api.task import task

@task()
def func():
    ...
```

Tip: The PyCOMPSs task api also provides the `@task` decorator in camelcase (`@Task`) with the same functionality.

The rationale of providing both `@task` and `@Task` relies on following the PEP8 naming convention. Decorators are usually defined using lowercase, but since the task decorator is implemented following the class pattern, its name is also available as camelcase.

Function parameters

The `@task` decorator does not interfere with the function parameters, Consequently, the user can define the function parameters as normal python functions ([Code 21](#)).

Code 21: Task function parameters example

```
@task()
def func(param1, param2):
    ...
```

The use of `*args` and `**kwargs` as function parameters is supported ([Code 22](#)).

Code 22: Python task `*args` and `**kwargs` example

```
@task(returns=int)
def argkwarg_func(*args, **kwargs):
    ...
```

And even with other parameters, such as usual parameters and *default defined arguments*. [Code 23](#) shows an example of a task with two three parameters (whose one of them ('s') has a default value), `*args` and `**kwargs`.

Code 23: Python task with default parameters example

```
@task(returns=int)
def multiarguments_func(v, w, s=2, *args, **kwargs):
    ...
```

Tasks within classes

Functions within classes can also be declared as tasks as normal functions. The main difference is the existence of the `self` parameter which enables to modify the callee object.

For tasks corresponding to instance methods, by default the task is assumed to modify the callee object (the object on which the method is invoked). The programmer can tell otherwise by setting the `target_direction` argument of the `@task` decorator to `IN` ([Code 24](#)).

Code 24: Python instance method example

```
class MyClass(object):
    ...
    @task(target_direction=IN)
    def instance_method(self):
        ... # self is NOT modified here
```

Class methods and static methods can also be declared as tasks. The only requirement is to place the `@classmethod` or `@staticmethod` over the `@task` decorator ([Code 25](#)). Note that there is no need to use the `target_direction` flag within the `@task` decorator.

Code 25: Python `@classmethod` and `@staticmethod` tasks example

```
class MyClass(object):
    ...
    @classmethod
    @task()
    def class_method(cls, a, b, c):
        ...
```

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```

@staticmethod
@task(returns=int)
def static_method(a, b, c):
    ...

```

Tip: Tasks inheritance and overriding supported!!!

Caution: The objects used as task parameters **MUST BE** serializable:

- Implement the `__getstate__` and `__setstate__` functions in their classes for those objects that are not automatically serializable.
- The classes must not be declared in the same file that contains the main method (if `__name__=='__main__'`) (known pickle issue).

Important: For instances of user-defined classes, the classes of these objects should have an empty constructor, otherwise the programmer will not be able to invoke task instance methods on those objects ([Code 26](#)).

Code 26: Using user-defined classes as task returns

```

# In file utils.py
from pycompss.api.task import task
class MyClass(object):
    def __init__(self): # empty constructor
        ...

    @task()
    def yet_another_task(self):
        # do something with the self attributes
        ...

...

# In file main.py
from pycompss.api.task import task
from utils import MyClass

@task(returns=MyClass)
def ret_func():
    ...
    myc = MyClass()
    ...
    return myc

def main():
    o = ret_func()
    # invoking a task instance method on a future object can only
    # be done when an empty constructor is defined in the object's
    # class
    o.yet_another_task()

if __name__=='__main__':
    main()

```

4.2.1.2 Task Parameters

The metadata corresponding to a parameter is specified as an argument of the `@task` decorator, whose name is the formal parameter's name and whose value defines the type and direction of the parameter. The parameter types and directions can be:

Types

- *Primitive types* (integer, long, float, boolean, strings)
- *Objects* (instances of user-defined classes, dictionaries, lists, tuples, complex numbers)
- *Files*
- *Collections* (instances of lists)
- *Dictionaries* (instances of dictionary)
- *Streams*
- *IO streams* (for binaries)

Direction

- Read-only (*IN* - default or *IN_DELETE*)
- Read-write (*INOUT*)
- Write-only (*OUT*)
- Concurrent (*CONCURRENT*)
- Commutative (*COMMUTATIVE*)

COMPSs is able to automatically infer the parameter type for primitive types, strings and objects, while the user needs to specify it for files. On the other hand, the direction is only mandatory for *INOUT* and *OUT* parameters.

Note: please note that in the following cases there is no need to include an argument in the `@task` decorator for a given task parameter:

- Parameters of primitive types (integer, long, float, boolean) and strings: the type of these parameters can be automatically inferred by COMPSs, and their direction is always *IN*.
 - Read-only object parameters: the type of the parameter is automatically inferred, and the direction defaults to *IN*.
-

The parameter metadata is available from the `pycompss` library ([Code 27](#))

Code 27: Python task parameters import

```
from pycompss.api.parameter import *
```

Objects

The default type for a parameter is object. Consequently, there is no need to use a specific keyword. However, it is necessary to indicate its direction (unless for input parameters):

PARAMETER	DESCRIPTION
<i>IN</i>	The parameter is read-only. The type will be inferred.
<i>IN_DELETE</i>	The parameter is read-only. The type will be inferred. Will be automatically removed after its usage.
<i>INOUT</i>	The parameter is read-write. The type will be inferred.
<i>OUT</i>	The parameter is write-only. The type will be inferred.
<i>CONCURRENT</i>	The parameter is read-write with concurrent access. The type will be inferred.
<i>COMMUTATIVE</i>	The parameter is read-write with commutative access. The type will be inferred.

Continuing with the example, in [Code 28](#) the decorator specifies that *func* has a parameter called *obj*, of type object and *INOUT* direction. Note how the second parameter, *i*, does not need to be specified, since its type (integer) and direction (*IN*) are automatically inferred by COMPSs.

Code 28: Python task example with input output object (*INOUT*) and input object (*IN*)

```
from pycompss.api.task import task
from pycompss.api.parameter import INOUT, IN

@task(obj=INOUT, i=IN)
def func(obj, i):
    ...
```

The previous task definition can be simplified due to the default *IN* direction for objects ([Code 29](#)):

Code 29: Python task example with input output object (*INOUT*) simplified

```
from pycompss.api.task import task
from pycompss.api.parameter import INOUT

@task(obj=INOUT)
def func(obj, i):
    ...
```

Tip: In order to choose the appropriate direction, a good exercise is to think if the function only consumes the object (*IN*), modifies the object (*INOUT*), or produces an object (*OUT*).

Tip: The *IN_DELETE* definition is intended to one use objects. Consequently, the information related to the object will be released as soon as possible.

The user can also define that the access to a object is concurrent with *CONCURRENT* ([Code 30](#)). Tasks that share a *CONCURRENT* parameter will be executed in parallel, if any other dependency prevents this. The *CONCURRENT* direction allows users to have access from multiple tasks to the same object/file during their executions.

Code 30: Python task example with *CONCURRENT*

```
from pycompss.api.task import task
from pycompss.api.parameter import CONCURRENT

@task(obj=CONCURRENT)
def func(obj, i):
    ...
```

Important: COMPSs does not manage the interaction with the objects used/modified concurrently. Taking care of the access/modification of the concurrent objects is responsibility of the developer.

Or even, the user can also define that the access to a parameter is commutative with *COMMUTATIVE* ([Code 31](#)). The execution order of tasks that share a *COMMUTATIVE* parameter can be changed by the runtime following the commutative property.

Code 31: Python task example with *COMMUTATIVE*

```
from pycompss.api.task import task
from pycompss.api.parameter import COMMUTATIVE

@task(obj=COMMUTATIVE)
def func(obj, i):
    ...
```

Files

It is possible to define that a parameter is a file (*FILE*), and its direction:

PARAMETER	DESCRIPTION
<i>FILE/FILE_IN</i>	The parameter is a file. The direction is assumed to be <i>IN</i> .
<i>FILE_INOUT</i>	The parameter is a read-write file.
<i>FILE_OUT</i>	The parameter is a write-only file.
<i>FILE_CONCURRENT</i>	The parameter is a concurrent read-write file.
<i>FILE_COMMUTATIVE</i>	The parameter is a commutative read-write file.

Continuing with the example, in [Code 32](#) the decorator specifies that `func` has a parameter called `f`, of type `FILE` and `INOUT` direction (`FILE_INOUT`).

Code 32: Python task example with input output file (*FILE_* - *INOUT*)

```
from pycompss.api.task import task
from pycompss.api.parameter import FILE_INOUT

@task(f=FILE_INOUT)
def func(f):
    fd = open(f, 'a+')
    ...
    # append something to fd
    ...
    fd.close()

def main():
    f = "/path/to/file.extension"
    # Populate f
    func(f)
```

Tip: The value for a `FILE` (e.g. `f`) is a string pointing to the file to be used at `func` task. However, it can also be `None` if it is optional. Consequently, the user can define task that can receive a `FILE` or not, and act accordingly. For example ([Code 33](#)):

Code 33: Python task example with optional input file (*FILE_IN*)

```
from pycompss.api.task import task
from pycompss.api.parameter import FILE_IN

@task(f=FILE_IN)
def func(f):
    if f:
```

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```

    # Do something with the file
    with open(f, 'r') as fd:
        num_lines = len(rd.readlines())
    return num_lines
else:
    # Do something when there is no input file
    return -1

def main():
    f = "/path/to/file.extension"
    # Populate f
    num_lines_f = func(f) # num_lines_f == actual number of lines of file.extension
    g = None
    num_lines_g = func(g) # num_lines_g == -1

```

The user can also define that the access to file parameter is concurrent with *FILE_CONCURRENT* (Code 34). Tasks that share a *FILE_CONCURRENT* parameter will be executed in parallel, if any other dependency prevents this. The *CONCURRENT* direction allows users to have access from multiple tasks to the same file during their executions.

Code 34: Python task example with *FILE_CONCURRENT*

```

from pycompss.api.task import task
from pycompss.api.parameter import FILE_CONCURRENT

@task(f=FILE_CONCURRENT)
def func(f, i):
    ...

```

Important: COMPSs does not manage the interaction with the files used/modified concurrently. Taking care of the access/modification of the concurrent files is responsibility of the developer.

Or even, the user can also define that the access to a parameter is a file *FILE_COMMUTATIVE* (Code 35). The execution order of tasks that share a *FILE_COMMUTATIVE* parameter can be changed by the runtime following the commutative property.

Code 35: Python task example with *FILE_COMMUTATIVE*

```

from pycompss.api.task import task
from pycompss.api.parameter import FILE_COMMUTATIVE

@task(f=FILE_COMMUTATIVE)
def func(f, i):
    ...

```

Directories

In addition to files, it is possible to define that a parameter is a directory (*DIRECTORY*), and its direction:

PARAMETER	DESCRIPTION
<i>DIRECTORY_IN</i>	The parameter is a directory and the direction is <i>IN</i> . The directory will be compressed before any transfer amongst nodes.
<i>DIRECTORY_INOUT</i>	The parameter is a read-write directory. The directory will be compressed before any transfer amongst nodes.
<i>DIRECTORY_OUT</i>	The parameter is a write-only directory. The directory will be compressed before any transfer amongst nodes.

The definition of a *DIRECTORY* parameter is shown in [Code 36](#). The decorator specifies that *func* has a parameter called *d*, of type *DIRECTORY* and *INOUT* direction.

Code 36: Python task example with input output directory (*DIRECTORY_INOUT*)

```

from pycompss.api.task import task
from pycompss.api.parameter import DIRECTORY_INOUT

@task(d=DIRECTORY_INOUT)
def func(d):
    ...

```

Collections

It is possible to specify that a parameter is a collection of elements (e.g. list) and its direction.

PARAMETER	DESCRIPTION
<i>COLLECTION_IN</i>	The parameter is read-only collection.
<i>COLLECTION_IN_DELETE</i>	The parameter is read-only collection for single usage (will be automatically removed after its usage).
<i>COLLECTION_INOUT</i>	The parameter is read-write collection.
<i>COLLECTION_OUT</i>	The parameter is write-only collection.

In this case ([Code 37](#)), the list may contain sub-objects that will be handled automatically by the runtime. It is important to annotate data structures as collections if in other tasks there are accesses to individual elements of these collections as parameters. Without this annotation, the runtime will not be able to identify data dependences between the collections and the individual elements.

Code 37: Python task example with *COLLECTION (IN)*

```

from pycompss.api.task import task
from pycompss.api.parameter import COLLECTION

@task(my_collection=COLLECTION)
def func(my_collection):
    for element in my_collection:
        ...

```

The sub-objects of the collection can be collections of elements (and recursively). In this case, the runtime also keeps track of all elements contained in all sub-collections. In order to improve the performance, the depth of the sub-objects can be limited through the use of the *depth* parameter (Code 38)

Code 38: Python task example with *COLLECTION_IN* and *Depth*

```

from pycompss.api.task import task
from pycompss.api.parameter import COLLECTION_IN

@task(my_collection={Type:COLLECTION_IN, Depth:2})
def func(my_collection):
    for inner_collection in my_collection:
        for element in inner_collection:
            # The contents of element will not be tracked
        ...

```

Tip: A collection can contain dictionaries, and will be analyzed automatically.

Tip: If the collection is intended to be used only once with IN direction, the *COLLECTION_IN_DELETE* type is recommended, since it automatically removes the entire collection after the task. This enables to release as soon as possible memory and storage.

Collections of files

It is also possible to specify that a parameter is a collection of files (e.g. list) and its direction.

PARAMETER	DESCRIPTION
<i>COLLECTION_FILE/COLLECTION_FILE_IN</i>	The parameter is read-only collection of files.
<i>COLLECTION_FILE_INOUT</i>	The parameter is read-write collection of files.
<i>COLLECTION_FILE_OUT</i>	The parameter is write-only collection of files.

In this case (Code 39), the list may contain files that will be handled automatically by the runtime. It is important to annotate data structures as collections if in other tasks there are accesses to individual elements of these collections as parameters. Without this annotation, the runtime will not be able to identify data dependences between the collections and the individual elements.

Code 39: Python task example with *COLLECTION_FILE (IN)*

```

from pycompss.api.task import task
from pycompss.api.parameter import COLLECTION_FILE

@task(my_collection=COLLECTION_FILE)

```

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```
def func(my_collection):
    for file in my_collection:
        ...
```

The file of the collection can be collections of elements (and recursively). In this case, the runtime also keeps track of all files contained in all sub-collections. In order to improve the performance, the depth of the sub-files can be limited through the use of the *depth* parameter as with objects ([Code 38](#))

Dictionaries

It is possible to specify that a parameter is a dictionary of elements (e.g. dict) and its direction.

PARAMETER	DESCRIPTION
<i>DICTIONARY_IN</i>	The parameter is read-only dictionary.
<i>DICTIONARY_IN_DELETE</i>	The parameter is read-only dictionary for single usage (will be automatically removed after its usage).
<i>DICTIONARY_INOUT</i>	The parameter is read-write dictionary.

As with the collections, it is possible to specify that a parameter is a dictionary of elements (e.g. dict) and its direction (*DICTIONARY_IN* or *DICTIONARY_INOUT*) ([Code 40](#)), whose sub-objects will be handled automatically by the runtime.

Code 40: Python task example with *DICTIONARY_IN*

```
from pycompss.api.task import task
from pycompss.api.parameter import DICTIONARY

@task(my_dictionary=DICTIONARY)
def func(my_dictionary):
    for k, v in my_dictionary.items():
        ...
```

The sub-objects of the dictionary can be collections or dictionary of elements (and recursively). In this case, the runtime also keeps track of all elements contained in all sub-collections/sub-dictionaries. In order to improve the performance, the depth of the sub-objects can be limited through the use of the *depth* parameter ([Code 41](#))

Code 41: Python task example with *DICTIONARY_IN* and *Depth*

```
from pycompss.api.task import task
from pycompss.api.parameter import DICTIONARY_IN

@task(my_dictionary={Type:DICTIONARY_IN, Depth:2})
def func(my_dictionary):
    for key, inner_dictionary in my_dictionary.items():
        for sub_key, sub_value in inner_dictionary.items():
            # The contents of element will not be tracked
        ...
```

Tip: A dictionary can contain collections, and will be analyzed automatically.

Tip: If the dictionary is intended to be used only once with *IN* direction, the *DICTIONARY_IN_DELETE* type is recommended, since it automatically removes the entire dictionary after the task. This enables to release as soon

as possible memory and storage.

Streams

It is possible to use streams as input or output of the tasks by defining that a parameter is *STREAM* and its direction.

PARAMETER	DESCRIPTION
<i>STREAM_IN</i>	The parameter is a read-only stream.
<i>STREAM_OUT</i>	The parameter is a write-only stream.

For example, [Code 42](#) shows an example using *STREAM_IN* or *STREAM_OUT* parameters. These parameters enable to mix a task-driven workflow with a data-driven workflow.

Code 42: Python task example with *STREAM_IN* and *STREAM_OUT*

```
from pycompss.api.task import task
from pycompss.api.parameter import STREAM_IN
from pycompss.api.parameter import STREAM_OUT

@task(ods=STREAM_OUT)
def write_objects(ods):
    ...
    for i in range(NUM_OBJECTS):
        # Build object
        obj = MyObject()
        # Publish object
        ods.publish(obj)
    ...
    # Mark the stream for closure
    ods.close()

@task(ods=STREAM_IN, returns=int)
def read_objects(ods):
    ...
    num_total = 0
    while not ods.is_closed():
        # Poll new objects
        new_objects = ods.poll()
        # Process files
        ...
        # Accumulate read files
        num_total += len(new_objects)
    ...
    # Return the number of processed files
    return num_total
```

The stream parameter also supports Files ([Code 43](#)).

Code 43: Python task example with *STREAM_IN* and *STREAM_OUT* for files

```
from pycompss.api.task import task
from pycompss.api.parameter import STREAM_IN
```

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```

from pycompss.api.parameter import STREAM_OUT

@task(fds=STREAM_OUT)
def write_files(fds):
    ...
    for i in range(NUM_FILES):
        file_name = str(uuid.uuid4())
        # Write file
        with open(file_path, 'w') as f:
            f.write("Test " + str(i))
        ...
    ...
    # Mark the stream for closure
    fds.close()

@task(fds=STREAM_IN, returns=int)
def read_files(fds):
    ...
    num_total = 0
    while not fds.is_closed():
        # Poll new files
        new_files = fds.poll()
        # Process files
        for nf in new_files:
            with open(nf, 'r') as f:
                ...
        # Accumulate read files
        num_total += len(new_files)
    ...
    # Return the number of processed files
    return num_total

```

In addition, the stream parameter can also be defined for binary tasks ([Code 44](#)).

Code 44: Python task example with *STREAM_OUT* for binaries

```

from pycompss.api.task import task
from pycompss.api.binary import binary
from pycompss.api.parameter import STREAM_OUT

@binary(binary="file_generator.sh")
@task(fds=STREAM_OUT)
def write_files(fds):
    # Equivalent to: ./file_generator.sh > fds
    pass

```

Standard Streams

Finally, a parameter can also be defined as the standard input, standard output, and standard error.

PARAMETER	DESCRIPTION
<i>STDIN</i>	The parameter is a IO stream for standard input redirection.
<i>STDOUT</i>	The parameter is a IO stream for standard output redirection.
<i>STDERR</i>	The parameter is a IO stream for standard error redirection.

Important: *STDIN*, *STDOUT* and *STDERR* are only supported in binary tasks

This is particularly useful with binary tasks that consume/produce from standard IO streams, and the user wants to redirect the standard input/output/error to a particular file. [Code 45](#) shows an example of a binary task that invokes *output_generator.sh* which produces the result in the standard output, and the task takes that output and stores it into *fds*.

Code 45: Python task example with *STDOUT* for binaries

```
from pycompss.api.task import task
from pycompss.api.binary import binary
from pycompss.api.parameter import STDOUT

@binary(binary="output_generator.sh")
@task(fds=STDOUT)
def write_files(fds):
    # Equivalent to: ./file_generator.sh > fds
    pass
```

4.2.1.3 Other Task Parameters

Task time out

The user is also able to define the time out of a task within the `@task` decorator with the `time_out=<TIME_IN_SECONDS>` hint. The runtime will cancel the task if the time to execute the task exceeds the time defined by the user. For example, [Code 46](#) shows how to specify that the `unknown_duration_task` maximum duration before canceling (if exceeded) is one hour.

Code 46: Python task *time_out* example

```
@task(time_out=3600)
def unknown_duration_task(self):
    ...
```

Scheduler hints

The programmer can provide hints to the scheduler through specific arguments within the `@task` decorator.

For instance, the programmer can mark a task as a high-priority task with the `priority` argument of the `@task` decorator ([Code 47](#)). In this way, when the task is free of dependencies, it will be scheduled before any of the available low-priority (regular) tasks. This functionality is useful for tasks that are in the critical path of the application's task dependency graph.

Code 47: Python task *priority* example

```
@task(priority=True)
def func():
    ...
```

Moreover, the user can also mark a task as distributed with the *is_distributed* argument or as replicated with the *is_replicated* argument (Code 48). When a task is marked with *is_distributed=True*, the method must be scheduled in a forced round robin among the available resources. On the other hand, when a task is marked with *is_replicated=True*, the method must be executed in all the worker nodes when invoked from the main application. The default value for these parameters is False.

Code 48: Python task *is_distributed* and *is_replicated* examples

```
@task(is_distributed=True)
def func():
    ...

@task(is_replicated=True)
def func2():
    ...
```

On failure task behaviour

In case a task fails, the whole application behaviour can be defined using the *@on_failure* decorator on top of the *@task* decorator (Code 49). It has four possible values that can be defined with the **management** parameter: **'RETRY'**, **'CANCEL_SUCCESSORS'**, **'FAIL'** and **'IGNORE'**. **'RETRY'** is the default behaviour, making the task to be executed again (on the same worker or in another worker if the failure remains). **'CANCEL_SUCCESSORS'** ignores the failed task and cancels the execution of the successor tasks, **'FAIL'** stops the whole execution once a task fails and **'IGNORE'** ignores the failure and continues with the normal execution.

Code 49: Python task *@on_failure* decorator example

```
from pycompss.api.task import task
from pycompss.api.on_failure import on_failure

@on_failure(management = 'CANCEL_SUCCESSORS')
@task()
def func():
    ...
```

Since the **'CANCEL_SUCCESSORS'** and **'IGNORE'** policies enable to continue the execution accepting that tasks may have failed, it is possible to define the value for the objects and/or files produced by the failed tasks (INOUT, OUT, FILE_INOUT, FILE_OUT and return). This is considered as the default output objects/files. For example, Code 50 shows a the *func* task which returns one integer. In the case of failure within *func*, the execution of the workflow will continue since the on failure management policy is set to **'IGNORE'**, with 0 as return value.

Code 50: Python task *@on_failure* example with default return value

```
from pycompss.api.task import task
from pycompss.api.on_failure import on_failure

@on_failure(management='IGNORE', returns=0)
@task(returns=int)
```

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```
def func():
    ...
```

For the INOUT parameters, the default value can be set by using the parameter name of `func` in the `@on_failure` decorator. [Code 51](#) shows how to define the default value for a `FILE_INOUT` parameter (named `f_inout`). The example is also valid for `FILE_OUT` values.

Code 51: Python task `@on_failure` example with default `FILE_INOUT` value

```
from pycompss.api.task import task
from pycompss.api.on_failure import on_failure
from pycompss.api.parameter import FILE_INOUT

@on_failure(management='IGNORE', f_inout="/path/to/default.file")
@task(f_inout=FILE_INOUT)
def func(f_inout):
    ...
```

Tip: The default `FILE_INOUT`/`FILE_OUT` can be generated at task generation time by calling a function instead of providing a static file path. [Code 52](#) shows an example of this case, where the default value for the output file produced by `func` is defined by the `generate_empty` function.

Code 52: Python task `@on_failure` example with default `FILE_OUT` value from function

```
from pycompss.api.task import task
from pycompss.api.on_failure import on_failure
from pycompss.api.parameter import FILE_OUT

def generate_empty(msg, name):
    empty_file = "/tmp/empty_file_" + name
    with open(empty_file, 'w') as f:
        f.write("EMPTY FILE " + msg)
    return empty_file

@on_failure(management='IGNORE', f_out=generate_empty("OUT", "out.tmp"))
@task(f_out=FILE_OUT)
def func(f_inout):
    ...
```

4.2.1.4 Task Parameters Summary

[Table 8](#) summarizes all arguments that can be found in the `@task` decorator.

Table 8: Arguments of the `@task` decorator

Argument	Value	
Formal parameter name	(default: empty)	The parameter is an object or a simple
	IN	Read-only parameter, all types.
	IN_DELETE	Read-only parameter, all types. Autom
	INOUT	Read-write parameter, all types except f
	OUT	Write-only parameter, all types except f
	CONCURRENT	Concurrent read-write parameter, all ty

Table 8 – continued from previous page

Argument	Value
	COMMUTATIVE
	FILE(_IN)
	FILE_INOUT
	FILE_OUT
	FILE_CONCURRENT
	FILE_COMMUTATIVE
	DIRECTORY(_IN)
	DIRECTORY_INOUT
	DIRECTORY_OUT
	COLLECTION(_IN)
	COLLECTION_IN_DELETE
	COLLECTION_INOUT
	COLLECTION_OUT
	COLLECTION_FILE(_IN)
	COLLECTION_FILE_INOUT
	COLLECTION_FILE_OUT
	DICTIONARY(_IN)
	DICTIONARY_IN_DELETE
	DICTIONARY_INOUT
	STREAM_IN
	STREAM_OUT
	STDIN
	STDOUT
	STDERR
	Explicit: {Type:(empty=object)/FILE/COLLECTION/DICTIONARY, Direction:(empty=IN)/DELETE/INOUT/OUT/CONCURRENT}
returns	int (for integer and boolean), long, float, str, dict, list, tuple, user-defined classes
target_direction	INOUT (default), IN or CONCURRENT
priority	True or False (default)
is_distributed	True or False (default)
is_replicated	True or False (default)
on_failure	'RETRY' (default), 'CANCEL_SUCCESSORS', 'FAIL' or 'IGNORE'
time_out	int (time in seconds)

4.2.1.5 Task Return

If the function or method returns a value, the programmer can use the *returns* argument within the *@task* decorator. In this argument, the programmer can specify the type of that value (Code 53).

Code 53: Python task returns example

```
@task(returns=int)
def ret_func():
    return 1
```

Moreover, if the function or method returns more than one value, the programmer can specify how many and their type in the *returns* argument. Code 54 shows how to specify that two values (an integer and a list) are returned.

Code 54: Python task with multireturn example

```
@task(returns=(int, list))
def ret_func():
    return 1, [2, 3]
```

Alternatively, the user can specify the number of return statements as an integer value (Code 55). This way of specifying the amount of return eases the *returns* definition since the user does not need to specify explicitly the

type of the return arguments. However, it must be considered that the type of the object returned when the task is invoked will be a future object. This consideration may lead to an error if the user expects to invoke a task defined within an object returned by a previous task. In this scenario, the solution is to specify explicitly the return type.

Code 55: Python task returns with integer example

```
@task(returns=1)
def ret_func():
    return "my_string"

@task(returns=2)
def ret_func():
    return 1, [2, 3]
```

Important: If the programmer selects as a task a function or method that returns a value, that value is not generated until the task executes (Code 56).

Code 56: Task return value generation

```
@task(return=MyClass)
def ret_func():
    return MyClass(...)

...

if __name__ == '__main__':
    o = ret_func()  # o is a future object
```

The object returned can be involved in a subsequent task call, and the COMPSs runtime will automatically find the corresponding data dependency. In the following example, the object *o* is passed as a parameter and callee of two subsequent (asynchronous) tasks, respectively (Code 57).

Code 57: Task return value subsequent usage

```
if __name__ == '__main__':
    # o is a future object
    o = ret_func()

    ...

    another_task(o)

    ...

    o.yet_another_task()
```

Tip: PyCOMPSs is able to infer if the task returns something and its amount in most cases. Consequently, the user can specify the task without *returns* argument. But this is discouraged since it requires code analysis, including an overhead that can be avoided by using the *returns* argument.

Tip: PyCOMPSs is compatible with Python 3 type hinting. So, if type hinting is present in the code, PyCOMPSs is able to detect the return type and use it (there is no need to use the *returns*):

Code 58: Python task returns with type hinting

```
@task()
def ret_func() -> str:
    return "my_string"

@task()
def ret_func() -> (int, list):
    return 1, [2, 3]
```

4.2.1.6 Other task types

In addition to this API functions, the programmer can use a set of decorators for other purposes.

For instance, there is a set of decorators that can be placed over the `@task` decorator in order to define the task methods as a **binary invocation** (with the [Binary decorator](#)), as a **OmpSs invocation** (with the [OmpSs decorator](#)), as a **MPI invocation** (with the [MPI decorator](#)), as a **COMPSs application** (with the [COMPSs decorator](#)), as a **task that requires multiple nodes** (with the [Multinode decorator](#)), or as a **Reduction task** that can be executed in parallel having a subset of the original input data as input (with the [Reduction decorator](#)). These decorators must be placed over the `@task` decorator, and under the `@constraint` decorator if defined.

Consequently, the task body will be empty and the function parameters will be used as invocation parameters with some extra information that can be provided within the `@task` decorator.

The following subparagraphs describe their usage.

Binary decorator

The `@binary` (or `@Binary`) decorator shall be used to define that a task is going to invoke a binary executable.

In this context, the `@task` decorator parameters will be used as the binary invocation parameters (following their order in the function definition). Since the invocation parameters can be of different nature, information on their type can be provided through the `@task` decorator.

Code 59 shows the most simple binary task definition without/with constraints (without parameters); please note that `@constraint` decorator has to be provided on top of the others.

Code 59: Binary task example

```
from pycompss.api.task import task
from pycompss.api.binary import binary

@binary(binary="mybinary.bin")
@task()
def binary_func():
    pass

@constraint(computingUnits="2")
@binary(binary="otherbinary.bin")
@task()
def binary_func2():
    pass
```

The invocation of these tasks would be equivalent to:

```
$ ./mybinary.bin
$ ./otherbinary.bin    # in resources that respect the constraint.
```

The `@binary` decorator supports the `working_dir` parameter to define the working directory for the execution of the defined binary.

Code 60 shows a more complex binary invocation, with files as parameters:

Code 60: Binary task example 2

```
from pycompss.api.task import task
from pycompss.api.binary import binary
from pycompss.api.parameter import *

@binary(binary="grep", working_dir=".")
@task(infile={Type:FILE_IN_STDIN}, result={Type:FILE_OUT_STDOUT})
def grepper():
    pass

# This task definition is equivalent to the following, which is more verbose:

@binary(binary="grep", working_dir=".")
@task(infile={Type:FILE_IN, StdIOStream:STDIN}, result={Type:FILE_OUT, StdIOStream:STDOUT})
def grepper(keyword, infile, result):
    pass

if __name__ == '__main__':
    infile = "infile.txt"
    outfile = "outfile.txt"
    grepper("Hi", infile, outfile)
```

The invocation of the *grepper* task would be equivalent to:

```
$ # grep keyword < infile > result
$ grep Hi < infile.txt > outfile.txt
```

Please note that the *keyword* parameter is a string, and it is respected as is in the invocation call.

Thus, PyCOMPSs can also deal with prefixes for the given parameters. Code 61 performs a system call (`ls`) with specific prefixes:

Code 61: Binary task example 3

```
from pycompss.api.task import task
from pycompss.api.binary import binary
from pycompss.api.parameter import *

@binary(binary="ls")
@task(hide={Type:FILE_IN, Prefix:"--hide="}, sort={Prefix:"--sort="})
def myLs(flag, hide, sort):
    pass

if __name__ == '__main__':
    flag = '-l'
    hideFile = "fileToHide.txt"
    sort = "time"
    myLs(flag, hideFile, sort)
```

The invocation of the *myLs* task would be equivalent to:

```
$ # ls -l --hide=hide --sort=sort
$ ls -l --hide=fileToHide.txt --sort=time
```

This particular case is intended to show all the power of the `@binary` decorator in conjunction with the `@task` decorator. Please note that although the `hide` parameter is used as a prefix for the binary invocation, the `fileToHide.txt` would also be transferred to the worker (if necessary) since its type is defined as `FILE_IN`. This feature enables to build more complex binary invocations.

In addition, the `@binary` decorator also supports the `fail_by_exit_value` parameter to define the failure of the task by the exit value of the binary ([Code 62](#)). It accepts a boolean (`True` to consider the task failed if the exit value is not 0, or `False` to ignore the failure by the exit value (**default**)), or a string to determine the environment variable that defines the fail by exit value (as boolean). The default behaviour (`fail_by_exit_value=False`) allows users to receive the exit value of the binary as the task return value, and take the necessary decisions based on this value.

Code 62: Binary task example with `fail_by_exit_value`

```
@binary(binary="mybinary.bin", fail_by_exit_value=True)
@task()
def binary_func():
    pass
```

OmpSs decorator

The `@ompss` (or `@OmpSs`) decorator shall be used to define that a task is going to invoke a OmpSs executable ([Code 63](#)).

Code 63: OmpSs task example

```
from pycompss.api.ompss import ompss

@ompss(binary="ompssApp.bin")
@task()
def ompss_func():
    pass
```

The OmpSs executable invocation can also be enriched with parameters, files and prefixes as with the `@binary` decorator through the function parameters and `@task` decorator information. Please, check [Binary decorator](#) for more details.

MPI decorator

The `@mpi` (or `@Mpi`) decorator shall be used to define that a task is going to invoke a MPI executable ([Code 64](#)).

Code 64: MPI task example

```
from pycompss.api.mpi import mpi

@mpi(binary="mpiApp.bin", runner="mpirun", processes=2)
@task()
def mpi_func():
    pass
```

The MPI executable invocation can also be enriched with parameters, files and prefixes as with the `@binary` decorator through the function parameters and `@task` decorator information. Please, check [Binary decorator](#) for more details.

The `@mpi` decorator can be also used to execute a MPI for python (mpi4py) code. To indicate it, developers only need to remove the binary field and include the Python MPI task implementation inside the function body as shown in the following example ([Code 65](#)).

Code 65: MPI task example with collections and data layout

```

from pycompss.api.mpi import mpi

@mpi(processes=4)
@task()
def layout_test_with_all():
    from mpi4py import MPI
    rank = MPI.COMM_WORLD.rank
    return rank

```

In both cases, users can also define, MPI + OpenMP tasks by using `processes` property to indicate the number of MPI processes and `computing_units` in the Task Constraints to indicate the number of OpenMP threads per MPI process.

The `@mpi` decorator can be combined with collections to allow the process of a list of parameters in the same MPI execution. By the default, all parameters of the list will be deserialized to all the MPI processes. However, a common pattern in MPI is that each MPI processes performs the computation in a subset of data. So, all data serialization is not needed. To indicate the subset used by each MPI process, developers can use the `data_layout` notation inside the MPI task declaration.

Code 66: MPI task example with collections and data layout

```

from pycompss.api.mpi import mpi

@mpi(processes=4, col_layout={block_count: 4, block_length: 2, stride: 1})
@task(col=COLLECTION_IN, returns=4)
def layout_test_with_all(col):
    from mpi4py import MPI
    rank = MPI.COMM_WORLD.rank
    return data[0]+data[1]+rank

```

Figure (Code 66) shows an example about how to combine MPI tasks with collections and data layouts. In this example, we have define a MPI task with an input collection (`col`). We have also defined a data layout with the property `<arg_name>_layout` and we specify the number of blocks (`block_count`), the elements per block (`block_length`), and the number of element between the starting block points (`stride`).

COMPSs decorator

The `@compss` (or `@COMPSs`) decorator shall be used to define that a task is going to be a COMPSs application (Code 67). It enables to have nested PyCOMPSs/COMPSs applications.

Code 67: COMPSs task example

```
from pycompss.api.compss import compss

@compss(runcompss="${RUNCOMPSS}", flags="-d",
        app_name="/path/to/simple_compss_nested.py", computing_nodes="2")
@task()
def compss_func():
    pass
```

The COMPSs application invocation can also be enriched with the flags accepted by the *runcompss* executable. Please, check execution manual for more details about the supported flags.

Multinode decorator

The *@multinode* (or *@Multinode*) decorator shall be used to define that a task is going to use multiple nodes (e.g. using internal parallelism) ([Code 68](#)).

Code 68: Multinode task example

```
from pycompss.api.multinode import multinode

@multinode(computing_nodes="2")
@task()
def multinode_func():
    pass
```

The only supported parameter is *computing_nodes*, used to define the number of nodes required by the task (the default value is 1). The mechanism to get the number of nodes, threads and their names to the task is through the *COMPSS_NUM_NODES*, *COMPSS_NUM_THREADS* and *COMPSS_HOSTNAMES* environment variables respectively, which are exported within the task scope by the COMPSs runtime before the task execution.

Reduction decorator

The *@reduction* (or *@Reduction*) decorator shall be used to define that a task is going to be subdivided into smaller tasks that take as input a subset of the input data. ([Code 69](#)).

Code 69: Reduction task example

```
from pycompss.api.reduction import reduction

@reduction(chunk_size="2")
@task()
def myreduction():
    pass
```

The only supported parameter is *chunk_size*, used to define the size of the data that the generated tasks will get as input parameter. The data given as input to the main reduction task is subdivided into chunks of the set size.

Container decorator

The `@container` (or `@Container`) decorator shall be used to define that a task is going to be executed within a container ([Code 70](#)).

Code 70: Container task example

```
from pycompss.api.compss import container
from pycompss.api.task import task
from pycompss.api.parameter import *
from pycompss.api.api import compss_wait_on

@container(engine="DOCKER",
           image="compss/compss")
@task(returns=1, num=IN, in_str=IN, fin=FILE_IN)
def container_fun(num, in_str, fin):
    # Sample task body:
    with open(fin, "r") as fd:
        num_lines = len(fd.readlines())
    str_len = len(in_str)
    result = num * str_len * num_lines

    # You can import and use libraries available in the container

    return result

if __name__ == '__main__':
    result = container_fun(5, "hello", "dataset.txt")
    result = compss_wait_on(result)
    print("result: %s" % result)
```

The *container_fun* task will be executed within the container defined in the *@container* decorator using the *docker* engine with the *compss/compss* image. This task is pure python and you can import and use any library available in the container

This feature allows to use specific containers for tasks where the library dependencies are met.

Tip: Singularity is also supported, and can be selected by setting the engine to SINGULARITY:

```
@container(engine=SINGULARITY)
```

In addition, the *@container* decorator can be placed on top of the *@binary*, *@ompss* or *@mpi* decorators. [Code 71](#) shows how to execute the same example described in the [Binary decorator](#) section, but within the *compss/compss* container using *docker*. This will execute the *binary/ompss/mpi* binary within the container.

Code 71: Container binary task example

```
from pycompss.api.compss import container
from pycompss.api.task import task
from pycompss.api.binary import binary
from pycompss.api.parameter import *

@container(engine="DOCKER",
           image="compss/compss")
@binary(binary="grep", working_dir=".")
@task(infile={Type:FILE_IN_STDIN}, result={Type:FILE_OUT_STDOUT})
def grepper():
    pass

if __name__ == '__main__':
    infile = "infile.txt"
    outfile = "outfile.txt"
    grepper("Hi", infile, outfile)
```

Other task types summary

Next tables summarizes the parameters of these decorators.

- @binary

Parameter	Description
binary	(Mandatory) String defining the full path of the binary that must be executed.
working_dir	Full path of the binary working directory inside the COMPSs Worker.

- @ompss

Parameter	Description
binary	(Mandatory) String defining the full path of the binary that must be executed.
working_dir	Full path of the binary working directory inside the COMPSs Worker.

- @mpi

Parameter	Description
binary	(Optional) String defining the full path of the binary that must be executed. Empty indicates python MPI code.
working_dir	Full path of the binary working directory inside the COMPSs Worker.
runner	(Mandatory) String defining the MPI runner command.
processes	Integer defining the number of computing nodes reserved for the MPI execution (only a single node is reserved by default).

- @compss

Parameter	Description
runcompss	(Mandatory) String defining the full path of the runcompss binary that must be executed.
flags	String defining the flags needed for the runcompss execution.
app_name	(Mandatory) String defining the application that must be executed.
computing_nodes	Integer defining the number of computing nodes reserved for the COMPSs execution (only a single node is reserved by default).

- @multinode

Parameter	Description
computing_nodes	Integer defining the number of computing nodes reserved for the task execution (only a single node is reserved by default).

- **@reduction**

Parameter	Description
chunk_size	Size of data fragments to be given as input parameter to the reduction function.

- **@container**

Parameter	Description
engine	Container engine to use (e.g. DOCKER or SINGULARITY).
image	Container image to be deployed and used for the task execution.

In addition to the parameters that can be used within the *@task* decorator, [Table 9](#) summarizes the *StdIOStream* parameter that can be used within the *@task* decorator for the function parameters when using the *@binary*, *@ompss* and *@mpi* decorators. In particular, the *StdIOStream* parameter is used to indicate that a parameter is going to be considered as a *FILE* but as a stream (e.g. *>*, *<* and *2 >* in bash) for the *@binary*, *@ompss* and *@mpi* calls.

Table 9: Supported StdIOStreams for the *@binary*, *@ompss* and *@mpi* decorators

Parameter	Description
(default: empty)	Not a stream.
STDIN	Standard input.
STDOUT	Standard output.
STDERR	Standard error.

Moreover, there are some shortcuts that can be used for files type definition as parameters within the *@task* decorator ([Table 10](#)). It is not necessary to indicate the *Direction* nor the *StdIOStream* since it may be already be indicated with the shortcut.

Table 10: File parameters definition shortcuts

Alias	Description
<code>COLLECTION(_IN)</code>	Type: COLLECTION, Direction: IN
<code>COLLECTION_IN_DELETE</code>	Type: COLLECTION, Direction: IN_DELETE
<code>COLLECTION_INOUT</code>	Type: COLLECTION, Direction: INOUT
<code>COLLECTION_OUT</code>	Type: COLLECTION, Direction: OUT
<code>DICTIONARY(_IN)</code>	Type: DICTIONARY, Direction: IN
<code>DICTIONARY_IN_DELETE</code>	Type: DICTIONARY, Direction: IN_DELETE
<code>DICTIONARY_INOUT</code>	Type: DICTIONARY, Direction: INOUT
<code>COLLECTION_FILE(_IN)</code>	Type: COLLECTION (File), Direction: IN
<code>COLLECTION_FILE_INOUT</code>	Type: COLLECTION (File), Direction: INOUT
<code>COLLECTION_FILE_OUT</code>	Type: COLLECTION (File), Direction: OUT
<code>FILE(_IN)_STDIN</code>	Type: File, Direction: IN, StdIOStream: STDIN
<code>FILE(_IN)_STDOUT</code>	Type: File, Direction: IN, StdIOStream: STDOUT
<code>FILE(_IN)_STDERR</code>	Type: File, Direction: IN, StdIOStream: STDERR
<code>FILE_OUT_STDIN</code>	Type: File, Direction: OUT, StdIOStream: STDIN
<code>FILE_OUT_STDOUT</code>	Type: File, Direction: OUT, StdIOStream: STDOUT
<code>FILE_OUT_STDERR</code>	Type: File, Direction: OUT, StdIOStream: STDERR
<code>FILE_INOUT_STDIN</code>	Type: File, Direction: INOUT, StdIOStream: STDIN
<code>FILE_INOUT_STDOUT</code>	Type: File, Direction: INOUT, StdIOStream: STDOUT
<code>FILE_INOUT_STDERR</code>	Type: File, Direction: INOUT, StdIOStream: STDERR
<code>FILE_CONCURRENT</code>	Type: File, Direction: CONCURRENT
<code>FILE_CONCURRENT_STDIN</code>	Type: File, Direction: CONCURRENT, StdIOStream: STDIN
<code>FILE_CONCURRENT_STDOUT</code>	Type: File, Direction: CONCURRENT, StdIOStream: STDOUT
<code>FILE_CONCURRENT_STDERR</code>	Type: File, Direction: CONCURRENT, StdIOStream: STDERR
<code>FILE_COMMUTATIVE</code>	Type: File, Direction: COMMUTATIVE
<code>FILE_COMMUTATIVE_STDIN</code>	Type: File, Direction: COMMUTATIVE, StdIOStream: STDIN
<code>FILE_COMMUTATIVE_STD- OUT</code>	Type: File, Direction: COMMUTATIVE, StdIOStream: STDOUT
<code>FILE_COMMUTATIVE_- STDERR</code>	Type: File, Direction: COMMUTATIVE, StdIOStream: STDERR

These parameter keys, as well as the shortcuts, can be imported from the PyCOMPSs library:

```
from pycompss.api.parameter import *
```

4.2.1.7 Task Constraints

It is possible to define constraints for each task. To this end, the `@constraint` (or `@Constraint`) decorator followed by the desired constraints needs to be placed ON TOP of the `@task` decorator ([Code 72](#)).

Important: Please note the the order of `@constraint` and `@task` decorators is important.

Code 72: Constrained task example

```
from pycompss.api.task import task
from pycompss.api.constraint import constraint
from pycompss.api.parameter import INOUT

@constraint(computing_units="4")
@task(c=INOUT)
def func(a, b, c):
    c += a * b
    ...
```

This decorator enables the user to set the particular constraints for each task, such as the amount of Cores required explicitly. Alternatively, it is also possible to indicate that the value of a constraint is specified in a environment variable ([Code 73](#)). A full description of the supported constraints can be found in [Table 14](#).

For example:

Code 73: Constrained task with environment variable example

```
from pycompss.api.task import task
from pycompss.api.constraint import constraint
from pycompss.api.parameter import INOUT

@constraint(computing_units="4",
            app_software="numpy, scipy, gnuplot",
            memory_size="$MIN_MEM_REQ")
@task(c=INOUT)
def func(a, b, c):
    c += a * b
    ...
```

Or another example requesting a CPU core and a GPU ([Code 74](#)).

Code 74: CPU and GPU constrained task example

```
from pycompss.api.task import task
from pycompss.api.constraint import constraint

@constraint(processors=[{'processorType': 'CPU', 'computingUnits': '1'},
                       {'processorType': 'GPU', 'computingUnits': '1'}])
@task(returns=1)
def func(a, b, c):
    ...
    return result
```

When the task requests a GPU, COMPSs provides the information about the assigned GPU through the *COMPSS_BINDED_GPUS*, *CUDA_VISIBLE_DEVICES* and *GPU_DEVICE_ORDINAL* environment variables. This information can be gathered from the task code in order to use the GPU.

Please, take into account that in order to respect the constraints, the peculiarities of the infrastructure must be defined in the *resources.xml* file.

4.2.1.8 Multiple Task Implementations

As in Java COMPSs applications, it is possible to define multiple implementations for each task. In particular, a programmer can define a task for a particular purpose, and multiple implementations for that task with the same objective, but with different constraints (e.g. specific libraries, hardware, etc). To this end, the *@implement* (or *@Implement*) decorator followed with the specific implementations constraints (with the *@constraint* decorator, see [Section \[subsubsec:constraints\]](#)) needs to be placed ON TOP of the *@task* decorator. Although the user only calls the task that is not decorated with the *@implement* decorator, when the application is executed in a heterogeneous distributed environment, the runtime will take into account the constraints on each implementation and will try to invoke the implementation that fulfills the constraints within each resource, keeping this management invisible to the user ([Code 75](#)).

Code 75: Multiple task implementations example

```
from pycompss.api.implement import implement

@implement(source_class="sourcemodule", method="main_func")
@constraint(app_software="numpy")
```

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```

@task(returns=list)
def myfunctionWithNumpy(list1, list2):
    # Operate with the lists using numpy
    return resultList

@task(returns=list)
def main_func(list1, list2):
    # Operate with the lists using built-int functions
    return resultList

```

Please, note that if the implementation is used to define a binary, OmpSs, MPI, COMPSs, multinode or reduction task invocation (see [Other task types](#)), the @implement decorator must be always on top of the decorators stack, followed by the @constraint decorator, then the @binary/@ompss/@mpi/@compss/@multinode decorator, and finally, the @task decorator in the lowest level.

4.2.1.9 API

PyCOMPSs provides an API for data synchronization and other functionalities, such as task group definition and automatic function parameter synchronization (local decorator).

Synchronization

The main program of the application is a sequential code that contains calls to the selected tasks. In addition, when synchronizing for task data from the main program, there exist six API functions that can be invoked:

- compss_open(file_name, mode='r')** Similar to the Python *open()* call. It synchronizes for the last version of file *file_name* and returns the file descriptor for that synchronized file. It can have an optional parameter *mode*, which defaults to 'r', containing the mode in which the file will be opened (the open modes are analogous to those of Python *open()*).
- compss_wait_on_file(*file_name)** Synchronizes for the last version of the file/s specified by *file_name*. Returns True if success (False otherwise).
- compss_wait_on_directory(*directory_name)** Synchronizes for the last version of the directory/ies specified by *directory_name*. Returns True if success (False otherwise).
- compss_barrier(no_more_tasks=False)** Performs a explicit synchronization, but does not return any object. The use of *compss_barrier()* forces to wait for all tasks that have been submitted before the *compss_barrier()* is called. When all tasks submitted before the *compss_barrier()* have finished, the execution continues. The *no_more_tasks* is used to specify if no more tasks are going to be submitted after the *compss_barrier()*.
- compss_barrier_group(group_name)** Performs a explicit synchronization over the tasks that belong to the group *group_name*, but does not return any object. The use of *compss_barrier_group()* forces to wait for all tasks that belong to the given group submitted before the *compss_barrier_group()* is called. When all group tasks submitted before the *compss_barrier_group()* have finished, the execution continues. See [Task Groups](#) for more information about task groups.
- compss_wait_on(*obj, mode='r' | 'rw')** Synchronizes for the last version of object/s specified by *obj* and returns the synchronized object. It can have an optional string parameter *mode*, which defaults to *rw*, that indicates whether the main program will modify the returned object. It is possible to wait on a list of objects. In this particular case, it will synchronize all future objects contained in the list recursively.

To illustrate the use of the aforementioned API functions, the following example ([Code 76](#)) first invokes a task *func* that writes a file, which is later synchronized by calling *compss_open()*. Later in the program, an object of class *MyClass* is created and a task method *method* that modifies the object is invoked on it; the object is then synchronized with *compss_wait_on*, so that it can be used in the main program from that point on.

Then, a loop calls again ten times to *func* task. Afterwards, the *compss_barrier()* call performs a synchronization, and the execution of the main user code will not continue until the ten *func* tasks have finished. This call does not retrieve any information.

Code 76: PyCOMPSs Synchronization API functions usage

```

from pycompss.api.api import compss_open
from pycompss.api.api import compss_wait_on
from pycompss.api.api import compss_wait_on_file
from pycompss.api.api import compss_wait_on_directory
from pycompss.api.api import compss_barrier

if __name__=='__main__':
    my_file = 'file.txt'
    func(my_file)
    fd = compss_open(my_file)
    ...

    my_file2 = 'file2.txt'
    func(my_file2)
    compss_wait_on_file(my_file2)
    ...

    my_directory = '/tmp/data'
    func_dir(my_directory)
    compss_wait_on_directory(my_directory)
    ...

    my_obj2 = MyClass()
    my_obj2.method()
    my_obj2 = compss_wait_on(my_obj2)
    ...

    for i in range(10):
        func(str(i) + my_file)
    compss_barrier()
    ...

```

The corresponding task definition for the example above would be ([Code 77](#)):

Code 77: PyCOMPSs Synchronization API usage tasks

```

@task(f=FILE_OUT)
def func(f):
    ...

class MyClass(object):
    ...

    @task()
    def method(self):
        ... # self is modified here

```

Tip: It is possible to synchronize a list of objects. This is particularly useful when the programmer expect to synchronize more than one elements (using the `compss_wait_on` function) ([Code 78](#)). This feature also works with dictionaries, where the value of each entry is synchronized. In addition, if the structure synchronized is a combination of lists and dictionaries, the `compss_wait_on` will look for all objects to be synchronized in the whole structure.

Code 78: Synchronization of a list of objects

```
if __name__=='__main__':
    # l is a list of objects where some/all of them may be future objects
    l = []
    for i in range(10):
        l.append(ret_func())

    ...

    l = compss_wait_on(l)
```

Important: In order to make the COMPSs Python binding function correctly, the programmer should not use relative imports in the code. Relative imports can lead to ambiguous code and they are discouraged in Python, as explained in: <http://docs.python.org/2/faq/programming.html#what-are-the-best-practices-for-using-import-in-a-module>

Local Decorator

Besides the synchronization API functions, the programmer has also a decorator for automatic function parameters synchronization at his disposal. The `@local` decorator can be placed over functions that are not decorated as tasks, but that may receive results from tasks (Code 79). In this case, the `@local` decorator synchronizes the necessary parameters in order to continue with the function execution without the need of using explicitly the `compss_wait_on` call for each parameter.

Code 79: @local decorator example

```
from pycompss.api.task import task
from pycompss.api.api import compss_wait_on
from pycompss.api.parameter import INOUT
from pycompss.api.local import local

@task(returns=list)
@task(v=INOUT)
def append_three_ones(v):
    v += [1, 1, 1]

@local
def scale_vector(v, k):
    return [k*x for x in v]

if __name__=='__main__':
    v = [1,2,3]
    append_three_ones(v)
    # v is automatically synchronized when calling the scale_vector function.
    w = scale_vector(v, 2)
```


File/Object deletion

PyCOMPSs also provides two functions within its API for object/file deletion. These calls allow the runtime to clean the infrastructure explicitly, but the deletion of the objects/files will be performed as soon as the objects/files dependencies are released.

compss_delete_file(*file_name) Notifies the runtime to delete a file/s.

compss_delete_object(*object) Notifies the runtime to delete all the associated files to a given object/s.

The following example ([Code 80](#)) illustrates the use of the aforementioned API functions.

Code 80: PyCOMPSs delete API functions usage

```
from pycompss.api.api import compss_delete_file
from pycompss.api.api import compss_delete_object

if __name__ == '__main__':
    my_file = 'file.txt'
    func(my_file)
    compss_delete_file(my_file)
    ...

    my_obj = MyClass()
    my_obj.method()
    compss_delete_object(my_obj)
    ...
```

The corresponding task definition for the example above would be ([Code 81](#)):

Code 81: PyCOMPSs delete API usage tasks

```
@task(f=FILE_OUT)
def func(f):
    ...

class MyClass(object):
    ...

    @task()
    def method(self):
        ... # self is modified here
```

Task Groups

COMPSs also enables to specify task groups. To this end, COMPSs provides the *TaskGroup* context ([Code 82](#)) which can be tuned with the group name, and a second parameter (boolean) to perform an implicit barrier for the whole group. Users can also define task groups within task groups.

TaskGroup(group_name, implicit_barrier=True) Python context to define a group of tasks. All tasks submitted within the context will belong to *group_name* context and are sensitive to wait for them while the rest are being executed. Tasks groups are depicted within a box into the generated task dependency graph.

Code 82: PyCOMPSs Task group definiton

```
from pycompss.api.task import task
from pycompss.api.api import TaskGroup
from pycompss.api.api import compss_barrier_group
```

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```
@task()
def func1():
    ...

@task()
def func2():
    ...

def test_taskgroup():
    # Creation of group
    with TaskGroup('Group1', False):
        for i in range(NUM_TASKS):
            func1()
            func2()
        ...
    ...
    compss_barrier_group('Group1')
    ...

if __name__ == '__main__':
    test_taskgroup()
```

Other

PyCOMPSs also provides other function within its API to check if a file exists.

compss_file_exists(*file_name) Checks if a file or files exist. If it does not exist, the function checks if the file has been accessed before by calling the runtime.

[Code 83](#) illustrates its usage.

Code 83: PyCOMPSs API file exists usage

```
from pycompss.api.api import compss_file_exists

if __name__ == '__main__':
    my_file = 'file.txt'
    func(my_file)
    if compss_file_exists(my_file):
        print("Exists")
    else:
        print("Not exists")
    ...
```

The corresponding task definition for the example above would be ([Code 84](#)):

Code 84: PyCOMPSs delete API usage tasks

```
@task(f=FILE_OUT)
def func(f):
    ...
```

API Summary

Finally, [Table 11](#) summarizes the API functions to be used in the main program of a COMPSs Python application.

Table 11: COMPSs Python API functions

Type	API Function	Description
Synchroniza- tion	compss_open(file_name, mode='r')	Synchronizes for the last version of a file and returns its file descriptor.
	compss_wait_on_file(*file_ name)	Synchronizes for the last version of the specified file/s.
	compss_wait_on_direct- ory(*directory_name)	Synchronizes for the last version of the specified direc- tory/ies.
	compss_barrier(no_more_ tasks=False)	Wait for all tasks submitted before the barrier.
	compss_barrier_group(group_ name)	Wait for all tasks that belong to <i>group_name</i> group sub- mitted before the barrier.
	compss_wait_on(*obj, mode="r" "rw")	Synchronizes for the last version of an object (or a list of objects) and returns it.
File/Object deletion	compss_delete_file(*file_name)	Notifies the runtime to remove the given file/s.
	compss_delete_object(*object)	Notifies the runtime to delete the associated file to the object/s.
Task Groups	TaskGroup(group_name, im- plicit_barrier=True)	Context to define a group of tasks. <i>implicit_barrier</i> forces waiting on context exit.
Other	compss_file_exists(*file_name)	Check if a file or files exist.

4.2.1.10 Failures and Exceptions

COMPSs is able to deal with failures and exceptions raised during the execution of the applications. In this case, if a user/python defined exception happens, the user can choose the task behaviour using the *on_failure* argument within the *@task* decorator.

The possible values are:

- **'RETRY'** (Default): The task is executed twice in the same worker and a different worker.
- **'CANCEL_SUCCESSORS'**: All successors of this task are canceled.
- **'FAIL'**: The task failure produces a failure of the whole application.
- **'IGNORE'**: The task failure is ignored and the output parameters are set with empty values.

A part from failures, COMPSs can also manage blocked tasks executions. Users can use the *time_out* property in the task definition to indicate the maximum duration of a task. If the task execution takes more seconds than the specified in the property. The task will be considered failed. This property can be combined with the *on_failure* mechanism.

Code 85: Task failures example

```
from pycompss.api.task import task

@task(time_out=60, on_failure='IGNORE')
def func(v):
    ...
```

COMPSs provides an special exception (`COMPSsException`) that the user can raise when necessary and can be caught in the main code for user defined behaviour management. [Code 86](#) shows an example of *COMPSsException* raising. In this case, the group definition is blocking, and waits for all task groups to finish. If a task of the group raises a *COMPSsException* it will be captured by the runtime. It will react to it by canceling the running and pending tasks of the group and raising the `COMPSsException` to enable the execution except clause. Consequently, the *COMPSsException* must be combined with task groups.

In addition, the tasks which belong to the group will be affected by the *on_failure* value defined in the `@task` decorator.

Code 86: COMPSs Exception with task group example

```
from pycompss.api.task import task
from pycompss.api.exceptions import COMPSsException
from pycompss.api.api import TaskGroup

@task()
def func(v):
    ...
    if v == 8:
        raise COMPSsException("8 found!")
    ...

if __name__ == '__main__':
    try:
        with TaskGroup('exceptionGroup1'):
            for i in range(10):
                func(i)
    except COMPSsException:
        ... # React to the exception (maybe calling other tasks or with other parameters)
```

It is possible to use a non-blocking task group for asynchronous behaviour (see [Code 87](#)). In this case, the *try-except* can be defined later in the code surrounding the *compss_barrier_group*, enabling to check exception from the defined groups without retrieving data while other tasks are being executed.

Code 87: Asynchronous COMPSs Exception with task group example

```
from pycompss.api.task import task
from pycompss.api.api import TaskGroup
from pycompss.api.api import compss_barrier_group

@task()
def func1():
    ...

@task()
def func2():
    ...

def test_taskgroup():
    # Creation of group
    for i in range(10):
        with TaskGroup('Group' + str(i), False):
            for i in range(NUM_TASKS):
                func1()
                func2()
```

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```

...
for i in range(10):
    try:
        compss_barrier_group('Group' + str(i))
    except COMPSsException:
        ... # React to the exception (maybe calling other tasks or with other parameters)
...

if __name__=='__main__':
    test_taskgroup()

```

4.2.2 Application Execution

The next subsections describe how to execute applications with the COMPSs Python binding.

4.2.2.1 Environment

The following environment variables must be defined before executing a COMPSs Python application:

JAVA_HOME Java JDK installation directory (e.g. /usr/lib/jvm/java-8-openjdk/)

4.2.2.2 Command

In order to run a Python application with COMPSs, the `runcompss` script can be used, like for Java and C/C++ applications. An example of an invocation of the script is:

```

compss@bsc:~$ runcompss \
    --lang=python \
    --pythonpath=$TEST_DIR \
    $TEST_DIR/application.py arg1 arg2

```

Or alternatively, use the `pycompss` module:

```

compss@bsc:~$ python -m pycompss \
    --pythonpath=$TEST_DIR \
    $TEST_DIR/application.py arg1 arg2

```

Tip: The `runcompss` command is able to detect the application language. Consequently, the `--lang=python` is not mandatory.

Tip: The `--pythonpath` flag enables the user to add directories to the `PYTHONPATH` environment variable and export them into the workers, so that the tasks can resolve successfully its imports.

Tip: PyCOMPSs applications can also be launched without parallelization (as a common python script) by avoiding the `-m pycompss` and its flags when using `python`:

```

compss@bsc:~$ python $TEST_DIR/application.py arg1 arg2

```

The main limitation is that the application must only contain `@task`, `@binary` and/or `@mpi` decorators and PyCOMPSs needs to be installed.

For full description about the options available for the `runcompss` command please check the [Executing COMPSs applications](#) Section.

4.2.3 Integration with Jupyter notebook

PyCOMPSs can also be used within Jupyter notebooks. This feature allows users to develop and run their PyCOMPSs applications in a Jupyter notebook, where it is possible to modify the code during the execution and experience an interactive behaviour.

4.2.3.1 Environment Variables

The following libraries must be present in the appropriate environment variables in order to enable PyCOMPSs within Jupyter notebook:

PYTHONPATH The path where PyCOMPSs is installed (e.g. `/opt/COMPSs/Bindings/python/`). Please, note that the path contains the folder 2 and/or 3. This is due to the fact that PyCOMPSs is able to choose the appropriate one depending on the kernel used with jupyter.

LD_LIBRARY_PATH The path where the `libbindings-commons.so` library is located (e.g. `<COMPSS_INSTALLATION_PATH>/Bindings/bindings-common/lib/`) and the path where the `libjvm.so` library is located (e.g. `/usr/lib/jvm/java-8-openjdk/jre/lib/amd64/server/`).

4.2.3.2 API calls

In this case, the user is responsible of **starting** and **stopping** the COMPSs runtime during the jupyter notebook execution. To this end, PyCOMPSs provides a module with two main API calls: one for starting the COMPSs runtime, and another for stopping it.

This module can be imported from the `pycompss` library:

```
import pycompss.interactive as ipycompss
```

And contains two main functions: `start` and `stop`. These functions can then be invoked as follows for the COMPSs runtime deployment with default parameters:

```
# Previous user code/cells

import pycompss.interactive as ipycompss
ipycompss.start()

# User code/cells that can benefit from PyCOMPSs

ipycompss.stop()

# Subsequent code/cells
```

Between the `start` and `stop` function calls, the user can write its own python code including PyCOMPSs imports, decorators and synchronization calls described in the [Programming Model](#) Section. The code can be splitted into multiple cells.

The `start` and `stop` functions accept parameters in order to customize the COMPSs runtime (such as the flags that can be selected with the `runcompss` command). [Table 12](#) summarizes the accepted parameters of the `start` function. [Table 13](#) summarizes the accepted parameters of the `stop` function.

Parameter Name	Parameter Type	Description
<code>log_level</code>	String	Log level Options: "off", "info" and "debug". (Default: "off")

Parameter Name	Parameter Type	Description
debug	Boolean	COMPSs runtime debug (Default: False) (overrides log level)
o_c	Boolean	Object conversion to string when possible (Default: False)
graph	Boolean	Task dependency graph generation (Default: False)
trace	Boolean	Paraver trace generation (Default: False)
monitor	Integer	Monitor refresh rate (Default: None - Monitoring disabled)
project_xml	String	Path to the project XML file (Default: "\$COMPSS/Runtime/configura
resources_xml	String	Path to the resources XML file (Default: "\$COMPSS/Runtime/configu
summary	Boolean	Show summary at the end of the execution (Default: False)
storage_impl	String	Path to an storage implementation (Default: None)
storage_conf	String	Storage configuration file path (Default: None)
task_count	Integer	Number of task definitions (Default: 50)
app_name	String	Application name (Default: " Interactive ")
uuid	String	Application uuid (Default: None - Will be random)
base_log_dir	String	Base directory to store COMPSs log files (a .COMPSs/ folder will be
specific_log_dir	String	Use a specific directory to store COMPSs log files (the folder MUST e
extrae_cfg	String	Sets a custom extrae config file. Must be in a shared disk between all
comm	String	Class that implements the adaptor for communications. Supported ad
conn	String	Class that implements the runtime connector for the cloud. Supported
master_name	String	Hostname of the node to run the COMPSs master (Default: "")
master_port	String	Port to run the COMPSs master communications (Only for NIO adap
scheduler	String	Class that implements the Scheduler for COMPSs. Supported schedul
jvm_workers	String	Extra options for the COMPSs Workers JVMs. Each option separed b
cpu_affinity	String	Sets the CPU affinity for the workers. Supported options: " disabled "
gpu_affinity	String	Sets the GPU affinity for the workers. Supported options: " disabled "
profile_input	String	Path to the file which stores the input application profile (Default: ""
profile_output	String	Path to the file to store the application profile at the end of the execu
scheduler_config	String	Path to the file which contains the scheduler configuration (Default: ""
external_adaptation	Boolean	Enable external adaptation (this option will disable the Resource Opti
propatage_virtual_environment	Boolean	Propagate the master virtual environment to the workers (Default: False)
verbose	Boolean	Verbose mode (Default: False)

Table 13: PyCOMPSs **stop** function for Jupyter notebook

Parameter Name	Parameter Type	Description
sync	Boolean	Synchronize the objects left on the user scope. (Default: False)

The following code snippet shows how to start a COMPSs runtime with tracing and graph generation enabled (with *trace* and *graph* parameters), as well as enabling the monitor with a refresh rate of 2 seconds (with the *monitor* parameter). It also synchronizes all remaining objects in the scope with the *sync* parameter when invoking the *stop* function.

```
# Previous user code

import pycompss.interactive as ipycompss
ipycompss.start(graph=True, trace=True, monitor=2000)

# User code that can benefit from PyCOMPSs

ipycompss.stop(sync=True)

# Subsequent code
```

Attention: Once the COMPSs runtime has been stopped it, the value of the variables that have not been synchronized will be lost.

4.2.3.3 Notebook execution

The application can be executed as a common Jupyter notebook by steps or the whole application.

Important: A message showing the failed task/s will pop up if an exception within them happens.

This pop up message will also allow you to continue the execution without PyCOMPSs, or to restart the COMPSs runtime. Please, note that in the case of COMPSs restart, the tracking of some objects may be lost (will need to be recomputed).

More information on the Notebook execution can be found in the Execution Environments [Jupyter Notebook](#) Section.

4.2.3.4 Notebook example

Sample notebooks can be found in the [PyCOMPSs Notebooks](#) Section.

4.2.4 Integration with Numba

PyCOMPSs can also be used with Numba. Numba (<http://numba.pydata.org/>) is an Open Source JIT compiler for Python which provides a set of decorators and functionalities to translate Python functions to optimized machine code.

4.2.4.1 Basic usage

PyCOMPSs' tasks can be decorated with Numba's `@jit`/`@njit` decorator (with the appropriate parameters) just below the `@task` decorator in order to apply Numba to the task.

```
from pycompss.api.task import task      # Import @task decorator
from numba import jit

@task(returns=1)
@jit()
def numba_func(a, b):
    ...
```

The task will be optimized by Numba within the worker node, enabling COMPSs to use the most efficient implementation of the task (and exploiting the compilation cache – any task that has already been compiled does not need to be recompiled in subsequent invocations).

4.2.4.2 Advanced usage

PyCOMPSs can be also used in conjunction with the Numba's `@vectorize`, `@guvectorize`, `@stencil` and `@cfunc`. But since these decorators do not preserve the original argument specification of the original function, their usage is done through the `numba` parameter with the `@task` decorator. The `numba` parameter accepts:

- **Boolean:** `True`: Applies *jit* to the function.
- **Dictionary{`k`, `v`}:** Applies *jit* with the dictionary parameters to the function (allows to specify specific jit parameters (e.g. `nopython=True`)).
- **String:**
 - `"jit"`: Applies *jit* to the function.
 - `"njit"`: Applies *jit* with `nopython=True` to the function.
 - `"generated_jit"`: Applies *generated_jit* to the function.
 - `"vectorize"`: Applies *vectorize* to the function. Needs some extra flags in the `@task` decorator:
 - * `numba_signature`: String with the *vectorize* signature.
 - `"guvectorize"`: Applies *guvectorize* to the function. Needs some extra flags in the `@task` decorator:
 - * `numba_signature`: String with the *guvectorize* signature.
 - * `numba_declaration`: String with the *guvectorize* declaration.
 - `"stencil"`: Applies *stencil* to the function.
 - `"cfunc"`: Applies *cfunc* to the function. Needs some extra flags in the `@task` decorator:
 - * `numba_signature`: String with the *cfunc* signature.

Moreover, the `@task` decorator also allows to define specific flags for the *jit*, *njit*, *generated_jit*, *vectorize*, *guvectorize* and *cfunc* functionalities with the `numba_flags` hint. This hint is used to declare a dictionary with the flags expected to use with these numba functionalities. The default flag included by PyCOMPSs is the `cache=True` in order to exploit the function caching of Numba across tasks.

For example, to apply Numba *jit* to a task:

```
from pycompss.api.task import task

@task(numba='jit') # Alternatively: @task(numba=True)
def jit_func(a, b):
    ...
```

And if the developer wants to use specific flags with *jit* (e.g. `parallel=True`), the `numba_flags` must be defined with a dictionary where the key is the numba flag name, and the value, the numba flag value to use):

```
from pycompss.api.task import task

@task(numba='jit', numba_flags={'parallel':True})
def jit_func(a, b):
    ...
```

Other Numba's functionalities require the specification of the function signature and declaration. In the next example a task that will use the *vectorize* with three parameters and a specific flag to target the CPU is shown:

```
from pycompss.api.task import task

@task(returns=1,
      numba='vectorize',
      numba_signature=['float32(float32, float32, float32)'],
      numba_flags={'target':'cpu'})
def vectorize_task(a, b, c):
    return a * b * c
```

Using Numba with GPUs

In addition, Numba is also able to optimize python code for GPUs that can be used within PyCOMPSs' tasks. [Task using Numba and a GPU](#) shows an example where the `calculate_wight` task has a constraint of one CPU and one GPU. This task first transfers the necessary data to the GPU using Numba's `cuda` module, then invokes the `calculate_weight_cuda` function (that is decorated with the Numba's `@vectorize` decorator defining its signature and the target specifically for GPU). When the execution in the GPU of the `calculate_weight_cuda` finishes, the result is transferred to the cpu with the `copy_to_host` function and the task result is returned.

Code 88: Task using Numba and a GPU

```
from pycompss.api.constraint import constraint
from pycompss.api.task import task
from pycompss.api.parameter import *
from numba import vectorize
from numba import cuda

@constraint(processors=[{'ProcessorType': 'CPU', 'ComputingUnits': '1'},
                       {'ProcessorType': 'GPU', 'ComputingUnits': '1'}])
@task(returns=1)
def calculate_weight(min_depth, max_depth, e3t, depth, mask):
    # Transfer data to the GPU
    gpu_mask = cuda.to_device(mask.data.astype(np.float32))
    gpu_e3t = cuda.to_device(e3t.data.astype(np.float32))
    gpu_depth = cuda.to_device(depth.data.astype(np.float32))
    # Invoke function compiled with Numba for GPU
    weight = calculate_weight_cuda(min_depth, max_depth,
                                   gpu_e3t, gpu_depth, gpu_mask)

    # Transfer result from GPU
    local_weight = weight.copy_to_host()
    return local_weight

@vectorize(['float32(int32, int32, float32, float32, float32)'], target='cuda')
def calculate_weight_cuda(min_depth, max_depth, e3t, depth, mask):
    """
    This code is compiled with Numba for GPU (cuda)
    """
    if not mask:
        return 0
    top = depth
    bottom = top + e3t
    if bottom < min_depth or top > max_depth:
        return 0
    else:
        if top < min_depth:
            top = min_depth
        if bottom > max_depth:
            bottom = max_depth

    return (bottom - top) * 1020 * 4000
```

Important: The function compiled with Numba for GPU can not be a task since the step to transfer the data to the GPU and backwards needs to be explicitly performed by the user.

For this reason, the appropriate structure is composed by a task that has the necessary constraints, deals with the data movements and invokes the function compiled with Numba for GPU.

The main application can then invoke the task.

More details about Numba and the specification of the signature, declaration and flags can be found in the Numba's webpage (<http://numba.pydata.org/>).

4.3 C/C++ Binding

COMPSs provides a binding for C and C++ applications. The new C++ version in the current release comes with support for objects as task parameters and the use of class methods as tasks.

4.3.1 Programming Model

As in Java, the application code is divided in 3 parts: the Task definition interface, the main code and task implementations. These files must have the following notation: `<app_ame>.idl`, for the interface file, `<app_name>.cc` for the main code and `<app_name>-functions.cc` for task implementations. Next paragraphs provide an example of how to define this files for matrix multiplication parallelised by blocks.

Task Definition Interface

As in Java the user has to provide a task selection by means of an interface. In this case the interface file has the same name as the main application file plus the suffix "idl", i.e. `Matmul.idl`, where the main file is called `Matmul.cc`.

Code 89: `Matmul.idl`

```
interface Matmul
{
    // C functions
    void initMatrix(inout Matrix matrix,
                   in int mSize,
                   in int nSize,
                   in double val);

    void multiplyBlocks(inout Block block1,
                      inout Block block2,
                      inout Block block3);
};
```

The syntax of the interface file is shown in the previous code. Tasks can be declared as classic C function prototypes, this allow to keep the compatibility with standard C applications. In the example, `initMatrix` and `multiplyBlocks` are functions declared using its prototype, like in a C header file, but this code is C++ as they have objects as parameters (objects of type `Matrix`, or `Block`).

The grammar for the interface file is:

```
["static"] return-type task-name ( parameter {, parameter }* );

return-type = "void" | type

ask-name = <qualified name of the function or method>

parameter = direction type parameter-name

direction = "in" | "out" | "inout"

type = "char" | "int" | "short" | "long" | "float" | "double" | "boolean" |
```

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```
"char[<size>]" | "int[<size>]" | "short[<size>]" | "long[<size>]" |  
"float[<size>]" | "double[<size>]" | "string" | "File" | class-name
```

```
class-name = <qualified name of the class>
```

Main Program

The following code shows an example of matrix multiplication written in C++.

Code 90: Matrix multiplication

```
#include "Matmul.h"  
#include "Matrix.h"  
#include "Block.h"  
int N; //MSIZE  
int M; //BSIZE  
double val;  
int main(int argc, char **argv)  
{  
    Matrix A;  
    Matrix B;  
    Matrix C;  
  
    N = atoi(argv[1]);  
    M = atoi(argv[2]);  
    val = atof(argv[3]);  
  
    compss_on();  
  
    A = Matrix::init(N,M,val);  
  
    initMatrix(&B,N,M,val);  
    initMatrix(&C,N,M,0.0);  
  
    cout << "Waiting for initialization...\n";  
  
    compss_wait_on(B);  
    compss_wait_on(C);  
  
    cout << "Initialization ends...\n";  
  
    C.multiply(A, B);  
  
    compss_off();  
    return 0;  
}
```

The developer has to take into account the following rules:

1. A header file with the same name as the main file must be included, in this case **Matmul.h**. This header file is automatically generated by the binding and it contains other includes and type-definitions that are required.
2. A call to the **compss_on** binding function is required to turn on the COMPSs runtime.
3. As in C language, out or inout parameters should be passed by reference by means of the “&” operator before the parameter name.
4. Synchronization on a parameter can be done calling the **compss_wait_on** binding function. The argument

- of this function must be the variable or object we want to synchronize.
5. There is an **implicit synchronization** in the `init` method of `Matrix`. It is not possible to know the address of “A” before exiting the method call and due to this it is necessary to synchronize before for the copy of the returned value into “A” for it to be correct.
 6. A call to the `compss_off` binding function is required to turn off the COMPSs runtime.

Functions file

The implementation of the tasks in a C or C++ program has to be provided in a functions file. Its name must be the same as the main file followed by the suffix “-functions”. In our case `Matmul-functions.cc`.

```
#include "Matmul.h"
#include "Matrix.h"
#include "Block.h"

void initMatrix(Matrix *matrix, int mSize, int nSize, double val){
    *matrix = Matrix::init(mSize, nSize, val);
}

void multiplyBlocks(Block *block1, Block *block2, Block *block3){
    block1->multiply(*block2, *block3);
}
```

In the previous code, class methods have been encapsulated inside a function. This is useful when the class method returns an object or a value and we want to avoid the explicit synchronization when returning from the method.

Additional source files

Other source files needed by the user application must be placed under the directory “**src**”. In this directory the programmer must provide a **Makefile** that compiles such source files in the proper way. When the binding compiles the whole application it will enter into the `src` directory and execute the `Makefile`.

It generates two libraries, one for the master application and another for the worker application. The directive `COMPSS_MASTER` or `COMPSS_WORKER` must be used in order to compile the source files for each type of library. Both libraries will be copied into the `lib` directory where the binding will look for them when generating the master and worker applications.

The following sections provide a more detailed view of the C++ Binding. It will include the available API calls, how to deal with objects and having tasks as method objects as well as how to define constraints and task versions.

4.3.1.1 Binding API

Besides the aforementioned `compss_on`, `compss_off` and `compss_wait_on` functions, the C/C++ main program can make use of a variety of other API calls to better manage the synchronization of data generated by tasks. These calls are as follows:

- void compss_ifstream(char * filename, ifstream* & * ifs)** Given an uninitialized input stream *ifs* and a file *filename*, this function will synchronize the content of the file and initialize *ifs* to read from it.
- void compss_ofstream(char * filename, ofstream* & * ofs)** Behaves the same way as *compss_ifstream*, but in this case the opened stream is an output stream, meaning it will be used to write to the file.
- FILE* compss_fopen(char * file_name, char * mode)** Similar to the C/C++ *fopen* call. Synchronizes with the last version of file *file_name* and returns the `FILE*` pointer to further reference it. As the mode parameter it takes the same that can be used in *fopen* (*r*, *w*, *a*, *r+*, *w+* and *a+*).
- void compss_wait_on(T** & * obj) or T compss_wait_on(T* & * obj)** Synchronizes for the last version of object *obj*, meaning that the execution will stop until the value of *obj* up to that point of the code is received (and thus all tasks that can modify it have ended).
- void compss_delete_file(char * file_name)** Makes an asynchronous delete of file *filename*. When all previous tasks have finished updating the file, it is deleted.

void compss_delete_object(T & * obj)** Makes an asynchronous delete of an object. When all previous tasks have finished updating the object, it is deleted.

void compss_barrier() Similarly to the Python binding, performs an explicit synchronization without a return. When a *compss_barrier* is encountered, the execution will not continue until all the tasks submitted before the *compss_barrier* have finished.

4.3.1.2 Functions file

The implementation of the tasks in a C or C++ program has to be provided in a functions file. Its name must be the same as the main file followed by the suffix “-functions”. In our case *Matmul-functions.cc*.

```
#include "Matmul.h"
#include "Matrix.h"
#include "Block.h"

void initMatrix(Matrix *matrix, int mSize, int nSize, double val){
    *matrix = Matrix::init(mSize, nSize, val);
}

void multiplyBlocks(Block *block1, Block *block2, Block *block3){
    block1->multiply(*block2, *block3);
}
```

In the previous code, class methods have been encapsulated inside a function. This is useful when the class method returns an object or a value and we want to avoid the explicit synchronization when returning from the method.

4.3.1.3 Additional source files

Other source files needed by the user application must be placed under the directory “**src**”. In this directory the programmer must provide a **Makefile** that compiles such source files in the proper way. When the binding compiles the whole application it will enter into the *src* directory and execute the *Makefile*.

It generates two libraries, one for the master application and another for the worker application. The directive *COMPSS_MASTER* or *COMPSS_WORKER* must be used in order to compile the source files for each type of library. Both libraries will be copied into the *lib* directory where the binding will look for them when generating the master and worker applications.

4.3.1.4 Class Serialization

In case of using an object as method parameter, as callee or as return of a call to a function, the object has to be serialized. The serialization method has to be provided inline in the header file of the object’s class by means of the “**boost**” library. The next listing contains an example of serialization for two objects of the *Block* class.

```
#ifndef BLOCK_H
#define BLOCK_H

#include <vector>
#include <boost/archive/text_iarchive.hpp>
#include <boost/archive/text_oarchive.hpp>
#include <boost/serialization/serialization.hpp>
#include <boost/serialization/access.hpp>
#include <boost/serialization/vector.hpp>

using namespace std;
using namespace boost;
using namespace serialization;
```

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```

class Block {
public:
    Block(){};
    Block(int bSize);
    static Block *init(int bSize, double initVal);
    void multiply(Block block1, Block block2);
    void print();

private:
    int M;
    std::vector< std::vector< double > > data;

    friend class::serialization::access;
    template<class Archive>
    void serialize(Archive & ar, const unsigned int version) {
        ar & M;
        ar & data;
    }
};
#endif

```

For more information about serialization using “boost” visit the related documentation at www.boost.org <www.boost.org>.

4.3.1.5 Method - Task

A task can be a C++ class method. A method can return a value, modify the *this* object, or modify a parameter.

If the method has a return value there will be an implicit synchronization before exit the method, but for the *this* object and parameters the synchronization can be done later after the method has finished.

This is because the *this* object and the parameters can be accessed inside and outside the method, but for the variable where the returned value is copied to, it can’t be known inside the method.

```

#include "Block.h"

Block::Block(int bSize) {
    M = bSize;
    data.resize(M);
    for (int i=0; i<M; i++) {
        data[i].resize(M);
    }
}

Block *Block::init(int bSize, double initVal) {
    Block *block = new Block(bSize);
    for (int i=0; i<bSize; i++) {
        for (int j=0; j<bSize; j++) {
            block->data[i][j] = initVal;
        }
    }
    return block;
}

#ifdef COMPSS_WORKER

```

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```

void Block::multiply(Block block1, Block block2) {
    for (int i=0; i<M; i++) {
        for (int j=0; j<M; j++) {
            for (int k=0; k<M; k++) {
                data[i][j] += block1.data[i][k] * block2.data[k][j];
            }
        }
    }
    this->print();
}

#endif

void Block::print() {
    for (int i=0; i<M; i++) {
        for (int j=0; j<M; j++) {
            cout << data[i][j] << " ";
        }
        cout << "\r\n";
    }
}

```

4.3.1.6 Task Constraints

The C/C++ binding also supports the definition of task constraints. The task definition specified in the IDL file must be decorated/annotated with the *@Constraints*. Below, you can find an example of how to define a task with a constraint of using 4 cores. The list of constraints which can be defined for a task can be found in Section [sec:Constraints]

```

interface Matmul
{
    @Constraints(ComputingUnits = 4)
    void multiplyBlocks(inout Block block1,
                       in Block block2,
                       in Block block3);
};

```

4.3.1.7 Task Versions

Another COMPSs functionality supported in the C/C++ binding is the definition of different versions for a tasks. The following code shows an IDL file where a function has two implementations, with their corresponding constraints. It shows an example where the *multiplyBlocks_GPU* is defined as an implementation of *multiplyBlocks* using the annotation/decoration *@Implements*. It also shows how to set a processor constraint which requires a GPU processor and a CPU core for managing the offloading of the computation to the GPU.

```

interface Matmul
{
    @Constraints(ComputingUnits=4);
    void multiplyBlocks(inout Block block1,
                       in Block block2,
                       in Block block3);
};

```

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```

// GPU implementation
@Constraints(processors={
    @Processor(ProcessorType=CPU, ComputingUnits=1)});
    @Processor(ProcessorType=GPU, ComputingUnits=1)});
@Implements(multiplyBlocks);
void multiplyBlocks_GPU(inout Block block1,
                        in Block block2,
                        in Block block3);
};

```

4.3.2 Use of programming models inside tasks

To improve COMPSs performance in some cases, C/C++ binding offers the possibility to use programming models inside tasks. This feature allows the user to exploit the potential parallelism in their application's tasks.

4.3.2.1 OmpSs

COMPSs C/C++ binding supports the use of the programming model OmpSs. To use OmpSs inside COMPSs tasks we have to annotate the implemented tasks. The implementation of tasks was described in section [sec:functionsfile]. The following code shows a COMPSs C/C++ task without the use of OmpSs.

```

void compss_task(int* a, int N) {
    int i;
    for (i = 0; i < N; ++i) {
        a[i] = i;
    }
}

```

This code will assign to every array element its position in it. A possible use of OmpSs is the following.

```

void compss_task(int* a, int N) {
    int i;
    for (i = 0; i < N; ++i) {
        #pragma omp task
        {
            a[i] = i;
        }
    }
}

```

This will result in the parallelization of the array initialization, of course this can be applied to more complex implementations and the directives offered by OmpSs are much more. You can find the documentation and specification in <https://pm.bsc.es/ompss>.

There's also the possibility to use a newer version of the OmpSs programming model which introduces significant improvements, OmpSs-2. The changes at user level are minimal, the following image shows the array initialization using OmpSs-2.

```

void compss_task(int* a, int N) {
    int i;

    for (i = 0; i < N; ++i) {
        #pragma omp taskwait
        {

```

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```
    a[i] = i;
  }
}
```

Documentation and specification of OmpSs-2 can be found in <https://pm.bsc.es/ompss-2>.

4.3.3 Application Compilation

To compile user's applications with the C/C++ binding two commands are used: The “**compss_build_app**” command allows to compile applications for a single architecture, and the “**compss_build_app_multi_arch**” command for multiple architectures. Both commands must be executed in the directory of the main application code.

4.3.3.1 Single architecture

The user command “**compss_build_app**” compiles both master and worker for a single architecture (e.g. x86-64, armhf, etc). Thus, whether you want to run your application in Intel based machine or ARM based machine, this command is the tool you need.

When the target is the native architecture, the command to execute is very simple;

```
$~/matmul_objects> compss_build_app Matmul
[ INFO ] Java libraries are searched in the directory: /usr/lib/jvm/java-1.8.0-openjdk-amd64//
→jre/lib/amd64/server
[ INFO ] Boost libraries are searched in the directory: /usr/lib/

...

[Info] The target host is: x86_64-linux-gnu

Building application for master...
g++ -g -O3 -I. -I/Bindings/c/share/c_build/worker/files/ -c Block.cc Matrix.cc
ar rvs libmaster.a Block.o Matrix.o
ranlib libmaster.a

Building application for workers...
g++ -DCOMPSS_WORKER -g -O3 -I. -I/Bindings/c/share/c_build/worker/files/ -c Block.cc -o Block.
→o
g++ -DCOMPSS_WORKER -g -O3 -I. -I/Bindings/c/share/c_build/worker/files/ -c Matrix.cc -o
→Matrix.o
ar rvs libworker.a Block.o Matrix.o
ranlib libworker.a

...

Command successful.
```

In order to build an application for a different architecture e.g. *armhf*, an environment must be provided, indicating the compiler used to cross-compile, and also the location of some COMPSs dependencies such as java or boost which must be compliant with the target architecture. This environment is passed by flags and arguments;

Please note that to use cross compilation features and multiple architecture builds, you need to do the proper installation of COMPSs, find more information in the builders README.

```

$~/matmul_objects> compss_build_app --cross-compile --cross-compile-prefix=arm-linux-
→gnueabihf --java_home=/usr/lib/jvm/java-1.8.0-openjdk-armhf Matmul
[ INFO ] Java libraries are searched in the directory: /usr/lib/jvm/java-1.8.0-openjdk-armhf/
→jre/lib/arm/server
[ INFO ] Boost libraries are searched in the directory: /usr/lib/
[ INFO ] You enabled cross-compile and the prefix to be used is: arm-linux-gnueabihf-

...

[ INFO ] The target host is: arm-linux-gnueabihf

Building application for master...
g++ -g -O3 -I. -I/Bindings/c/share/c_build/worker/files/ -c Block.cc Matrix.cc
ar rvs libmaster.a Block.o Matrix.o
ranlib libmaster.a

Building application for workers...
g++ -DCOMPSS_WORKER -g -O3 -I. -I/Bindings/c/share/c_build/worker/files/ -c Block.cc -o Block.
→o
g++ -DCOMPSS_WORKER -g -O3 -I. -I/Bindings/c/share/c_build/worker/files/ -c Matrix.cc -o
→Matrix.o
ar rvs libworker.a Block.o Matrix.o
ranlib libworker.a

...

Command successful.

```

[The previous outputs have been cut for simplicity]

The **–cross-compile** flag is used to indicate the users desire to cross-compile the application. It enables the use of **–cross-compile-prefix** flag to define the prefix for the cross-compiler. Setting `$CROSS_COMPILE` environment variable will also work (in case you use the environment variable, the prefix passed by arguments is overridden with the variable value). This prefix is added to `$CC` and `$CXX` to be used by the user *Makefile* and lastly by the *GNU toolchain*. Regarding java and boost, **–java_home** and **–boostlib** flags are used respectively. In this case, users can also use the `$JAVA_HOME` and `$BOOST_LIB` variables to indicate the java and boost for the target architecture. Note that these last arguments are purely for linkage, where `$LD_LIBRARY_PATH` is used by *Unix/Linux* systems to find libraries, so feel free to use it if you want to avoid passing some environment arguments.

4.3.3.2 Multiple architectures

The user command “**compss_build_app_multi_arch**” allows a to compile an application for several architectures. Users are able to compile both master and worker for one or more architectures. Environments for the target architectures are defined in a file specified by ***c*fg** flag. Imagine you wish to build your application to run the master in your Intel-based machine and the worker also in your native machine and in an ARM-based machine, without this command you would have to execute several times the command for a single architecture using its cross compile features. With the multiple architecture command is done in the following way.

```

$~/matmul_objects> compss_build_app_multi_arch --master=x86_64-linux-gnu --worker=arm-linux-
→gnueabihf,x86_64-linux-gnu Matmul

[ INFO ] Using default configuration file: /opt/COMPSs/Bindings/c/cfgs/compssrc.
[ INFO ] Java libraries are searched in the directory: /usr/lib/jvm/java-1.8.0-openjdk-amd64/
→jre/lib/amd64/server
[ INFO ] Boost libraries are searched in the directory: /usr/lib/

```

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```

...

Building application for master...
g++ -g -O3 -I. -I/Bindings/c/share/c_build/worker/files/ -c Block.cc Matrix.cc
ar rvs libmaster.a Block.o Matrix.o
ranlib libmaster.a

Building application for workers...
g++ -DCOMPSS_WORKER -g -O3 -I. -I/Bindings/c/share/c_build/worker/files/ -c Block.cc -o Block.
↪o
g++ -DCOMPSS_WORKER -g -O3 -I. -I/Bindings/c/share/c_build/worker/files/ -c Matrix.cc -o↪
↪Matrix.o
ar rvs libworker.a Block.o Matrix.o
ranlib libworker.a

...

Command successful. # The master for x86_64-linux-gnu compiled successfully

...

[ INFO ] Java libraries are searched in the directory: /usr/lib/jvm/java-1.8.0-openjdk-armhf/
↪jre/lib/arm/server
[ INFO ] Boost libraries are searched in the directory: /opt/install-arm/libboost

...

Building application for master...
arm-linux-gnueabi-g++ -g -O3 -I. -I/Bindings/c/share/c_build/worker/files/ -c Block.cc↪
↪Matrix.cc
ar rvs libmaster.a Block.o Matrix.o
ranlib libmaster.a

Building application for workers...
arm-linux-gnueabi-g++ -DCOMPSS_WORKER -g -O3 -I. -I/Bindings/c/share/c_build/worker/files/ -
↪c Block.cc -o Block.o
arm-linux-gnueabi-g++ -DCOMPSS_WORKER -g -O3 -I. -I/Bindings/c/share/c_build/worker/files/ -
↪c Matrix.cc -o Matrix.o
ar rvs libworker.a Block.o Matrix.o
ranlib libworker.a

...

Command successful. # The worker for arm-linux-gnueabi compiled successfully

...

[ INFO ] Java libraries are searched in the directory: /usr/lib/jvm/java-1.8.0-openjdk-amd64/
↪jre/lib/amd64/server
[ INFO ] Boost libraries are searched in the directory: /usr/lib/

...

Building application for master...
g++ -g -O3 -I. -I/Bindings/c/share/c_build/worker/files/ -c Block.cc Matrix.cc
ar rvs libmaster.a Block.o Matrix.o

```

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```

ranlib libmaster.a

Building application for workers...
g++ -DCOMPSS_WORKER -g -O3 -I. -I/Bindings/c/share/c_build/worker/files/ -c Block.cc -o Block.o
g++ -DCOMPSS_WORKER -g -O3 -I. -I/Bindings/c/share/c_build/worker/files/ -c Matrix.cc -o Matrix.o
ar rvs libworker.a Block.o Matrix.o
ranlib libworker.a

...

Command successful. # The worker for x86_64-linux-gnu compiled successfully

```

[The previous output has been cut for simplicity]

Building for single architectures would lead to a directory structure quite different than the one obtained using the script for multiple architectures. In the single architecture case, only one master and one worker directories are expected. In the multiple architectures case, one master and one worker is expected per architecture.

```

.
|-- arm-linux-gnueabi
|   |-- worker
|       |-- gsbuild
|           |-- autom4te.cache
|-- src
|-- x86_64-linux-gnu
|   |-- master
|       |-- gsbuild
|           |-- autom4te.cache
|   |-- worker
|       |-- gsbuild
|           |-- autom4te.cache
|-- xml

```

(Note than only directories are shown).

4.3.3.3 Using OmpSs

As described in section [sec:ompss] applications can use OmpSs and OmpSs-2 programming models. The compilation process differs a little bit compared with a normal COMPSs C/C++ application. Applications using OmpSs must be compiled using the `--ompss` option in the `compss_build_app` command.

```
$~/matmul_objects> compss_build_app --ompss Matmul
```

Executing the previous command will start the compilation of the application. Sometimes due to configuration issues OmpSs can not be found, the option `--with_ompss=/path/to/ompss` specifies the OmpSs path that the user wants to use in the compilation.

Applications using OmpSs-2 are similarly compiled. The options to compile with OmpSs-2 are `--ompss-2` and `--with_ompss-2=/path/to/ompss-2`

```
$~/matmul_objects> compss_build_app --with_ompss-2=/home/mdomingu/ompss-2 --ompss-2 Matmul
```

Remember that additional source files can be used in COMPSs C/C++ applications, if the user expects OmpSs or OmpSs-2 to be used in those files she, must be sure that the files are properly compiled with OmpSs or OmpSs-2.

4.3.4 Application Execution

The following environment variables must be defined before executing a COMPSs C/C++ application:

JAVA_HOME Java JDK installation directory (e.g. /usr/lib/jvm/java-8-openjdk/)

After compiling the application, two directories, master and worker, are generated. The master directory contains a binary called as the main file, which is the master application, in our example is called Matmul. The worker directory contains another binary called as the main file followed by the suffix “-worker”, which is the worker application, in our example is called Matmul-worker.

The `runcompss` script has to be used to run the application:

```
$ runcompss /home/compss/tutorial_apps/c/matmul_objects/master/Matmul 3 4 2.0
```

The complete list of options of the `runcompss` command is available in Section [Executing COMPSs applications](#).

4.3.5 Task Dependency Graph

COMPSs can generate a task dependency graph from an executed code. It is indicating by a

```
$ runcompss -g /home/compss/tutorial_apps/c/matmul_objects/master/Matmul 3 4 2.0
```

The generated task dependency graph is stored within the `$HOME/.COMPSs/<APP_NAME>_<00-99>/monitor` directory in dot format. The generated graph is `complete_graph.dot` file, which can be displayed with any dot viewer. COMPSs also provides the `compss_gengraph` script which converts the given dot file into pdf.

```
$ cd $HOME/.COMPSs/Matmul_02/monitor
$ compss_gengraph complete_graph.dot
$ evince complete_graph.pdf # or use any other pdf viewer you like
```

The following figure depicts the task dependency graph for the Matmul application in its object version with 3x3 blocks matrices, each one containing a 4x4 matrix of doubles. Each block in the result matrix accumulates three block multiplications, i.e. three multiplications of 4x4 matrices of doubles.

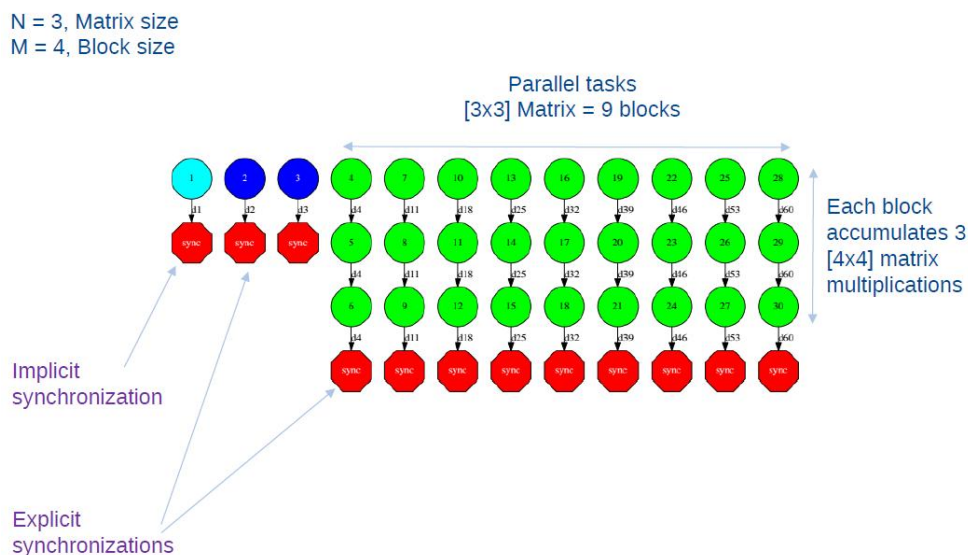


Figure 6: Matmul Execution Graph.

The light blue circle corresponds to the initialization of matrix “A” by means of a method-task and it has an implicit synchronization inside. The dark blue circles correspond to the other two initializations by means of

function-tasks; in this case the synchronizations are explicit and must be provided by the developer after the task call. Both implicit and explicit synchronizations are represented as red circles.

Each green circle is a partial matrix multiplication of a set of 3. One block from matrix “A” and the correspondent one from matrix “B”. The result is written in the right block in “C” that accumulates the partial block multiplications. Each multiplication set has an explicit synchronization. All green tasks are method-tasks and they are executed in parallel.

4.4 Constraints

This section provides a detailed information about all the supported constraints by the COMPSs runtime for **Java**, **Python** and **C/C++** languages. The constraints are defined as key-value pairs, where the key is the name of the constraint. [Table 14](#) details the available constraints names for *Java*, *Python* and *C/C++*, its value type, its default value and a brief description.

Table 14: Arguments of the *@constraint* decorator

Java	Python	C / C++	Value type	Default value	Description
computingUnits	computing_ - units	ComputingU- nits	<string>	"1"	Required num- ber of comput- ing units
processorName	processor_ - name	ProcessorName	<string>	"[unassigned]"	Required pro- cessor name
processorSpeed	processor_ - speed	ProcessorSpeed	<string>	"[unassigned]"	Required pro- cessor speed
processorArchi- tecture	processor_ ar- chitecture	ProcessorArchi- tecture	<string>	"[unassigned]"	Required pro- cessor architec- ture
processorType	processor_ type	ProcessorType	<string>	"[unassigned]"	Required pro- cessor type
processorProp- ertyName	processor_ - property_ name	ProcessorProp- ertyName	<string>	"[unassigned]"	Required pro- cessor property
processorProp- ertyValue	processor_ - property_ value	ProcessorProp- ertyValue	<string>	"[unassigned]"	Required pro- cessor property value
processorInter- nalMemorySize	processor_ in- ternal_ mem- ory_ size	ProcessorInter- nalMemorySize	<string>	"[unassigned]"	Required inter- nal device mem- ory
processors	processors	•	List<@Processor>	"{"	Required pro- cessors (check Table 15 for Processor de- tails)
memorySize	memory_ size	MemorySize	<string>	"[unassigned]"	Required mem- ory size in GBs
memoryType	memory_ type	MemoryType	<string>	"[unassigned]"	Required memory type (SRAM, DRAM, etc.)
storageSize	storage_ size	StorageSize	<string>	"[unassigned]"	Required stor- age size in GBs
storageType	storage_ type	StorageType	<string>	"[unassigned]"	Required stor- age type (HDD, SSD, etc.)
operatingSys- temType	operating_ sys- tem_ type	OperatingSys- temType	<string>	"[unassigned]"	Required op- erating system type (Windows, MacOS, Linux, etc.)
operatingSys- temDistribution	operating_ sys- tem_ distribu- tion	OperatingSys- temDistribution	<string>	"[unassigned]"	Required op- erating system distribution (XP, Sierra, openSUSE, etc.)
operatingSys- temVersion	operating_ sys- tem_ version	OperatingSys- temVersion	<string>	"[unassigned]"	Required op- erating system version
wallClockLimit	wall_ clock_ - limit	WallClockLimit	<string>	"[unassigned]"	Maximum wall clock time
hostQueues	host_ queues	HostQueues	<string>	"[unassigned]"	Required queues
appSoftware	app_ software	AppSoftware	<string>	"[unassigned]"	Required ap- plications that must be avail- able within the remote node for the task

All constraints are defined with a simple value except the *HostQueue* and *AppSoftware* constraints, which allow multiple values.

The *processors* constraint allows the users to define multiple processors for a task execution. This constraint is specified as a list of @Processor annotations that must be defined as shown in [Table 15](#)

Table 15: Arguments of the @Processor decorator

Annotation	Value type	Default value	Description
processorType	<string>	“CPU”	Required processor type (e.g. CPU or GPU)
computingUnits	<string>	“1”	Required number of computing units
name	<string>	“[unassigned]”	Required processor name
speed	<string>	“[unassigned]”	Required processor speed
architecture	<string>	“[unassigned]”	Required processor architecture
propertyName	<string>	“[unassigned]”	Required processor property
propertyValue	<string>	“[unassigned]”	Required processor property value
internalMemorySize	<string>	“[unassigned]”	Required internal device memory

Chapter 5

Execution Environments

This section is intended to show how to execute the COMPSs applications.

5.1 Master-Worker Deployments

This section is intended to show how to execute the COMPSs applications deploying COMPSs as a master-worker structure.

5.1.1 Local

This section is intended to walk you through the COMPSs usage in local machines.

5.1.1.1 Executing COMPSs applications

Prerequisites

Prerequisites vary depending on the application's code language: for Java applications the users need to have a **jar archive** containing all the application classes, for Python applications there are no requirements and for C/C++ applications the code must have been previously compiled by using the *buildapp* command.

For further information about how to develop COMPSs applications please refer to [Application development](#).

Runcompss command

COMPSs applications are executed using the **runcompss** command:

```
compss@bsc:~$ runcompss [options] application_name [application_arguments]
```

The application name must be the fully qualified name of the application in Java, the path to the *.py* file containing the main program in Python and the path to the master binary in C/C++.

The application arguments are the ones passed as command line to main application. This parameter can be empty.

The **runcompss** command allows the users to customize a COMPSs execution by specifying different options. For clarity purposes, parameters are grouped in *Runtime configuration*, *Tools enablers* and *Advanced options*.

```
compss@bsc:~$ runcompss -h
```

```
Usage: /opt/COMPSs/Runtime/scripts/user/runcompss [options] application_name application_
→arguments
```

* Options:

General:

```
--help, -h          Print this help message

--opts              Show available options

--version, -v       Print COMPSs version
```

Tools enablers:

```
--graph=<bool>, --graph, -g      Generation of the complete graph (true/false)
                                   When no value is provided it is set to true
                                   Default: false

--tracing=<level>, --tracing, -t  Set generation of traces and/or tracing level ( [
→true | basic ] | advanced | scorep | arm-map | arm-ddt | false)
                                   True and basic levels will produce the same
→traces.
                                   When no value is provided it is set to 1
                                   Default: 0

--monitoring=<int>, --monitoring, -m Period between monitoring samples (milliseconds)
                                   When no value is provided it is set to 2000
                                   Default: 0

--external_debugger=<int>,
--external_debugger              Enables external debugger connection on the
→specified port (or 9999 if empty)
                                   Default: false

--jmx_port=<int>                 Enable JVM profiling on specified port
```

Runtime configuration options:

```
--task_execution=<compss|storage> Task execution under COMPSs or Storage.
                                   Default: compss

--storage_impl=<string>           Path to an storage implementation. Shortcut to
→setting pypath and classpath. See Runtime/storage in your installation folder.

--storage_conf=<path>            Path to the storage configuration file
                                   Default: null

--project=<path>                 Path to the project XML file
                                   Default: /opt/COMPSs//Runtime/configuration/xml/
→projects/default_project.xml

--resources=<path>               Path to the resources XML file
                                   Default: /opt/COMPSs//Runtime/configuration/xml/
→resources/default_resources.xml

--lang=<name>                    Language of the application (java/c/python)
                                   Default: Inferred is possible. Otherwise: java
                                   Displays a task execution summary at the end of
→the application execution
                                   Default: false

--log_level=<level>, --debug, -d Set the debug level: off | info | api | debug |
→trace
                                   Warning: Off level compiles with -O2 option
→disabling asserts and __debug__
                                   Default: off
```

Advanced options:

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<code>--extrae_config_file=<path></code> → shared disk between all COMPSs workers.	Sets a custom extrae config file. Must be in a Default: null
<code>--extrae_config_file_python=<path></code> → be in a shared disk between all COMPSs workers.	Sets a custom extrae config file for python. Must Default: null
<code>--trace_label=<string></code> → used in the case of tracing is activated.	Add a label in the generated trace file. Only Default: None
<code>--comm=<ClassName></code> → communications	Class that implements the adaptor for Supported adaptors: es.bsc.compss.nio.master.NIOAdaptor es.bsc.compss.gat.master.GATAdaptor Default: es.bsc.compss.nio.master.NIOAdaptor
<code>--conn=<className></code> → the cloud	Class that implements the runtime connector for Supported connectors: es.bsc.compss.connectors. es.bsc.compss.connectors. Default: es.bsc.compss.connectors.
→ DefaultSSHConnector	
→ DefaultNoSSHConnector	
→ DefaultSSHConnector	
<code>--streaming=<type></code>	Enable the streaming mode for the given type. Supported types: FILES, OBJECTS, PSCOS, ALL, NONE Default: NONE
<code>--streaming_master_name=<str></code>	Use an specific streaming master node name. Default: null
<code>--streaming_master_port=<int></code>	Use an specific port for the streaming master. Default: null
<code>--scheduler=<className></code>	Class that implements the Scheduler for COMPSs Supported schedulers: es.bsc.compss.scheduler. es.bsc.compss.scheduler.fifonew. es.bsc.compss.scheduler.fifodatanew. es.bsc.compss.scheduler.lifonew. es.bsc.compss.components.impl. es.bsc.compss.scheduler.loadbalancing.
→ fifodatalocation.FIFODataLocationScheduler	
→ FIFOScheduler	
→ FIFODataScheduler	
→ LIFOScheduler	
→ TaskScheduler	
→ LoadBalancingScheduler	
→ LoadBalancingScheduler	
<code>--scheduler_config_file=<path></code> → configuration.	Path to the file which contains the scheduler Default: Empty
<code>--library_path=<path></code> → (e.g. Java JVM library, Python library, C binding library)	Non-standard directories to search for libraries Default: Working Directory
<code>--classpath=<path></code>	Path for the application classes / modules Default: Working Directory
<code>--appdir=<path></code>	Path for the application class folder.

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<code>--pythonpath=<path></code> →PYTHONPATH	Default: /home/user Additional folders or paths to add to the
<code>--env_script=<path></code> →environment variables are defined.	Default: /home/user Path to the script file where the application
<code>--application.</code>	COMPSs sources this script before running the
<code>--base_log_dir=<path></code> →COMPSs/ folder will be created inside this location)	Default: Empty Base directory to store COMPSs log files (a .
<code>--specific_log_dir=<path></code> →files (no sandbox is created)	Default: User home Use a specific directory to store COMPSs log
<code>--uuid=<int></code>	Warning: Overwrites --base_log_dir option Default: Disabled Preset an application UUID
<code>--master_name=<string></code>	Default: Automatic random generation Hostname of the node to run the COMPSs master
<code>--master_port=<int></code>	Default: Port to run the COMPSs master communications. Only for NIO adaptor
<code>--jvm_master_opts=<string></code> →option separated by "," and without blank spaces (Notice the quotes)	Default: [43000,44000] Extra options for the COMPSs Master JVM. Each
<code>--jvm_workers_opts=<string></code> →option separated by "," and without blank spaces (Notice the quotes)	Default: Extra options for the COMPSs Workers JVMs. Each
<code>--cpu_affinity=<string></code> →defined map of the form "0-8/9,10,11/12-14,15,16"	Default: -Xms1024m,-Xmx1024m,-Xmn400m Sets the CPU affinity for the workers Supported options: disabled, automatic, user
<code>--gpu_affinity=<string></code> →defined map of the form "0-8/9,10,11/12-14,15,16"	Default: automatic Sets the GPU affinity for the workers Supported options: disabled, automatic, user
<code>--fpga_affinity=<string></code> →defined map of the form "0-8/9,10,11/12-14,15,16"	Default: automatic Sets the FPGA affinity for the workers Supported options: disabled, automatic, user
<code>--fpga_reprogram=<string></code> →executed to reprogram the FPGA with the desired bitstream. The location must be an absolute →path.	Default: automatic Specify the full command that needs to be
<code>--io_executors=<int></code>	Default: 0 IO Executors per worker
<code>--task_count=<int></code> →different functions/methods, invoked from	Default: 0 Only for C/Python Bindings. Maximum number of
<code>--input_profile=<path></code> →application profile	Default: 50 Path to the file which stores the input
<code>--output_profile=<path></code> →at the end of the execution	Default: Empty Path to the file to store the application profile
	Default: Empty

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```

--PyObject_serialize=<bool>          Only for Python Binding. Enable the object
↪serialization to string when possible (true/false).
                                     Default: false

--persistent_worker_c=<bool>         Only for C Binding. Enable the persistent worker
↪in c (true/false).
                                     Default: false

--enable_external_adaptation=<bool>  Enable external adaptation. This option will
↪disable the Resource Optimizer.
                                     Default: false

--gen_coredump                       Enable master coredump generation
                                     Default: false

--keep_workingdir                   Do not remove the worker working directory after
↪the execution
                                     Default: false

--python_interpreter=<string>        Python interpreter to use (python/python2/
↪python3).
                                     Default: python Version:

--python_propagate_virtual_environment=<true> Propagate the master virtual environment
↪to the workers (true/false).
                                     Default: true

--python_mpi_worker=<false>          Use MPI to run the python worker instead of
↪multiprocessing. (true/false).
                                     Default: false

--python_memory_profile             Generate a memory profile of the master.
                                     Default: false

--python_worker_cache=<string>       Python worker cache (true/size/false).
                                     Only for NIO without mpi worker and python >= 3.8.
                                     Default: false

--wall_clock_limit=<int>             Maximum duration of the application (in seconds).
                                     Default: 0

* Application name:
  For Java applications:  Fully qualified name of the application
  For C applications:    Path to the master binary
  For Python applications: Path to the .py file containing the main program

* Application arguments:
  Command line arguments to pass to the application. Can be empty.

```

Running a COMPSs application

Before running COMPSs applications the application files **must** be in the **CLASSPATH**. Thus, when launching a COMPSs application, users can manually pre-set the **CLASSPATH** environment variable or can add the **--classpath** option to the **runcompss** command.

The next three sections provide specific information for launching COMPSs applications developed in different code languages (Java, Python and C/C++). For clarity purposes, we will use the *Simple* application (developed in Java, Python and C++) available in the COMPSs Virtual Machine or at <https://compss.bsc.es/projects/bar> webpage. This application takes an integer as input parameter and increases it by one unit using a task. For further details about the codes please refer to [Sample Applications](#).

Tip: For further information about applications scheduling refer to [Schedulers](#).

Running Java applications

A Java COMPSs application can be launched through the following command:

```
compss@bsc:~$ cd tutorial_apps/java/simple/jar/
compss@bsc:~/tutorial_apps/java/simple/jar$ runcompss simple.Simple <initial_number>
```

```
compss@bsc:~/tutorial_apps/java/simple/jar$ runcompss simple.Simple 1
[ INFO] Using default execution type: compss
[ INFO] Using default location for project file: /opt/COMPSs/Runtime/configuration/xml/
→projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSs/Runtime/configuration/xml/
→resources/default_resources.xml
[ INFO] Using default language: java

----- Executing simple.Simple -----

WARNING: COMPSs Properties file is null. Setting default values
[(1066)  API] - Starting COMPSs Runtime v<version>
Initial counter value is 1
Final counter value is 2
[(4740)  API] - Execution Finished

-----
```

In this first execution we use the default value of the `--classpath` option to automatically add the jar file to the classpath (by executing `runcompss` in the directory which contains the jar file). However, we can explicitly do this by exporting the **CLASSPATH** variable or by providing the `--classpath` value. Next, we provide two more ways to perform the same execution:

```
compss@bsc:~$ export CLASSPATH=$CLASSPATH:/home/compss/tutorial_apps/java/simple/jar/simple.
→jar
compss@bsc:~$ runcompss simple.Simple <initial_number>
```

```
compss@bsc:~$ runcompss --classpath=/home/compss/tutorial_apps/java/simple/jar/simple.jar \
simple.Simple <initial_number>
```

Running Python applications

To launch a COMPSs Python application users have to provide the `--lang=python` option to the `runcompss` command. If the extension of the main file is a regular Python extension (`.py` or `.pyc`) the `runcompss` command can also infer the application language without specifying the `lang` flag.

```
compss@bsc:~$ cd tutorial_apps/python/simple/
compss@bsc:~/tutorial_apps/python/simple$ runcompss --lang=python ./simple.py <initial_number>
```

```
compss@bsc:~/tutorial_apps/python/simple$ runcompss simple.py 1
[ INFO] Using default execution type: compss
[ INFO] Using default location for project file: /opt/COMPSs/Runtime/configuration/xml/
→projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSs/Runtime/configuration/xml/
→resources/default_resources.xml
[ INFO] Inferred PYTHON language

----- Executing simple.py -----
```

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```

WARNING: COMPSs Properties file is null. Setting default values
[(616)   API] - Starting COMPSs Runtime v<version>
Initial counter value is 1
Final counter value is 2
[(4297)  API] - Execution Finished
-----

```

Attention: Executing without debug (e.g. default log level or `--log_level=off`) uses `-O2` compiled sources, disabling `asserts` and `__debug__`.

Alternatively, it is possible to execute the a COMPSs Python application using `pycompss` as module:

```
compss@bsc:~$ python -m pycompss <runcompss_flags> <application> <application_parameters>
```

Consequently, the previous example could also be run as follows:

```

compss@bsc:~$ cd tutorial_apps/python/simple/
compss@bsc:~/tutorial_apps/python/simple$ python -m pycompss simple.py <initial_number>

```

If the `-m pycompss` is not set, the application will be run ignoring all PyCOMPSs imports, decorators and API calls, that is, sequentially.

In order to run a COMPSs Python application with a different interpreter, the `runcompss` command provides a specific flag:

```

compss@bsc:~$ cd tutorial_apps/python/simple/
compss@bsc:~/tutorial_apps/python/simple$ runcompss --python_interpreter=python3 ./simple.py
→<initial_number>

```

However, when using the `pycompss` module, it is inferred from the python used in the call:

```

compss@bsc:~$ cd tutorial_apps/python/simple/
compss@bsc:~/tutorial_apps/python/simple$ python3 -m pycompss simple.py <initial_number>

```

Finally, both `runcompss` and `pycompss` module provide a particular flag for virtual environment propagation (`--python_propagate_virtual_environment=<bool>`). This, flag is intended to activate the current virtual environment in the worker nodes when set to true.

Specific flags

Some of the `runcompss` flags are only for PyCOMPSs application execution:

- `--pythonpath=<path>` Additional folders or paths to add to the PYTHONPATH Default: `/home/user`
- `--PyObject_serialize=<bool>` Only for Python Binding. Enable the object serialization to string when possible (true/false). Default: false
- `--python_interpreter=<string>` Python interpreter to use (python/python2/python3). Default: "python" version
- `--python_propagate_virtual_environment=<true>` Propagate the master virtual environment to the workers (true/false). Default: true
- `--python_mpi_worker=<false>` Use MPI to run the python worker instead of multiprocessing. (true/false). Default: false

`--python_memory_profile` Generate a memory profile of the master. Default: false

See: [Memory Profiling](#)

`--python_worker_cache=<string>` Python worker cache (true/true:size/false). Only for NIO without mpi worker and python ≥ 3.8 . Default: false

See: [Worker cache](#)

Worker cache

The `--python_worker_cache` is used to enable a cache between processes on each worker node. More specifically, this flag enables a shared memory space between the worker processes, so that they can share objects between processes in order to leverage the deserialization overhead.

The possible values are:

`--python_worker_cache=false` Disable the cache. This is the default value.

`--python_worker_cache=true` Enable the cache. The default cache size is 25% of the worker node memory.

`--python_worker_cache=true:<SIZE>` Enable the cache with specific cache size (in bytes).

During execution, each worker will try to store automatically the parameters and return objects, so that next tasks can make use of them without needing to deserialize from file.

Important: The supported objects to be stored in the cache is **limited** to: **python primitives** (int, float, bool, str (less than 10 Mb), bytes (less than 10 Mb) and None), **lists** (composed by python primitives), **tuples** (composed by python primitives) and **Numpy ndarrays**.

It is important to take into account that storing the objects in cache has some non negligible overhead that can be representative, while getting objects from cache shows to be more efficient than deserialization. Consequently, the applications that most benefit from the cache are the ones that reuse many times the same objects.

Avoiding to store an object into the cache is possible by setting **Cache** to **False** into the `@task` decorator for the parameter. For example, [Code 91](#) shows how to avoid caching the **value** parameter.

Code 91: Avoid parameter caching

```
from pycompss.api.task import task
from pycompss.api.parameter import *

@task(value={Cache: False})
def mytask(value):
    ...
```

Additional features

Concurrent serialization

It is possible to perform concurrent serialization of the objects in the master when using Python 3. To this end, just export the `COMPSS_THREADED_SERIALIZATION` environment variable with any value:

```
compss@bsc:~$ export COMPSS_THREADED_SERIALIZATION=1
```

Caution: Please, make sure that the `COMPSS_THREADED_SERIALIZATION` environment variable is not in the environment (`env`) to avoid the concurrent serialization of the objects in the master.

Tip: This feature can also be used within supercomputers in the same way.

Running C/C++ applications

To launch a COMPSs C/C++ application users have to compile the C/C++ application by means of the `buildapp` command. For further information please refer to [C/C++ Binding](#). Once compiled, the `--lang=c` option must be provided to the `runcompss` command. If the main file is a C/C++ binary the `runcompss` command can also infer the application language without specifying the `lang` flag.

```
compss@bsc:~$ cd tutorial_apps/c/simple/
compss@bsc:~/tutorial_apps/c/simple$ runcompss --lang=c simple <initial_number>
```

```
compss@bsc:~/tutorial_apps/c/simple$ runcompss ~/tutorial_apps/c/simple/master/simple 1
[ INFO] Using default execution type: compss
[ INFO] Using default location for project file: /opt/COMPSs/Runtime/configuration/xml/
->projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSs/Runtime/configuration/xml/
->resources/default_resources.xml
[ INFO] Inferred C/C++ language

----- Executing simple -----

JVM_OPTIONS_FILE: /tmp/tmp.ItT1tQfKgP
COMPSS_HOME: /opt/COMPSs
Args: 1

WARNING: COMPSs Properties file is null. Setting default values
[(650)   API] - Starting COMPSs Runtime v<version>
Initial counter value is 1
[ BINDING] - @compss_wait_on - Entry.filename: counter
[ BINDING] - @compss_wait_on - Runtime filename: dlV2_1497432831496.IT
Final counter value is 2
[(4222)  API] - Execution Finished

-----
```

Walltime

The `runcompss` command provides the `--wall_clock_limit` for the users to specify the maximum execution time for the application (in seconds). If the time is reached, the execution is stopped.

Tip: This flag enables to stop the execution of an application in a controlled way if the execution is taking more than expected.

Additional configurations

The COMPSs runtime has two configuration files: `resources.xml` and `project.xml`. These files contain information about the execution environment and are completely independent from the application.

For each execution users can load the default configuration files or specify their custom configurations by using, respectively, the `--resources=<absolute_path_to_resources.xml>` and the `--project=<absolute_path_to_project.xml>` in the `runcompss` command. The default files are located in the `/opt/COMPSs/Runtime/configuration/xml/` path. Users can manually edit these files or can use the *Eclipse IDE* tool developed for COMPSs. For further information about the *Eclipse IDE* please refer to [COMPSs IDE](#) Section.

For further details please check the [Configuration Files](#).

5.1.1.2 Results and logs

Results

When executing a COMPSs application we consider different type of results:

- **Application Output:** Output generated by the application.
- **Application Files:** Files used or generated by the application.
- **Tasks Output:** Output generated by the tasks invoked from the application.

Regarding the application output, COMPSs will preserve the application output but will add some pre and post output to indicate the COMPSs Runtime state. [Figure 7](#) shows the standard output generated by the execution of the Simple Java application. The green box highlights the application `stdout` while the rest of the output is produced by COMPSs.

```
compss@bsc:~/tutorial_apps/java/simple/jar$ runcompss simple.Simple 1
[ INFO] Using default execution type: compss
[ INFO] Using default location for project file: /opt/COMPSs/Runtime/configuration/xml/projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSs/Runtime/configuration/xml/resources/default_resources.xml

----- Executing simple.Simple -----

WARNING: IT Properties file is null. Setting default values
[(1046) API] - Starting COMPSs Runtime
Initial counter value is 1
Final counter value is 2
[(4107) API] - Execution Finished

-----
```

Figure 7: Output generated by the execution of the *Simple* Java application with COMPSs

Regarding the application files, COMPSs **does not modify** any of them and thus, the results obtained by executing the application with COMPSs are the same than the ones generated by the sequential execution of the application.

Regarding the tasks output, COMPSs introduces some modifications due to the fact that tasks can be executed in remote machines. After the execution, COMPSs stores the `stdout` and the `stderr` of each job (a task execution) inside the ```/home/$USER/.COMPSs/$APPNAME/$EXEC_NUMBER/jobs/``` directory of the main application node.

[Figure 8](#) and [Figure 9](#) show an example of the results obtained from the execution of the *Hello* Java application. While [Figure 8](#) provides the output of the sequential execution of the application (without COMPSs), [Figure 9](#) provides the output of the equivalent COMPSs execution. Please note that the sequential execution produces the `Hello World! (from a task)` message in the `stdout` while the COMPSs execution stores the message inside the `job1_NEW.out` file.

```
compss@bsc:~/workspace_java/hello/jar$ java -cp hello.jar hello.Hello
Hello World! (from main application)
Hello World! (from a task)
```

Figure 8: Sequential execution of the *Hello* java application

```

compss@bsc:~/tutorial_apps/java/hello/jar$ runcompss -d hello.Hello
[ INFO] Using default execution type: compss
[ INFO] Using default location for project file: /opt/COMPSs/Runtime/configuration/xml/projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSs/Runtime/configuration/xml/resources/default_resources.xml

----- Executing hello.Hello -----

WARNING: IT Properties file is null. Setting default values
[[744)  API] - Deploying COMPSs Runtime
[[747)  API] - Starting COMPSs Runtime
[[747)  API] - Initializing components
[[1193) API] - Ready to process tasks
Hello World! (from main application)
[[1203) API] - Creating task from method sayHello in hello.HelloImpl
[[1203) API] - There is 0 parameter
[[1235) API] - No more tasks for app 1
[[3776) API] - Getting Result Files 1
[[3777) API] - Stop IT reached
[[3778) API] - Stopping AP...
[[3779) API] - Stopping TD...
[[3932) API] - Stopping Comm...
[[3934) API] - Runtime stopped
[[3934) API] - Execution Finished

-----
compss@bsc:~/tutorial_apps/java/hello/jar$ more ~/.COMPSs/hello.Hello_01/jobs/job1_NEW.out
[JAVA EXECUTOR] executeTask - Begin task execution
WORKER - Parameters of execution:
* Method type: METHOD
* Method definition: [DECLARING CLASS=hello.HelloImpl, METHOD NAME=sayHello]
* Parameter types:
* Parameter values:
Hello World! (from a task)
[JAVA EXECUTOR] executeTask - End task execution

```

Figure 9: COMPSs execution of the *Hello* java application

Logs

COMPSs includes three log levels for running applications but users can modify them or add more levels by editing the logger files under the `/opt/COMPSs/Runtime/configuration/log/` folder. Any of these log levels can be selected by adding the `--log_level=<debug | info | off>` flag to the `runcompss` command. The default value is `off`.

The logs generated by the `NUM_EXEC` execution of the application APP by the user USER are stored under `/home/$USER/.COMPSs/$APP/$EXEC_NUMBER/` folder (from this point on: **base log folder**). The `EXEC_NUMBER` execution number is automatically used by COMPSs to prevent mixing the logs of data of different executions.

When running COMPSs with **log level off** only the errors are reported. This means that the *base log folder* will contain two empty files (`runtime.log` and `resources.log`) and one empty folder (`jobs`). If somehow the application has failed, the `runtime.log` and/or the `resources.log` will not be empty and a new file per failed job will appear inside the `jobs` folder to store the `stdout` and the `stderr`. Figure 10 shows the logs generated by the execution of the Simple java application (without errors) in **off** mode.

```

.COMPSs/
├── [4.0K] simple.Simple_01
│   ├── [4.0K] jobs
│   ├── [ 0] resources.log
│   ├── [ 0] runtime.log
│   └── [4.0K] tmpFiles

```

Figure 10: Structure of the logs folder for the Simple java application in **off** mode

When running COMPSs with **log level info** the *base log folder* will contain two files (`runtime.log` and `resources.log`) and one folder (`jobs`). The `runtime.log` file contains the execution information retrieved from the master resource, including the file transfers and the job submission details. The `resources.log` file contains information about the available resources such as the number of processors of each resource (slots), the information about running or pending tasks in the resource queue and the created and destroyed resources. The `jobs` folder will be empty unless there has been a failed job. In this case it will store, for each failed job, one file for the `stdout` and another for the `stderr`. As an example, Figure 11 shows the logs generated by the same execution than the previous case but with **info** mode.

The `runtime.log` and `resources.log` are quite large files, thus they should be only checked by advanced users. For an easier interpretation of these files the COMPSs Framework includes a monitor tool. For further information about the COMPSs Monitor please check [COMPSs Monitor](#).

Figure 11: Structure of the logs folder for the Simple java application in **info** mode

Figure 12 and Figure 13 provide the content of these two files generated by the execution of the *Simple* java application.

```
compss@bsc:~/COMPSs/simple.Simple_02$ cat runtime.log
[[732](2015-08-20 16:34:30,731) TaskScheduler] @<init> - Initialization finished
[[738](2015-08-20 16:34:30,737) TaskScheduler] @<init> - Initialization finished
[[742](2015-08-20 16:34:30,741) JobManager] @<init> - Initialization finished
[[742](2015-08-20 16:34:30,741) TaskDispatcher] @<init> - Initialization finished
[[748](2015-08-20 16:34:30,747) TaskAnalyser] @<init> - Initialization finished
[[753](2015-08-20 16:34:30,752) TaskScheduler] @resourcesCreated - Resource http://bscgrid05.bsc.es:20390/hmmerobj/hmmerobj?wsdl
created
[[753](2015-08-20 16:34:30,752) DataInfoProvider] @<init> - Initialization finished
[[787](2015-08-20 16:34:30,786) TaskAnalyser] @processTask - New method task(increment), ID = 1
[[791](2015-08-20 16:34:30,790) TaskScheduler] @scheduleTask - Blocked: Task(1, increment)
[[1479](2015-08-20 16:34:31,478) Communication] @getWorkerIsReady - Notifying that worker is ready localhost
[[1892](2015-08-20 16:34:31,891) TaskScheduler] @resourcesCreated - Resource localhost created
[[1893](2015-08-20 16:34:31,892) TaskScheduler] @asksForResource - Available Resource: localhost. Task: 1, score: 0
[[1894](2015-08-20 16:34:31,893) JobManager] @processJob - New Job 1 (Task: 1)
[[1894](2015-08-20 16:34:31,893) JobManager] @processJob - * Method name: increment
[[1895](2015-08-20 16:34:31,894) JobManager] @processJob - * Target host: localhost
[[1899](2015-08-20 16:34:31,898) Communication] @submit - Submit NIOJob with ID 1
[[1944](2015-08-20 16:34:31,943) JobManager] @completedJob - Received a notification for job 1 with state OK
[[1945](2015-08-20 16:34:31,944) TaskProcessor] @notifyTaskEnd - Notification received for task 1 with end status FINISHED
[[1946](2015-08-20 16:34:31,945) TaskProcessor] @waitForTask - End of waited task for data 1
[[1955](2015-08-20 16:34:31,954) TaskProcessor] @noMoreTasks - All tasks finished
[[1962](2015-08-20 16:34:31,961) TaskProcessor] @run - AccessProcessor shutdown
[[1965](2015-08-20 16:34:31,964) Communication] @stop - Shutting down localhost:43001
```

Figure 12: runtime.log generated by the execution of the *Simple* java application

Running COMPSs with **log level debug** generates the same files as the info log level but with more detailed information. Additionally, the **jobs** folder contains two files per **submitted** job; one for the **stdout** and another for the **stderr**. In the other hand, the COMPSs Runtime state is printed out on the **stdout**. Figure 14 shows the logs generated by the same execution than the previous cases but with **debug** mode.

The runtime.log and the resources.log files generated in this mode can be **extremely large**. Consequently, the users should take care of their quota and manually erase these files if needed.

When running Python applications a **pycompss.log** file is written inside the *base log folder* containing debug information about the specific calls to PyCOMPSs.

Furthermore, when running **runcompss** with additional flags (such as monitoring or tracing) additional folders will appear inside the *base log folder*. The meaning of the files inside these folders is explained in [COMPSs Tools](#).

5.1.1.3 COMPSs Tools

Application graph

At the end of the application execution a dependency graph can be generated representing the order of execution of each type of task and their dependencies. To allow the final graph generation the **-g** flag has to be passed to the **runcompss** command; the graph file is written in the *base_log_folder/monitor/complete_graph.dot* at the end of the execution.

Figure 15 shows a dependency graph example of a *SparseLU* java application. The graph can be visualized by running the following command:

```
compss@bsc:~$ compss_gengraph ~/.COMPSs/sparseLU.arrays.SparseLU_01/monitor/complete_graph.dot
```

```

compss@bsc:~/COMPSs/simple.Simple_02$ cat resources.log
TIMESTAMP = 1440081270727
INFO_MSG = [New resource available in the pool. Name = http://bscgrid05.bsc.es:20390/hmmerobj/hmmerobj?wsdl]
TIMESTAMP = 1440081270752
LOAD_INFO = [
  CORE_INFO = [
    COREID = 0
    NO_RESOURCE = 0
    TO_RESCHEDULE = 0
    ORDINARY = 0
    MIN = 100
    MEAN = 100
    MAX = 100
  ]
]

TIMESTAMP = 1440081271891
INFO_MSG = [New resource available in the pool. Name = localhost]
TIMESTAMP = 1440081271962
INFO_MSG = [Stopping all workers]
TIMESTAMP = 1440081271962
LOAD_INFO = [
  CORE_INFO = [
    COREID = 0
    NO_RESOURCE = 0
    TO_RESCHEDULE = 0
    ORDINARY = 0
    MIN = 56
    MEAN = 56
    MAX = 56
  ]
]

```

Figure 13: resources.log generated by the execution of the *Simple* java application

```

.COMPSs/
├── [4.0K] simple.Simple_03
│   ├── [4.0K] jobs
│   │   ├── [ 0] job1_NEW.err
│   │   └── [380] job1_NEW.out
│   ├── [ 612] resources.log
│   ├── [ 70K] runtime.log
│   └── [4.0K] tmpFiles

```

Figure 14: Structure of the logs folder for the Simple java application in **debug** mode

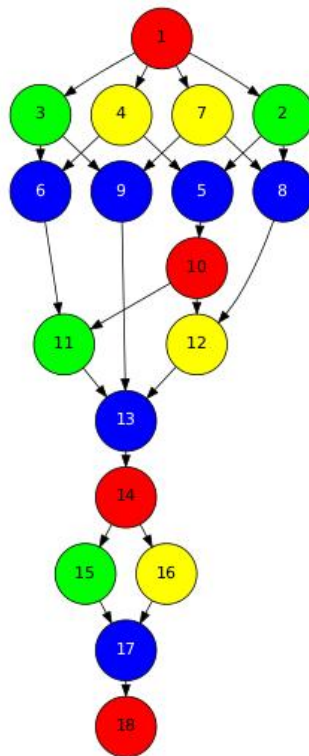


Figure 15: The dependency graph of the SparseLU application

COMPSs Monitor

The COMPSs Framework includes a Web graphical interface that can be used to monitor the execution of COMPSs applications. COMPSs Monitor is installed as a service and can be easily managed by running any of the following commands:

```
compss@bsc:~$ /etc/init.d/compss-monitor usage
Usage: compss-monitor {start | stop | reload | restart | try-restart | force-reload | status}
```

Service configuration

The COMPSs Monitor service can be configured by editing the `/opt/COMPSs/Tools/monitor/apache-tomcat/conf/compss-monitor.conf` file which contains one line per property:

COMPSS_MONITOR Default directory to retrieve monitored applications (defaults to the `.COMPSs` folder inside the `root` user).

COMPSs_MONITOR_PORT Port where to run the `compss-monitor` web service (defaults to 8080).

COMPSs_MONITOR_TIMEOUT Web page timeout between browser and server (defaults to 20s).

Usage

In order to use the COMPSs Monitor users need to start the service as shown in [Figure 16](#).

```
compss@bsc:~$ /etc/init.d/compss-monitor start
* Starting COMPSS Monitor
* Checking JAVA Installation...
Warning: JRE_HOME not defined
Info: JAVA_HOME found.
  Loading JRE_HOME from JAVA_HOME
  Success
* Checking IT_HOME...
WARNING: IT_HOME not defined. Trying default location /opt/COMPSs/
  Success
* Checking IT_MONITOR...
  IT_MONITOR=/home/compss/.COMPSs/
  Success
* Checking COMPSS Monitor Port...
Warning: COMPSS_MONITOR_PORT not defined.
  Loading from configuration file.
  COMPSS_MONITOR_PORT=8080
  Success
* Checking COMPSS Monitor Timeout...
Warning: COMPSS_MONITOR_TIMEOUT not defined.
  Loading from configuration file.
  COMPSS_MONITOR_TIMEOUT=20000
  Success
* Configuring COMPSS Monitor service...
  Success
Using CATALINA_BASE:   /opt/COMPSs/Tools/monitor/apache-tomcat
Using CATALINA_HOME:   /opt/COMPSs/Tools/monitor/apache-tomcat
Using CATALINA_TMPDIR: /opt/COMPSs/Tools/monitor/apache-tomcat/temp
Using JRE_HOME:        /usr/lib/jvm/java-8-openjdk-amd64/jre
Using CLASSPATH:       /opt/COMPSs/Tools/monitor/apache-tomcat/bin/bootstrap.jar:/opt/COMPSs/Tools/monitor/apache-tomcat/bin/tomcat-juli.jar
Tomcat started.
```

Figure 16: COMPSs Monitor start command

And use a web browser to open the specific URL:

```
compss@bsc:~$ firefox http://localhost:8080/compss-monitor &
```

The COMPSs Monitor allows to monitor applications from different users and thus, users need to first login to access their applications. As shown in [Figure 17](#), the users can select any of their executed or running COMPSs applications and display it.

To enable **all** the COMPSs Monitor features, applications must run the `runcompss` command with the `-m` flag. This flag allows the COMPSs Runtime to store special information inside the `log_base_folder` under the `monitor` folder (see [Figure 17](#) and [Figure 18](#)). Only advanced users should modify or delete any of these files. If the application that a user is trying to monitor has not been executed with this flag, some of the COMPSs Monitor features will be disabled.

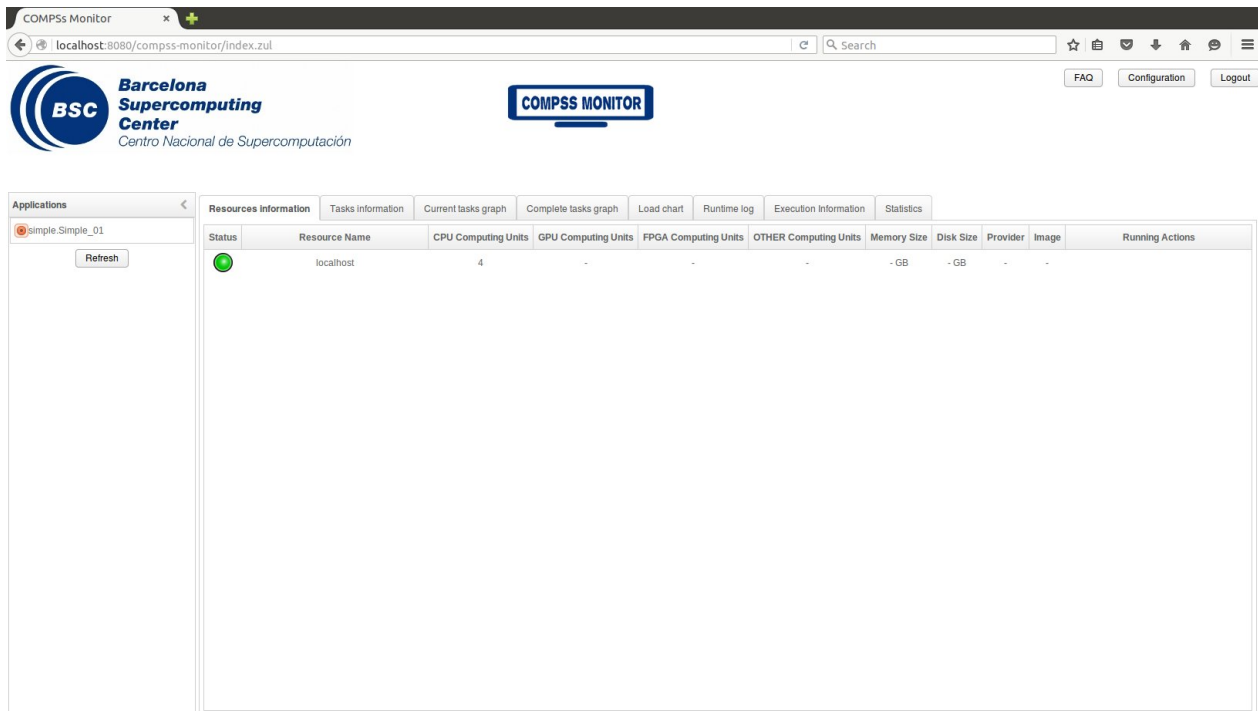


Figure 17: COMPSs monitoring interface

```
compss@bsc:~/tutorial_apps/java/simple/jar$ runcompss -dm simple.Simple 1
[ INFO] Using default execution type: compss
[ INFO] Using default location for project file: /opt/COMPSs/Runtime/configuration/xml/
->projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSs/Runtime/configuration/xml/
->resources/default_resources.xml
[ INFO] Using default language: java

----- Executing simple.Simple -----

WARNING: COMPSs Properties file is null. Setting default values
[(799)   API] - Deploying COMPSs Runtime v<version>
[(801)   API] - Starting COMPSs Runtime v<version>
[(801)   API] - Initializing components
[(1290)  API] - Ready to process tasks
[(1293)  API] - Opening /home/compss/tutorial_apps/java/simple/jar/counter in mode OUT
[(1338)  API] - File target Location: /home/compss/tutorial_apps/java/simple/jar/counter
Initial counter value is 1
[(1340)  API] - Creating task from method increment in simple.SimpleImpl
[(1340)  API] - There is 1 parameter
[(1341)  API] - Parameter 1 has type FILE_T
Final counter value is 2
[(4307)  API] - No more tasks for app 1
[(4311)  API] - Getting Result Files 1
[(4340)  API] - Stop IT reached
[(4344)  API] - Stopping Graph generation...
[(4344)  API] - Stopping Monitor...
[(6347)  API] - Stopping AP...
[(6348)  API] - Stopping TD...
[(6509)  API] - Stopping Comm...
[(6510)  API] - Runtime stopped
```

(continues on next page)

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```
[(6510)    API] - Execution Finished
```

```
compss@bsc:~$ cd .COMPSs/
compss@bsc:~/.COMPSs$ tree
.
├── simple.Simple_01
│   ├── jobs
│   │   ├── job1_NEW.err
│   │   └── job1_NEW.out
│   └── monitor
│       ├── complete_graph.dot
│       ├── COMPSs_state.xml
│       └── current_graph.dot
├── resources.log
├── runtime.log
└── tmpFiles
```

Figure 18: Logs generated by the Simple java application with the monitoring flag enabled

Graphical Interface features

In this section we provide a summary of the COMPSs Monitor supported features available through the graphical interface:

- **Resources information** Provides information about the resources used by the application
- **Tasks information** Provides information about the tasks definition used by the application
- **Current tasks graph** Shows the tasks dependency graph currently stored into the COMPSs Runtime
- **Complete tasks graph** Shows the complete tasks dependency graph of the application
- **Load chart** Shows different dynamic charts representing the evolution over time of the resources load and the tasks load
- **Runtime log** Shows the runtime log
- **Execution Information** Shows specific job information allowing users to easily select failed or uncompleted jobs
- **Statistics** Shows application statistics such as the accumulated cloud cost.

Important: To enable all the COMPSs Monitor features applications must run with the `-m` flag.

The webpage also allows users to configure some performance parameters of the monitoring service by accessing the *Configuration* button at the top-right corner of the web page.

For specific COMPSs Monitor feature configuration please check our *FAQ* section at the top-right corner of the web page.

Application tracing

COMPSs Runtime can generate a post-execution trace of the execution of the application. This trace is useful for performance analysis and diagnosis.

A trace file may contain different events to determine the COMPSs master state, the task execution state or the file-transfers. The current release does not support file-transfers informations.

During the execution of the application, an XML file is created in the worker nodes to keep track of these events. At the end of the execution, all the XML files are merged to get a final trace file.

In this manual we only provide information about how to obtain a trace and about the available Paraver (the tool used to analyze the traces) configurations. For further information about the application instrumentation or the trace visualization and configurations please check the [Tracing](#) Section.

Trace Command

In order to obtain a post-execution trace file one of the following options `-t`, `--tracing`, `--tracing=true`, `--tracing=basic` must be added to the `runcompss` command. All this options activate the basic tracing mode; the advanced mode is activated with the option `--tracing=advanced`. For further information about advanced mode check the [COMPSs applications tracing](#) Section. Next, we provide an example of the command execution with the basic tracing option enabled for a java K-Means application.

```
compss@bsc:~$ runcompss -t kmeans.Kmeans
*** RUNNING JAVA APPLICATION KMEANS
[ INFO] Relative Classpath resolved: /path/to/jar/kmeans.jar

----- Executing kmeans.Kmeans -----

Welcome to Extrae VERSION
Extrae: Parsing the configuration file (/opt/COMPSs/Runtime/configuration/xml/tracing/extrae_
→basic.xml) begins
Extrae: Warning! <trace> tag has no <home> property defined.
Extrae: Generating intermediate files for Paraver traces.
Extrae: <cpu> tag at <counters> level will be ignored. This library does not support CPU HW.
Extrae: Tracing buffer can hold 100000 events
Extrae: Circular buffer disabled.
Extrae: Dynamic memory instrumentation is disabled.
Extrae: Basic I/O memory instrumentation is disabled.
Extrae: System calls instrumentation is disabled.
Extrae: Parsing the configuration file (/opt/COMPSs/Runtime/configuration/xml/tracing/extrae_
→basic.xml) has ended
Extrae: Intermediate traces will be stored in /user/folder
Extrae: Tracing mode is set to: Detail.
Extrae: Successfully initiated with 1 tasks and 1 threads

WARNING: COMPSs Properties file is null. Setting default values
[(751)   API] - Deploying COMPSs Runtime v<version>
[(753)   API] - Starting COMPSs Runtime v<version>
[(753)   API] - Initializing components
[(1142)  API] - Ready to process tasks
...
...
...
merger: Output trace format is: Paraver
merger: Extrae 3.3.0 (revision 3966 based on extrae/trunk)
mpi2prv: Assigned nodes < Marginis >
mpi2prv: Assigned size per processor < <1 Mbyte >
mpi2prv: File set-0/TRACE@Marginis.000000190400000000000000.mpit is object 1.1.1 on node_
→Marginis assigned to processor 0
mpi2prv: File set-0/TRACE@Marginis.000000190400000000000001.mpit is object 1.1.2 on node_
→Marginis assigned to processor 0
mpi2prv: File set-0/TRACE@Marginis.000000190400000000000002.mpit is object 1.1.3 on node_
→Marginis assigned to processor 0
mpi2prv: File set-0/TRACE@Marginis.00000019800000001000000.mpit is object 1.2.1 on node_
→Marginis assigned to processor 0
mpi2prv: File set-0/TRACE@Marginis.000000198000000010000001.mpit is object 1.2.2 on node_
→Marginis assigned to processor 0
mpi2prv: File set-0/TRACE@Marginis.000000198000000010000002.mpit is object 1.2.3 on node_
→Marginis assigned to processor 0
mpi2prv: File set-0/TRACE@Marginis.000000198000000010000003.mpit is object 1.2.4 on node_
→Marginis assigned to processor 0
```

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```

mpi2prv: File set-0/TRACE@Marginis.0000001980000001000004.mpit is object 1.2.5 on node_
→Marginis assigned to processor 0
mpi2prv: Time synchronization has been turned off
mpi2prv: A total of 9 symbols were imported from TRACE.sym file
mpi2prv: 0 function symbols imported
mpi2prv: 9 HWC counter descriptions imported
mpi2prv: Checking for target directory existence... exists, ok!
mpi2prv: Selected output trace format is Paraver
mpi2prv: Stored trace format is Paraver
mpi2prv: Searching synchronization points... done
mpi2prv: Time Synchronization disabled.
mpi2prv: Circular buffer enabled at tracing time? NO
mpi2prv: Parsing intermediate files
mpi2prv: Progress 1 of 2 ... 5% 10% 15% 20% 25% 30% 35% 40% 45% 50% 55% 60% 65% 70% 75% 80% 85
→% 90% 95% done
mpi2prv: Processor 0 succeeded to translate its assigned files
mpi2prv: Elapsed time translating files: 0 hours 0 minutes 0 seconds
mpi2prv: Elapsed time sorting addresses: 0 hours 0 minutes 0 seconds
mpi2prv: Generating tracefile (intermediate buffers of 838848 events)
        This process can take a while. Please, be patient.
mpi2prv: Progress 2 of 2 ... 5% 10% 15% 20% 25% 30% 35% 40% 45% 50% 55% 60% 65% 70% 75% 80% 85
→% 90% 95% done
mpi2prv: Warning! Clock accuracy seems to be in microseconds instead of nanoseconds.
mpi2prv: Elapsed time merge step: 0 hours 0 minutes 0 seconds
mpi2prv: Resulting tracefile occupies 991743 bytes
mpi2prv: Removing temporal files... done
mpi2prv: Elapsed time removing temporal files: 0 hours 0 minutes 0 seconds
mpi2prv: Congratulations! ./trace/kmeans.Kmeans_compss_trace_1460456106.prv has been_
→generated.
[  API] - Execution Finished
-----

```

At the end of the execution the trace will be stored inside the **trace** folder under the application log directory.

```

compss@bsc:~$ cd .COMPSs/kmeans.Kmeans_01/trace/
compss@bsc:~$ ls -l
kmeans.Kmeans_compss_trace_1460456106.pcf
kmeans.Kmeans_compss_trace_1460456106.prv
kmeans.Kmeans_compss_trace_1460456106.row

```

Trace visualization

The traces generated by an application execution are ready to be visualized with *Paraver*. *Paraver* is a powerful tool developed by *BSC* that allows users to show many views of the trace data by means of different configuration files. Users can manually load, edit or create configuration files to obtain different trace data views.

If *Paraver* is installed, issue the following command to visualize a given tracefile:

```
compss@bsc:~$ wxparaver path/to/trace/trace_name.prv
```

For further information about *Paraver* please visit the following site: <http://www.bsc.es/computer-sciences/performance-tools/paraver>

COMPSs IDE

COMPSs IDE is an Integrated Development Environment to develop, compile, deploy and execute COMPSs applications. It is available through the *Eclipse Market* as a plugin and provides an even easier way to work with COMPSs.

For further information please check the *COMPSs IDE User Guide* available at: <http://compss.bsc.es>.

5.1.2 Supercomputers

This section is intended to walk you through the COMPSs usage in Supercomputers.

5.1.2.1 Executing COMPSs applications

Loading the COMPSs Environment

Depending on the supercomputer installation, COMPSs can be loaded by an environment script, or an Environment Module. The following paragraphs provide the details about how to load the COMPSs environment in the different situations.

COMPSs Environment Script

After a successful installation from the supercomputers package, users can find the *compssenv* script in the folder where COMPSs was installed. This script can be used to load the COMPSs environment in the system as indicated below.

```
$ source <COMPSS_INSTALLATION_DIR>/compssenv
```

COMPSs Environment Module

In BSC supercomputers, COMPSs is configured as an Environment Module. As shown in next Figure, users can type the `module available COMPSs` command to list the supported COMPSs modules in the supercomputer. The users can also execute the `module load COMPSs/<version>` command to load an specific COMPSs module.

```
$ module available COMPSs
----- /apps/modules/modulefiles/tools -----
COMPSs/1.3
COMPSs/1.4
COMPSs/2.0
COMPSs/2.1
COMPSs/2.2
COMPSs/2.3
COMPSs/2.4
COMPSs/2.5
COMPSs/2.6
COMPSs/2.7
COMPSs/2.8
COMPSs/2.9
COMPSs/release(default)
COMPSs/trunk

$ module load COMPSs/release
```

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```
load java/1.8.0u66 (PATH, MANPATH, JAVA_HOME, JAVA_ROOT, JAVA_BINDIR,  
                  SDK_HOME, JDK_HOME, JRE_HOME)  
load MKL/11.0.1 (LD_LIBRARY_PATH)  
load PYTHON/2.7.3 (PATH, MANPATH, LD_LIBRARY_PATH, C_INCLUDE_PATH)  
load COMPSs/release (PATH, MANPATH, COMPSS_HOME)
```

The following command can be run to check if the correct COMPSs version has been loaded:

```
$ enqueue_compss --version  
COMPSs version <version>
```

Configuration Notes

The COMPSs module contains **all** the COMPSs dependencies, including Java, Python and MKL. Modifying any of these dependencies can cause execution failures and thus, we **do not** recommend to change them. Before running any COMPSs job please check your environment and, if needed, comment out any line inside the `.bashrc` file that loads custom COMPSs, Java, Python and/or MKL modules.

The COMPSs environment needs to be loaded in all the nodes that will run COMPSs jobs. Some queue system (such as Slurm) already forward the environment in the allocated nodes. If it is not the case, the `module load` or the `compssenv` script **must** be included in your `.bashrc` file. To do so, please run the following command with the corresponding COMPSs version:

```
$ cat "module load COMPSs/release" >> ~/.bashrc
```

Log out and back in again to check that the file has been correctly edited. The next listing shows an example of the output generated by well loaded COMPSs installation.

```
$ exit  
$ ssh USER@SC  
load java/1.8.0u66 (PATH, MANPATH, JAVA_HOME, JAVA_ROOT, JAVA_BINDIR,  
                  SDK_HOME, JDK_HOME, JRE_HOME)  
load MKL/11.0.1 (LD_LIBRARY_PATH)  
load PYTHON/2.7.3 (PATH, MANPATH, LD_LIBRARY_PATH, C_INCLUDE_PATH)  
load COMPSs/release (PATH, MANPATH, COMPSS_HOME)  
  
USER@SC$ enqueue_compss --version  
COMPSs version <version>
```

Important: Please remember that PyCOMPSs uses Python 2.7 by default. In order to use Python 3, the Python 2.7 module **must** be unloaded after loading COMPSs module, and then load the Python 3 module.

COMPSs Job submission

COMPSs jobs can be easily submitted by running the `enqueue_compss` command. This command allows to configure any `runcompss` ([Runcompss command](#)) option and some particular queue options such as the queue system, the number of nodes, the wallclock time, the master working directory, the workers working directory and number of tasks per node.

Next, we provide detailed information about the `enqueue_compss` command:

```
$ enqueue_compss -h
```

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```

Usage: /apps/COMPSs/2.9/Runtime/scripts/user/enqueue_compss [queue_system_options] [COMPSs_
→options] application_name application_arguments

* Options:
  General:
    --help, -h                Print this help message
    --heterogeneous           Indicates submission is going to be heterogeneous
                                Default: Disabled

  Queue system configuration:
    --sc_cfg=<name>           SuperComputer configuration file to use. Must
→exist inside queues/cfgs/
                                Default: default

  Submission configuration:
  General submission arguments:
    --exec_time=<minutes>     Expected execution time of the application (in
→minutes)
                                Default: 10
    --job_name=<name>         Job name
                                Default: COMPSs
    --queue=<name>            Queue name to submit the job. Depends on the
→queue system.
                                For example (MN3): bsc_cs | bsc_debug | debug |
→interactive
                                Default: default
    --reservation=<name>      Reservation to use when submitting the job.
                                Default: disabled
    --env_script=<path/to/script> Script to source the required environment for the
→application.
                                Default: Empty
    --extra_submit_flag=<flag> Flag to pass queue system flags not supported by
→default command flags.
                                Spaces must be added as '#'
                                Default: Empty
    --cpus_per_task           Number of cpus per task the queue system must
→allocate per task.
                                Note that this will be equal to the cpus_per_node
→in a worker node and
                                equal to the worker_in_master_cpus in a master
→node respectively.
                                Default: false
    --job_dependency=<jobID>   Postpone job execution until the job dependency
→has ended.
                                Default: None
    --forward_time_limit=<true|false> Forward the queue system time limit to the
→runtime.
                                It will stop the application in a controlled way.
                                Default: true
    --storage_home=<string>    Root installation dir of the storage
→implementation
                                Default: null
    --storage_props=<string>   Absolute path of the storage properties file
                                Mandatory if storage_home is defined

  Agents deployment arguments:
    --agents=<string>          Hierarchy of agents for the deployment. Accepted
→values: plain|tree

```

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<code>--agents</code>	Default: tree
<code>→ classic Master-Worker deployment.</code>	Deploys the runtime as agents instead of the <code>U</code>
	Default: disabled
Homogeneous submission arguments:	
<code>--num_nodes=<int></code>	Number of nodes to use
	Default: 2
<code>--num_switches=<int></code>	Maximum number of different switches. Select 0 <code>U</code>
<code>→ for no restrictions.</code>	
	Maximum nodes per switch: 18
	Only available for at least 4 nodes.
	Default: 0
Heterogeneous submission arguments:	
<code>--type_cfg=<file_location></code>	Location of the file with the descriptions of <code>U</code>
<code>→ node type requests</code>	
	File should follow the following format:
	type_X(){
	cpus_per_node=24
	node_memory=96
	...
	}
	type_Y(){
	...
	}
<code>--master=<master_node_type></code>	Node type for the master
	(Node type descriptions are provided in the --
<code>→ type_cfg flag)</code>	
<code>--workers=type_X:nodes,type_Y:nodes</code>	Node type and number of nodes per type for the <code>U</code>
<code>→ workers</code>	
	(Node type descriptions are provided in the --
<code>→ type_cfg flag)</code>	
Launch configuration:	
<code>--cpus_per_node=<int></code>	Available CPU computing units on each node
	Default: 32
<code>--gpus_per_node=<int></code>	Available GPU computing units on each node
	Default: 0
<code>--fpgas_per_node=<int></code>	Available FPGA computing units on each node
	Default:
<code>--io_executors=<int></code>	Number of IO executors on each node
	Default: 0
<code>--fpga_reprogram=<string></code>	Specify the full command that needs to be <code>U</code>
<code>→ executed to reprogram the FPGA with</code>	
<code>→ absolute path.</code>	the desired bitstream. The location must be an <code>U</code>
<code>--max_tasks_per_node=<int></code>	Default:
<code>→ node</code>	Maximum number of simultaneous tasks running on a <code>U</code>
<code>--node_memory=<MB></code>	Default: -1
	Maximum node memory: disabled <int> (MB)
	Default: disabled
<code>--node_storage_bandwidth=<MB></code>	Maximum node storage bandwidth: <int> (MB)
	Default:
<code>--network=<name></code>	Communication network for transfers: default <code>U</code>
<code>→ ethernet infiniband data.</code>	

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	Default: ethernet
<code>--prolog=<string></code> →the quotes)	Task to execute before launching COMPSs (Notice
→rather than spaces.	If the task has arguments split them by ","
→than one prolog action	This argument can appear multiple times for more
<code>--epilog=<string></code> →application (Notice the quotes)	Default: Empty Task to execute after executing the COMPSs
→rather than spaces.	If the task has arguments split them by ","
→than one epilog action	This argument can appear multiple times for more
	Default: Empty
<code>--master_working_dir=<path></code>	Working directory of the application Default: .
<code>--worker_working_dir=<name path></code> →<path>	Worker directory. Use: local_disk shared_disk Default: local_disk
<code>--worker_in_master_cpus=<int></code> →master node can run as worker. Cannot exceed cpus_per_node.	Maximum number of CPU computing units that the Default: 0
<code>--worker_in_master_memory=<int> MB</code> →worker. Cannot exceed the node_memory.	Maximum memory in master node assigned to the Mandatory if worker_in_master_cpus is specified. Default: disabled
<code>--worker_port_range=<min>,<max></code> →side	Port range used by the NIO adaptor at the worker Default: 43001,43005
<code>--jvm_worker_in_master_opts=<string></code> →the Master Node.	Extra options for the JVM of the COMPSs Worker in Each option separated by "," and without blank
→spaces (Notice the quotes)	Default: Runs the application by means of a container
<code>--container_image=<path></code> →engine image	Default: Empty Path where compss is installed in the container
<code>--container_compss_path=<path></code> →image	Default: /opt/COMPSs Options to pass to the container engine Default: empty
<code>--container_opts=<string></code>	Activate elasticity specifying the maximum extra →nodes (ONLY AVAILABLE FORM SLURM CLUSTERS WITH NIO ADAPTOR) Default: 0
<code>--elasticity=<max_extra_nodes></code> →nodes (ONLY AVAILABLE FORM SLURM CLUSTERS WITH NIO ADAPTOR)	Default: 0 Enable or disable the runtime automatic scaling
<code>--automatic_scaling=<bool></code> →(for elasticity)	Default: true Swap the COMPSs master initialization with
<code>--jupyter_notebook=<path>,<path></code> →jupyter notebook from the specified path.	Default: false Swap the COMPSs master initialization with
<code>--jupyter_notebook</code> →ipython.	

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	Default: empty
Runcompss configuration:	
Tools enablers:	
--graph=<bool>, --graph, -g	Generation of the complete graph (true/false) When no value is provided it is set to true Default: false
--tracing=<level>, --tracing, -t →true basic] advanced scorep arm-map arm-ddt false) →traces.	Set generation of traces and/or tracing level ([True and basic levels will produce the same When no value is provided it is set to 1 Default: 0
--monitoring=<int>, --monitoring, -m	Period between monitoring samples (milliseconds) When no value is provided it is set to 2000 Default: 0
--external_debugger=<int>, --external_debugger →specified port (or 9999 if empty)	Enables external debugger connection on the Default: false
--jmx_port=<int>	Enable JVM profiling on specified port
Runtime configuration options:	
--task_execution=<compss storage>	Task execution under COMPSs or Storage. Default: compss
--storage_impl=<string> →setting pypath and classpath. See Runtime/storage in your installation folder.	Path to an storage implementation. Shortcut to Path to the storage configuration file Default: null
--storage_conf=<path>	Path to the project XML file Default: /opt/COMPSs//Runtime/configuration/xml/ →projects/default_project.xml
--project=<path> →resources/default_resources.xml	Path to the resources XML file Default: /opt/COMPSs//Runtime/configuration/xml/ →resources/default_resources.xml
--lang=<name>	Language of the application (java/c/python) Default: Inferred is possible. Otherwise: java
--summary →the application execution	Displays a task execution summary at the end of Default: false
--log_level=<level>, --debug, -d →trace	Set the debug level: off info api debug Warning: Off level compiles with -O2 option Default: off
→disabling asserts and __debug__	
Advanced options:	
--extrae_config_file=<path> →shared disk between all COMPSs workers.	Sets a custom extrae config file. Must be in a Default: null
--extrae_config_file_python=<path> →be in a shared disk between all COMPSs workers.	Sets a custom extrae config file for python. Must Default: null

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<code>--trace_label=<string></code> →used in the case of tracing is activated.	Add a label in the generated trace file. Only Default: None
<code>--comm=<ClassName></code> →communications	Class that implements the adaptor for Supported adaptors: es.bsc.compss.nio.master.NIOAdaptor es.bsc.compss.gat.master.GATAdaptor Default: es.bsc.compss.nio.master.NIOAdaptor
<code>--conn=<className></code> →the cloud	Class that implements the runtime connector for Supported connectors: es.bsc.compss.connectors. es.bsc.compss.connectors.
→DefaultSSHConnector	
→DefaultNoSSHConnector	
→DefaultSSHConnector	
<code>--streaming=<type></code>	Enable the streaming mode for the given type. Supported types: FILES, OBJECTS, PSCOS, ALL, NONE Default: NONE
<code>--streaming_master_name=<str></code>	Use an specific streaming master node name. Default: null
<code>--streaming_master_port=<int></code>	Use an specific port for the streaming master. Default: null
<code>--scheduler=<className></code>	Class that implements the Scheduler for COMPSs Supported schedulers: es.bsc.compss.scheduler. es.bsc.compss.scheduler.fifonew. es.bsc.compss.scheduler.fifodatanew. es.bsc.compss.scheduler.lifonew. es.bsc.compss.components.impl. es.bsc.compss.scheduler.loadbalancing.
→fifodatalocation.FIFODataLocationScheduler	
→FIFOScheduler	
→FIFODataScheduler	
→LIFOScheduler	
→TaskScheduler	
→LoadBalancingScheduler	
→LoadBalancingScheduler	
<code>--scheduler_config_file=<path></code> →configuration.	Path to the file which contains the scheduler Default: Empty
<code>--library_path=<path></code> →(e.g. Java JVM library, Python library, C binding library)	Non-standard directories to search for libraries Default: Working Directory
<code>--classpath=<path></code>	Path for the application classes / modules Default: Working Directory
<code>--appdir=<path></code>	Path for the application class folder. Default: /home/user
<code>--pythonpath=<path></code> →PYTHONPATH	Additional folders or paths to add to the Default: /home/user
<code>--env_script=<path></code> →environment variables are defined.	Path to the script file where the application

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→application.	COMPSs sources this script before running the
--base_log_dir=<path>	Default: Empty
→COMPSs/ folder will be created inside this location)	Base directory to store COMPSs log files (a .
--specific_log_dir=<path>	Default: User home
→files (no sandbox is created)	Use a specific directory to store COMPSs log
	Warning: Overwrites --base_log_dir option
--uuid=<int>	Default: Disabled
	Preset an application UUID
--master_name=<string>	Default: Automatic random generation
	Hostname of the node to run the COMPSs master
--master_port=<int>	Default:
	Port to run the COMPSs master communications.
	Only for NIO adaptor
	Default: [43000,44000]
--jvm_master_opts="<string>"	Extra options for the COMPSs Master JVM. Each
→option separated by "," and without blank spaces (Notice the quotes)	Default:
--jvm_workers_opts="<string>"	Extra options for the COMPSs Workers JVMs. Each
→option separated by "," and without blank spaces (Notice the quotes)	Default: -Xms1024m,-Xmx1024m,-Xmn400m
--cpu_affinity="<string>"	Sets the CPU affinity for the workers
→defined map of the form "0-8/9,10,11/12-14,15,16"	Supported options: disabled, automatic, user
--gpu_affinity="<string>"	Default: automatic
→defined map of the form "0-8/9,10,11/12-14,15,16"	Sets the GPU affinity for the workers
--fpga_affinity="<string>"	Supported options: disabled, automatic, user
→defined map of the form "0-8/9,10,11/12-14,15,16"	Default: automatic
--fpga_reprogram="<string>"	Sets the FPGA affinity for the workers
→executed to reprogram the FPGA with the desired bitstream. The location must be an absolute	Supported options: disabled, automatic, user
→path.	Default: automatic
--io_executors=<int>	Specify the full command that needs to be
	Default: 0
--task_count=<int>	IO Executors per worker
→different functions/methods, invoked from the application, that have been selected as tasks	Default: 0
--input_profile=<path>	Only for C/Python Bindings. Maximum number of
→application profile	Default: 50
	Path to the file which stores the input
--output_profile=<path>	Default: Empty
→at the end of the execution	Path to the file to store the application profile
--PyObject_serialize=<bool>	Default: Empty
→serialization to string when possible (true/false).	Only for Python Binding. Enable the object
--persistent_worker_c=<bool>	Default: false
→in c (true/false).	Only for C Binding. Enable the persistent worker
	Default: false

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<code>--enable_external_adaptation=<bool></code> →disable the Resource Optimizer.	Enable external adaptation. This option will Default: false
<code>--gen_coredump</code>	Enable master coredump generation Default: false
<code>--keep_workingdir</code> →the execution	Do not remove the worker working directory after Default: false
<code>--python_interpreter=<string></code> →python3).	Python interpreter to use (python/python2/ Default: python Version:
<code>--python_propagate_virtual_environment=<true></code> →to the workers (true/false).	Propagate the master virtual environment Default: true
<code>--python_mpi_worker=<false></code> →multiprocessing. (true/false).	Use MPI to run the python worker instead of Default: false
<code>--python_memory_profile</code>	Generate a memory profile of the master. Default: false
<code>--python_worker_cache=<string></code>	Python worker cache (true/size/false). Only for NIO without mpi worker and python >= 3.8. Default: false
<code>--wall_clock_limit=<int></code>	Maximum duration of the application (in seconds). Default: 0
* Application name:	
For Java applications: Fully qualified name of the application	
For C applications: Path to the master binary	
For Python applications: Path to the .py file containing the main program	
* Application arguments:	
Command line arguments to pass to the application. Can be empty.	

Tip: For further information about applications scheduling refer to [Schedulers](#).

Attention: From COMPSs 2.8 version, the `worker_working_dir` has changed its built-in values to be more generic. The current values are: `local_disk` which substitutes the former `scratch` value; and `shared_disk` which replaces the `gpfs` value.

Walltime

As with the `runcompss` command, the `enqueue_compss` command also provides the `--wall_clock_limit` for the users to specify the maximum execution time for the application (in seconds). If the time is reached, the execution is stopped.

Do not confuse with `--exec_time`, since `exec_time` indicates the walltime for the queuing system, whilst `wall_clock_limit` is for COMPSs. Consequently, if the `exec_time` is reached, the queuing system will arise an exception and the execution will be stopped suddenly (potentially causing loose of data). However, if the `wall_clock_limit` is reached, the COMPSs runtime stops and grabs all data safely.

Tip: It is a good practice to define the `--wall_clock_limit` with less time than defined for `--exec_time`, so

that the COMPSs runtime can stop the execution safely and ensure that no data is lost.

PyCOMPSs within interactive jobs

PyCOMPSs can be used in interactive jobs through the use of `ipython`. To this end, the first thing is to request an interactive job. For example, an interactive job with Slurm for one node with 48 cores (as in MareNostrum 4) can be requested as follows:

```
$ salloc --qos=debug -N1 -n48

salloc: Pending job allocation 12189081
salloc: job 12189081 queued and waiting for resources
salloc: job 12189081 has been allocated resources
salloc: Granted job allocation 12189081
salloc: Waiting for resource configuration
salloc: Nodes s02r2b27 are ready for job
```

When the job starts running, the terminal directly opens within the given node.

Then, it is necessary to start the COMPSs infrastructure in the given nodes. To this end, the following command will start one worker with 24 cores (default worker in master), and then launch the *ipython* interpreter:

```
$ launch_compss \
--sc_cfg=mn.cfg \
--master_node="$SLURMD_NODENAME" \
--worker_nodes="" \
--ipython \
--pythonpath=$(pwd) \
"dummy"
```

Note that the *launch_compss* command requires the supercomputing configuration file, which in the MareNostrum 4 case is *mn.cfg* (more information about the supercomputer configuration can be found in [Configuration Files](#)). In addition, requires to define which node is going to be the master, and which ones the workers (if none, takes the default worker in master). Finally, the *-ipython* flag indicates that use *ipython* is expected.

When *ipython* is started, the COMPSs infrastructure is ready, and the user can start running interactive commands considering the PyCOMPSs API for jupyter notebook (see Jupyter [API calls](#)).

5.1.2.2 MareNostrum 4

Basic queue commands

The MareNostrum supercomputer uses the SLURM (Simple Linux Utility for Resource Management) workload manager. The basic commands to manage jobs are listed below:

- **sbatch** Submit a batch job to the SLURM system
- **scancel** Kill a running job
- **squeue -u <username>** See the status of jobs in the SLURM queue

For more extended information please check the *SLURM: Quick start user guide* at <https://slurm.schedmd.com/quickstart.html>.

Tracking COMPSs jobs

When submitting a COMPSs job a temporal file will be created storing the job information. For example:

```
$ enqueue_compss \
--exec_time=15 \
--num_nodes=3 \
--cpus_per_node=16 \
--master_working_dir=. \
--worker_working_dir=shared_disk \
--lang=python \
--log_level=debug \
<APP> <APP_PARAMETERS>

SC Configuration:      default.cfg
Queue:                 default
Reservation:           disabled
Num Nodes:             3
Num Switches:          0
GPUs per node:         0
Job dependency:        None
Exec-Time:             00:15
Storage Home:          null
Storage Properties:    null
Other:
  --sc_cfg=default.cfg
  --cpus_per_node=48
  --master_working_dir=.
  --worker_working_dir=shared_disk
  --lang=python
  --classpath=.
  --library_path=.
  --comm=es.bsc.compss.nio.master.NIOAdaptor
  --tracing=false
  --graph=false
  --pythonpath=.
  <APP> <APP_PARAMETERS>

Temp submit script is: /scratch/tmp/tmp.pBG5yfFxEO

$ cat /scratch/tmp/tmp.pBG5yfFxEO
#!/bin/bash
#
#SBATCH --job-name=COMPSs
#SBATCH --workdir=.
#SBATCH -o compss-%J.out
#SBATCH -e compss-%J.err
#SBATCH -N 3
#SBATCH -n 144
#SBATCH --exclusive
#SBATCH -t00:15:00
...
```

In order to track the jobs state users can run the following command:

```
$ squeue
```

JOBID	PARTITION	NAME	USER	TIME_LEFT	TIME_LIMIT	START_TIME	ST	NODES	CPUS	NODELIST
474130	main	COMPSs	XX	0:15:00	0:15:00	N/A	PD	3	144	-

The specific COMPSs logs are stored under the `~/COMPSs/` folder; saved as a local *runcompss* execution. For further details please check the [Executing COMPSs applications](#) Section.

5.1.2.3 MinoTauro

Basic queue commands

The MinoTauro supercomputer uses the SLURM (Simple Linux Utility for Resource Management) workload manager. The basic commands to manage jobs are listed below:

- **sbatch** Submit a batch job to the SLURM system
- **scancel** Kill a running job
- **squeue -u <username>** See the status of jobs in the SLURM queue

For more extended information please check the *SLURM: Quick start user guide* at <https://slurm.schedmd.com/quickstart.html>.

Tracking COMPSs jobs

When submitting a COMPSs job a temporal file will be created storing the job information. For example:

```
$ enqueue_compss \  
--exec_time=15 \  
--num_nodes=3 \  
--cpus_per_node=16 \  
--master_working_dir=. \  
--worker_working_dir=shared_disk \  
--lang=python \  
--log_level=debug \  
<APP> <APP_PARAMETERS>  
  
SC Configuration:      default.cfg  
Queue:                 default  
Reservation:           disabled  
Num Nodes:             3  
Num Switches:          0  
GPUs per node:         0  
Job dependency:         None  
Exec-Time:             00:15  
Storage Home:          null  
Storage Properties:    null  
Other:  
    --sc_cfg=default.cfg  
    --cpus_per_node=16  
    --master_working_dir=.  
    --worker_working_dir=shared_disk  
    --lang=python  
    --classpath=.  
    --library_path=.  
    --comm=es.bsc.compss.nio.master.NIOAdaptor  
    --tracing=false  
    --graph=false  
    --pythonpath=.  
    <APP> <APP_PARAMETERS>  
Temp submit script is: /scratch/tmp/tmp.pBG5yfFxEO
```

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```
$ cat /scratch/tmp/tmp.pBG5yfFxEO
#!/bin/bash
#
#SBATCH --job-name=COMPSs
#SBATCH --workdir=.
#SBATCH -o compss-%J.out
#SBATCH -e compss-%J.err
#SBATCH -N 3
#SBATCH -n 48
#SBATCH --exclusive
#SBATCH -t00:15:00
...
```

In order to track the jobs state users can run the following command:

```
$ squeue
JOBID PARTITION NAME USER ST TIME NODES NODELIST (REASON)
XXXX projects COMPSs XX R 00:02 3 nvb[6-8]
```

The specific COMPSs logs are stored under the `~/COMPSs/` folder; saved as a local `runcompss` execution. For further details please check the [Executing COMPSs applications](#) Section.

5.1.2.4 Nord 3

Basic queue commands

The Nord3 supercomputer uses the LSF (Load Sharing Facility) workload manager. The basic commands to manage jobs are listed below:

- **bsub** Submit a batch job to the LSF system
- **bkill** Kill a running job
- **bjobs** See the status of jobs in the LSF queue
- **bqueues** Information about LSF batch queues

For more extended information please check the *IBM Platform LSF Command Reference* at https://www.ibm.com/support/knowledgecenter/en/SSETD4_9.1.2/lfs_kc_cmd_ref.html.

Tracking COMPSs jobs

When submitting a COMPSs job a temporal file will be created storing the job information. For example:

```
$ enqueue_compss \
--exec_time=15 \
--num_nodes=3 \
--cpus_per_node=16 \
--master_working_dir=. \
--worker_working_dir=shared_disk \
--lang=python \
--log_level=debug \
<APP> <APP_PARAMETERS>

SC Configuration:      default.cfg
Queue:                default
```

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```

Reservation:           disabled
Num Nodes:            3
Num Switches:         0
GPUs per node:        0
Job dependency:       None
Exec-Time:            00:15
Storage Home:         null
Storage Properties:    null
Other:
    --sc_cfg=default.cfg
    --cpus_per_node=16
    --master_working_dir=.
    --worker_working_dir=shared_disk
    --lang=python
    --classpath=.
    --library_path=.
    --comm=es.bsc.compss.nio.master.NIOAdaptor
    --tracing=false
    --graph=false
    --pythonpath=.
    <APP> <APP_PARAMETERS>
Temp submit script is: /scratch/tmp/tmp.pBG5yfFxEO

$ cat /scratch/tmp/tmp.pBG5yfFxEO
#!/bin/bash
#
#BSUB -J COMPSs
#BSUB -cwd .
#BSUB -oo compss-%J.out
#BSUB -eo compss-%J.err
#BSUB -n 3
#BSUB -R "span[ptile=1]"
#BSUB -W 00:15
...

```

In order to trac the jobs state users can run the following command:

```

$ bjobs
JOBID  USER  STAT  QUEUE  FROM_HOST  EXEC_HOST  JOB_NAME  SUBMIT_TIME
XXXX   bscXX  PEND  XX     login1     XX         COMPSs    Month Day Hour

```

The specific COMPSs logs are stored under the `~/COMPSs/` folder; saved as a local *runcompss* execution. For further details please check the [Executing COMPSs applications](#) Section.

5.1.2.5 Enabling COMPSs Monitor

Configuration

As supercomputer nodes are connection restricted, the better way to enable the *COMPSs Monitor* is from the users local machine. To do so please install the following packages:

- COMPSs Runtime
- COMPSs Monitor
- sshfs

For further details about the COMPSs packages installation and configuration please refer to [Installation and Administration](#) Section. If you are not willing to install COMPSs in your local machine please consider to download

our Virtual Machine available at our webpage.

Once the packages have been installed and configured, users need to mount the sshfs directory as follows. The SC_USER stands for your supercomputer's user, the SC_ENDPOINT to the supercomputer's public endpoint and the TARGET_LOCAL_FOLDER to the local folder where you wish to deploy the supercomputer files):

```
compss@bsc:~$ scp $HOME/.ssh/id_rsa.pub ${SC_USER}@mn1.bsc.es:~/id_rsa_local.pub
compss@bsc:~$ ssh SC_USER@SC_ENDPOINT \
    "cat ~/id_rsa_local.pub >> ~/.ssh/authorized_keys; \
    rm ~/id_rsa_local.pub"
compss@bsc:~$ mkdir -p TARGET_LOCAL_FOLDER/.COMPSs
compss@bsc:~$ sshfs -o IdentityFile=$HOME/.ssh/id_rsa -o allow_other \
    SC_USER@SC_ENDPOINT:~/id_rsa_local.pub \
    TARGET_LOCAL_FOLDER/.COMPSs
```

Whenever you wish to unmount the sshfs directory please run:

```
compss@bsc:~$ sudo umount TARGET_LOCAL_FOLDER/.COMPSs
```

Execution

Access the COMPSs Monitor through its webpage (<http://localhost:8080/compss-monitor> by default) and log in with the TARGET_LOCAL_FOLDER to enable the COMPSs Monitor for MareNostrum.

Please remember that to enable **all** the COMPSs Monitor features applications must be ran with the *-m* flag. For further details please check the *Executing COMPSs applications* Section.

Figure 19 illustrates how to login and Figure 20 shows the COMPSs Monitor main page for an application run inside a Supercomputer.

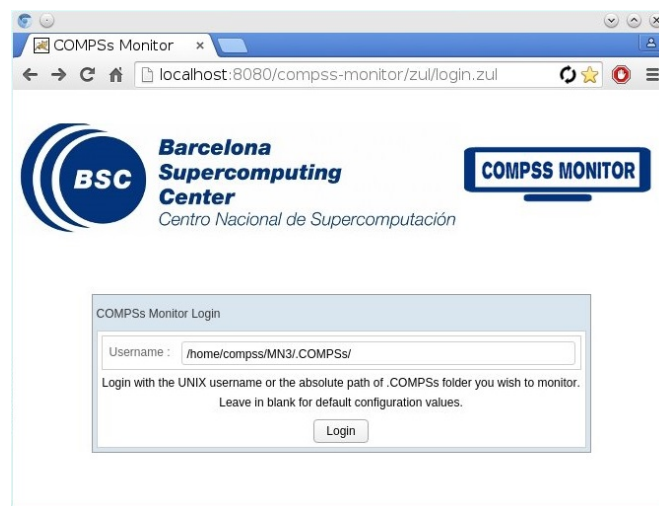


Figure 19: COMPSs Monitor login for Supercomputers

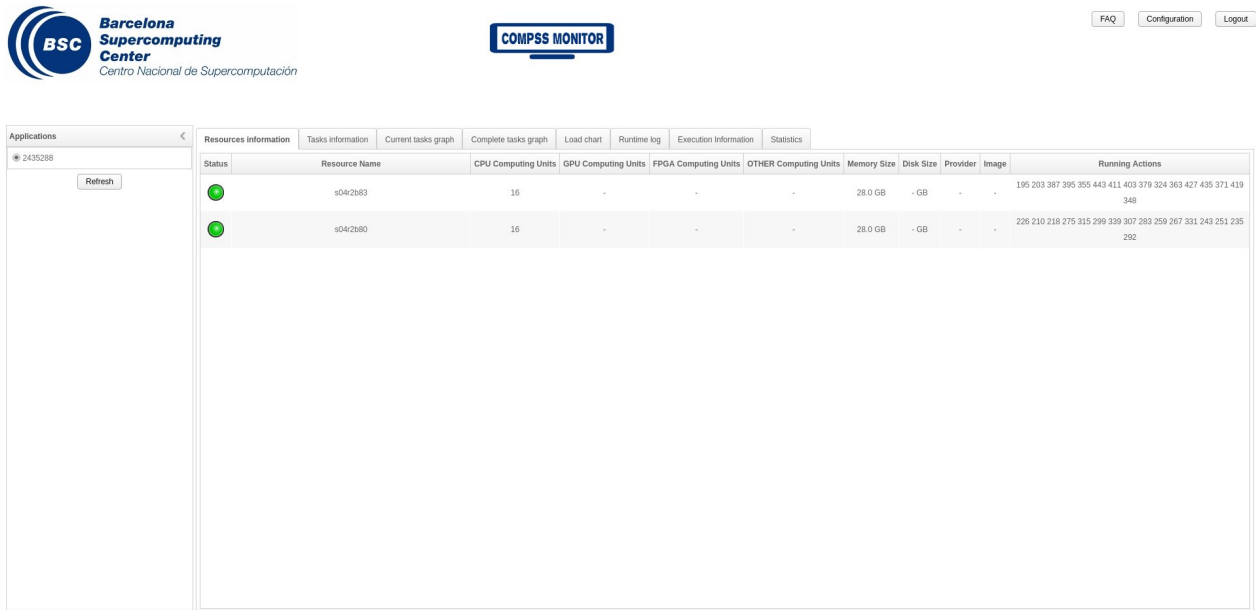


Figure 20: COMPSs Monitor main page for a test application at Supercomputers

5.1.3 Docker

5.1.3.1 What is Docker?

Docker is an open-source project that automates the deployment of applications inside software containers, by providing an additional layer of abstraction and automation of operating-system-level virtualization on Linux. In addition to the Docker container engine, there are other Docker tools that allow users to create complex applications (Docker-Compose) or to manage a cluster of Docker containers (Docker Swarm).

COMPSs supports running a distributed application in a Docker Swarm cluster.

5.1.3.2 Requirements

In order to use COMPSs with Docker, some requirements must be fulfilled:

- Have **Docker** and **Docker-Compose** installed in your local machine.
- Have an available **Docker Swarm cluster** and its Swarm manager ip and port to access it remotely.
- A **Dockerhub account**. Dockerhub is an online repository for Docker images. We don't currently support another sharing method besides uploading to Dockerhub, so you will need to create a personal account. This has the advantage that it takes very little time either upload or download the needed images, since it will reuse the existing layers of previous images (for example the COMPSs base image).

5.1.3.3 Execution in Docker

The runcompss-docker execution workflow uses Docker-Compose, which is in charge of spawning the different application containers into the Docker Swarm manager. Then the Docker Swarm manager schedules the containers to the nodes and the application starts running. The COMPSs master and workers will run in the nodes Docker Swarm decides. To see where the masters and workers are located in runtime, you can use:

```
$ docker -H '<swarm_manager_ip:swarm_port>' ps -a
```

The execution of an application using Docker containers with COMPSs consists of 2 steps:

Execution step 1: Creation of the application image

The very first step to execute a COMPSs application in Docker is creating your application Docker image.

This must be done **only once** for every new application, and then you can run it as many times as needed. If the application is updated for whatever reason, this step must be done again to create and share the updated image.

In order to do this, you must use the `compss_docker_gen_image` tool, which is available in the standard COMPSs application. This tool is the responsible of taking your application, create the needed image, and upload it to Dockerhub to share it.

The image is created injecting your application into a COMPSs base image. This base image is available in Dockerhub. In case you need it, you can pull it using the following command:

```
$ docker pull compss/compss
```

The `compss_docker_gen_image` script receives 2 parameters:

--c, --context-dir Specifies the **context directory** path of the application. This path **MUST BE ABSOLUTE**, not relative. The context directory is a local directory that **must contain the needed binaries and input files of the app (if any)**. In its simplest case, it will contain the executable file (a .jar for example). Keep the context-directory as lightest as possible.

For example: `--context-dir='/home/compss-user/my-app-dir'` (where 'my-app-dir' contains 'app.jar', 'data1.dat' and 'data2.csv'). For more details, this context directory will be recursively copied into a COMPSs base image. Specifically, it will create all the path down to the context directory inside the image.

--image-name Specifies a name for the created image. It **MUST** have this format: 'DOCKERHUB-USERNAME/image-name'. The `DOCKERHUB_USERNAME` must be the username of your personal Dockerhub account. The *image_name* can be whatever you want, and will be used as the identifier for the image in Dockerhub. This name will be the one you will use to execute the application in Docker. For example, if my Dockerhub username is john123 and I want my image to be named "my-image-app": `--image-name='john123/my-image-app'`.

As stated before, this is needed to share your container application image with the nodes that need it. Image tags are also supported (for example "john123/my-image-app:1.23").

Important: After creating the image, be sure to write down the absolute context-directory and the absolute classpath (the absolute path to the executable jar). You will need it to run the application using `runcompss-docker`. In addition, if you plan on distributing the application, you can use the Dockerhub image's information tab to write them, so the application users can retrieve them.

Execution step 2: Run the application

To execute COMPSs in a Docker Swarm cluster, you must use the `runcompss-docker` command, instead of `runcompss`.

The command `runcompss-docker` has some **additional arguments** that will be needed by COMPSs to run your application in a distributed Docker Swarm cluster environment. The rest of typical arguments (classpath for example) will be delegated to `runcompss` command.

These additional arguments must go before the typical `runcompss` arguments. The `runcompss-docker` additional arguments are:

- w, --worker-containers** Specifies the number of **worker containers** the app will execute on. One more container will be created to host the **master**. If you have enough nodes in the Swarm cluster, each container will be executed by one node. This is the default schedule strategy used by Swarm. For example: `--worker-containers=3`
- s, --swarm-manager** Specifies the Swarm manager ip and port (format: ip:port). For example: `--swarm-manager='129.114.108.8:4000'`
- i, --image-name** Specify the image name of the application image in Dockerhub. Remember you must generate this with `compss_docker_gen_image`. Remember as well that the format must be: `'DOCKERHUB_USERNAME/APP_IMAGE_NAME:TAG'` (the `:TAG` is optional). For example: `--image-name='john123/my-compss-application:1.9'`
- c, --context-dir** Specifies the **context directory** of the app. It must be specified by the application image provider. For example: `--context-dir='/home/compss-user/my-app-context-dir'`

As **optional** arguments:

- c-cpu-units** Specifies the number of cpu units used by each container (default value is 4). For example: `*--c-cpu-units:=16`
- c-memory** Specifies the physical memory used by each container in GB (default value is 8 GB). For example, in this case, each container would use as maximum 32 GB of physical memory: `--c-memory=32`

Here is the **format** you must use with `runcompss-docker` command:

```
$ runcompss-docker --worker-containers=N \
  --swarm-manager='<ip>:<port>' \
  --image-name='DOCKERHUB_USERNAME/image_name' \
  --context-dir='CTX_DIR' \
  [rest of classic runcompss args]
```

Or alternatively, in its shortest form:

```
$ runcompss-docker --w=N --s='<ip>:<port>' --i='DOCKERHUB_USERNAME/image_name' --c='CTX_DIR' \
  [rest of classic runcompss args]
```

5.1.3.4 Execution with TLS

If your cluster uses **TLS** or has been created using **Docker-Machine**, you will have to **export two environment variables** before using `runcompss-docker`:

On one hand, **DOCKER_TLS_VERIFY** environment variable will tell Docker that you are using TLS:

```
export DOCKER_TLS_VERIFY="1"
```

On the other hand, **DOCKER_CERT_PATH** variable will tell Docker where to find your TLS certificates. As an example:

```
export DOCKER_CERT_PATH="/home/compss-user/.docker/machine/machines/my-manager-node"
```

In case you have created your cluster using `docker-machine`, in order to know what your **DOCKER_CERT_PATH** is, you can use this command:

```
$ docker-machine env my-swarm-manager-node-name | grep DOCKER_CERT_PATH
```

In which *swarm-manager-node-name* must be changed by the name `docker-machine` has assigned to your swarm manager node. With these environment variables set, you are ready to use `runcompss-docker` in a cluster using TLS.

5.1.3.5 Execution results

The execution results will be retrieved from the master container of your application.

If your context-directory name is **'matmul'**, then your results will be saved in the **'matmul-results'** directory, which will be located in the same directory you executed runcompss-docker on.

Inside the **'matmul-results'** directory you will have:

- A folder named **'matmul'** with all the result files that were in the same directory as the executable when the application execution ended. More precisely, this will contain the context-directory state right after finishing your application execution. Additionally, and for more advanced debug purposes, you will have some intermediate files created by runcompss-docker (Dockerfile, project.xml, resources.xml), in case you want to check for more complex errors or details.
- A folder named **'debug'**, which (in case you used the runcompss debug option (-d)), will contain the **'COMPSs'** directory, which contains another directory in which there are the typical debug files runtime.log, jobs, etc. Remember **.COMPSs** is a **hidden** directory, take this into account if you do **ls** inside the debug directory (add the **-a** option).

To make it simpler, we provide a **tree visualization** of an example of what your directories should look like after the execution. In this case we executed the **Matmul example application** that we provide you:

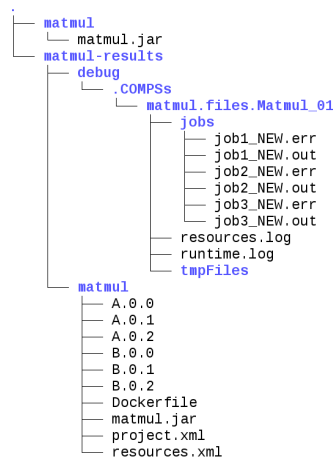


Figure 21: Result and log folders of a *Matmul* execution with COMPSs and Docker

5.1.3.6 Execution examples

Next we will use the *Matmul* application as an example of a Java application running with COMPSs and Docker.

Imagine we have our Matmul application in `/home/john/matmul` and inside the `matmul` directory we only have the file `matmul.jar`.

We have created a Dockerhub account with username 'john123'.

The first step will be creating the image:

```
$ compss_docker_gen_image --context-dir='/home/john/matmul' \
                          --image-name='john123/matmul-example'
```

Now, we write down the context-dir (`/home/john/matmul`) and the classpath (`/home/john/matmul/matmul.jar`). We do this because they will be needed for future executions. Since the image is created and uploaded, we won't need to do this step anymore.

Now we are going to execute our Matmul application in a Docker cluster.

Take as assumptions:

- We will use **5 worker docker containers**.

- The **swarm-manager ip** will be 129.114.108.8, with the Swarm manager listening to the **port** 4000.
- We will use **debug (-d)**.
- Finally, as we would do with the typical runcompss, we specify the **main class** name and its **parameters** (16 and 4 in this case).

In addition, we know from the former step that the image name is `john123/matmul-example`, the **context directory** is `/home/john/matmul`, and the classpath is `/home/john/matmul/matmul.jar`. And this is how you would run `runcompss-docker`:

```
$ runcompss-docker --worker-containers=5 \  
                  --swarm-manager='129.114.108.8:4000' \  
                  --context-dir='/home/john/matmul' \  
                  --image-name='john123/matmul-example' \  
                  --classpath=/home/john/matmul/matmul.jar \  
                  -d \  
                  matmul.objects.Matmul 16 4
```

Here we show another example using the short arguments form, with the KMeans example application, that is also provided as an example COMPSs application to you:

First step, create the image once:

```
$ compss_docker_gen_image --context-dir='/home/laura/apps/kmeans' \  
                        --image-name='laura-67/my-kmeans'
```

And now execute with 30 worker containers, and Swarm located in '110.3.14.159:26535'.

```
$ runcompss-docker --w=30 \  
                  --s='110.3.14.159:26535' \  
                  --c='/home/laura/apps/kmeans' \  
                  --image-name='laura-67/my-kmeans' \  
                  --classpath=/home/laura/apps/kmeans/kmeans.jar \  
                  kmeans.KMeans
```

5.1.4 Chameleon

5.1.4.1 What is Chameleon?

The Chameleon project is a configurable experimental environment for large-scale cloud research based on a *OpenStack* KVM Cloud. With funding from the *National Science Foundation (NSF)*, it provides a large-scale platform to the open research community allowing them explore transformative concepts in deeply programmable cloud services, design, and core technologies. The Chameleon testbed, is deployed at the *University of Chicago* and the *Texas Advanced Computing Center* and consists of 650 multi-core cloud nodes, 5PB of total disk space, and leverage 100 Gbps connection between the sites.

The project is led by the *Computation Institute* at the *University of Chicago* and partners from the *Texas Advanced Computing Center* at the *University of Texas* at Austin, the *International Center for Advanced Internet Research* at *Northwestern University*, the *Ohio State University*, and *University of Texas* at *San Antoni*, comprising a highly qualified and experienced team. The team includes members from the *NSF* supported *FutureGrid* project and from the *GENI* community, both forerunners of the *NSFCloud* solicitation under which this project is funded. Chameleon will also sets of partnerships with commercial and academic clouds, such as *Rackspace*, *CERN* and *Open Science Data Cloud (OSDC)*.

For more information please check <https://www.chameleoncloud.org/> .

5.1.4.2 Execution in Chameleon

Currently, COMPSs can only handle the Chameleon infrastructure as a cluster (deployed inside a lease). Next, we provide the steps needed to execute COMPSs applications at Chameleon:

- Make a lease reservation with 1 minimum node (for the COMPSs master instance) and a maximum number of nodes equal to the number of COMPSs workers needed plus one
- Instantiate the master image (based on the published image *COMPSs__CC-CentOS7*)
- Attach a public IP and login to the master instance (the instance is correctly contextualized for COMPSs executions if you see a COMPSs login banner)
- Set the instance as COMPSs master by running `/etc/init.d/chameleon_init start`
- Copy your CH file (API credentials) to the Master and source it
- Run the `chameleon_cluster_setup` script and fill the information when prompted (you will be asked for the name of the master instance, the reservation id and number of workers). This scripts may take several minutes since it sets up the all cluster.
- Execute your COMPSs applications normally using the `runcompss` script

As an example you can check this video <https://www.youtube.com/watch?v=BrQ6anPHjAU> performing a full setup and execution of a COMPSs application at Chameleon.

5.1.5 Jupyter Notebook

5.1.5.1 Notebook execution

The jupyter notebook can be executed as a common Jupyter notebook by steps or the whole application.

Important: A message showing the failed task/s will pop up if an exception within them happens.

This pop up message will also allow you to continue the execution without PyCOMPSs, or to restart the COMPSs runtime. Please, note that in the case of COMPSs restart, the tracking of some objects may be lost (will need to be recomputed).

5.1.5.2 Notebook example

Sample notebooks can be found in the *PyCOMPSs Notebooks* Section.

5.1.5.3 Tips and Tricks

Tasks information

It is possible to show task related information with `tasks_info` function.

```
# Previous user code

import pycompss.interactive as ipycompss
ipycompss.start(graph=True)

# User code that calls tasks

# Check the current tasks info
ipycompss.tasks_info()

ipycompss.stop(sync=True)

# Subsequent code
```

Important: The tasks information will not be displayed if the `monitor` option at `ipycompss.start` is not set (to a refresh value).

The `tasks_info` function provides a widget that can be updated while running other cells from the notebook, and will keep updating every second until stopped. Alternatively, it will show a snapshot of the tasks information status if `ipywidgets` is not available.

The information displayed is composed by two plots: the left plot shows the average time per task, while the right plot shows the amount of tasks. Then, a table with the specific number of number of executed tasks, maximum execution time, mean execution time and minimum execution time, per task is shown.

Tasks status

It is possible to show task status (running or completed) tasks with the `tasks_status` function.

```
# Previous user code

import pycompss.interactive as ipycompss
ipycompss.start(graph=True)

# User code that calls tasks

# Check the current tasks info
ipycompss.tasks_status()

ipycompss.stop(sync=True)

# Subsequent code
```

Important: The tasks information will not be displayed if the `monitor` option at `ipycompss.start` is not set (to a refresh value).

The `tasks_status` function provides a widget that can be updated while running other cells from the notebook, and will keep updating every second until stopped. Alternatively, it will show a snapshot of the tasks status if `ipywidgets` is not available.

The information displayed is composed by a pie chart and a table showing the number of running tasks, and the number of completed tasks.

Resources status

It is possible to show resources status with the `resources_status` function.

```
# Previous user code

import pycompss.interactive as ipycompss
ipycompss.start(graph=True)

# User code that calls tasks

# Check the current tasks info
ipycompss.resources_status()

ipycompss.stop(sync=True)
```

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```
# Subsequent code
```

Important: The tasks information will not be displayed if the `monitor` option at `ipycompss.start` is not set (to a refresh value).

The `resources_status` function provides a widget that can be updated while running other cells from the notebook, and will keep updating every second until stopped. Alternatively, it will show a snapshot of the resources status if ipywidgets is not available.

The information displayed is a table showing the number of computing units, gpus, fpgas, other computing units, amount of memory, amount of disk, status and actions.

Current task graph

It is possible to show the current task graph with the `current_task_graph` function.

```
# Previous user code

import pycompss.interactive as ipycompss
ipycompss.start(graph=True)

# User code that calls tasks

# Check the current task graph
ipycompss.current_task_graph()

ipycompss.stop(sync=True)

# Subsequent code
```

Important: The graph will not be displayed if the `graph` option at `ipycompss.start` is not set to `true`.

In addition, the `current_task_graph` has some options. Specifically, its full signature is:

```
current_task_graph(fit=False, refresh_rate=1, timeout=0)
```

Parameters:

- `fit` Adjust the size to the available space in jupyter if set to true. Display full size if set to false (default).
- `refresh_rate` When `timeout` is set to a value different from 0, it defines the number of seconds between graph refresh.
- `timeout` Check the current task graph during the `timeout` value (seconds). During the `timeout` value, it refresh the graph considering the `refresh_rate` value. It can be stopped with the stop button of Jupyter. Does not update the graph if set to 0 (default).

Caution: The graph can be empty if all pending tasks have been completed.

Complete task graph

It is possible to show the complete task graph with the `complete_task_graph` function.

```
# Previous user code

import pycompss.interactive as ipycompss
ipycompss.start(graph=True)

# User code that calls tasks

# Check the current task graph
ipycompss.complete_task_graph()

ipycompss.stop(sync=True)

# Subsequent code
```

Important: The graph will not be displayed if the `graph` option at `ipycompss.start` is not set to `true`.

In addition, the `complete_task_graph` has some options. Specifically, its full signature is:

```
complete_task_graph(fit=False, refresh_rate=1, timeout=0)
```

Parameters:

- `fit` Adjust the size to the available space in jupyter if set to true. Display full size if set to false (default).
- `refresh_rate` When `timeout` is set to a value different from 0, it defines the number of seconds between graph refresh.
- `timeout` Check the current task graph during the `timeout` value (seconds). During the `timeout` value, it refresh the graph considering the `refresh_rate` value. It can be stopped with the stop button of Jupyter. Does not update the graph if set to 0 (default).

Caution: The graph may be empty or raise an exception if the graph has not been updated by the runtime (may happen if there are too few tasks). In this situation, stop the compss runtime (synchronizing the remaining objects if intended to start the runtime afterwards) and try again.

5.2 Agents Deployments

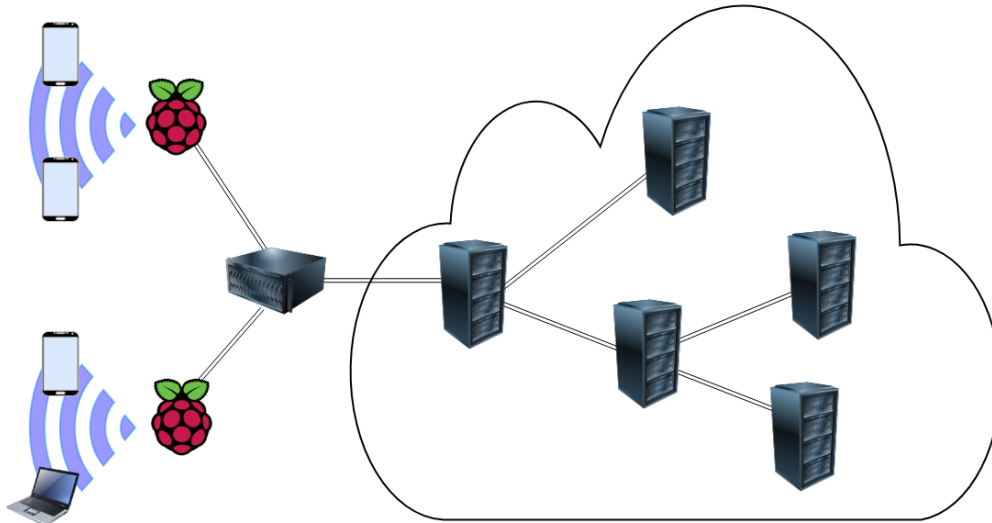
Opposing to well-established deployments with an almost-static set of computing resources and hardly-varying interconnection conditions such as a single-computer, a cluster or a supercomputer; dynamic infrastructures, like Fog environments, require a different kind of deployment able to adapt to rapidly-changing conditions. Such infrastructures are likely to comprise several mobile devices whose connectivity to the infrastructure is temporary. When the device is within the network range, it joins an already existing COMPSs deployment and interacts with the other resources to offload tasks onto them or viceversa. Eventually, the connectivity of that mobile device could be disrupted to never reestablish. If the leaving device was used as a worker node, the COMPSs master needs to react to the departure and reassign the tasks running on that node. If the device was the master node, it should be able to carry on with the computation being isolated from the rest of the infrastructure or with another set of available resources.

COMPSs Agents is a deployment approach especially designed to fit in this kind of environments. Each device is an autonomous individual with processing capabilities hosting the execution of a COMPSs runtime as a background service. Applications - running on that device or on another - can contact this service to request the execution of a function in a serverless, stateless manner (resembling the Function-as-a-Service model). If the requested function

follows the COMPSs programming model, the runtime will parallelise its execution as if it were the main function of a regular COMPSs application.

Agents can associate with other agents by offering their embedded computing resources to execute functions to achieve a greater purpose; in exchange, they receive a platform where they can offload their computation in the same manner, and, thus, achieve lower response times. As opposed to the master-worker approach followed by the classic COMPSs deployment, where a single node produces all the workload, in COMPSs Agents deployments, any of the nodes within the platform becomes a potential source of computation to distribute. Therefore, this master-centric approach where workload producer to orchestrate holistically the execution is no longer valid. Besides, concentrating all the knowledge of several applications and handling the changes of infrastructure represents an important computational burden for the resource assuming the master role, especially if it is a resource-scarce device like a mobile. For these two reasons, COMPSs agents propose a hierarchic approach to organize the nodes. Each node will only be aware of some devices with which it has direct connection and only decides whether the task runs on its embedded computing devices or if the responsibility of executing the task is delegated onto one of the other agents. In the latter case, the receiver node will face the same problem and decide whether it should host the execution or forward it to a different node.

The following image illustrates an example of a COMPSs agents hierarchy that could be deployed in any kind of facilities; for instance, a university campus. In this case, students only interact directly with their mobile phones and laptops to run their applications; however, the computing workload produced by them is distributed across the whole system. To do so, the mobile devices need to connect to one of the edge devices (in the example, raspberry Pi) which runs a COMPSs agent. To submit the operation execution to the platform, mobile devices can either contact a COMPSs agent running in the device or the application can directly contact the remote agent running on the rPi. All rPi agents are connected to an on-premise server within the campus that also runs a COMPSs Agent. Upon an operation request by a user device, the rPi can host the computation on its own devices or forward the request to one of its neighbouring agents: the on-premise server or another user's device running a COMPSs agent. In the case that the rPi decides to move up the request through the hierarchy, the on-premise server faces a similar problem: hosting the computation on its local devices, delegating the execution onto one of the rPi – which in turn could forward the execution back to another user's device –, or submit the request to a cloud. Internally, the Cloud can also be organized with COMPSs Agents hierarchy; thus, one of its nodes can act as the gateway to receive external requests and share the workload across the whole system.



5.2.1 Local

This section is intended to show how to execute COMPSs applications deploying the runtime as an agent in local machines.

5.2.1.1 Deploying a COMPSs Agent

COMPSs Agents are deployed using the `compss_agent_start` command:

```
compss@bsc:~$ compss_agent_start [OPTION]
```

There is one mandatory parameter `--hostname` that indicates the name that other agents and itself use to refer to the agent. Bear in mind that agents are not able to dynamically modify its classpath; therefore, the `--classpath` parameter becomes important to indicate the application available on the agent. Any public method available on the classpath is an execution request candidate.

The following command raises an agent with name 192.168.1.100 and any of the public methods of the classes encapsulated in the jarfile `/app/path.jar` can be executed.

```
compss@bsc:~$ compss_agent_start --hostname=192.168.1.100 --classpath=/app/path.jar
```

The `compss_agent_start` command allows users to set up the COMPSs runtime by specifying different options in the same way as done for the `runcompss` command. To indicate the available resources, the device administrator can use the `--project` and `--resources` option exactly in the same way as for the `runcompss` command. For further details on how to dynamically modify the available resources, please, refer to section [Modifying the available resources](#).

Currently, COMPSs agents allow interaction through two interfaces: the Comm interface and the REST interface. The Comm interface leverages on a proprietary protocol to submit operations and request updates on the current resource configuration of the agent. Although users and applications can use this interface, its design purpose is to enable high-performance interactions among agents rather than supporting user interaction. The REST interface takes the completely opposed approach; Users should interact with COMPSs agents through it rather than submitting tasks with the Comm interface. The COMPSs agent allows to enact both interfaces at a time; thus, users can manually submit operations using the REST interface, while other agents can use the Comm interface. However, the device owner can decide at deploy time which of the interfaces will be available on the agent and through which port the API will be exposed using the `rest_port` and `comm_port` options of the `compss_agent_start` command. Other agents can be configured to interact with the agent through any of the interfaces. For further details on how to configure the interaction with another agent, please, refer to section [Modifying the available resources](#).

```
compss@bsc:~$ compss_agent_start -h
```

```
Usage: /opt/COMPSs/Runtime/scripts/user/compss_agent_start [OPTION]...
```

COMPSs options:

<code>--appdir=<path></code>	Path for the application class folder. Default: <code>/home/flordan/git/compss/framework/</code>
<code>↪builders</code>	
<code>--classpath=<path></code>	Path for the application classes / modules Default: Working Directory
<code>--comm=<className></code>	Class that implements the adaptor for
<code>↪communications with other nodes</code>	
	Supported adaptors:
	— <code>es.bsc.compss.nio.master.NIOAdaptor</code>
	— <code>es.bsc.compss.gat.master.GATAdaptor</code>

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	es.bsc.compss.agent.rest.Adaptor es.bsc.compss.agent.comm.CommAgentAdaptor Default: es.bsc.compss.agent.comm.CommAgentAdaptor
--comm_port=<int> ↪(<=0: Disabled)	Port on which the agent sets up a Comm interface.↵
-d, --debug	Enable debug. (Default: disabled)
--hostname ↪identify the agent.	Name with which itself and other agents will↵
--jvm_opts="string" ↪option separated by "," and without blank spaces (Notice the quotes)	Extra options for the COMPSs Runtime JVM. Each↵
--library_path=<path> ↪(e.g. Java JVM library, Python library, C binding library)	Non-standard directories to search for libraries↵ Default: Working Directory
--log_dir=<path>	Log directory. (Default: /tmp/)
--log_level=<level> ↪trace	Set the debug level: off info api debug ↵ Default: off
--master_port=<int> ↪used. The value is overridden by the comm_port value.)	Port to run the COMPSs master communications. (Only when es.bsc.compss.nio.master.NIOAdaptor is↵ Default: [43000,44000]
--pythonpath=<path> ↪PYTHONPATH ↪builders	Additional folders or paths to add to the↵ Default: /home/flordan/git/compss/framework/
--python_interpreter=<string> ↪python3).	Python interpreter to use (python/python2/ Default: python Version:
--python_propagate_virtual_environment=<true> ↪to the workers (true/false).	Propagate the master virtual environment↵ Default: true
--python_mpi_worker=<false> ↪multiprocessing. (true/false).	Use MPI to run the python worker instead of↵ Default: false
--python_memory_profile	Generate a memory profile of the master. Default: false
--python_worker_cache=<string>	Python worker cache (true/size/false). Only for NIO without mpi worker and python >= 3.8. Default: false
--project=<path> ↪projects/examples/local/project.xml)	Path of the project file (Default: /opt/COMPSs/Runtime/configuration/xml/

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<code>--resources=<path></code> <code>→resources/examples/local/resources.xml)</code>	Path of the resources file (Default: /opt/COMPSs/Runtime/configuration/xml/
<code>--rest_port=<int></code> <code>→(<=0: Disabled)</code>	Port on which the agent sets up a REST interface. <code>␣</code>
<code>--reuse_resources_on_block=<boolean></code> <code>→to a task when its execution stalls.</code>	Enables/Disables reusing the resources assigned <code>␣</code> (Default:true)
<code>--scheduler=<className></code> <code>→FIFODataLocationScheduler</code> <code>→FIFOScheduler</code> <code>→FIFODataScheduler</code> <code>→LIFOScheduler</code> <code>→TaskScheduler</code> <code>→LoadBalancingScheduler</code> <code>→LoadBalancingScheduler</code>	Class that implements the Scheduler for COMPSs Supported schedulers: ├ es.bsc.compss.scheduler.fifodatalocation. ├ es.bsc.compss.scheduler.fifonew. ├ es.bsc.compss.scheduler.fifodatanew. ├ es.bsc.compss.scheduler.lifonew. ├ es.bsc.compss.components.impl. └ es.bsc.compss.scheduler.loadbalancing. Default: es.bsc.compss.scheduler.loadbalancing.
<code>--scheduler_config_file=<path></code> <code>→configuration.</code>	Path to the file which contains the scheduler <code>␣</code> Default: Empty
<code>--input_profile=<path></code> <code>→application profile</code>	Path to the file which stores the input <code>␣</code> Default: Empty
<code>--output_profile=<path></code> <code>→at the end of the execution</code>	Path to the file to store the application profile <code>␣</code> Default: Empty
<code>--summary</code> <code>→the application execution</code>	Displays a task execution summary at the end of <code>␣</code> Default: false
<code>--tracing=<level>, --tracing, -t</code> <code>→true basic] advanced scorep arm-map arm-ddt false)</code> <code>→traces.</code>	Set generation of traces and/or tracing level (<code>␣</code> True and basic levels will produce the same <code>␣</code> When no value is provided it is set to 1 Default: 0
<code>--trace_label=<string></code> <code>→used in the case of tracing is activated.</code>	Add a label in the generated trace file. Only <code>␣</code> Default: None

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Other options:	
--help	prints this message

5.2.1.2 Executing an operation

The **compss_agent_call_operation** commands interacts with the REST interface of the COMPSs agent to submit an operation.

```
compss@bsc:~$ compss_agent_call_operation [options] application_name application_arguments
```

The command has two mandatory flags **--master_node** and **--master_port** to indicate the endpoint of the COMPSs Agent. By default, the command submits an execution of the **main** method of the Java class with the name passed in as the **application_name** and gathering all the application arguments in a single `String[]` instance. To execute Python methods, the user can use the **--lang=PYTHON** option and the Agent will execute the python script with the name passed in as **application_name**. Operation invocations can be customized by using other options of the command. The **--method_name** option allow to execute a specific method; in the case of specifying a method, each of the parameters will be passed in as a different parameter to the function and it is necessary to indicate the **--array** flag to encapsulate all the parameters as an array.

Additionally, the command offers two options to shutdown a whole agents deployment upon the operation completion. The flag **--stop** indicates that, at the end of the operation, the agent receiving the operation request will stop. For shutting down the rest of the deployment, the command offers the option **--forward_to** to indicate a list of IP:port pairs. Upon the completion of the operation, the agent receiving the request will forward the stop command to all the nodes specified in such option.

```
compss@bsc.es:~$ compss_agent_call_operation -h

Usage: compss_agent_call_operation [options] application_name application_arguments

* Options:
General:
  --help, -h                Print this help message
  --opts                    Show available options
  --version, -v             Print COMPSs version
  --master_node=<string>    Node where to run the COMPSs Master
                           Mandatory
  --master_port=<string>    Node where to run the COMPSs Master
                           Mandatory
  --stop                    Stops the agent after the execution
                           of the task.
  --forward_to=<list>       Forwards the stop action to other
                           agents, the list shoud follow the
                           format:
                           <ip1>:<port1>;<ip2>:<port2>...

Launch configuration:
  --cei=<string>            Canonical name of the interface declaring the
  ↪ methods                Default: No interface declared
  --lang=<string>          Language implementing the operation
```

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	Default: JAVA
<code>--method_name=<string></code>	Name of the method to invoke Default: main and enables array parameter
<code>--parameters_array, --array</code>	Parameters are encapsulated as an array Default: disabled

For example, to submit the execution of the `demoFunction` method from the `es.bsc.compss.tests.DemoClass` class passing in a single parameter with value 1 on the agent 127.0.0.1 with a REST interface listening on port 46101, the user should execute the following example command:

```
compss@bsc.es:~$ compss_agent_call_operation --master_node="127.0.0.1" --master_port="46101" -
↪--method_name="demoFunction" es.bsc.compss.test.DemoClass 1
```

For the agent to detect inner tasks within the operation execution, the COMPSs Programming model requires an interface selecting the methods to be replaced by asynchronous task creations. An invoker should use the `--cei` option to specify the name of the interface selecting the tasks.

5.2.1.3 Modifying the available resources

Finally, the COMPSs framework offers three commands to control dynamically the pool of resources available for the runtime on one agent. These commands are `compss_agent_add_resources`, `compss_agent_reduce_resources` and `compss_agent_lost_resources`.

The `compss_agent_add_resources` command interacts with the REST interface of the COMPSs agent to attach new resources to the Agent.

```
compss@bsc.es:~$ compss_agent_add_resources [options] resource_name [<adaptor_property_
↪name=adaptor_property_value>]
```

By default, the command modifies the resource pool of the agent deployed on the node running the command listening on port 46101; however, this can be modified by using the options `--agent_node` and `--agent_port` to indicate the endpoint of the COMPSs Agent. The other options passed in to the command modify the characteristics of the resources to attach; by default, it adds one single CPU core. However, it also allows to modify the amount of GPU cores, FPGAs, memory type and size and OS details.

```
compss@bsc.es:~$ compss_agent_add_resources -h

Usage: compss_agent_add_resources [options] resource_name [<adaptor_property_name=adaptor_
↪property_value>]

* Options:
General:
  --help, -h                Print this help message

  --opts                    Show available options

  --version, -v             Print COMPSs version

  --agent_node=<string>     Name of the node where to add the resource
                          Default:

  --agent_port=<string>     Port of the node where to add the resource
                          Default:

Resource description:
```

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<code>--comm=<string></code> →with the resource	Canonical class name of the adaptor to interact Default: <code>es.bsc.compss.agent.comm.CommAgentAdaptor</code>
<code>--cpu=<integer></code>	Number of cpu cores available on the resource Default: 1
<code>--gpu=<integer></code>	Number of gpus devices available on the resource Default: 0
<code>--fpga=<integer></code>	Number of fpga devices available on the resource Default: 0
<code>--mem_type=<string></code>	Type of memory used by the resource Default: [unassigned]
<code>--mem_size=<string></code>	Size of the memory available on the resource Default: -1
<code>--os_type=<string></code>	Type of operating system managing the resource Default: [unassigned]
<code>--os_distr=<string></code> →resource	Distribution of the operating system managing the Default: [unassigned]
<code>--os_version=<string></code> →resource	Version of the operating system managing the Default: [unassigned]

If `resource_name` matches the name of the Agent, the capabilities of the device are increased according to the description; otherwise, the runtime adds a remote worker to the resource pool with the specified characteristics. Notice that, if there is another resource within the pool with the same name, the agent will increase the resources of such node instead of adding it as a new one. The `--comm` option is used for selecting which adaptor is used for interacting with the remote node; the default adaptor (CommAgent) interacts with the remote node through the Comm interface of the COMPSs agent.

The following command adds a new Agent onto the pool of resources of the Agent deployed at IP 192.168.1.70 with a REST Interface on port 46101. The new agent, which has 4 CPU cores, is deployed on IP 192.168.1.72 and has a Comm interface endpoint on port 46102.

```
compss@bsc.es:~$ compss_agent_add_resources --agent_node=192.168.1.70 --agent_port=46101 --
→cpu=4 192.168.1.72 Port=46102
```

Conversely, the `compss_agent_reduce_resources` command allows to reduce the number of resources configured in an agent. Executing the command causes the target agent to reduce the specified amount of resources from one of its configured neighbors. At the moment of the reception of the resource removal request, the agent might be actively using those remote resources by executing some tasks. If that is the case, the agent will register the resource reduction request, stop submitting more workload to the corresponding node, and, when the idle resources of the node match the request, the agent removes them from the pool. If upon the completion of the `compss_agent_reduce_resources` command no resources are associated to the reduced node, the node is completely removed from the resource pool of the agent. The options and default values are the same than for the `compss_agent_add_resources` command. Notice that `--comm` option is not available because only one resource can be associated to that name regardless the selected adaptor.

```
compss@bsc.es:~$ compss_agent_reduce_resources -h
```

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```

Usage: compss_agent_reduce_resources [options] resource_name

* Options:
General:
  --help, -h                Print this help message

  --opts                    Show available options

  --version, -v             Print COMPSs version

  --agent_node=<string>     Name of the node where to add the resource
                           Default:

  --agent_port=<string>     Port of the node where to add the resource
                           Default:

Resource description:
  --cpu=<integer>           Number of cpu cores available on the resource
                           Default: 1

  --gpu=<integer>           Number of gpus devices available on the resource
                           Default: 0

  --fpga=<integer>          Number of fpga devices available on the resource
                           Default: 0

  --mem_type=<string>       Type of memory used by the resource
                           Default: [unassigned]

  --mem_size=<string>       Size of the memory available on the resource
                           Default: -1

  --os_type=<string>        Type of operating system managing the resource
                           Default: [unassigned]

  --os_distr=<string>       Distribution of the operating system managing the
↪ resource
                           Default: [unassigned]

  --os_version=<string>     Version of the operating system managing the
↪ resource
                           Default: [unassigned]

```

Finally, the last command to control the pool of resources configured, `compss_agent_lost_resources`, immediately removes from an agent's pool all the resources corresponding to the remote node associated to that name.

```
compss@bsc.es:~$ compss_agent_lost_resources [options] resource_name
```

In this case, the only available options are those used for identifying the endpoint of the agent: `--agent_node` and `--agent_port`. As with the previous commands, by default, the request is submitted to the agent deployed on the IP address 127.0.0.1 and listening on port 46101.

5.2.2 Supercomputers

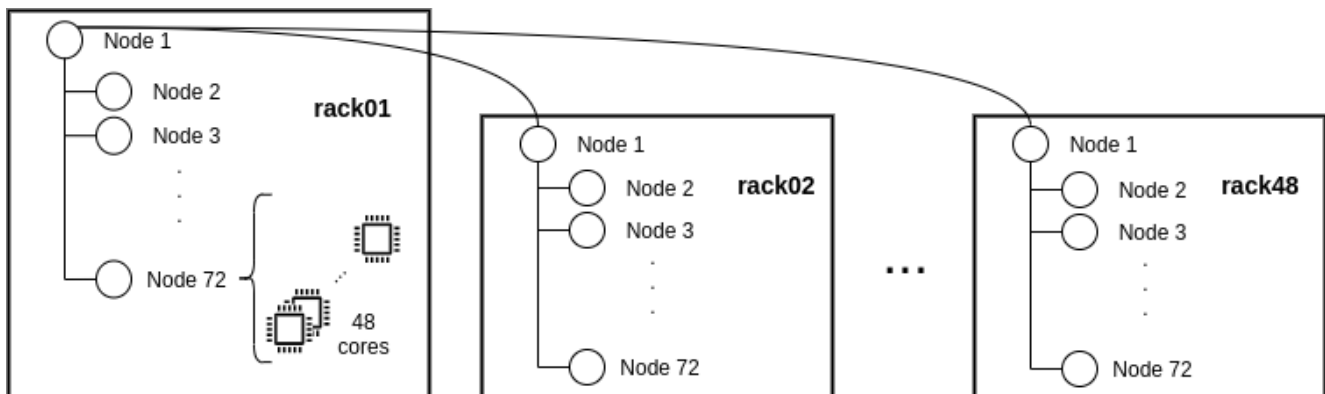
Similar to Section [Supercomputers](#) for Master-Worker deployments, this section is intended to walk you through the COMPSs usage with agents in Supercomputers. All the configuration and commands to install COMPSs on the Supercomputer, load the environment and submitting a job remain exactly the same as described in Sections [Supercomputers](#).

The only difference to submit jobs with regards the COMPSs Master-Worker approach is to enact the **agents** option of the **enqueue_compss** command. When this option is enabled, the whole COMPSs deployment changes and, instead of deploying the COMPSs master in one node and workers in the remaining ones, it deploys an agent in each node provided by the queue system. When all the agents have been deployed, COMPSs' internal scripts handling the job execution will submit the operation using the REST API of the one of the agent. Although COMPSs agents allow any method of the application to be the starting point of the execution, to maintain the similarities between the scripts when deploying COMPSs following the Master-Worker or the Agents approaches, the execution will start with the main method of the class/module passed in as a parameter to the script.

The main advantage of using the Agents approach in Supercomputers is the ability to define different topologies. For that purpose, the **--agents** option of the **enqueue_compss** script allows to choose two different options **--agents=plain** and **--agents=tree**.

The **Plain** topology configures the deployment resembling the Master-worker approach. One of the agents is selected as the master and has all the other agents as workers where to offload tasks; the agents acting as workers also host a COMPSs runtime and, therefore, they can detect nested tasks on the tasks offloaded onto them. However, nested tasks will always be executed on the worker agent detecting them.

The **Tree** topology is the default topology when using agent deployments on Supercomputers. This option tries to create a three-layer topology that aims to exploit data locality and reduce the workload of the scheduling problem. Such topology consists in deploying an agent on each node managing only the resources available within the node. Then, the script groups all the nodes by rack and selects a representative node for each group that will orchestrate all the resources within it and offload tasks onto the other agents. Finally, the script picks one of these representative agents as the main agent of the hierarchy; this main agent is configured to be able to offload tasks onto the representative agents for all other racks; it will be onto this node that the script will call the main method of the execution. The following image depicts an example of such topology on Marenstrum.



To ensure that no resources are wasted waiting from the execution end until the wall clock limit, the **enqueue_compss** script submits the invocation enabling the **--stop** and **--forward** options to stop all the deployed agents for the execution.

5.3 Schedulers

This section provides detailed information about all the schedulers that are implemented in COMPSs and can be used for the executions of the applications. Depending on the scheduler selected for your executions the tasks will be scheduled in a way or another and this will result in different execution times depending on the scheduler used.

Table 16: Schedulers

Scheduler name	Class name	Type	Description	Recommendations
LoadBalancingScheduler (default)	es.bsc.compss.scheduler.loadbalancing	Ready	Ready Load Balancing Scheduler and then (FIFO) task generation	
FIFODataLocationScheduler	es.bsc.compss.scheduler.fifodatalocation	Ready	FIFODataLocationScheduler then data location and then the (FIFO) task generation	SCS when using local disk
FIFOScheduler	es.bsc.compss.scheduler.fifonew	Ready	FIFOScheduler prioritizes the (FIFO) generation order of the tasks	
FIFO-DataScheduler	es.bsc.compss.scheduler.fifodatanew	Ready	FIFO-DataScheduler prioritizes dependencies and then the (FIFO) task generation	SCS when using shared disk
LIFOScheduler	es.bsc.compss.scheduler.lifonew	Ready	LIFOScheduler prioritizes the (LIFO) generation order of the tasks	
MOScheduler (Experimental)	es.bsc.compss.scheduler.multiobjective	Full	Schedules all tasks based on a multiobjective function (time, energy and cost estimation)	

Chapter 6

Tracing

COMPSs is instrumented with EXTRAЕ, which enables to produce PARAVЕR traces for performance profiling. This section is intended to walk you through the tracing of your COMPSs applications in order to analyse the performance with great detail.

6.1 COMPSs applications tracing

COMPSs Runtime has a built-in instrumentation system to generate post-execution tracefiles of the applications' execution. The tracefiles contain different events representing the COMPSs master state, the tasks' execution state, and the data transfers (transfers' information is only available when using NIO adaptor), and are useful for both visual and numerical performance analysis and diagnosis. The instrumentation process essentially intercepts and logs different events, so it adds overhead to the execution time of the application.

The tracing system uses Extrae¹ to generate tracefiles of the execution that, in turn, can be visualized with Paraver². Both tools are developed and maintained by the Performance Tools team of the BSC and are available on its web page <http://www.bsc.es/computer-sciences/performance-tools>.

For each worker node and the master, Extrae keeps track of the events in an intermediate format file (with *.mpit* extension). At the end of the execution, all intermediate files are gathered and merged with Extrae's `mpi2prv` command in order to create the final tracefile, a Paraver format file (*.prv*). See the [Visualization](#) Section for further information about the Paraver tool.

When instrumentation is activated, Extrae outputs several messages corresponding to the tracing initialization, intermediate files' creation, and the merging process.

At present time, COMPSs tracing features two execution modes:

Basic Aimed at COMPSs applications developers

Advanced For COMPSs developers and users with access to its source code or custom installations

Next sections describe the information provided by each mode and how to use them.

¹ For more information: <https://www.bsc.es/computer-sciences/extrae>

² For more information: <https://www.bsc.es/computer-sciences/performance-tools/paraver>

6.1.1 Basic Mode

This mode is aimed at COMPSs' apps users and developers. It instruments computing threads and some management resources providing information about tasks' executions, data transfers, and hardware counters if PAPI is available (see [PAPI: Hardware Counters](#) for more info).

6.1.1.1 Basic Mode Usage

In order to activate basic tracing one needs to provide one of the following arguments to the execution command:

- -t
- --tracing
- --tracing=basic
- --tracing=true

Example:

```
$ runcompss --tracing application_name application_args
```

When tracing is activated, Extrae generates additional output to help the user ensure that instrumentation is turned on and working without issues. On basic mode this is the output users should see when tracing is working correctly:

```
$ runcompss --tracing kmeans.py -n 102400000 -f 8 -d 3 -c 8 -i 10

[ INFO] Inferred PYTHON language
[ INFO] Using default location for project file: /opt/COMPSs//Runtime/configuration/xml/
→projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSs//Runtime/configuration/xml/
→resources/default_resources.xml
[ INFO] Using default execution type: compss

----- Executing kmeans.py -----

Welcome to Extrae 3.8.3
Extrae: Parsing the configuration file (/opt/COMPSs//Runtime/configuration/xml/tracing/extrae_
→basic.xml) begins
Extrae: Warning! <trace> tag has no <home> property defined.
Extrae: Generating intermediate files for Paraver traces.

PAPI Error: Error finding event OFFCORE_RESPONSE_0:SNP_FWD, it is used in derived event PAPI_
→CA_ITV.
Extrae: PAPI domain set to ALL for HWC set 1
Extrae: HWC set 1 contains following counters < PAPI_TOT_INS (0x80000032) PAPI_TOT_CYC_
→(0x8000003b) PAPI_L1_DCM (0x80000000) PAPI_L2_DCM (0x80000002) PAPI_L3_TCM (0x80000008)_
→PAPI_BR_INS (0x80000037) PAPI_BR_MSP (0x8000002e) RESOURCE_STALLS (0x4000002f) > - never_
→changes
Extrae: Tracing buffer can hold 100000 events
Extrae: Circular buffer disabled.
Extrae: Warning! <input-output> tag will be ignored. This library does not support_
→instrumenting I/O calls.
Extrae: Dynamic memory instrumentation is disabled.
Extrae: Basic I/O memory instrumentation is disabled.
Extrae: System calls instrumentation is disabled.
Extrae: Parsing the configuration file (/opt/COMPSs//Runtime/configuration/xml/tracing/extrae_
→basic.xml) has ended
Extrae: Intermediate traces will be stored in /home/user/temp/documentation
Extrae: Tracing mode is set to: Detail.
```

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```

Extrae: Error! Hardware counter PAPI_BR_INS (0x80000037) cannot be added in set 1 (task 0,
↳thread 0)
Extrae: Error! Hardware counter PAPI_BR_MSP (0x8000002e) cannot be added in set 1 (task 0,
↳thread 0)
Extrae: Error! Hardware counter RESOURCE_STALLS (0x4000002f) cannot be added in set 1 (task 0,
↳ thread 0)
Extrae: Successfully initiated with 1 tasks and 1 threads

PAPI Error: Error finding event OFFCORE_RESPONSE_0:SNP_FWD, it is used in derived event PAPI_
↳CA_ITV.
Extrae: Error! Hardware counter PAPI_BR_INS (0x80000037) cannot be added in set 1 (task 0,
↳thread 0)
Extrae: Error! Hardware counter PAPI_BR_MSP (0x8000002e) cannot be added in set 1 (task 0,
↳thread 0)
Extrae: Error! Hardware counter RESOURCE_STALLS (0x4000002f) cannot be added in set 1 (task 0,
↳ thread 0)
pyextrae: Loading tracing library 'libseqtrace.so'
WARNING: COMPSs Properties file is null. Setting default values
Loading LogManager
[(419)   API] - Starting COMPSs Runtime v2.9.rc2107 (build 20210720-1547.
↳r81bdafc6f06a7680a344ae434a467473ecbaf27e)
Generation/Load done
Starting kmeans
Doing iteration #1/10
Doing iteration #2/10
Doing iteration #3/10
Doing iteration #4/10
Doing iteration #5/10
Doing iteration #6/10
Doing iteration #7/10
Doing iteration #8/10
Doing iteration #9/10
Doing iteration #10/10
Ending kmeans
-----
----- RESULTS -----
-----
Initialization time: 55.369870
Kmeans time: 117.859757
Total time: 173.229627
-----
CENTRES:
[[0.69757475 0.74511351 0.48157611]
[0.54683653 0.20274669 0.2117475 ]
[0.24194863 0.74448094 0.75633981]
[0.21854362 0.67072938 0.23273541]
[0.77272546 0.68522249 0.16245965]
[0.22683962 0.23359743 0.67203863]
[0.75351606 0.73746265 0.83339847]
[0.75838884 0.23805883 0.71538748]]
-----
Extrae: Intermediate raw trace file created : /home/user/temp/documentation/set-0/TRACE@linux-
↳2e63.000002702900000000000002.mpit
Extrae: Intermediate raw trace file created : /home/user/temp/documentation/set-0/TRACE@linux-
↳2e63.000002702900000000000001.mpit

```

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```

Extrae: Intermediate raw trace file created : /home/user/temp/documentation/set-0/TRACE@linux-
↪2e63.000002702900000000000000.mpit
Extrae: Intermediate raw sym file created : /home/user/temp/documentation/set-0/TRACE@linux-
↪2e63.000002702900000000000000.sym
Extrae: Deallocating memory.
Extrae: Application has ended. Tracing has been terminated.
merger: Output trace format is: Paraver
merger: Extrae 3.8.3
mpi2prv: Assigned nodes < linux-2e63 >
mpi2prv: Assigned size per processor < 1 Mbytes >
mpi2prv: File set-0/TRACE@linux-2e63.0000027148000001000000.mpit is object 1.2.1 on node_
↪linux-2e63 assigned to processor 0
mpi2prv: File set-0/TRACE@linux-2e63.0000027148000001000001.mpit is object 1.2.2 on node_
↪linux-2e63 assigned to processor 0
mpi2prv: File set-0/TRACE@linux-2e63.0000027148000001000002.mpit is object 1.2.3 on node_
↪linux-2e63 assigned to processor 0
mpi2prv: File set-0/TRACE@linux-2e63.0000027148000001000003.mpit is object 1.2.4 on node_
↪linux-2e63 assigned to processor 0
mpi2prv: File set-0/TRACE@linux-2e63.0000027148000001000004.mpit is object 1.2.5 on node_
↪linux-2e63 assigned to processor 0
mpi2prv: File set-0/TRACE@linux-2e63.0000027148000001000005.mpit is object 1.2.6 on node_
↪linux-2e63 assigned to processor 0
mpi2prv: File set-0/TRACE@linux-2e63.0000027148000001000006.mpit is object 1.2.7 on node_
↪linux-2e63 assigned to processor 0
mpi2prv: File set-0/TRACE@linux-2e63.0000027029000000000000.mpit is object 1.1.1 on node_
↪linux-2e63 assigned to processor 0
mpi2prv: File set-0/TRACE@linux-2e63.000002702900000000000001.mpit is object 1.1.2 on node_
↪linux-2e63 assigned to processor 0
mpi2prv: File set-0/TRACE@linux-2e63.000002702900000000000002.mpit is object 1.1.3 on node_
↪linux-2e63 assigned to processor 0
mpi2prv: A total of 8 symbols were imported from TRACE.sym file
mpi2prv: 0 function symbols imported
mpi2prv: 8 HWC counter descriptions imported
mpi2prv: Checking for target directory existence... exists, ok!
mpi2prv: Selected output trace format is Paraver
mpi2prv: Stored trace format is Paraver
mpi2prv: Searching synchronization points... done
mpi2prv: Time Synchronization disabled.
mpi2prv: Circular buffer enabled at tracing time? NO
mpi2prv: Parsing intermediate files
mpi2prv: Progress 1 of 2 ... 5% 10% 15% 20% 25% 30% 35% 40% 45% 50% 55% 60% 65% 70% 75% 80% 85
↪% 90% 95% done
mpi2prv: Processor 0 succeeded to translate its assigned files
mpi2prv: Elapsed time translating files: 0 hours 0 minutes 0 seconds
mpi2prv: Elapsed time sorting addresses: 0 hours 0 minutes 0 seconds
mpi2prv: Generating tracefile (intermediate buffers of 671078 events)
    This process can take a while. Please, be patient.
mpi2prv: Progress 2 of 2 ... 5% 10% 15% 20% 25% 30% 35% 40% 45% 50% 55% 60% 65% 70% 75% 80% 85
↪% 90% 95% done
mpi2prv: Elapsed time merge step: 0 hours 0 minutes 0 seconds
mpi2prv: Resulting tracefile occupies 664068 bytes
mpi2prv: Removing temporal files... mpi2prv: Warning! Clock accuracy seems to be in_
↪microseconds instead of nanoseconds.
done
mpi2prv: Elapsed time removing temporal files: 0 hours 0 minutes 0 seconds
mpi2prv: Congratulations! ./trace/kmeans.py_compss.prv has been generated.

```

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```
[(189793)    API] - Execution Finished
-----
```

The output contains diverse information about the tracing, for example, Extrae version used (VERSION will be replaced by the actual number during executions), the XML configuration file used (/opt/COMPSs/Runtime/configuration/xml/tracing/extrae_basic.xml – if using python, the extrae_python_worker.xml located in the same folder will be used in the workers), the amount of threads instrumented (objects through 1.1.1 to 1.2.7), available hardware counters (PAPI_TOT_INS (0x80000032) ... PAPI_L3_TCM (0x80000008)) or the name of the generated tracefile (./trace/ kmeans.py_compss.prv). When using NIO communications adaptor with debug activated, the log of each worker also contains the Extrae initialization information.

Tip: The extrae configuration files used in basic mode are:

- \$COMPSS_HOME/Runtime/configuration/xml/tracing/extrae_basic.xml
- \$COMPSS_HOME/Runtime/configuration/xml/tracing/extrae_python_worker.xml (when using Python)

Tip: [Figure 22](#) was generated with this execution.

Important: COMPSs needs to perform an extra merging step when using Python in order to add the Python-produced events to the main tracefile. If Python events are not shown, check *runtime.log* file and search for the following expected output of this merging process to find possible errors:

```
[(189467)(2021-07-21 08:09:33,292)      Tracing]    @teMasterPackage - Tracing:␣
→generating master package: package
[(189468)(2021-07-21 08:09:33,293)      Tracing]    @run          - Starting␣
→stream goobler
[(189469)(2021-07-21 08:09:33,294)      Tracing]    @run          - Starting␣
→stream goobler
[(189501)(2021-07-21 08:09:33,326)      Tracing]    @erMasterPackage - Tracing:␣
→Transferring master package
[(189503)(2021-07-21 08:09:33,328)      Tracing]    @generateTrace - Tracing:␣
→Generating trace with mode gentrace
[(189503)(2021-07-21 08:09:33,328)      Tracing]    @run          - Starting␣
→stream goobler
[(189504)(2021-07-21 08:09:33,329)      Tracing]    @run          - Starting␣
→stream goobler
[(189589)(2021-07-21 08:09:33,414)      Tracing]    @<init>       - Trace's␣
→merger initialization successful
[(189589)(2021-07-21 08:09:33,414)      Tracing]    @umAndSyncEvents - Parsing␣
→master sync events
[(189589)(2021-07-21 08:09:33,414)      Tracing]    @getSyncEvents - Getting sync␣
→events from: /home/user/.COMPSs/kmeans.py_01/trace/kmeans.py_compss.prv for worker -1
[(189745)(2021-07-21 08:09:33,570)      Tracing]    @umAndSyncEvents - Merging task␣
→traces into master which contains 1 lines.
[(189745)(2021-07-21 08:09:33,570)      Tracing]    @umAndSyncEvents - Merging␣
→worker /home/user/.COMPSs/kmeans.py_01/trace/python/1_python_trace.prv
[(189745)(2021-07-21 08:09:33,570)      Tracing]    @getWorkerEvents - Getting␣
→worker events from: /home/user/.COMPSs/kmeans.py_01/trace/python/1_python_trace.prv
[(189751)(2021-07-21 08:09:33,576)      Tracing]    @getSyncEvents - Getting sync␣
→events from: /home/user/.COMPSs/kmeans.py_01/trace/python/1_python_trace.prv for worker 2
[(189852)(2021-07-21 08:09:33,677)      Tracing]    @iteWorkerEvents - Writing 4089␣
→lines from worker 2 with 4 threads
```

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```

[(189872)(2021-07-21 08:09:33,697)      Tracing]    @ardwareCounters - Merging PCF␣
↪Hardware Counters into master
[(189872)(2021-07-21 08:09:33,697)      Tracing]    @getHWCounters  - Getting pcf␣
↪hw counters from: /home/user/.COMPSs/kmeans.py_01/trace/kmeans.py_compss.pcf
[(189872)(2021-07-21 08:09:33,697)      Tracing]    @getHWCounters  - Getting pcf␣
↪hw counters from: /home/user/.COMPSs/kmeans.py_01/trace/python/1_python_trace.pcf
[(189873)(2021-07-21 08:09:33,698)      Tracing]    @ardwareCounters - Analised␣
↪worker had 0 lines to be included
[(189873)(2021-07-21 08:09:33,698)      Tracing]    @ardwareCounters - No hardware␣
↪counters to include in PCF.
[(189873)(2021-07-21 08:09:33,698)      Tracing]    @merge          - Merging␣
↪finished.
[(189873)(2021-07-21 08:09:33,698)      Tracing]    @updateThreads  - Tracing:␣
↪Updating thread labels
[(189914)(2021-07-21 08:09:33,739)      Tracing]    @latedPrvThreads - Tracing:␣
↪Updating thread identifiers in .prv file
[(189959)(2021-07-21 08:09:33,784)      Tracing]    @anMasterPackage - Tracing:␣
↪Removing tracing master package: /home/user/documentation/master_compss_trace.tar.gz
[(189959)(2021-07-21 08:09:33,784)      Tracing]    @anMasterPackage - Deleted␣
↪master tracing package.

```

6.1.1.2 Instrumented Threads in Basic Mode

Basic traces instrument the following threads:

- Master node (3 threads)
 - COMPSs runtime (main application thread)
 - Access Processor thread
 - Task Dispatcher thread
- Worker node (3 + Computing Units)
 - Worker main thread
 - Worker File system thread
 - Worker timer thread
 - Number of threads available for computing

6.1.1.3 Information Available in Basic Traces

The basic mode tracefiles contain three kinds of information:

Events Marking diverse situations such as the runtime start, tasks' execution or synchronization points.

Communications Showing the transfers and requests of the parameters needed by COMPSs tasks.

Hardware counters Of the execution obtained with Performance API (see *PAPI: Hardware Counters*)

6.1.1.4 Basic Trace Example

Figure 22 is a tracefile generated by the execution of a k-means clustering algorithm. Each timeline contains information of a different resource, and each event's name is on the legend. Depending on the number of computing threads specified for each worker, the number of timelines varies. However the following threads are always shown:

Master - Thread 1.1.1 This timeline shows the actions performed by the main thread of the COMPSs application

Access Processor - Thread 1.1.2 All the events related to the tasks' parameters management, such as dependencies or transfers are shown in this thread.

Task Dispatcher - Thread 1.1.3 Shows information about the state and scheduling of the tasks to be executed.

Worker X Master - Thread X.1.1 This thread is the master of each worker and handles the computing resources and transfers. It is repeated for each available resource. All data events of the worker, such as requests, transfers and receives are marked on this timeline (when using the appropriate configurations).

Worker X File system - Thread X.1.2 This thread manages the synchronous file system operations (e.g. copy file) performed by the worker.

Worker X Timer - Thread X.1.3 This thread manages the cancellation of the tasks when the wall-clock limit is reached.

Worker X Executor Y - Thread X.2.Y Shows the actual tasks execution information and is repeated as many times as computing threads has the worker X

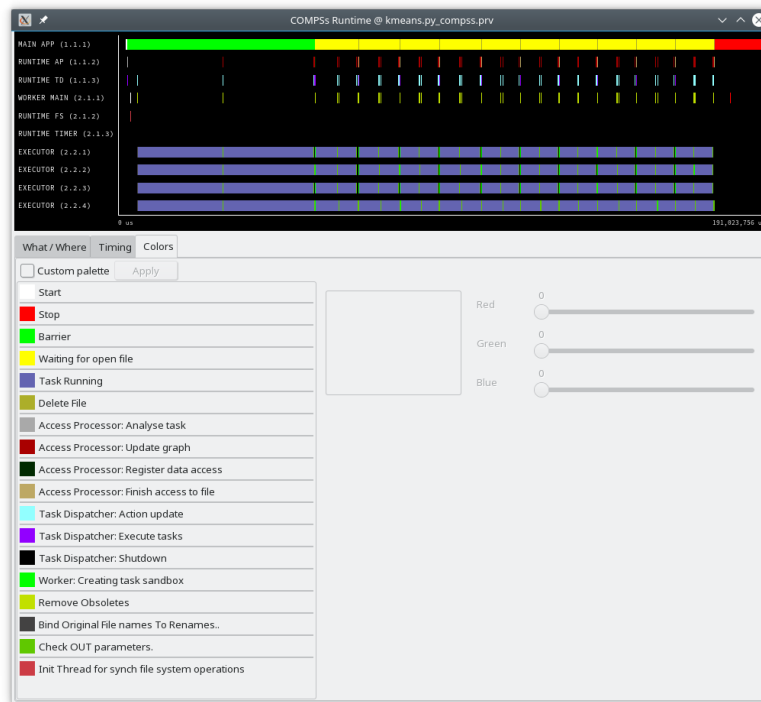


Figure 22: Basic mode tracefile for a k-means algorithm visualized with compss_runtime.cfg

6.1.2 Advanced Mode

This mode is for more advanced COMPSs' users and developers who want to customize further the information provided by the tracing or need rawer information like pthreads calls or Java garbage collection. With it, every single thread created during the execution is traced.

Important: The extra information provided by the advanced mode is only available on the workers when using NIO adaptor.

6.1.2.1 Advanced Mode Usage

In order to activate the advanced tracing add the following option to the execution:

- `--tracing=advanced`

Example:

```
$ runcompss --tracing=advanced application_name application_args
```

When advanced tracing is activated, the configuration file reported on the output is `$COMPSS_HOME/Runtime/configuration/xml/tracing/extrae_advanced.xml`.

```
$ runcompss --tracing=advanced kmeans.py -n 102400000 -f 8 -d 3 -c 8 -i 10

[ INFO] Inferred PYTHON language
[ INFO] Using default location for project file: /opt/COMPSSs/Runtime/configuration/xml/
→projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSSs/Runtime/configuration/xml/
→resources/default_resources.xml
[ INFO] Using default execution type: compss

----- Executing kmeans.py -----

Welcome to Extrae 3.8.3
Extrae: Parsing the configuration file (/opt/COMPSSs/Runtime/configuration/xml/tracing/extrae_
→advanced.xml) begins
...
...
...
```

This is the default file used for advanced tracing as well as `extrae_python_worker.xml` if using Python. However, advanced users can modify it in order to customize the information provided by Extrae. The configuration file is read first by the master on the `runcompss` script. When using NIO adaptor for communication, the configuration file is also read when each worker is started (on `persistent_worker.sh` or `persistent_worker_starter.sh` depending on the execution environment).

Tip: The extrae configuration files used in advanced mode are:

- `$COMPSS_HOME/Runtime/configuration/xml/tracing/extrae_advanced.xml`
 - `$COMPSS_HOME/Runtime/configuration/xml/tracing/extrae_python_worker.xml` (when using Python)
-

Tip: [Figure 23](#) was generated with this execution.

If the `extrae_advanced.xml` file is modified, the changes always affect the master, and also the workers when using NIO. Modifying the scripts which turn on the master and the workers is possible to achieve different instrumentations for master/workers. However, not all Extrae available XML configurations work with COMPSs, some of them can make the runtime or workers crash so modify them at your discretion and risk. More information about instrumentation XML configurations on Extrae User Guide at: <https://www.bsc.es/computer-sciences/performance-tools/trace-generation/extrae/extrae-user-guide>.

6.1.2.2 Instrumented Threads in Advanced Mode

Advanced mode instruments all the pthreads created during the application execution. It contains all the threads shown on basic traces plus extra ones used to call command-line commands, I/O streams managers and all actions which create a new process. Due to the temporal nature of many of this threads, they may contain little information or appear just at specific parts of the execution pipeline.

6.1.2.3 Information Available in Advanced Traces

The advanced mode tracefiles contain the same information as the basic ones:

Events Marking diverse situations such as the runtime start, tasks' execution or synchronization points.

Communications Showing the transfers and requests of the parameters needed by COMPSs tasks.

Hardware counters Of the execution obtained with Performance API (see [PAPI: Hardware Counters](#))

6.1.2.4 Advanced Trace Example

Figure 23 shows the total completed instructions for a sample program executed with the advanced tracing mode. Note that the thread - resource correspondence described on the basic trace example is no longer static and thus cannot be inferred. Nonetheless, they can be found thanks to the named events shown in other configurations such as `compss_runtime.cfg`.

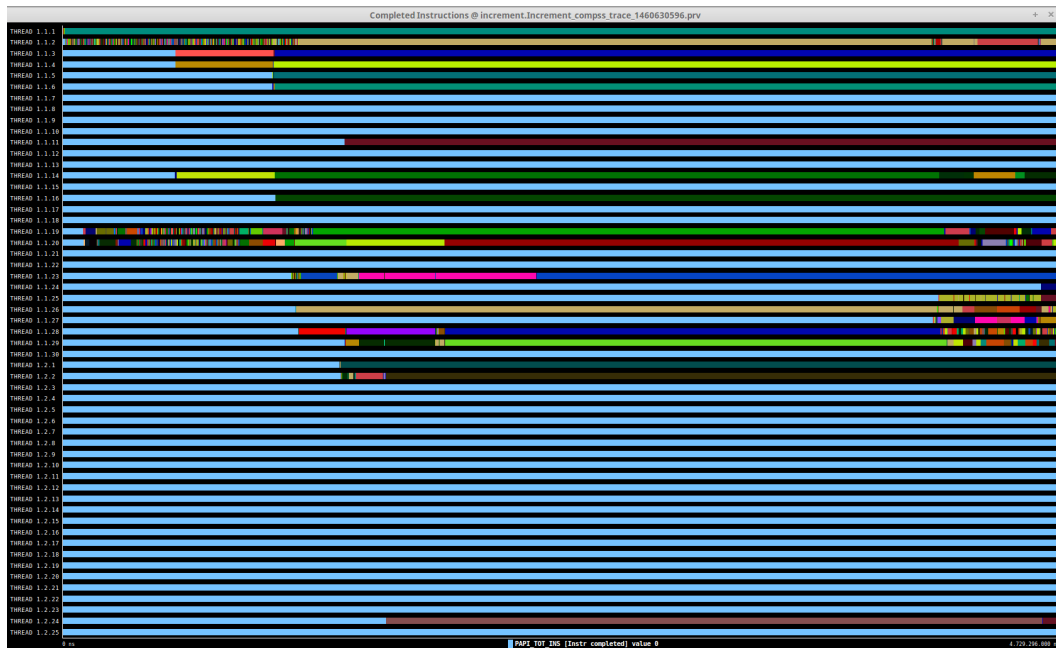


Figure 23: Advanced mode tracefile for a testing program showing the total completed instructions

For further information about Extrae, please visit the following site:

<http://www.bsc.es/computer-science/extrae>

6.1.3 Trace for Agents

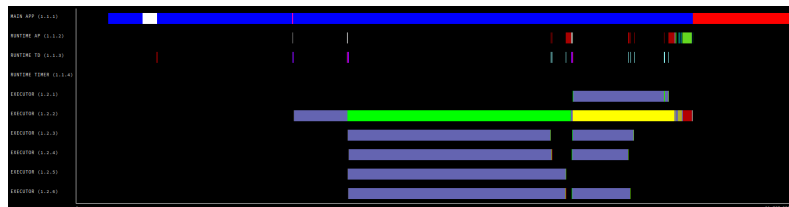
Applications deployed as COMPSs Agents can also be traced. Unlike master-worker COMPSs applications, where the trace contains the events for all the nodes within the infrastructure, with the Agents approach, each Agent generates its own trace.

To activate the tracing – either basic or advanced mode –, the `compss_agent_start` command allows the `-t`, `--tracing` and `--tracing=<level>` options with the same meaning as with the master-worker approach. For example:

```
$ compss_agent_start \
  --hostname="COMPSsWorker01" \
  --pythonpath="/python/path" \
  --log_dir="/agent1/log" \
  --rest_port="46101" \
  --comm_port="46102" \
  -d -t \
  --project="/project.xml" \
  --resources="/resources.xml"&
```

Upon the completion of an operation submitted with the `--stop` flag, the agent stops and generates a trace folder within his log folder, containing the `prv`, `pcf` and `row` files.

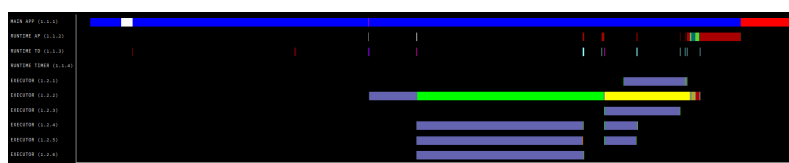
```
$ compss_agent_call_operation" \
  --lang="PYTHON" \
  --master_node="127.0.0.1" \
  --master_port="46101" \
  --method_name="kmeans" \
  --stop \
  "kmeans"
```

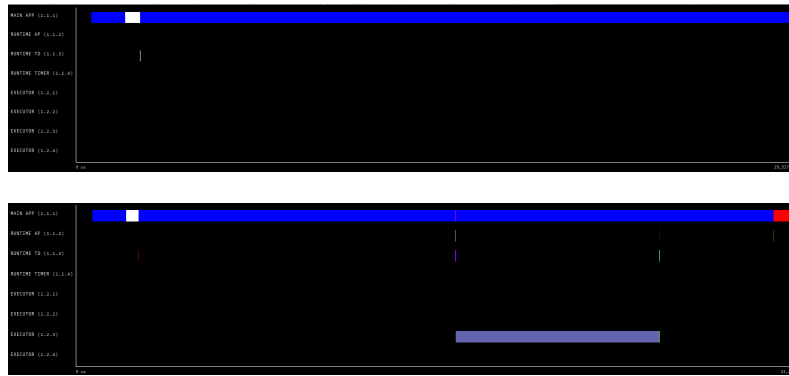


When multiple agents are involved in an application's execution, the stop command must be forwarded to all the other agents with the `--forward` parameter.

```
$ compss_agent_call_operation" \
  --lang="PYTHON" \
  --master_node="127.0.0.1" \
  --master_port="46101" \
  --method_name="kmeans" \
  --stop \
  --forward_to="COMPSsWorker02:46201;COMPSsWorker03:46301" \
  "kmeans"
```

Upon the completion of the last operation submitted and the shutdown of all involved agents, all agent will have generated their own individual trace.





In order to merge this traces the script `compss_agent_merge_traces` can be used. The script takes as parameters the folders of the log dirs of the agents with the traces to merge.

```
$ compss_agent_merge_traces -h
/opt/COMPSs/Runtime/scripts/user/compss_agent_merge_traces <options> <log_dir1> <log_dir2>
↪<log_dir3> ...

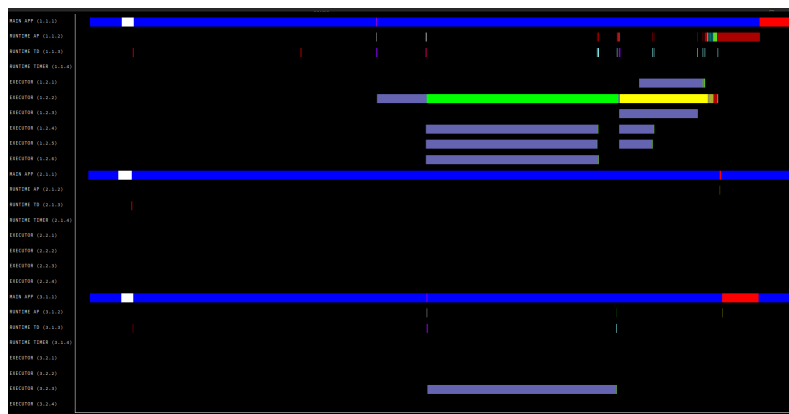
Merges the traces of the specified agents into a new trace created at the directory <output_
↪dir>

options:
    -h/--help                shows this message
    --output_dir=<output_dir> the directory where to store the
↪merged traces
    -f/--force_override      overrides output_dir if it already
↪exists without asking
    --result_trace_name=<result_trace_name> the name of the generated trace
```

Usage example:

```
$ compss_agent_merge_traces \
  --result_trace_name=merged_kmeans \
  ~/.COMPSs/1agent_python3_01/agent1 \
  ~/.COMPSs/1agent_python3_01/agent2 \
  ~/.COMPSs/1agent_python3_01/agent3
```

The script will put the merged trace in the specified `output_dir` or in the current directory inside a folder named `compss_agent_merge_traces` by default



6.1.4 Custom Installation and Configuration

6.1.4.1 Custom Extrae

COMPSs uses the environment variable `EXTRAЕ_HOME` to get the reference to its installation directory (by default: `/opt/COMPSs/Dependencies/extrae`). However, if the variable is already defined once the runtime is started, COMPSs will not override it. User can take advantage of this fact in order to use custom extrae installations. Just set the `EXTRAЕ_HOME` environment variable to the directory where your custom package is, and make sure that it is also set for the worker's environment. Be aware that using different Extrae packages can break the runtime and executions so you may change it at your own risk.

6.1.4.2 Custom Configuration file

COMPSs offers the possibility to specify an extrae custom configuration file in order to harness all the tracing capabilities further tailoring which information about the execution is displayed (except for Python workers). To do so just indicate the file as an execution parameter as follows:

```
--extrae_config_file=/path/to/config/file.xml
```

In addition, there is also the possibility to specify an extrae custom configuration file for the Python workers as follows:

```
--extrae_config_file_python=/path/to/config/file_python.xml
```

The configuration files must be in a shared disk between all COMPSs workers because a file's copy is not distributed among them, just the path to that file.

Tip: The default configuration files are in:

- `$COMPSS_HOME/Runtime/configuration/xml/tracing/extrae_advanced.xml`
- `$COMPSS_HOME/Runtime/configuration/xml/tracing/extrae_python_worker.xml` (when using Python)

The can be taken as base for customization.

6.2 Visualization

Paraver is the BSC tool for trace visualization. Trace events are encoded in Paraver format (`.prv`) by the Extrae tool. Paraver is a powerful tool and allows users to show many views of the trace data using different configuration files. Users can manually load, edit or create configuration files to obtain different tracing views.

The following subsections explain how to load a trace file into Paraver, open the task events view using an already predefined configuration file, and how to adjust the view to display the data properly.

For further information about Paraver, please visit the following site:

<http://www.bsc.es/computer-sciences/performance-tools/paraver>

6.2.1 Trace Loading

The final trace file in Paraver format (`.prv`) is at the base log folder of the application execution inside the trace folder. The fastest way to open it is calling the Paraver binary directly using the tracefile name as the argument.

```
$ wxparaver /path/to/trace/trace.prv
```

Tip: The path where the traces are usually located is `${HOME}/.COMPSs/<APPLICATION_NAME_INFO>/trace/`.

Where `<APPLICATION_NAME_INFO>` represents the executed application name and some information, such as the execution number or deployment information (e.g. number of nodes) and the generation time.

6.2.2 Configurations

To see the different events, counters and communications that the runtime generates, diverse configurations are available with the COMPSs installation. To open one of them, go to the “Load Configuration” option in the main window and select “File”. The configuration files are under the following path for the default installation `/opt/COMPSs/Dependencies/paraver/cfgs/`. A detailed list of all the available configurations can be found in [Paraver: configurations](#).

The following guide uses a kmeans trace (result from executing the [Kmeans](#) sample code with the `--tracing` flag.) with the `compss_tasks.cfg` configuration file as an example to illustrate the basic usage of Paraver. After accepting the load of the configuration file, another window appears showing the view. [Figure 24](#) and [Figure 25](#) show an example of this process.

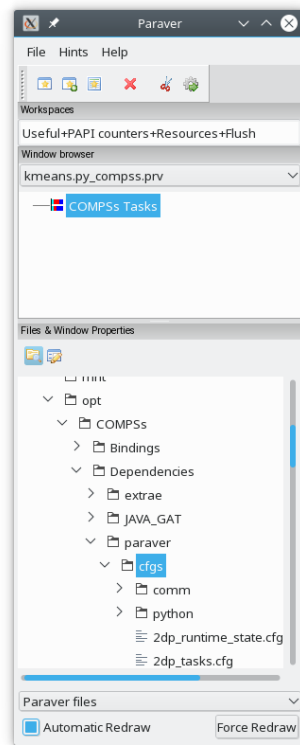


Figure 24: Paraver menu

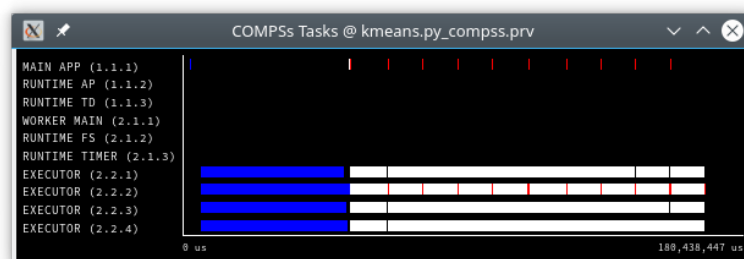


Figure 25: Kmeans Trace file

Caution: In a Paraver view, a red exclamation sign may appear in the bottom-left corner. This means that some event values are not being shown (because they are out of the current view scope), so little adjustments must be made to view the trace correctly:

- Fit window: modifies the view scope to fit and display all the events in the current window.
 - Right click on the trace window
 - Choose the option Fit Semantic Scale / Fit Both

6.2.3 View Adjustment

- View Event Flags: marks with a green flag all the emitted events.
 - Right click on the trace window
 - Chose the option View / Event Flags

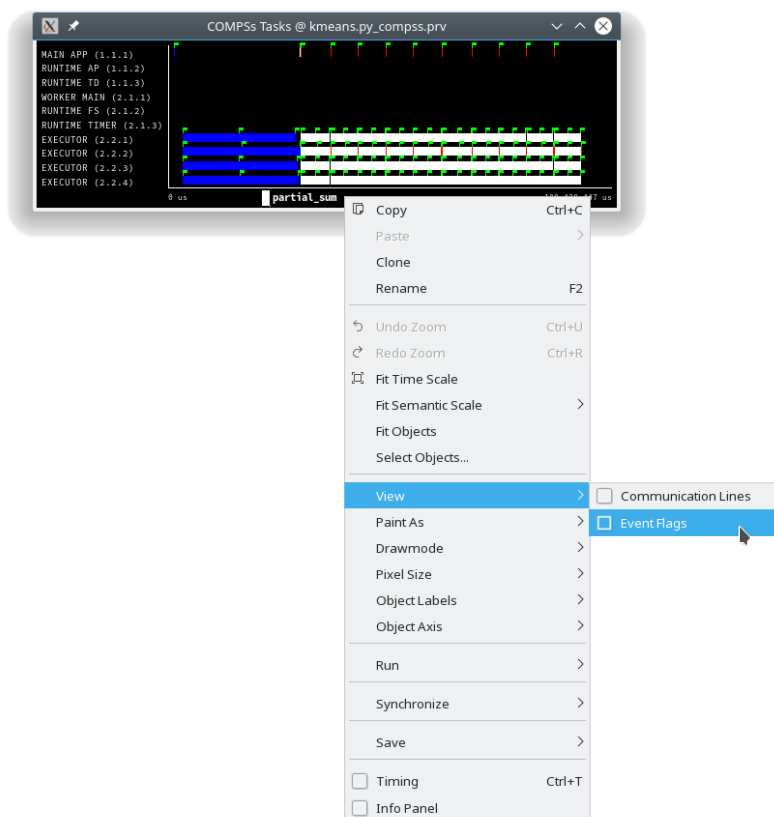


Figure 26: Paraver view adjustment: View Event Flags

- Show Info Panel: display the information panel. In the tab “Colors” we can see the legend of the colors shown in the view.
 - Right click on the trace window
 - Check the Info Panel option
 - Select the Colors tab in the panel
- Zoom: explore the tracefile more in-depth by zooming into the most relevant sections.
 - Select a region in the trace window to see that region in detail
 - Repeat the previous step as many times as needed
 - The undo-zoom option is in the right click panel

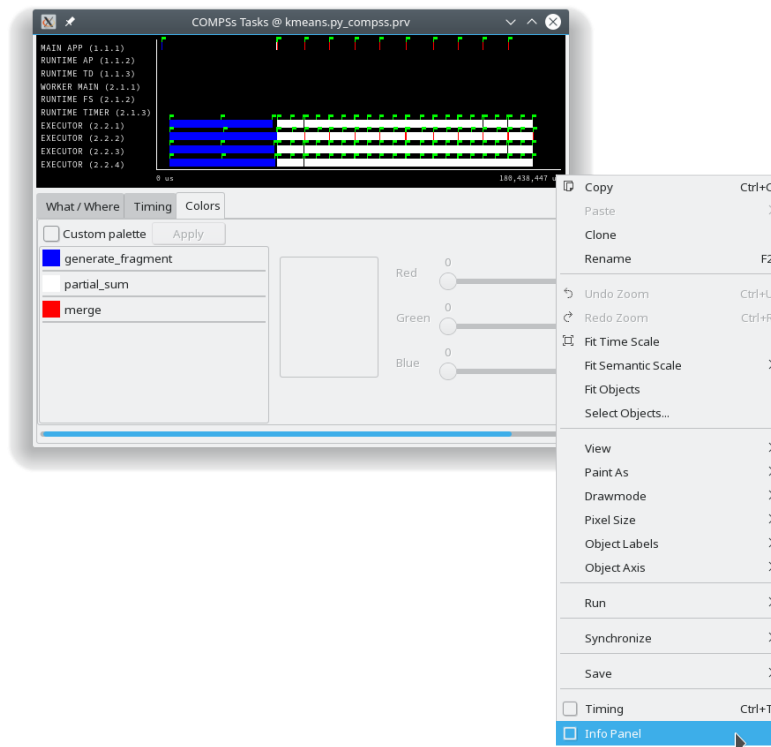


Figure 27: Paraver view adjustment: Show info panel

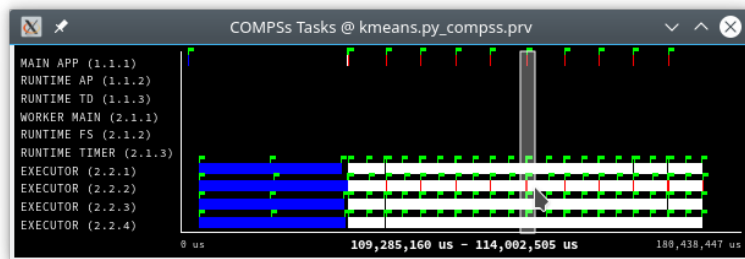


Figure 28: Paraver view adjustment: Zoom configuration

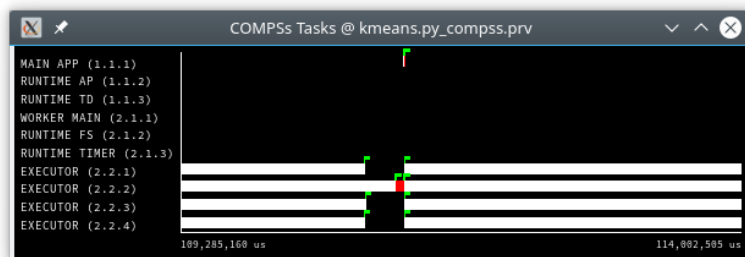


Figure 29: Paraver view adjustment: Zoom result

6.3 Interpretation

This section explains how to interpret a trace view once it has been adjusted as described in the previous section.

- The trace view has on its horizontal axis the execution time and on the vertical axis one line for the master at the top, and below it, one line for each of the workers.
- In a line, the black color is associated with an idle state, i.e. there is no event at that time.
- Whenever an event starts or ends a flag is shown.
- In the middle of an event, the line shows a different color. Colors are assigned depending on the event type.
- The info panel contains the legend of the assigned colors to each event type.

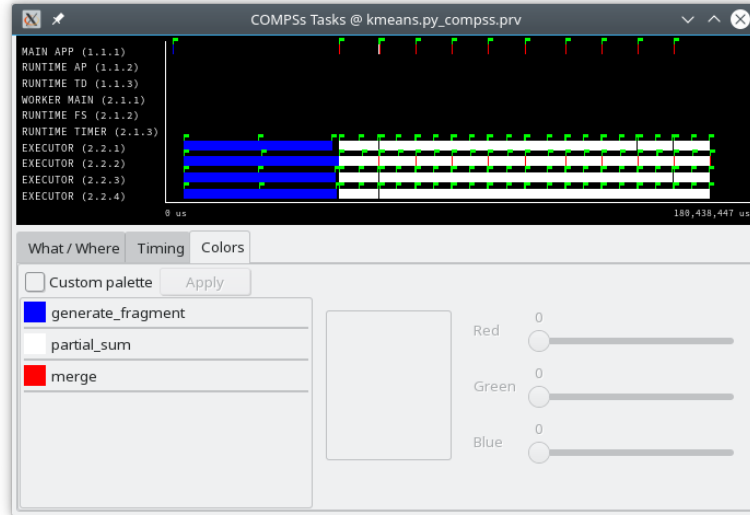


Figure 30: Trace interpretation

6.4 Analysis

This section gives some tips to analyze a COMPSs trace from two different points of view: graphically and numerically.

6.4.1 Graphical Analysis

The main concept is that computational events, the task events in this case, must be well distributed among all workers to have a good parallelism, and the duration of task events should be also balanced, this means, the duration of computational bursts.

In the previous trace view, all the tasks of type “generate_fragment” in dark blue appear to be well distributed among the four workers, each worker executor executes two “generate_fragment” tasks.

Next, a set of “partial_sum” tasks, coloured in white, are distributed across the four workers. In particular, eight “partial_sum” tasks are executed per kmeans iteration, so each worker executor executes two “partial_sum” tasks per iteration. This trace shows the execution of ten iterations. Note that all “partial_sum” tasks are very similar in time. This means that there is not much variability among them, and consequently not imbalance.

Finally, there is a “merge” task at the end of each iteration (coloured in red). This task is executed by one of the worker executors, and gathers the result from the previous eight “partial_sum” tasks. This task can be better displayed thanks to zoom.

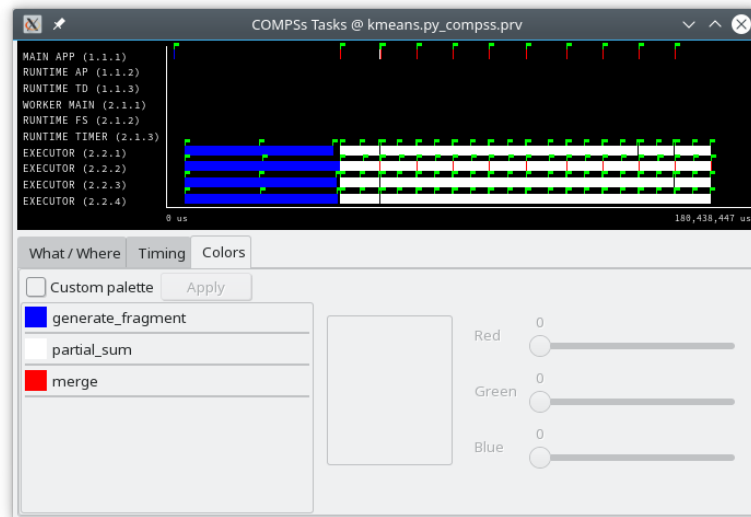


Figure 31: Basic trace view of a Kmeans execution.

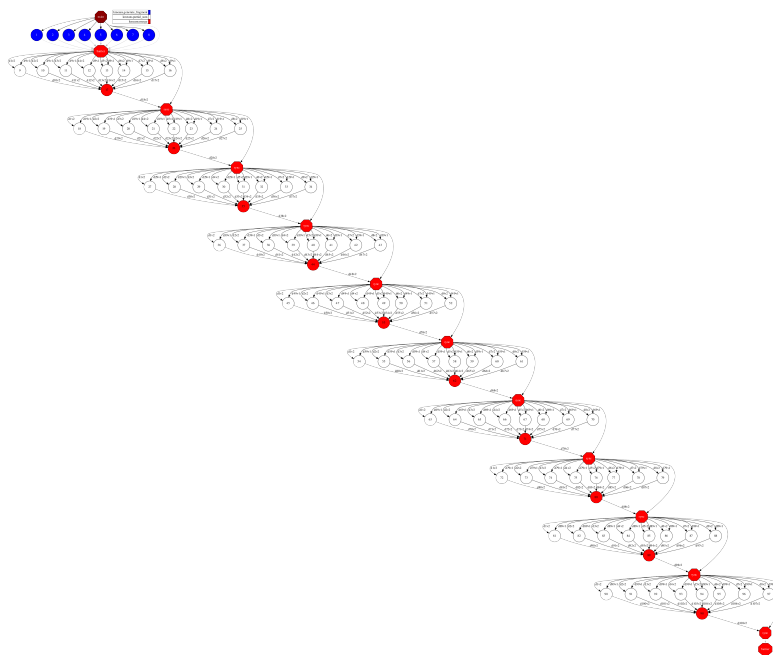


Figure 32: Data dependencies graph of a Kmeans execution.

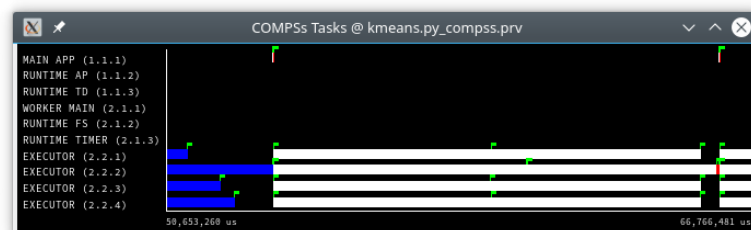


Figure 33: Zoomed in view of a Kmeans execution (first iteration).

6.4.2 Numerical Analysis

Here we analyze the Kmeans trace numerically.

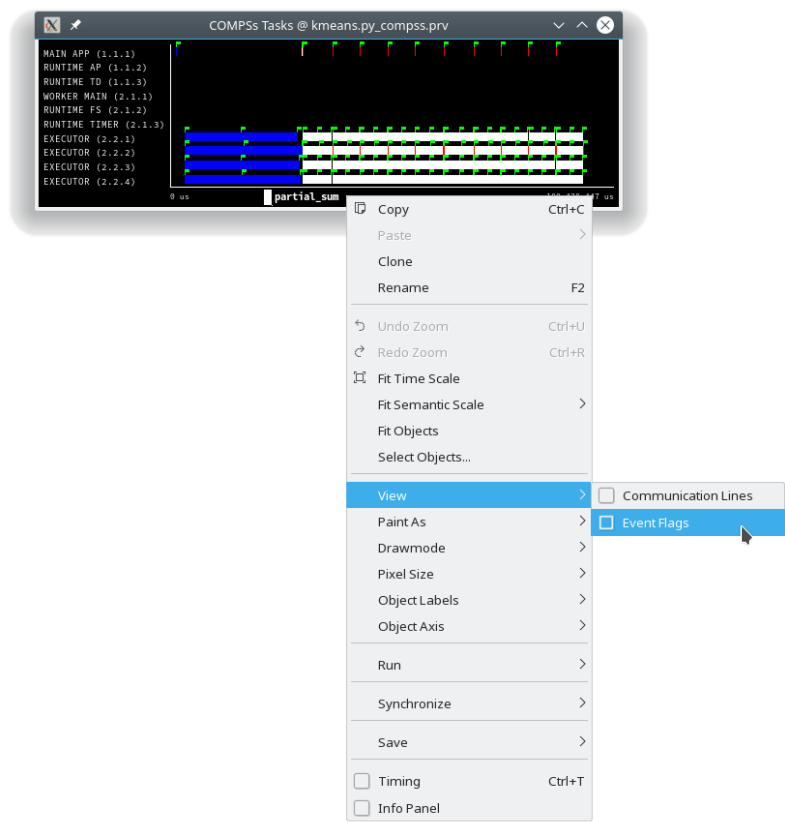


Figure 34: Original sample trace of a Kmeans execution to be analyzed

Paraver offers the possibility of having different histograms of the trace events. Click the “New Histogram” button in the main window and accept the default options in the “New Histogram” window that will appear.



Figure 35: Paraver Menu - New Histogram

After that, the following table is shown. In this case for each worker, the time spent executing each type of task is shown in gradient from light green to dark-blue for higher ones. The values corresponding to the colours and task names can be shown by clicking in the gray magnifying glass button. And the task corresponding to each task column can also be shown by clicking in the colour bars button.

The time spent executing each type of task is shown, and task names appear in the same color than in the trace view. The color of the cells in a row is kept, conforming a color based histogram.

The previous table also gives, at the end of each column, some extra statistical information for each type of tasks (as the total, average, maximum or minimum values, etc.).

In the window properties of the main window (Button [Figure 39](#)), it is possible to change the semantic of the statistics to see other factors rather than the time, for example, the number of bursts ([Figure 40](#)).

In the same way as before, the following table shows for each worker the number of bursts for each type of task, this is, the number or tasks executed of each type. Notice the gradient scale from light-green to dark-blue changes with the new values.

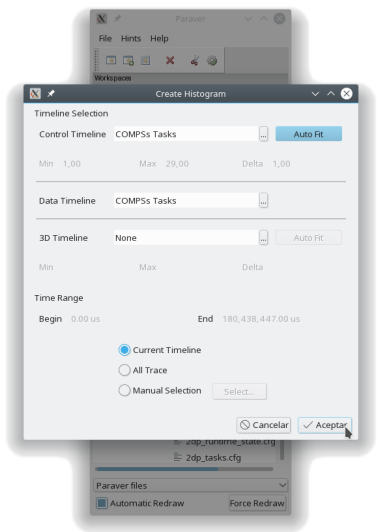


Figure 36: Histogram configuration (Accept default values)

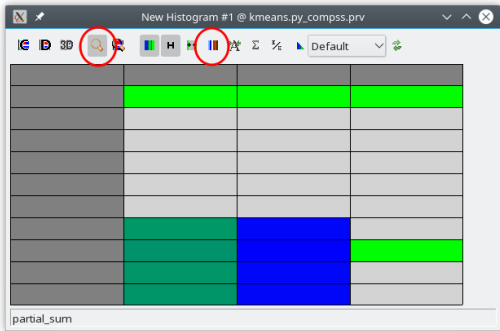


Figure 37: Kmeans histogram corresponding to previous trace

	generate_fragment	partial_sum	merge
MAIN APP (1.1.1)	12,465 us	62,958 us	88,148 us
RUNTIME AP (1.1.2)	-	-	-
RUNTIME TD (1.1.3)	-	-	-
WORKER MAIN (2.1.1)	-	-	-
RUNTIME FS (2.1.2)	-	-	-
RUNTIME TIMER (2.1.3)	-	-	-
EXECUTOR (2.2.1)	45,663,980 us	110,485,332 us	-
EXECUTOR (2.2.2)	48,012,074 us	113,531,033 us	608,829 us
EXECUTOR (2.2.3)	46,535,929 us	110,674,004 us	-
EXECUTOR (2.2.4)	46,951,813 us	110,773,953 us	-
Total	187,176,261 us	445,527,280 us	696,977 us
Average	37,435,252.20 us	89,105,456 us	348,488.50 us
Maximum	48,012,074 us	113,531,033 us	608,829 us
Minimum	12,465 us	62,958 us	88,148 us
StdDev	18,726,630.08 us	44,535,380.06 us	260,340.50 us
Avg/Max	0.78	0.78	0.57

Figure 38: Kmeans numerical histogram corresponding to previous trace

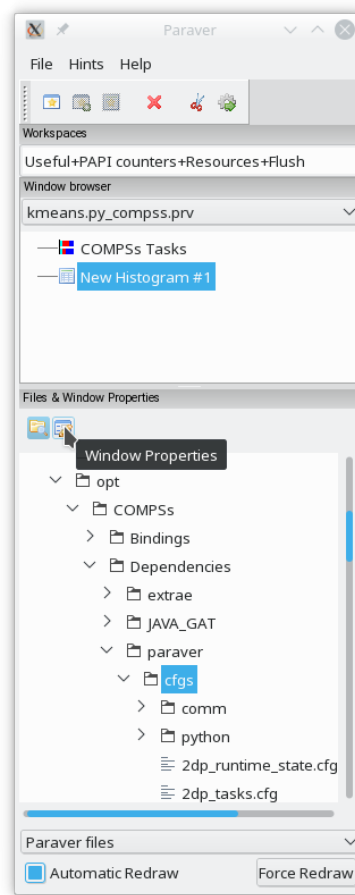


Figure 39: Paraver window properties button

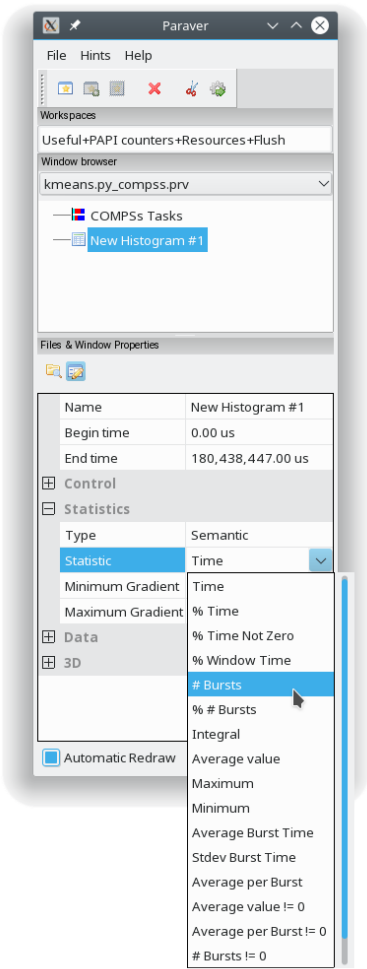


Figure 40: Paraver histogram options menu

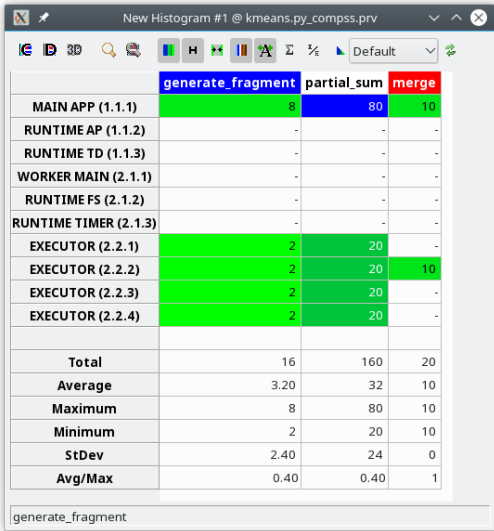


Figure 41: Kmeans histogram with the number of bursts

6.5 PAPI: Hardware Counters

The applications instrumentation supports hardware counters through the performance API (PAPI). In order to use it, PAPI needs to be present on the machine before installing COMPSs.

During COMPSs installation it is possible to check if PAPI has been detected in the Extrae config report:

```
Package configuration for Extrae VERSION based on extrae/trunk rev. XXXX:
-----
Installation prefix: /opt/COMPSs/Dependencies/extrae
Cross compilation: no
...
...
...

Performance counters: yes
  Performance API: PAPI
  PAPI home: /usr
  Sampling support: yes
```

Caution: PAPI detection is only performed in the machine where COMPSs is installed. User is responsible of providing a valid PAPI installation to the worker machines to be used (if they are different from the master), otherwise workers will crash because of the missing *libpapi.so*.

PAPI installation and requirements depend on the OS. On Ubuntu 14.04 it is available under *papi-tools* package; on OpenSuse *libpapi*, *papi* and *papi-devel* packages. For more information check https://icl.cs.utk.edu/projects/papi/wiki/Installing_PAPI.

Extrae only supports 8 active hardware counters at the same time. Both basic and advanced mode have the same default counters list:

PAPI_TOT_INS Instructions completed
PAPI_TOT_CYC Total cycles
PAPI_LD_INS Load instructions
PAPI_SR_INS Store instructions
PAPI_BR_UCN Unconditional branch instructions
PAPI_BR_CN Conditional branch instructions
PAPI_VEC_SP Single precision vector/SIMD instructions
RESOURCE_STALLS Cycles Allocation is stalled due to Resource Related reason

The XML config file contains a secondary set of counters. In order to activate it just change the *starting-set-distribution* from 2 to 1 under the *cpu* tag. The second set provides the following information:

PAPI_TOT_INS Instructions completed
PAPI_TOT_CYC Total cycles
PAPI_L1_DCM Level 1 data cache misses
PAPI_L2_DCM Level 2 data cache misses
PAPI_L3_TCM Level 3 cache misses
PAPI_FP_INS Floating point instructions

Tip: To find the available PAPI counters on a given computer issue the command:

```
$ papi_avail -a
```

And for more hardware counters:

```
$ papi_native_avail
```

To further customize the tracked counters, modify the XML to suit your needs. For more information about Extrae's XML configuration refer to <https://www.bsc.es/computer-sciences/performance-tools/trace-generation/extrae/extrae-user-guide>.

6.6 Paraver: configurations

Table 17, Table 18 and Table 19 provide information about the different pre-build configurations that are distributed with COMPSs and that can be found under the `/opt/COMPSs/Dependencies/paraver/cfgs/` folder. The `cfgs` folder contains all the basic views, the `python` folder contains the configurations for Python events, and finally the `comm` folder contains the configurations related to communications.

Additionally, it can be shown the data transfers and the task dependencies. To see them it is needed to show communication lines in the paraver windows, to only see the task dependencies are needed to put in Filter > Communications > Comm size, the size equal to 0. Some of the dependencies between tasks may be lost.

Table 17: General paraver configurations for COMPSs Applications

Configuration File Name	Description
2dp_runtime_state.cfg	2D plot of runtime state
2dp_tasks.cfg	2D plot of tasks duration
3dh_duration_runtime.cfg	3D Histogram of runtime execution
3dh_duration_tasks.cfg	3D Histogram of tasks duration
compss_cpu_constraints.cfg	Shows tasks cpu constraints
compss_executors.cfg	Shows the number of executor threads in each node
compss_runtime.cfg	Shows COMPSs Runtime events (master and workers)
compss_runtime_master.cfg	Shows COMPSs Runtime master events
compss_storage.cfg	Shows COMPSs persistent storage events
compss_tasks_and_binding.cfg	Shows COMPSs Binding events (master and workers) and tasks execution
compss_tasks_and_runtime.cfg	Shows COMPSs Runtime events (master and workers) and tasks execution
compss_tasks.cfg	Shows tasks execution and tasks instantiation in master nodes
compss_tasks_cpu_affinity.cfg	Shows tasks CPU affinity
compss_tasks_gpu_affinity.cfg	Shows tasks GPU affinity
compss_tasks_id.cfg	Shows tasks execution by task id
compss_tasks_runtime_&_agents.cfg	Shows COMPSs Agent and Runtime events and tasks execution
compss_waiting_tasks.cfg	Shows waiting tasks
histograms_HW_counters.cfg	Shows hardware counters histograms
instantiation_time.cfg	Shows the instantiation time
Interval_between_runtime.cfg	Interval between runtime events
nb_executing_tasks.cfg	Number of executing tasks
nb_requested_cpus.cfg	Number of requested CPUs
nb_requested_disk_bw.cfg	Number of requested disk bandwidth
nb_requested_gpus.cfg	Number of requested GPUs
nb_executing_mem.cfg	Number of executing memory
nb_tasks_in_graph.cfg	Number of executing tasks
number_executors.cfg	Number of executors
task_duration.cfg	Shows tasks duration
thread_cpu.cfg	Shows the initial executing CPU
thread_identifiers.cfg	Shows the type of each thread
time_btw_tasks.cfg	Shows the time between tasks
user_events.cfg	Shows the user events (type 9000000)

Table 18: Available paraver configurations for Python events of COMPSs Applications

Configuration File Name	Description
3dh_events_inside_task.cfg	3D Histogram of python events
3dh_tasks_phase.cfg	3D Histogram of execution functions
deserialization_object_number.cfg	Shows the numbers of the objects that are being deserialized
deserialization_size.cfg	Shows the size of the objects that are being deserialized (Bytes)
events_inside_tasks.cfg	Events showing python information such as user function execution time, modules imports, or serializations
events_in_workers.cfg	Events showing python binding information in worker
nb_user_code_executing.cfg	Number of user code executing
serdes_bw.cfg	Serialization and deserializations bandwidth (MB/s)
serdes_cache_bw.cfg	Serialization and deserializations to cache bandwidth (MB/s)
serialization_object_number.cfg	Shows the numbers of the objects that are being serialized
serialization_size.cfg	Shows the size of the objects that are being serialized (Bytes)
nb_user_code_executing.cfg	Number of user code executing
tasks_cpu_affinity.cfg	Events showing the CPU affinity of the tasks (shows only the first core if multiple assigned)
tasks_gpu_affinity.cfg	Events showing the GPU affinity of the tasks (shows only the first GPU if multiple assigned)
Time_between_events_inside_tasks.cfg	Shows the time between events inside tasks

Table 19: Available paraver configurations for COMPSs Applications

Configuration File Name	Description
communication_matrix.cfg	Table view of communications between each node
compss_data_transfers.cfg	Shows data transfers for each task's parameter
compss_tasksID_transfers.cfg	Task's transfers request for each task (task with its IDs are also shown)
process_bandwidth.cfg	Send/Receive bandwidth table for each node
receive_bandwidth.cfg	Receive bandwidth view for each node
send_bandwidth.cfg	Send bandwidth view for each node
sr_bandwidth.cfg	Send/Receive bandwidth view for each node

6.7 User Events in Python

Users can emit custom events inside their python **tasks**. Thanks to the fact that python is not a compiled language, users can emit events inside their own tasks using the available EXTRAE instrumentation object because it is already loaded and available in the PYTHONPATH when running with tracing enabled.

To emit an event first import pyextrae:

- `import pyextrae.sequential as pyextrae` to emit events from the main code.
- `import pyextrae.multiprocessing as pyextrae` to emit events within tasks code.

And then just use the call `pyextrae.event(type, id)` (or `pyextrae.eventandcounters (type, id)` if you also want to emit PAPI hardware counters).

Tip: It must be used a type number higher than 8000050 in order to avoid type conflicts.

We suggest to use 9000000 since we provide the `user_events.cfg` configuration file to visualize the user events of this type in PARAVER.

6.7.1 Events in main code

The following code snippet shows how to emit an event from the main code (or any other code which is not within a task). In this case it is necessary to import `pyextrae.sequential`.

```
from pycompss.api.api import compss_wait_on
from pycompss.api.task import task
import pyextrae.sequential as pyextrae

@task(returns=1)
def increment(value):
    return value + 1

def main():
    value = 1
    pyextrae.eventandcounters(9000000, 2)
    result = increment(value)
    result = compss_wait_on(result)
    pyextrae.eventandcounters(9000000, 0)
    print("result: " + str(result))

if __name__ == "__main__":
    main()
```

6.7.2 Events in task code

The following code snippet shows how to emit an event from the task code. In this case it is necessary to import `pyextrae.multiprocessing`.

```
from pycompss.api.task import task

@task()
def compute():
    import pyextrae.multiprocessing as pyextrae
    pyextrae.eventandcounters(9000000, 2)
    ...
    # Code to wrap within event 2
    ...
    pyextrae.eventandcounters(9000000, 0)
```

Caution: Please, note that the `import pyextrae.multiprocessing as pyextrae` is performed within the task. If the user needs to add more events to tasks within the same module (excluding the applicatin main module) and wants to put this import in the top of the module making `pyextrae` available for all of them, it is necessary to enable the tracing hook on the tasks that emit events:

```
from pycompss.api.task import task
import pyextrae.multiprocessing as pyextrae

@task(tracing_hook=True)
def compute():
    pyextrae.eventandcounters(9000000, 2)
    ...
    # Code to wrap within event 2
    ...
    pyextrae.eventandcounters(9000000, 0)
```

The `tracing_hook` is disabled by default in order to reduce the overhead introduced by tracing avoiding to intercept all function calls within the task code.

6.7.3 Result trace

The events will appear automatically on the generated trace. In order to visualize them, just load the `user_events.cfg` configuration file in PARAVR.

If a different type value is choosen, take the same `user_events.cfg` and go to **Window Properties -> Filter -> Events -> Event Type** and change the value labeled *Types* for your custom events type.

Tip: If you want to name the events, you will need to manually add them to the `.pcf` file with the corresponding name for each value.

6.7.4 Practical example

Consider the following application where we define an event in the main code (1) and another within the task (2). The `increment` task is invoked 8 times (with a mimic computation time of the value received as parameter.)

```
from pycompss.api.api import compss_wait_on
from pycompss.api.task import task
import time

@task(returns=1)
def increment(value):
    import pyextrae.multiprocessing as pyextrae
    pyextrae.eventandcounters(9000000, 2)
    time.sleep(value) # mimic some computation
    pyextrae.eventandcounters(9000000, 0)
    return value + 1

def main():
    import pyextrae.sequential as pyextrae
    elements = [1, 2, 3, 4, 5, 6, 7, 8]
    results = []
    pyextrae.eventandcounters(9000000, 1)
    for element in elements:
        results.append(increment(element))
    results = compss_wait_on(results)
    pyextrae.eventandcounters(9000000, 0)
    print("results: " + str(results))

if __name__ == "__main__":
    main()
```

After launching with tracing enabled (`-t` flag), the trace has been generated into the logs folder:

- `$HOME/.COMPSs/events.py_01/trace` if using `runcompss`.
- `$HOME/.COMPSs/<JOB_ID>/trace` if using `enqueue_compss`.

Now it is time to modify the `.pcf` file including the folling text at the end of the file with your favourite text editor:


```

EVENT_TYPE
0      9000000    User events
VALUES
0      End
1      Main code event
2      Task event

```

Caution: Keep value 0 with the End message.

Add all values defined in the application with a descriptive short name to ease the event identification in PARAVR.

Open PARAVR, load the tracefile (.prv) and open the `user_events.cfg` configuration file. The result (see [Figure 42](#)) shows that there are 8 “Task event” (in white), and 1 “Main code event” (in blue) as we expected. Their length can be seen with the event flags (green flags), and measured by double clicking on the event of interest.

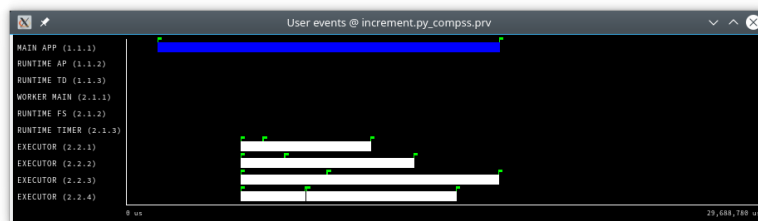


Figure 42: User events trace file

Paraver uses by default the .pcf with the same name as the tracefile so if you add them to one, you can reuse it just by changing its name to the tracefile.

Chapter 7

Persistent Storage

COMPSs is able to interact with Persistent Storage frameworks. To this end, it is necessary to take some considerations in the application code and on its execution. This section is intended to walk you through the COMPSs' storage interface and its integration with some Persistent Storage frameworks.

7.1 First steps

COMPSs relies on a Storage API to enable the interaction with persistent storage frameworks (Figure 43), which is composed by two main modules: *Storage Object Interface* (SOI) and *Storage Runtime Interface* (SRI)

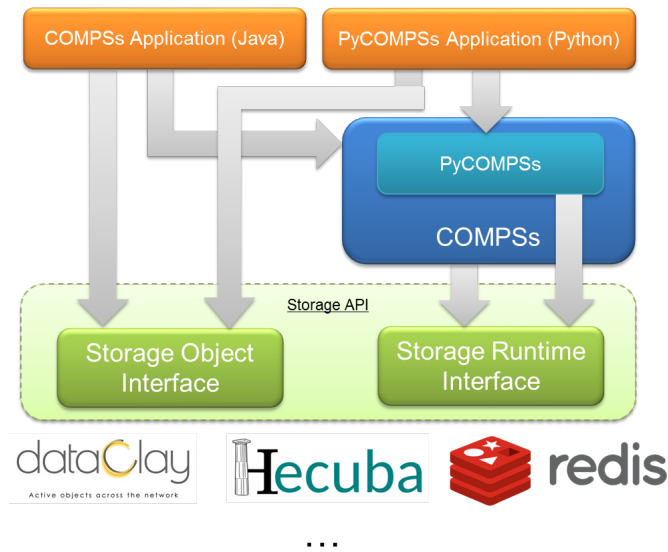


Figure 43: COMPSs with persistent storage architecture

Any COMPSs application aimed at using a persistent storage framework has to include calls to:

- The SOI in order to define the data model (see [Defining the data model](#)), and relies on COMPSs, which interacts with the persistent storage framework through the SRI.
- The SRI in order to interact directly with the storage backend (e.g. retrieve data, etc.) (see [Interacting with the persistent storage](#)).

In addition, it must be taken into account that the execution of an application using a persistent storage framework requires some specific flags in `runcompss` and `enqueue_compss` (see [Running with persistent storage](#)).

Currently, there exists storage interfaces for [dataClay](#), [Hecuba](#) and [Redis](#). They are thoroughly described from the developer and user point of view in Sections:

- [COMPSs + dataClay](#)
- [COMPSs + Hecuba](#)
- [COMPSs + Redis](#)

The interface is open to any other storage framework by implementing the required functionalities described in [Implement your own Storage interface for COMPSs](#).

7.1.1 Defining the data model

The data model consists of a set of related classes programmed in one of the supported languages aimed at representing the objects used in the application (e.g. in a wordcount application, the data model would be text).

In order to define that the application objects are going to be stored in the underlying persistent storage backend, the data model must be enriched with the *Storage Object Interface* (SOI).

The SOI provides a set of functionalities that all objects stored in the persistent storage backend will need. Consequently, the user must inherit the SOI on its data model classes, and give some insights of the class attributes.

The following subsections detail how to enrich the data model in Java and Python applications.

7.1.1.1 Java

To define that a class object is going to be stored in the persistent storage backend, the class must extend the `StorageObject` class (as well as implement the `Serializable` interface). This class is provided by the persistent storage backend.

```
import storage.StorageObject;
import java.io.Serializable;

class MyClass extends StorageObject implements Serializable {

    private double[] vector;

    /**
     * Write here your class-specific
     * constructors, attributes and methods.
     */
}
```

The `StorageObject` object enriches the class with some methods that allow the user to interact with the persistent storage backend. These methods can be found in [Table 20](#).

Table 20: Available methods from StorageObject

Name	Returns	Comments
<code>makePersistent(String id)</code>	Nothing	Inserts the object in the database with the id. If id is null, a random UUID will be computed instead.
<code>deletePersistent()</code>	Nothing	Removes the object from the storage. It does nothing if it was not already there.
<code>getID()</code>	String	Returns the current object identifier if the object is not persistent (null instead).

These functions can be used from the application in order to persist an object (pushing the object into the persistent storage) with `make_persistent`, remove it from the persistent storage with `delete_persistent` or getting the object identifier with `getID` for the later interaction with the storage backend.

```
import MyPackage.MyClass;

class Test{
    // ...
    public static void main(String args[]){
        // ...
        MyClass my_obj = new MyClass();
        my_obj.matrix = new double[10];
        my_obj.makePersistent();           // make persistent without parameter
        String obj_id = my_obj.getID();    // get the identifier provided by the storage framework
        // ...
        my_obj.deletePersistent();
        // ...
        MyClass my_obj2 = new MyClass();
        my_obj2.matrix = new double[20];
        my_obj2.makePersistent("obj2");    // make persistent providing identifier
        // ...
        my_obj2.delete_persistent();
        // ...
    }
}
```

7.1.1.2 Python

To define that a class objects are going to be stored in the persistent storage backend, the class must inherit the `StorageObject` class. This class is provided by the persistent storage backend.

```
from storage.api import StorageObject

class MyClass(StorageObject):
    ...
```

In addition, the user has to give details about the class attributes using the class documentation. For example, if the user wants to define a class containing a numpy ndarray as attribute, the user has to specify this attribute starting with `@ClassField` followed by the attribute name and type:

```
from storage.api import StorageObject

class MyClass(StorageObject):
    """
    @ClassField matrix numpy.ndarray
    """
    pass
```

Important: Methods inside the class are not supported by all storage backends. `dataClay` is currently the only backend that provides support for them (see [Enabling COMPSs applications with dataClay](#)).

Then, the user can use the instantiated object normally:

```
from MyFile import MyClass
import numpy as np

my_obj = MyClass()
my_obj.matrix = np.random.rand(10, 2)
...
```

The following code snippet gives some examples of several types of attributes:

```
from storage.api import StorageObject

class MyClass(StorageObject):
    """
    # Elemental types
    @ClassField field1 int
    @ClassField field2 str
    @ClassField field3 np.ndarray

    # Structured types
    @ClassField field4 list <int>
    @ClassField field5 set <list<float>>

    # Another class instance as attribute
    @ClassField field6 AnotherClassName

    # Complex dictionaries:
    @ClassField field7 dict <<int,str>, dict<<int>, list<str>>>
    @ClassField field8 dict <<int>, AnotherClassName>

    # Dictionary with structured value:
```

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```

@ClassField field9 dict <<k1: int, k2: int>, tuple<v1: int, v2: float, v3: text>>
# Plain definition of the same dictionary:
@ClassField field10 dict <<int,int>, str>
"""
pass

```

Finally, the `StorageObject` class includes some functions in the class that will be available from the instantiated objects (Table 21).

Table 21: Available methods from `StorageObject` in Python

Name	Returns	Comments
<code>make_persistent(String id)</code>	Nothing	Inserts the object in the database with the id. If id is null, a random UUID will be computed instead.
<code>delete_persistent()</code>	Nothing	Removes the object from the storage. It does nothing if it was not already there.
<code>getID()</code>	String	Returns the current object identifier if the object is not persistent (None instead).

These functions can be used from the application in order to persist an object (pushing the object into the persistent storage) with `make_persistent`, remove it from the persistent storage with `delete_persistent` or getting the object identifier with `getID` for the later interaction with the storage backend.

```

import numpy as np

my_obj = MyClass()
my_obj.matrix = np.random.rand(10, 2)
my_obj.make_persistent() # make persistent without parameter
obj_id = my_obj.getID() # get the identifier provided by the storage framework
...
my_obj.delete_persistent()
...
my_obj2 = MyClass()
my_obj2.matrix = np.random.rand(10, 3)
my_obj2.make_persistent('obj2') # make persistent providing identifier
...
my_obj2.delete_persistent()
...

```

7.1.1.3 C/C++

Unsupported

Persistent storage is not supported with C/C++ COMPSs applications.

7.1.2 Interacting with the persistent storage

The **Storage Runtime Interface** (SRI) provides some functions to interact with the storage backend. All of them are aimed at enabling the COMPSs runtime to deal with persistent data across the infrastructure.

However, the function to retrieve an object from the storage backend from its identifier can be useful for the user. Consequently, users can import the SRI and use the `getByID` function when needed necessary. This function requires a String parameter with the object identifier, and returns the object associated with that identifier (`null` or `None` otherwise).

The following subsections detail how to call the `getByID` function in Java and Python applications.

7.1.2.1 Java

Import the `getByID` function from the storage api and use it:

```
import storage.StorageItf;
import MyPackage.MyClass;

class Test{
    // ...
    public static void main(String args[]){
        // ...
        obj = StorageItf.getByID("my_obj");
        // ...
    }
}
```

7.1.2.2 Python

Import the `getByID` function from the storage api and use it:

```
from storage.api import getByID

..
obj = getByID('my_obj')
...
```


7.1.2.3 C/C++

Unsupported

Persistent storage is not supported with C/C++ COMPSs applications.

7.1.3 Running with persistent storage

7.1.3.1 Local

In order to run a COMPSs application locally, the `runcompss` command is used.

The `runcompss` command includes some flags to execute the application considering a running persistent storage framework. These flags are: `--classpath`, `--pythonpath` and `--storage_conf`.

Consequently, the `runcompss` requirements to run an application with a running persistent storage backend are:

<code>--classpath</code>	Add the <code>--classpath=\${path_to_storage_api.jar}</code> flag to the <code>runcompss</code> command.
<code>--pythonpath</code>	If you are running a python application, also add the <code>--pythonpath=\${path_to_the_storage_api}/python</code> flag to the <code>runcompss</code> command.
<code>--storage_conf</code>	Add the flag <code>--storage_conf=\${path_to_your_storage_conf_dot_cfg_file}</code> to the <code>runcompss</code> command. The storage configuration file (usually <code>storage_conf.cfg</code>) contains the configuration parameters needed by the storage framework for the execution (it depends on the storage framework).

As usual, the `project.xml` and `resources.xml` files must be correctly set.

7.1.3.2 Supercomputer

In order to run a COMPSs application in a Supercomputer or cluster, the `enqueue_compss` command is used.

The `enqueue_compss` command includes some flags to execute the application considering a running persistent storage framework. These flags are: `--classpath`, `--pythonpath`, `--storage-home` and `--storage-props`.

Consequently, the `enqueue_compss` requirements to run an application with a running persistent storage backend are:

<code>--classpath</code>	<code>--classpath=\${path_to_storage_interface.jar}</code> As with the <code>runcompss</code> command, the JAR with the storage API must be specified. It is usually available in a environment variable (check the persistent storage framework).
<code>--pythonpath</code>	If you are running a Python application, also add the <code>--pythonpath=\${path_to_the_storage_api}/python</code> flag. It is usually available in a environment variable (check the persistent storage framework).
<code>--storage-home</code>	<code>--storage-home=\${path_to_the_storage_api}</code> This must point to the root of the storage folder. This folder must contain a <code>scripts</code> folder where the scripts to start and stop the persistent framework are. It is usually available in a environment variable (check the persistent storage framework).
<code>--storage-props</code>	<code>--storage-props=\${path_to_the_storage_props_file}</code> This must point to the storage properties configuration file (usually <code>storage_props.cfg</code>) It contains the configuration parameters needed by the storage framework for the execution (it depends on the storage framework).

7.2 COMPSs + dataClay

Warning: Under construction

7.2.1 COMPSs + dataClay Dependencies

7.2.1.1 dataClay

7.2.1.2 Other dependencies

7.2.2 Enabling COMPSs applications with dataClay

7.2.2.1 Java

7.2.2.2 Python

7.2.2.3 C/C++

Unsupported

C/C++ COMPSs applications are not supported with dataClay.

7.2.3 Executing a COMPSs application with dataClay

7.2.3.1 Launching using an existing dataClay deployment

7.2.3.2 Launching on queue system based environments

7.3 COMPSs + Hecuba

Warning: Under construction

7.3.1 COMPSs + Hecuba Dependencies

7.3.1.1 Hecuba

7.3.1.2 Other dependencies

7.3.2 Enabling COMPSs applications with Hecuba

7.3.2.1 Java

Unsupported

Java COMPSs applications are not supported with Hecuba.

7.3.2.2 Python

7.3.2.3 C/C++

Unsupported

C/C++ COMPSs applications are not supported with Hecuba.

7.3.3 Executing a COMPSs application with Hecuba

7.3.3.1 Launching using an existing Hecuba deployment

7.3.3.2 Launching on queue system based environments

7.4 COMPSs + Redis

COMPSs provides a built-in interface to use Redis as persistent storage from COMPSs' applications.

Note: We assume that COMPSs is already installed. See [Installation and Administration](#)

The next subsections focus on how to install the Redis utilities and the storage API for COMPSs.

Hint: It is advisable to read the Redis Cluster tutorial for beginners¹ in order to understand all the terminology that is used.

7.4.1 COMPSs + Redis Dependencies

The required dependencies are:

- [Redis Server](#)
- [Redis Cluster script](#)
- [COMPSs-Redis Bundle](#)

7.4.1.1 Redis Server

`redis-server` is the core Redis program. It allows to create standalone Redis instances that may form part of a cluster in the future. `redis-server` can be obtained by following these steps:

1. Go to <https://redis.io/download> and download the last stable version. This should download a `redis- $\{version\}$ .tar.gz` file to your computer, where $\{version\}$ is the current latest version.
2. Unpack the compressed file to some directory, open a terminal on it and then type `sudo make install` if you want to install Redis for all users. If you want to have it installed only for yourself you can simply type `make redis-server`. This will leave the `redis-server` executable file inside the directory `src`, allowing you to move it to a more convenient place. By *convenient place* we mean a folder that is in your `PATH` environment variable. It is advisable to not delete the uncompressed folder yet.
3. If you want to be sure that Redis will work well on your machine then you can type `make test`. This will run a very exhaustive test suite on Redis features.

Important: Do not delete the uncompressed folder yet.

¹ <https://redis.io/topics/cluster-tutorial>

7.4.1.2 Redis Cluster script

Redis needs an additional script to form a cluster from various Redis instances. This script is called `redis-trib.rb` and can be found in the same tar.gz file that contains the sources to compile `redis-server` in `src/redis-trib.rb`. Two things must be done to make this script work:

1. Move it to a convenient folder. By *convenient folder* we mean a folder that is in your `PATH` environment variable.
2. Make sure that you have Ruby and `gem` installed. Type `gem install redis`.
3. In order to use COMPSs + Redis with Python you must also install the `redis` and `redis-py-cluster` PyPI packages.

Hint: It is also advisable to have the PyPI package `hiredis`, which is a library that makes the interactions with the storage to go faster.

7.4.1.3 COMPSs-Redis Bundle

COMPSs-Redis Bundle is a software package that contains the following:

1. A java JAR file named `compss-redisPSCO.jar`. This JAR contains the implementation of a Storage Object that interacts with a given Redis backend. We will discuss the details later.
2. A folder named `scripts`. This folder contains a bunch of scripts that allows a COMPSs-Redis app to create a custom, in-place cluster for the application.
3. A folder named `python` that contains the Python equivalent to `compss-redisPSCO.jar`

This package can be obtained from the COMPSs source as follows:

1. Go to `trunk/utils/storage/redisPSCO`
2. Type `./make_bundle`. This will leave a folder named `COMPSs-Redis-bundle` with all the bundle contents.

7.4.2 Enabling COMPSs applications with Redis

7.4.2.1 Java

This section describes how to develop Java applications with the Redis storage. The application project should have the dependency induced by `compss-redisPSCO.jar` satisfied. That is, it should be included in the application's `pom.xml` if you are using Maven, or it should be listed in the dependencies section of the used development tool.

The application is almost identical to a regular COMPSs application except for the presence of Storage Objects. A Storage Object is an object that it is capable to interact with the storage backend. If a custom object extends the Redis Storage Object and implements the `Serializable` interface then it will be ready to be stored and retrieved from a Redis database. An example signature could be the following:

```
import storage.StorageObject;
import java.io.Serializable;

/**
 * A PSCO that contains a KD point
 */
class RedisPoint
extends StorageObject implements Serializable {

    // Coordinates of our point
    private double[] coordinates;
    /**
     * Write here your class-specific
     * constructors, attributes and methods.
```

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```

    */
    double getManhattanDistance(RedisPoint other) {
        ...
    }
}

```

The `StorageObject` object has some inherited methods that allow the user to write custom objects that interact with the Redis backend. These methods can be found in [Table 22](#).

Table 22: Available methods from `StorageObject`

Name	Returns	Comments
<code>makePersistent(String id)</code>	Nothing	Inserts the object in the database with the id. If id is null, a random UUID will be computed instead.
<code>deletePersistent()</code>	Nothing	Removes the object from the storage. It does nothing if it was not already there.
<code>getID()</code>	String	Returns the current object identifier if the object is not persistent (null instead).

Caution: Redis Storage Objects that are used as INOUTs must be manually updated. This is due to the fact that COMPSs does not know the exact effects of the interaction between the object and the storage, so the runtime cannot know if it is necessary to call `makePersistent` after having used an INOUT or not (other storage approaches do live modifications to its storage objects). The following example illustrates this situation:

```

/**
 * A is passed as INOUT
 */
void accumulativePointSum(RedisPoint a, RedisPoint b) {
    // This method computes the coordinate-wise sum between a and b
    // and leaves the result in a
    for(int i=0; i<a.getCoordinates().length; ++i) {
        a.setComponent(i, a.getComponent(i) + b.getComponent(i));
    }
    // Delete the object from the storage and
    // re-insert the object with the same old identifier
    String objectIdentifier = a.getID();
    // Redis contains the old version of the object
    a.deletePersistent();
    // Now we will insert the updated one
    a.makePersistent(objectIdentifier);
}

```

If the last three statements were not present, the changes would never be reflected on the `RedisPoint a` object.

7.4.2.2 Python

Redis is also available for Python. As happens with Java, we first need to define a custom Storage Object. Let's suppose that we want to write an application that multiplies two matrices A , and B by blocks. We can define a `Block` object that lets us store and write matrix blocks in our Redis backend:

```
from storage.storage_object import StorageObject
import storage.api

class Block(StorageObject):
    def __init__(self, block):
        super(Block, self).__init__()
        self.block = block

    def get_block(self):
        return self.block

    def set_block(self, new_block):
        self.block = new_block
```

Let's suppose that we are multiplying our matrices in the usual blocked way:

```
for i in range(MSIZE):
    for j in range(MSIZE):
        for k in range(MSIZE):
            multiply(A[i][k], B[k][j], C[i][j])
```

Where A and B are `Block` objects and C is a regular Python object (e.g: a Numpy matrix), then we can define `multiply` as a task as follows:

```
@task(c = INOUT)
def multiply(a_object, b_object, c, MKLProc):
    c += a_object.block * b_object.block
```

Let's also suppose that we are interested to store the final result in our storage. A possible solution is the following:

```
for i in range(MSIZE):
    for j in range(MSIZE):
        persist_result(C[i][j])
```

Where `persist_result` can be defined as a task as follows:

```
@task()
def persist_result(obj):
    to_persist = Block(obj)
    to_persist.make_persistent()
```

This way is preferred for two main reasons:

- we avoid to bring the resulting matrix to the master node,
- and we can exploit the data locality by executing the task in the node where last version of `obj` is located.

7.4.2.3 C/C++

Unsupported

C/C++ COMPSs applications are not supported with Redis.

7.4.3 Executing a COMPSs application with Redis

7.4.3.1 Launching using an existing Redis Cluster

If there is already a running Redis Cluster on the node/s where the COMPSs application will run then only the following steps must be followed:

1. Create a `storage_conf.cfg` file that lists, one per line, the nodes where the storage is present. Only hostnames or IPs are needed, ports are not necessary here.
2. Add the flag `--classpath=${path_to_COMPSs-redisPSCO.jar}` to the `runcompss` command that launches the application.
3. Add the flag `--storage_conf=${path_to_your_storage_conf_dot_cfg_file}` to the `runcompss` command that launches the application.
4. If you are running a python app, also add the `--pythonpath=${app_path}:${path_to_the_bundle_folder}/python` flag to the `runcompss` command that launches the application.

As usual, the `project.xml` and `resources.xml` files must be correctly set. It must be noted that there can be Redis nodes that are not COMPSs nodes (although **this is a highly unrecommended practice**). As a requirement, **there must be at least one Redis instance on each COMPSs node listening to the official Redis port 6379²**. This is required because nodes without running Redis instances would cause a great amount of transfers (they will **always** need data that must be transferred from another node). Also, any locality policy will likely cause this node to have a very low workload, rendering it almost useless.

7.4.3.2 Launching on queue system based environments

COMPSs-Redis-Bundle also includes a collection of scripts that allow the user to create an in-place Redis cluster with his/her COMPSs application. These scripts will create a cluster using only the COMPSs nodes provided by the queue system (e.g. SLURM, PBS, etc.). Some parameters can be tuned by the user via a `storage_props.cfg` file. This file must have the following form:

```
REDIS_HOME=some_path
REDIS_NODE_TIMEOUT=some_nonnegative_integer_value
REDIS_REPLICAS=some_nonnegative_integer_value
```

There are some observations regarding to this configuration file:

- REDIS_HOME** Must be equal to a path to some location that is **not** shared between nodes. This is the location where the Redis sandboxes for the instances will be created.
- REDIS_NODE_TIMEOUT** Must be a nonnegative integer number that represents the amount of milliseconds that must pass before Redis declares the cluster broken in the case that some instance is not available.
- REDIS_REPLICAS** Must be equal to a nonnegative integer. This value will represent the amount of replicas that a given shard will have. If possible, Redis will ensure that all replicas of a given shard will be on different nodes.

In order to run a COMPSs + Redis application on a queue system the user must add the following flags to the `enqueue_compss` command:

1. `--storage-home=${path_to_the_bundle_folder}` This must point to the root of the COMPSs-Redis bundle.

² https://en.wikipedia.org/wiki/List_of_TCP_and_UDP_port_numbers

2. `--storage-props=${path_to_the_storage_props_file}` This must point to the `storage_props.cfg` mentioned above.
3. `--classpath=${path_to_COMPSs-redisPSCO.jar}` As in the previous section, the JAR with the storage API must be specified.
4. If you are running a Python application, also add the `--pythonpath=${app_path}:${path_to_the_bundle_folder}` flag

Caution: As a requirement, the supercomputer **MUST NOT** kill daemonized processes running on the provided computing nodes during the execution.

7.5 Implement your own Storage interface for COMPSs

In order to implement an interface for a Storage framework, it is necessary to implement the Java SRI (mandatory), and depending on the desired language, implement the Python SRI and the specific SOI inheriting from the generic SOI provided by COMPSs.

7.5.1 Generic Storage Object Interface

Table 23 shows the functions that must exist in the storage object interface, that enables the object that inherits it to interact with the storage framework.

Table 23: SCO object definition

Name	Returns	Comments
Constructor	Nothing	Instantiates the object.
<code>get_by_alias(String id)</code>	Object	Retrieve the object with alias “name”.
<code>makePersistent(String id)</code>	Nothing	Inserts the object in the storage framework with the id. If id is null, a random UUID will be computed instead.
<code>deletePersistent()</code>	Nothing	Removes the object from the storage. It does nothing if it was not already there.
<code>getID()</code>	String	Returns the current object identifier if the object is not persistent (null instead).

For example, the **makePersistent** function is intended to store the object content into the persistent storage, **deletePersistent** to remove it, and **getID** to provide the object identifier.

Important: An object will be considered persisted if the `getID` function retrieves something different from `None`.

This interface must be implemented in the target language desired (e.g. Java or Python).

7.5.2 Generic Storage Runtime Interfaces

[Table 24](#) shows the functions that must exist in the storage runtime interface, that enables the COMPSs runtime to interact with the storage framework.

Table 24: Java API

Name	Returns	Comments	Signature
init(String storage_conf)	Nothing	Do any initialization action before starting to execute the application. Receives the storage configuration file path defined in the runcompss or enqueue_composs command.	public static void init(String storageConf) throws StorageException {}
finish()	Nothing	Do any finalization action after executing the application.	public static void finish() throws StorageException
getLocations(String id)	List<String>	Retrieve the locations where a particular object is from its identifier.	public static List<String> getLocations(String id) throws StorageException
getByID(String id)	Object	Retrieve an object from its identifier.	public static Object getByID(String id) throws StorageException
newReplica(String id, String hostName)	String	Create a new replica of an object in the storage framework.	public static void newReplica(String id, String hostName) throws StorageException
newVersion(String id, String hostname)	String	Create a new version of an object in the storage framework.	public static String newVersion(String id, String hostName) throws StorageException
consolidateVersion(String id)	Nothing	Consolidate a version of an object in the storage framework.	public static void consolidateVersion(String id-Final) throws StorageException
executeTask(String id, ...)	String	Execute the task into the datastore.	public static String executeTask(String id, String descriptor, Object[] values, String hostName, CallbackHandler callback) throws StorageException
getResult(CallbackEvent event())	Object	Retrieve the result of the execution into the storage framework.	public static Object getResult(CallbackEvent event) throws StorageException

This functions enable the COMPSs runtime to keep the data consistency through the distributed execution.

In addition, [Table 25](#) shows the functions that must exist in the storage runtime interface, that enables the COMPSs Python binding to interact with the storage framework. It is only necessary if the target language is Python.

Table 25: Python API

Name	Returns	Comments	Signature
init(String storage_conf)	Nothing	Do any initialization action before starting to execute the application. Receives the storage configuration file path defined in the <code>runcompss</code> or <code>enqueue_composs</code> command.	<pre>def initWorker(config_ - file_path=None, **kwargs) # Does not return</pre>
finish()	Nothing	Do any finalization action after executing the application.	<pre>def finishWorker(**kwargs) # Does not return</pre>
getByID(String id)	Object	Retrieve an object from its identifier.	<pre>def getByID(id) # Returns the object with Id 'id'</pre>
TaskContext	Context	Define a task context (task enter/exit actions).	<pre>class TaskContext(object): def __init__(self, logger, values, config_file_ - path=None, **kwargs): self.logger = logger self.values = values self.config_ - file_path = config_file_ - path def __enter__(self): # Do something for task prolog def __exit__(self, type, value, traceback): # Do something for task epilog</pre>

7.5.3 Storage Interface usage

7.5.3.1 Using runcompss

The first consideration is to deploy the storage framework, and then follow the next steps:

1. Create a `storage_conf.cfg` file with the configuration required by the `init` SRI's functions.
2. Add the flag `--classpath=${path_to_SRI.jar}` to the `runcompss` command.
3. Add the flag `--storage_conf="path to storage_conf.cfg file"` to the `runcompss` command.
4. If you are running a Python app, also add the `--pythonpath=${app_path}:${path_to_the_bundle_folder}/python` flag to the `runcompss` command.

As usual, the `project.xml` and `resources.xml` files must be correctly set. It must be noted that there can be nodes that are not COMPSs nodes (although **this is a highly unrecommended** practice since they will **always** need data that must be transferred from another node). Also, any locality policy will likely cause this node to have a very low workload.

7.5.3.2 Using enqueue_compss

In order to run a COMPSs + your storage on a queue system the user must add the following flags to the `enqueue_compss` command:

1. `--storage-home=${path_to_the_user_storage_folder}` This must point to the root of the user storage folder, where the scripts for starting (`storage_init.sh`) and stopping (`storage_stop.sh`) the storage framework must exist.
 - **storage_init.sh is called before the application execution and it is intended to deploy the storage framework within the nodes provided by the queuing system.** The parameters that receives are (in order):
 - JOBID** The job identifier provided by the queuing system.
 - MASTER_NODE** The name of the master node considered by COMPSs.
 - STORAGE_MASTER_NODE** The name of the node to be considered the master for the Storage framework.
 - WORKER_NODES** The set of nodes provided by the queuing system that will be considered as worker nodes by COMPSs.
 - NETWORK** Network interface (e.g. `ib0`)
 - STORAGE_PROPS** Storage properties file path (defined as `enqueue_compss` flag).
 - VARIABLES_TO_BE_SOURCED** If environment variables for the Storage framework need to be defined COMPSs provides an empty file to be filled by the `storage_init.sh` script, that will be sourced afterwards. This file is cleaned immediately after sourcing it.
 - **storage_stop.sh is called after the application execution and it is intended to stop the storage framework within the nodes provided by the queuing system.** The parameters that receives are (in order):
 - JOBID** The job identifier provided by the queuing system.
 - MASTER_NODE** The name of the master node considered by COMPSs.
 - STORAGE_MASTER_NODE** The name of the node to be considered the master for the Storage framework.
 - WORKER_NODES** The set of nodes provided by the queuing system that will be considered as worker nodes by COMPSs.
 - NETWORK** Network interface (e.g. `ib0`)
 - STORAGE_PROPS** Storage properties file path (defined as `enqueue_compss` flag).
2. `--storage-props=${path_to_the_storage_props_file}` This must point to the `storage_props.cfg` specific for the storage framework that will be used by the start and stop scripts provided in the `--storage-home` path.
3. `--classpath=${path_to_SRI.jar}` As in the previous section, the JAR with the Java SRI must be specified.
4. If you are running a Python application, also add the `--pythonpath=${app_path}:${path_to_the_user_storage_folder}` flag, where the SOI for Python must exist.

Chapter 8

Sample Applications

This section is intended to walk you through some COMPSs applications.

8.1 Java Sample applications

The first two examples in this section are simple applications developed in COMPSs to easily illustrate how to code, compile and run COMPSs applications. These applications are executed locally and show different ways to take advantage of all the COMPSs features.

The rest of the examples are more elaborated and consider the execution in a cloud platform where the VMs mount a common storage on `/sharedDisk` directory. This is useful in the case of applications that require working with big files, allowing to transfer data only once, at the beginning of the execution, and to enable the application to access the data directly during the rest of the execution.

The Virtual Machine available at our webpage (<http://compss.bsc.es/>) provides a development environment with all the applications listed in the following sections. The codes of all the applications can be found under the `/home/compss/tutorial_apps/java/` folder.

8.1.1 Hello World

The Hello World is a Java application that creates a task and prints a Hello World! message. Its purpose is to clarify that the COMPSs tasks output is redirected to the job files and it is **not** available at the standard output.

Next we provide the important parts of the application's code.

```
// hello.Hello

public static void main(String[] args) throws Exception {
    // Check and get parameters
    if (args.length != 0) {
        usage();
        throw new Exception("[ERROR] Incorrect number of parameters");
    }

    // Hello World from main application
    System.out.println("Hello World! (from main application)");

    // Hello World from a task
    HelloImpl.sayHello();
}
```

As shown in the main code, this application has no input arguments.

```
// hello.HelloImpl

public static void sayHello() {
    System.out.println("Hello World! (from a task)");
}
```

Remember that, to run with COMPSs, java applications must provide an interface. For simplicity, in this example, the content of the interface only declares the task which has no parameters:

```
// hello.HelloItf

@Method(declaringClass = "hello.HelloImpl")
void sayHello(
);
```

Notice that there is a first Hello World message printed from the main code and, a second one, printed inside a task. When executing sequentially this application users will be able to see both messages at the standard output. However, when executing this application with COMPSs, users will only see the message from the main code at the standard output. The message printed from the task will be stored inside the job log files.

Let's try it. First we proceed to compile the code by running the following instructions:

```
compss@bsc:~$ cd ~/tutorial_apps/java/hello/src/main/java/hello/
compss@bsc:~/tutorial_apps/java/hello/src/main/java/hello$ javac *.java
compss@bsc:~/tutorial_apps/java/hello/src/main/java/hello$ cd ..
compss@bsc:~/tutorial_apps/java/hello/src/main/java$ jar cf hello.jar hello
compss@bsc:~/tutorial_apps/java/hello/src/main/java$ mv hello.jar ~/tutorial_apps/java/hello/
→jar/
```

Alternatively, this example application is prepared to be compiled with *maven*:

```
compss@bsc:~$ cd ~/tutorial_apps/java/hello/
compss@bsc:~/tutorial_apps/java/hello$ mvn clean package
```

Once done, we can sequentially execute the application by directly invoking the *jar* file.

```
compss@bsc:~$ cd ~/tutorial_apps/java/hello/jar/
compss@bsc:~/tutorial_apps/java/hello/jar$ java -cp hello.jar hello.Hello
Hello World! (from main application)
Hello World! (from a task)
```

And we can also execute the application with COMPSs:

```
compss@bsc:~$ cd ~/tutorial_apps/java/hello/jar/
compss@bsc:~/tutorial_apps/java/hello/jar$ runcompss -d hello.Hello
[ INFO] Using default execution type: compss
[ INFO] Using default location for project file: /opt/COMPSs/Runtime/configuration/xml/
→projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSs/Runtime/configuration/xml/
→resources/default_resources.xml

----- Executing hello.Hello -----

WARNING: COMPSs Properties file is null. Setting default values
[(928)   API] - Deploying COMPSs Runtime v<version>
[(931)   API] - Starting COMPSs Runtime v<version>
[(931)   API] - Initializing components
[(1472)  API] - Ready to process tasks
```

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```

Hello World! (from main application)
[(1474)   API] - Creating task from method sayHello in hello.HelloImpl
[(1474)   API] - There is 0 parameter
[(1477)   API] - No more tasks for app 1
[(4029)   API] - Getting Result Files 1
[(4030)   API] - Stop IT reached
[(4030)   API] - Stopping AP...
[(4031)   API] - Stopping TD...
[(4161)   API] - Stopping Comm...
[(4163)   API] - Runtime stopped
[(4166)   API] - Execution Finished
-----

```

Notice that the COMPSs execution is using the `-d` option to allow the job logging. Thus, we can check out the application jobs folder to look for the task output.

```

compss@bsc:~$ cd ~/.COMPSs/hello.Hello_01/jobs/
compss@bsc:~/.COMPSs/hello.Hello_01/jobs$ ls -l
job1_NEW.err
job1_NEW.out
compss@bsc:~/.COMPSs/hello.Hello_01/jobs$ cat job1_NEW.out
[JAVA EXECUTOR] executeTask - Begin task execution
WORKER - Parameters of execution:
  * Method type: METHOD
  * Method definition: [DECLARING CLASS=hello.HelloImpl, METHOD NAME=sayHello]
  * Parameter types:
  * Parameter values:
Hello World! (from a task)
[JAVA EXECUTOR] executeTask - End task execution

```

8.1.2 Simple

The Simple application is a Java application that increases a counter by means of a task. The counter is stored inside a file that is transferred to the worker when the task is executed. Thus, the tasks interface is defined as follows:

```

// simple.SimpleItf

@Method(declaringClass = "simple.SimpleImpl")
void increment(
    @Parameter(type = Type.FILE, direction = Direction.INOUT) String file
);

```

Next we also provide the invocation of the task from the main code and the increment's method code.

```

// simple.Simple

public static void main(String[] args) throws Exception {
    // Check and get parameters
    if (args.length != 1) {
        usage();
        throw new Exception("[ERROR] Incorrect number of parameters");
    }
    int initialValue = Integer.parseInt(args[0]);
}

```

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```

// Write value
FileOutputStream fos = new FileOutputStream(fileName);
fos.write(initialValue);
fos.close();
System.out.println("Initial counter value is " + initialValue);

//Execute increment
SimpleImpl.increment(fileName);

// Write new value
FileInputStream fis = new FileInputStream(fileName);
int finalValue = fis.read();
fis.close();
System.out.println("Final counter value is " + finalValue);
}

```

```

// simple.SimpleImpl

public static void increment(String counterFile) throws FileNotFoundException, IOException {
    // Read value
    FileInputStream fis = new FileInputStream(counterFile);
    int count = fis.read();
    fis.close();

    // Write new value
    FileOutputStream fos = new FileOutputStream(counterFile);
    fos.write(++count);
    fos.close();
}

```

Finally, to compile and execute this application users must run the following commands:

```

compss@bsc:~$ cd ~/tutorial_apps/java/simple/src/main/java/simple/
compss@bsc:~/tutorial_apps/java/simple/src/main/java/simple$ javac *.java
compss@bsc:~/tutorial_apps/java/simple/src/main/java/simple$ cd ..
compss@bsc:~/tutorial_apps/java/simple/src/main/java$ jar cf simple.jar simple
compss@bsc:~/tutorial_apps/java/simple/src/main/java$ mv simple.jar ~/tutorial_apps/java/
→simple.jar/

compss@bsc:~$ cd ~/tutorial_apps/java/simple.jar
compss@bsc:~/tutorial_apps/java/simple.jar$ runcompss simple.Simple 1
compss@bsc:~/tutorial_apps/java/simple.jar$ runcompss simple.Simple 1
[ INFO] Using default execution type: compss
[ INFO] Using default location for project file: /opt/COMPSs/Runtime/configuration/xml/
→projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSs/Runtime/configuration/xml/
→resources/default_resources.xml

----- Executing simple.Simple -----

WARNING: COMPSs Properties file is null. Setting default values
[(772)   API] - Starting COMPSs Runtime v<version>
Initial counter value is 1
Final counter value is 2
[(3813)  API] - Execution Finished

```

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8.1.3 Increment

The Increment application is a Java application that increases N times three different counters. Each increase step is developed by a separated task. The purpose of this application is to show parallelism between the three counters.

Next we provide the main code of this application. The code inside the *increment* task is the same than the previous example.

```
// increment.Increment

public static void main(String[] args) throws Exception {
    // Check and get parameters
    if (args.length != 4) {
        usage();
        throw new Exception("[ERROR] Incorrect number of parameters");
    }
    int N = Integer.parseInt(args[0]);
    int counter1 = Integer.parseInt(args[1]);
    int counter2 = Integer.parseInt(args[2]);
    int counter3 = Integer.parseInt(args[3]);

    // Initialize counter files
    System.out.println("Initial counter values:");
    initializeCounters(counter1, counter2, counter3);

    // Print initial counters state
    printCounterValues();

    // Execute increment tasks
    for (int i = 0; i < N; ++i) {
        IncrementImpl.increment(fileName1);
        IncrementImpl.increment(fileName2);
        IncrementImpl.increment(fileName3);
    }

    // Print final counters state (sync)
    System.out.println("Final counter values:");
    printCounterValues();
}
```

As shown in the main code, this application has 4 parameters that stand for:

1. **N**: Number of times to increase a counter
2. **InitialValue1**: Initial value for counter 1
3. **InitialValue2**: Initial value for counter 2
4. **InitialValue3**: Initial value for counter 3

Next we will compile and run the Increment application with the *-g* option to be able to generate the final graph at the end of the execution.

```
compss@bsc:~$ cd ~/tutorial_apps/java/increment/src/main/java/increment/
compss@bsc:~/tutorial_apps/java/increment/src/main/java/increment$ javac *.java
```

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```

compss@bsc:~/tutorial_apps/java/increment/src/main/java/increment$ cd ..
compss@bsc:~/tutorial_apps/java/increment/src/main/java$ jar cf increment.jar increment
compss@bsc:~/tutorial_apps/java/increment/src/main/java$ mv increment.jar ~/tutorial_apps/
↳ java/increment/jar/

compss@bsc:~$ cd ~/tutorial_apps/java/increment/jar
compss@bsc:~/tutorial_apps/java/increment/jar$ runcompss -g increment.Increment 10 1 2 3
[ INFO] Using default execution type: compss
[ INFO] Using default location for project file: /opt/COMPSs/Runtime/configuration/xml/
↳ projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSs/Runtime/configuration/xml/
↳ resources/default_resources.xml

----- Executing increment.Increment -----

WARNING: COMPSs Properties file is null. Setting default values
[(1028)   API] - Starting COMPSs Runtime v<version>
Initial counter values:
- Counter1 value is 1
- Counter2 value is 2
- Counter3 value is 3
Final counter values:
- Counter1 value is 11
- Counter2 value is 12
- Counter3 value is 13
[(4403)   API] - Execution Finished

-----

```

By running the *compss_gengraph* command users can obtain the task graph of the above execution. Next we provide the set of commands to obtain the graph show in [Figure 44](#).

```

compss@bsc:~$ cd ~/.COMPSs/increment.Increment_01/monitor/
compss@bsc:~/.COMPSs/increment.Increment_01/monitor$ compss_gengraph complete_graph.dot
compss@bsc:~/.COMPSs/increment.Increment_01/monitor$ evince complete_graph.pdf

```

8.1.4 Matrix multiplication

The Matrix Multiplication (Matmul) is a pure Java application that multiplies two matrices in a direct way. The application creates 2 matrices of N x N size initialized with values, and multiply the matrices by blocks.

This application provides three different implementations that only differ on the way of storing the matrix:

matmul.objects.Matmul Matrix stored by means of objects

matmul.files.Matmul Matrix stored in files

matmul.arrays.Matmul Matrix represented by an array

In all the implementations the multiplication is implemented in the *multiplyAccumulative* method that is thus selected as the task to be executed remotely. As example, we provide next the task implementation and the tasks interface for the objects implementation.

```

// matmul.objects.Block

public void multiplyAccumulative(Block a, Block b) {
    for (int i = 0; i < M; i++) {
        for (int j = 0; j < M; j++) {

```

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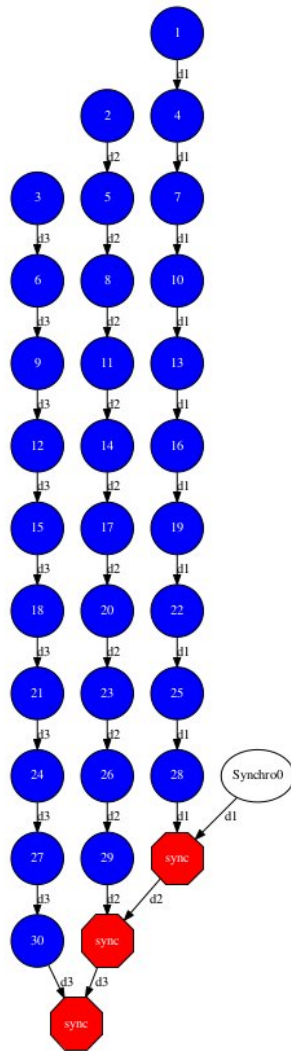


Figure 44: Java increment tasks graph

$$\begin{array}{c} a_1 \\ a_2 \\ \vdots \\ a_m \end{array} \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{bmatrix} \begin{bmatrix} \begin{array}{c} b_1 \\ b_{11} \\ b_{21} \\ \vdots \\ b_{n1} \end{array} & \begin{array}{c} b_2 \\ b_{12} \\ b_{22} \\ \vdots \\ b_{n2} \end{array} & \dots & \begin{array}{c} b_p \\ b_{1p} \\ b_{2p} \\ \vdots \\ b_{np} \end{array} \end{bmatrix} = \begin{bmatrix} a_1 \cdot b_1 & a_1 \cdot b_2 & \dots & a_1 \cdot b_p \\ a_2 \cdot b_1 & a_2 \cdot b_2 & \dots & a_2 \cdot b_p \\ \vdots & \vdots & \ddots & \vdots \\ a_m \cdot b_1 & a_m \cdot b_2 & \dots & a_m \cdot b_p \end{bmatrix}$$

Figure 45: Matrix multiplication

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```

        for (int k = 0; k < M; k++) {
            data[i][j] += a.data[i][k]*b.data[k][j];
        }
    }
}

```

```

// matmul.objects.MatmulItf

@Method(declaringClass = "matmul.objects.Block")
void multiplyAccumulative(
    @Parameter Block a,
    @Parameter Block b
);

```

In order to run the application the matrix dimension (number of blocks) and the dimension of each block have to be supplied. Consequently, any of the implementations must be executed by running the following command.

```
compss@bsc:~$ runcompss matmul.<IMPLEMENTATION_TYPE>.Matmul <matrix_dim> <block_dim>
```

Finally, we provide an example of execution for each implementation.

```

compss@bsc:~$ cd ~/tutorial_apps/java/matmul/jar/
compss@bsc:~/tutorial_apps/java/matmul/jar$ runcompss matmul.objects.Matmul 8 4
[ INFO] Using default execution type: compss
[ INFO] Using default location for project file: /opt/COMPSs/Runtime/configuration/xml/
->projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSs/Runtime/configuration/xml/
->resources/default_resources.xml

----- Executing matmul.objects.Matmul -----

WARNING: COMPSs Properties file is null. Setting default values
[(887)   API] - Starting COMPSs Runtime v<version>
[LOG] MSIZE parameter value = 8
[LOG] BSIZE parameter value = 4
[LOG] Allocating A/B/C matrix space
[LOG] Computing Result
[LOG] Main program finished.
[(7415)  API] - Execution Finished

-----

```

```

compss@bsc:~$ cd ~/tutorial_apps/java/matmul/jar/
compss@bsc:~/tutorial_apps/java/matmul/jar$ runcompss matmul.files.Matmul 8 4
[ INFO] Using default execution type: compss
[ INFO] Using default location for project file: /opt/COMPSs/Runtime/configuration/xml/
->projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSs/Runtime/configuration/xml/
->resources/default_resources.xml

----- Executing matmul.files.Matmul -----

WARNING: COMPSs Properties file is null. Setting default values
[(907)   API] - Starting COMPSs Runtime v<version>
[LOG] MSIZE parameter value = 8

```

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```
[LOG] BSIZE parameter value = 4
[LOG] Computing result
[LOG] Main program finished.
[(9925)   API] - Execution Finished

-----
```

```
compss@bsc:~$ cd ~/tutorial_apps/java/matmul/jar/
compss@bsc:~/tutorial_apps/java/matmul/jar$ runcompss matmul.arrays.Matmul 8 4
[ INFO] Using default execution type: compss
[ INFO] Using default location for project file: /opt/COMPSs/Runtime/configuration/xml/
->projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSs/Runtime/configuration/xml/
->resources/default_resources.xml

----- Executing matmul.arrays.Matmul -----

WARNING: COMPSs Properties file is null. Setting default values
[(1062)   API] - Starting COMPSs Runtime v<version>
[LOG] MSIZE parameter value = 8
[LOG] BSIZE parameter value = 4
[LOG] Allocating C matrix space
[LOG] Computing Result
[LOG] Main program finished.
[(7811)   API] - Execution Finished

-----
```

8.1.5 Sparse LU decomposition

SparseLU multiplies two matrices using the factorization method of LU decomposition, which factorizes a matrix as a product of a lower triangular matrix and an upper one.

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}.$$

Figure 46: Sparse LU decomposition

The matrix is divided into N x N blocks on where 4 types of operations will be applied modifying the blocks: **lu0**, **fwd**, **bdiv** and **bmod**. These four operations are implemented in four methods that are selected as the tasks that will be executed remotely. In order to run the application the matrix dimension has to be provided.

As the previous application, the sparseLU is provided in three different implementations that only differ on the way of storing the matrix:

1. **sparseLU.objects.SparseLU** Matrix stored by means of objects
2. **sparseLU.files.SparseLU** Matrix stored in files
3. **sparseLU.arrays.SparseLU** Matrix represented by an array

Thus, the commands needed to execute the application is with each implementation are:

```
compss@bsc:~$ cd tutorial_apps/java/sparseLU/jar/
compss@bsc:~/tutorial_apps/java/sparseLU/jar$ runcompss sparseLU.objects.SparseLU 16 8
[ INFO] Using default execution type: compss
```

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```
[ INFO] Using default location for project file: /opt/COMPSs/Runtime/configuration/xml/
→projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSs/Runtime/configuration/xml/
→resources/default_resources.xml

----- Executing sparseLU.objects.SparseLU -----

WARNING: COMPSs Properties file is null. Setting default values
[(1221)   API] - Starting COMPSs Runtime v<version>
[LOG] Running with the following parameters:
[LOG] - Matrix Size: 16
[LOG] - Block Size:  8
[LOG] Initializing Matrix
[LOG] Computing SparseLU algorithm on A
[LOG] Main program finished.
[(13642)   API] - Execution Finished

-----
```

```
compss@bsc:~$ cd tutorial_apps/java/sparseLU/jar/
compss@bsc:~/tutorial_apps/java/sparseLU/jar$ runcompss sparseLU.files.SparseLU 4 8
[ INFO] Using default execution type: compss
[ INFO] Using default location for project file: /opt/COMPSs/Runtime/configuration/xml/
→projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSs/Runtime/configuration/xml/
→resources/default_resources.xml

----- Executing sparseLU.files.SparseLU -----

WARNING: COMPSs Properties file is null. Setting default values
[(1082)   API] - Starting COMPSs Runtime v<version>
[LOG] Running with the following parameters:
[LOG] - Matrix Size: 16
[LOG] - Block Size:  8
[LOG] Initializing Matrix
[LOG] Computing SparseLU algorithm on A
[LOG] Main program finished.
[(13605)   API] - Execution Finished

-----
```

```
compss@bsc:~$ cd tutorial_apps/java/sparseLU/jar/
compss@bsc:~/tutorial_apps/java/sparseLU/jar$ runcompss sparseLU.arrays.SparseLU 8 8
[ INFO] Using default execution type: compss
[ INFO] Using default location for project file: /opt/COMPSs/Runtime/configuration/xml/
→projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSs/Runtime/configuration/xml/
→resources/default_resources.xml

----- Executing sparseLU.arrays.SparseLU -----

WARNING: COMPSs Properties file is null. Setting default values
[(1082)   API] - Starting COMPSs Runtime v<version>
[LOG] Running with the following parameters:
[LOG] - Matrix Size: 16
```

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```
[LOG] - Block Size: 8
[LOG] Initializing Matrix
[LOG] Computing SparseLU algorithm on A
[LOG] Main program finished.
[(13605)  API] - Execution Finished
```

8.1.6 BLAST Workflow

BLAST is a widely-used bioinformatics tool for comparing primary biological sequence information, such as the amino-acid sequences of different proteins or the nucleotides of DNA sequences with sequence databases, identifying sequences that resemble the query sequence above a certain threshold. The work performed by the COMPSs Blast workflow is computationally intensive and embarrassingly parallel.

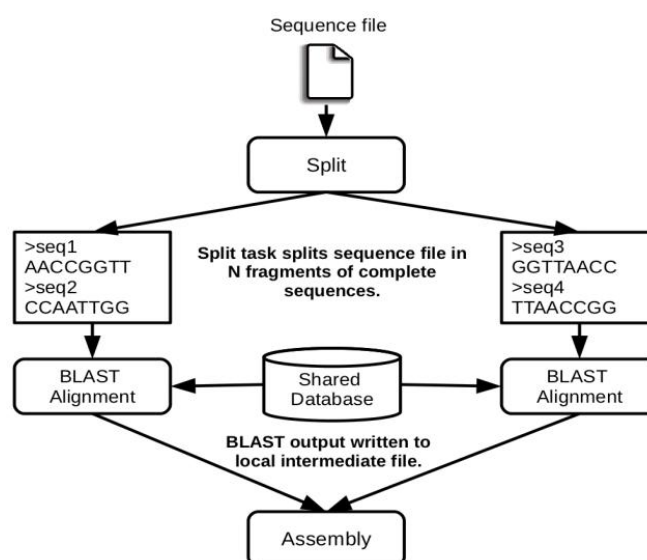


Figure 47: The COMPSs Blast workflow

The workflow describes the three blocks of the workflow implemented in the **Split**, **Align** and **Assembly** methods. The second one is the only method that is chosen to be executed remotely, so it is the unique method defined in the interface file. The **Split** method chops the query sequences file in N fragments, **Align** compares each sequence fragment against the database by means of the Blast binary, and **Assembly** combines all intermediate files into a single result file.

This application uses a database that will be on the shared disk space avoiding transferring the entire database (which can be large) between the virtual machines.

```
compss@bsc:~$ cp ~/workspace/blast/package/Blast.tar.gz /home/compss/
compss@bsc:~$ tar xzf Blast.tar.gz
```

The command line to execute the workflow:

```
compss@bsc:~$ runcompss blast.Blast <debug> \
                                     <bin_location> \
                                     <database_file> \
                                     <sequences_file> \
                                     <frag_number> \
                                     <tmpdir> \
                                     <output_file>
```

Where:

- **debug**: The debug flag of the application (true or false).
- **bin_location**: Path of the Blast binary.
- **database_file**: Path of database file; the shared disk **/sharedDisk/** is suggested to avoid big data transfers.
- **sequences_file**: Path of sequences file.
- **frag_number**: Number of fragments of the original sequence file, this number determines the number of parallel Align tasks.
- **tmpdir**: Temporary directory (**/home/compss/tmp/**).
- **output_file**: Path of the result file.

Example:

```
compss@bsc:~$ runcompss blast.Blast true \  
    /home/compss/tutorial_apps/java/blast/binary/blastall \  
    /sharedDisk/Blast/databases/swissprot/swissprot \  
    /sharedDisk/Blast/sequences/sargasso_test.fasta \  
    4 \  
    /tmp/ \  
    /home/compss/out.txt
```

8.2 Python Sample applications

The first two examples in this section are simple applications developed in COMPSs to easily illustrate how to code, compile and run COMPSs applications. These applications are executed locally and show different ways to take advantage of all the COMPSs features.

The rest of the examples are more elaborated and consider the execution in a cloud platform where the VMs mount a common storage on **/sharedDisk** directory. This is useful in the case of applications that require working with big files, allowing to transfer data only once, at the beginning of the execution, and to enable the application to access the data directly during the rest of the execution.

The Virtual Machine available at our webpage (<http://compss.bsc.es/>) provides a development environment with all the applications listed in the following sections. The codes of all the applications can be found under the **/home/compss/tutorial_apps/python/** folder.

8.2.1 Simple

The Simple application is a Python application that increases a counter by means of a task. The counter is stored inside a file that is transferred to the worker when the task is executed. Next, we provide the main code and the task declaration:

```
from pycompss.api.task import task  
from pycompss.api.parameter import FILE_INOUT  
  
@task(filePath = FILE_INOUT)  
def increment(filePath):  
    # Read value  
    fis = open(filePath, 'r')  
    value = fis.read()  
    fis.close()  
  
    # Write value  
    fos = open(filePath, 'w')  
    fos.write(str(int(value) + 1))  
    fos.close()
```

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```

def main_program():
    from pycompss.api.api import compss_open

    # Check and get parameters
    if len(sys.argv) != 2:
        exit(-1)
    initialValue = sys.argv[1]

    fileName="counter"

    # Write value
    fos = open(fileName, 'w')
    fos.write(initialValue)
    fos.close()
    print "Initial counter value is " + initialValue

    # Execute increment
    increment(fileName)

    # Write new value
    fis = compss_open(fileName, 'r+')
    finalValue = fis.read()
    fis.close()
    print "Final counter value is " + finalValue

if __name__=='__main__':
    main_program()

```

The simple application can be executed by invoking the `runcompss` command with the application file name and the initial counter value.

The following lines provide an example of its execution.

```

compss@bsc:~$ cd ~/tutorial_apps/python/simple/
compss@bsc:~/tutorial_apps/python/simple$ runcompss ~/tutorial_apps/python/simple/simple.py 1
[ INFO] Using default execution type: compss
[ INFO] Using default location for project file: /opt/COMPSs/Runtime/configuration/xml/
->projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSs/Runtime/configuration/xml/
->resources/default_resources.xml

----- Executing simple.py -----

WARNING: COMPSs Properties file is null. Setting default values
[(639)   API] - Starting COMPSs Runtime v<version>
Initial counter value is 1
Final counter value is 2
[(6230)  API] - Execution Finished

-----

```

8.2.2 Increment

The Increment application is a Python application that increases N times three different counters. Each increase step is developed by a separated task. The purpose of this application is to show parallelism between the three counters.

Next we provide the main code of this application. The code inside the *increment* task is the same than the previous example.

```
from pycompss.api.task import task
from pycompss.api.parameter import FILE_INOUT

@task(filePath = FILE_INOUT)
def increment(filePath):
    # Read value
    fis = open(filePath, 'r')
    value = fis.read()
    fis.close()

    # Write value
    fos = open(filePath, 'w')
    fos.write(str(int(value) + 1))
    fos.close()

def main_program():
    # Check and get parameters
    if len(sys.argv) != 5:
        exit(-1)
    N = int(sys.argv[1])
    counter1 = int(sys.argv[2])
    counter2 = int(sys.argv[3])
    counter3 = int(sys.argv[4])

    # Initialize counter files
    initializeCounters(counter1, counter2, counter3)
    print "Initial counter values:"
    printCounterValues()

    # Execute increment
    for i in range(N):
        increment(FILENAME1)
        increment(FILENAME2)
        increment(FILENAME3)

    # Write final counters state (sync)
    print "Final counter values:"
    printCounterValues()

if __name__ == '__main__':
    main_program()
```

As shown in the main code, this application has 4 parameters that stand for:

N Number of times to increase a counter

counter1 Initial value for counter 1

counter2 Initial value for counter 2

counter3 Initial value for counter 3

Next we run the Increment application with the **-g** option to be able to generate the final graph at the end of the execution.

```

compss@bsc:~/tutorial_apps/python/increment$ runcompss --lang=python -g ~/tutorial_apps/
python/increment/increment.py 10 1 2 3
[ INFO] Using default execution type: compss
[ INFO] Using default location for project file: /opt/COMPSs/Runtime/configuration/xml/
projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSs/Runtime/configuration/xml/
resources/default_resources.xml

----- Executing increment.py -----

WARNING: COMPSs Properties file is null. Setting default values
[(670)   API] - Starting COMPSs Runtime v<version>
Initial counter values:
- Counter1 value is 1
- Counter2 value is 2
- Counter3 value is 3
Final counter values:
- Counter1 value is 11
- Counter2 value is 12
- Counter3 value is 13
[(7390)   API] - Execution Finished

-----

```

By running the `compss_gengraph` command users can obtain the task graph of the above execution. Next we provide the set of commands to obtain the graph show in [Figure 48](#).

```

compss@bsc:~$ cd ~/.COMPSs/increment.py_01/monitor/
compss@bsc:~/COMPSs/increment.py_01/monitor$ compss_gengraph complete_graph.dot
compss@bsc:~/COMPSs/increment.py_01/monitor$ evince complete_graph.pdf

```

8.2.3 Kmeans

KMeans is machine-learning algorithm (NP-hard), popularly employed for cluster analysis in data mining, and interesting for benchmarking and performance evaluation.

The objective of the Kmeans algorithm to group a set of multidimensional points into a predefined number of clusters, in which each point belongs to the closest cluster (with the nearest mean distance), in an iterative process.

```

import numpy as np
import time

from sklearn.metrics import pairwise_distances
from sklearn.metrics.pairwise import paired_distances

from pycompss.api.task import task
from pycompss.api.api import compss_wait_on
from pycompss.api.api import compss_barrier

@task(returns=np.ndarray)
def partial_sum(fragment, centres):
    partials = np.zeros((centres.shape[0], 2), dtype=object)
    close_centres = pairwise_distances(fragment, centres).argmin(axis=1)
    for center_idx, _ in enumerate(centres):
        indices = np.argwhere(close_centres == center_idx).flatten()

```

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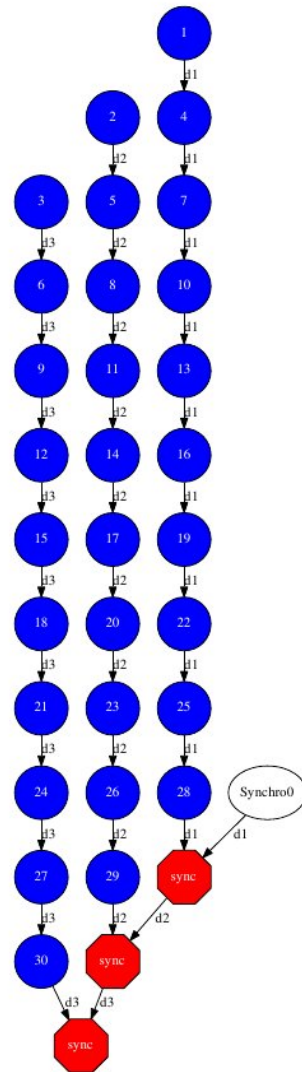


Figure 48: Python increment tasks graph

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```

        partials[center_idx][0] = np.sum(fragment[indices], axis=0)
        partials[center_idx][1] = indices.shape[0]
    return partials

@task(returns=dict)
def merge(*data):
    accum = data[0].copy()
    for d in data[1:]:
        accum += d
    return accum

def converged(old_centres, centres, epsilon, iteration, max_iter):
    if old_centres is None:
        return False
    dist = np.sum(paired_distances(centres, old_centres))
    return dist < epsilon ** 2 or iteration >= max_iter

def recompute_centres(partial, old_centres, arity):
    centres = old_centres.copy()
    while len(partial) > 1:
        partial_subset = partial[:arity]
        partial = partial[arity:]
        partial.append(merge(*partial_subset))
    partial = compss_wait_on(partial)
    for idx, sum_ in enumerate(partial[0]):
        if sum_[1] != 0:
            centres[idx] = sum_[0] / sum_[1]
    return centres

def kmeans_frag(fragments, dimensions, num_centres=10, iterations=20,
                seed=0., epsilon=1e-9, arity=50):
    """
    A fragment-based K-Means algorithm.
    Given a set of fragments, the desired number of clusters and the
    maximum number of iterations, compute the optimal centres and the
    index of the centre for each point.
    :param fragments: Number of fragments
    :param dimensions: Number of dimensions
    :param num_centres: Number of centres
    :param iterations: Maximum number of iterations
    :param seed: Random seed
    :param epsilon: Epsilon (convergence distance)
    :param arity: Reduction arity
    :return: Final centres
    """
    # Set the random seed
    np.random.seed(seed)
    # Centres is usually a very small matrix, so it is affordable to have it in
    # the master.
    centres = np.asarray(
        [np.random.random(dimensions) for _ in range(num_centres)]
    )

```

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```

# Note: this implementation treats the centres as files, never as PSCOs.
old_centres = None
iteration = 0
while not converged(old_centres, centres, epsilon, iteration, iterations):
    print("Doing iteration #%d/%d" % (iteration + 1, iterations))
    old_centres = centres.copy()
    partials = []
    for frag in fragments:
        partial = partial_sum(frag, old_centres)
        partials.append(partial)
    centres = recompute_centres(partial, old_centres, arity)
    iteration += 1
return centres

def parse_arguments():
    """
    Parse command line arguments. Make the program generate
    a help message in case of wrong usage.
    :return: Parsed arguments
    """
    import argparse
    parser = argparse.ArgumentParser(description='KMeans Clustering.')
    parser.add_argument('-s', '--seed', type=int, default=0,
                        help='Pseudo-random seed. Default = 0')
    parser.add_argument('-n', '--numpoints', type=int, default=100,
                        help='Number of points. Default = 100')
    parser.add_argument('-d', '--dimensions', type=int, default=2,
                        help='Number of dimensions. Default = 2')
    parser.add_argument('-c', '--num_centres', type=int, default=5,
                        help='Number of centres. Default = 2')
    parser.add_argument('-f', '--fragments', type=int, default=10,
                        help='Number of fragments.' +
                             ' Default = 10. Condition: fragments < points')
    parser.add_argument('-m', '--mode', type=str, default='uniform',
                        choices=['uniform', 'normal'],
                        help='Distribution of points. Default = uniform')
    parser.add_argument('-i', '--iterations', type=int, default=20,
                        help='Maximum number of iterations')
    parser.add_argument('-e', '--epsilon', type=float, default=1e-9,
                        help='Epsilon. Kmeans will stop when: ' +
                             ' |old - new| < epsilon.')
    parser.add_argument('-a', '--arity', type=int, default=50,
                        help='Arity of the reduction carried out during \
                             the computation of the new centroids')
    return parser.parse_args()

@task(returns=1)
def generate_fragment(points, dim, mode, seed):
    """
    Generate a random fragment of the specified number of points using the
    specified mode and the specified seed. Note that the generation is
    distributed (the master will never see the actual points).
    :param points: Number of points
    :param dim: Number of dimensions

```

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```

:param mode: Dataset generation mode
:param seed: Random seed
:return: Dataset fragment
"""
# Random generation distributions
rand = {
    'normal': lambda k: np.random.normal(0, 1, k),
    'uniform': lambda k: np.random.random(k),
}
r = rand[mode]
np.random.seed(seed)
mat = np.asarray(
    [r(dim) for __ in range(points)]
)
# Normalize all points between 0 and 1
mat -= np.min(mat)
mx = np.max(mat)
if mx > 0.0:
    mat /= mx

return mat

def main(seed, numpoints, dimensions, num_centres, fragments, mode, iterations,
        epsilon, arity):
    """
    This will be executed if called as main script. Look at the kmeans_frag
    for the KMeans function.
    This code is used for experimental purposes.
    I.e it generates random data from some parameters that determine the size,
    dimensionality and etc and returns the elapsed time.
    :param seed: Random seed
    :param numpoints: Number of points
    :param dimensions: Number of dimensions
    :param num_centres: Number of centres
    :param fragments: Number of fragments
    :param mode: Dataset generation mode
    :param iterations: Number of iterations
    :param epsilon: Epsilon (convergence distance)
    :param arity: Reduction arity
    :return: None
    """
    start_time = time.time()

    # Generate the data
    fragment_list = []
    # Prevent infinite loops
    points_per_fragment = max(1, numpoints // fragments)

    for l in range(0, numpoints, points_per_fragment):
        # Note that the seed is different for each fragment.
        # This is done to avoid having repeated data.
        r = min(numpoints, l + points_per_fragment)

        fragment_list.append(
            generate_fragment(r - 1, dimensions, mode, seed + 1)

```

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```

    )

    compss_barrier()
    print("Generation/Load done")
    initialization_time = time.time()
    print("Starting kmeans")

    # Run kmeans
    centres = kmeans_frag(fragments=fragment_list,
                          dimensions=dimensions,
                          num_centres=num_centres,
                          iterations=iterations,
                          seed=seed,
                          epsilon=epsilon,
                          arity=arity)

    compss_barrier()
    print("Ending kmeans")
    kmeans_time = time.time()

    print("-----")
    print("----- RESULTS -----")
    print("-----")
    print("Initialization time: %f" % (initialization_time - start_time))
    print("Kmeans time: %f" % (kmeans_time - initialization_time))
    print("Total time: %f" % (kmeans_time - start_time))
    print("-----")
    centres = compss_wait_on(centres)
    print("CENTRES:")
    print(centres)
    print("-----")

if __name__ == "__main__":
    options = parse_arguments()
    main(**vars(options))

```

The kmeans application can be executed by invoking the `runcompss` command with the desired parameters (in this case we use `-g` to generate the task dependency graph) and application. The following lines provide an example of its execution considering 10M points, of 3 dimensions, divided into 8 fragments, looking for 8 clusters and a maximum number of iterations set to 10.

```

compss@bsc:~$ runcompss -g kmeans.py -n 10240000 -f 8 -d 3 -c 8 -i 10

[ INFO] Inferred PYTHON language
[ INFO] Using default location for project file: /opt/COMPSs/Runtime/configuration/xml/
→projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSs/Runtime/configuration/xml/
→resources/default_resources.xml
[ INFO] Using default execution type: compss

----- Executing kmeans.py -----

WARNING: COMPSs Properties file is null. Setting default values
[(436)   API] - Starting COMPSs Runtime v2.7 (build 20200519-1005.
→r6093e5ac94d67250e097a6fad9d3ec00d676fe6c)
Generation/Load done

```

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```

Starting kmeans
Doing iteration #1/5
Doing iteration #2/5
Doing iteration #3/5
Doing iteration #4/5
Doing iteration #5/5
Ending kmeans
-----
----- RESULTS -----
-----
Initialization time: 8.625658
Kmeans time: 6.110023
Total time: 14.735682
-----
CENTRES:
[[0.72244748 0.73760837 0.47839032]
 [0.555741 0.20736841 0.21758715]
 [0.25766653 0.73309038 0.77668994]
 [0.20623714 0.67588471 0.25750168]
 [0.73305652 0.7013741 0.15204797]
 [0.22431367 0.22614948 0.66875431]
 [0.76540302 0.75721277 0.83083206]
 [0.75688812 0.24817146 0.72752128]]
-----
[(16137) API] - Execution Finished
-----

```

Figure 49 depicts the generated task dependency graph. The dataset generation can be identified in the 8 blue tasks, while the five iterations appear next. Between the iteration there is a synchronization which corresponds to the convergence/max iterations check.

8.2.4 Kmeans with Persistent Storage

KMeans is machine-learning algorithm (NP-hard), popularly employed for cluster analysis in data mining, and interesting for benchmarking and performance evaluation.

The objective of the Kmeans algorithm to group a set of multidimensional points into a predefined number of clusters, in which each point belongs to the closest cluster (with the nearest mean distance), in an iterative process.

In this application we make use of the persistent storage API. In particular, the dataset fragments are considered **StorageObject**, delegating its content into the persistent framework. Since the data model (object declared as storage object) includes functions, it can run efficiently with dataClay.

First, lets see the data model (`storage_model/fragment.py`)

```

from storage.api import StorageObject

try:
    from pycompss.api.task import task
    from pycompss.api.parameter import IN
except ImportError:
    # Required since the pycompss module is not ready during the registry
    from dataclay.contrib.dummy_pycompss import task, IN

from dataclay import dclayMethod

```

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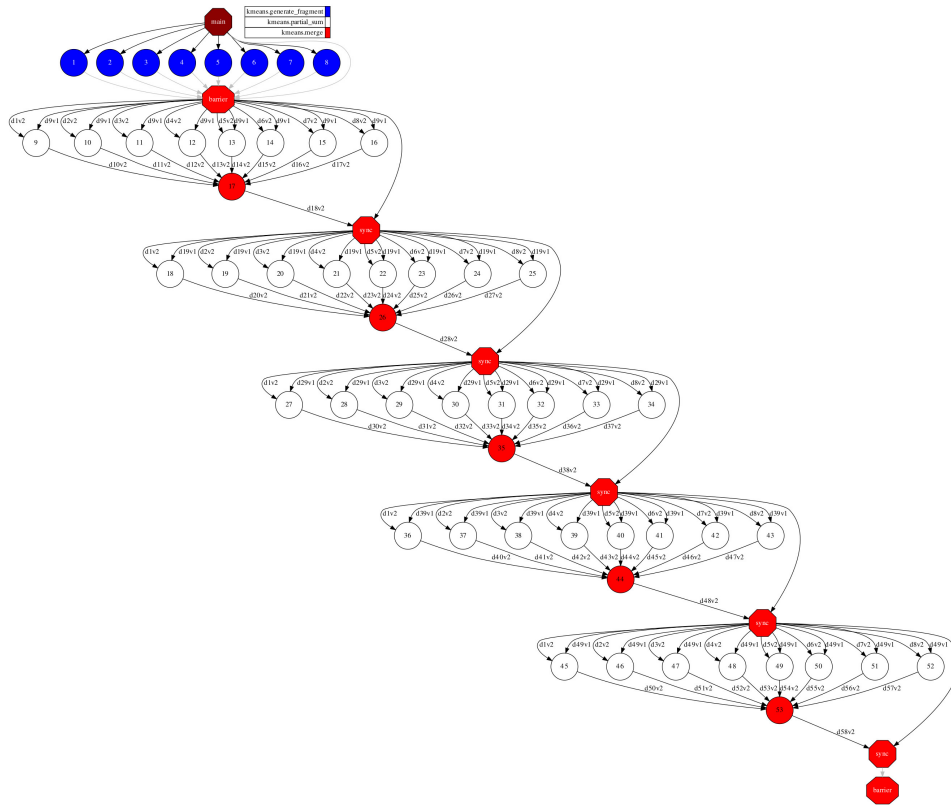


Figure 49: Python kmeans tasks graph

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```

import numpy as np
from sklearn.metrics import pairwise_distances

class Fragment(StorageObject):
    """
    @ClassField points numpy.ndarray

    @dclayImport numpy as np
    @dclayImportFrom sklearn.metrics import pairwise_distances
    """
    @dclayMethod()
    def __init__(self):
        super(Fragment, self).__init__()
        self.points = None

    @dclayMethod(num_points='int', dim='int', mode='str', seed='int')
    def generate_points(self, num_points, dim, mode, seed):
        """
        Generate a random fragment of the specified number of points using the
        specified mode and the specified seed. Note that the generation is
        distributed (the master will never see the actual points).
        :param num_points: Number of points
        :param dim: Number of dimensions
        :param mode: Dataset generation mode

```

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```

:param seed: Random seed
:return: Dataset fragment
"""
# Random generation distributions
rand = {
    'normal': lambda k: np.random.normal(0, 1, k),
    'uniform': lambda k: np.random.random(k),
}
r = rand[mode]
np.random.seed(seed)
mat = np.asarray(
    [r(dim) for __ in range(num_points)]
)
# Normalize all points between 0 and 1
mat -= np.min(mat)
mx = np.max(mat)
if mx > 0.0:
    mat /= mx

self.points = mat

@task(returns=np.ndarray, target_direction=IN)
@dclayMethod(centres='numpy.ndarray', return_='anything')
def partial_sum(self, centres):
    partials = np.zeros((centres.shape[0], 2), dtype=object)
    arr = self.points
    close_centres = pairwise_distances(arr, centres).argmin(axis=1)
    for center_idx, _ in enumerate(centres):
        indices = np.argwhere(close_centres == center_idx).flatten()
        partials[center_idx][0] = np.sum(arr[indices], axis=0)
        partials[center_idx][1] = indices.shape[0]
    return partials

```

Now we can focus in the main kmeans application (kmeans.py):

```

import time
import numpy as np

from pycompss.api.task import task
from pycompss.api.api import compss_wait_on
from pycompss.api.api import compss_barrier

from storage_model.fragment import Fragment

from sklearn.metrics.pairwise import paired_distances

@task(returns=dict)
def merge(*data):
    accum = data[0].copy()
    for d in data[1:]:
        accum += d
    return accum

def converged(old_centres, centres, epsilon, iteration, max_iter):

```

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```

if old_centres is None:
    return False
dist = np.sum(paired_distances(centres, old_centres))
return dist < epsilon ** 2 or iteration >= max_iter

def recompute_centres(partials, old_centres, arity):
    centres = old_centres.copy()
    while len(partials) > 1:
        partials_subset = partials[:arity]
        partials = partials[arity:]
        partials.append(merge(*partials_subset))
    partials = compss_wait_on(partials)
    for idx, sum_ in enumerate(partials[0]):
        if sum_[1] != 0:
            centres[idx] = sum_[0] / sum_[1]
    return centres

def kmeans_frag(fragments, dimensions, num_centres=10, iterations=20,
                seed=0., epsilon=1e-9, arity=50):
    """
    A fragment-based K-Means algorithm.
    Given a set of fragments (which can be either PSCOs or future objects that
    point to PSCOs), the desired number of clusters and the maximum number of
    iterations, compute the optimal centres and the index of the centre
    for each point.
    PSCO.mat must be a NxD float np.ndarray, where D = dimensions
    :param fragments: Number of fragments
    :param dimensions: Number of dimensions
    :param num_centres: Number of centres
    :param iterations: Maximum number of iterations
    :param seed: Random seed
    :param epsilon: Epsilon (convergence distance)
    :param arity: Arity
    :return: Final centres and labels
    """
    # Set the random seed
    np.random.seed(seed)
    # Centres is usually a very small matrix, so it is affordable to have it in
    # the master.
    centres = np.asarray(
        [np.random.random(dimensions) for _ in range(num_centres)]
    )
    # Note: this implementation treats the centres as files, never as PSCOs.
    old_centres = None
    iteration = 0
    while not converged(old_centres, centres, epsilon, iteration, iterations):
        print("Doing iteration #%d/%d" % (iteration + 1, iterations))
        old_centres = centres.copy()
        partials = []
        for frag in fragments:
            partial = frag.partial_sum(old_centres)
            partials.append(partial)
        centres = recompute_centres(partials, old_centres, arity)
        iteration += 1

```

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```

return centres

def parse_arguments():
    """
    Parse command line arguments. Make the program generate
    a help message in case of wrong usage.
    :return: Parsed arguments
    """
    import argparse
    parser = argparse.ArgumentParser(description='KMeans Clustering.')
    parser.add_argument('-s', '--seed', type=int, default=0,
                        help='Pseudo-random seed. Default = 0')
    parser.add_argument('-n', '--numpoints', type=int, default=100,
                        help='Number of points. Default = 100')
    parser.add_argument('-d', '--dimensions', type=int, default=2,
                        help='Number of dimensions. Default = 2')
    parser.add_argument('-c', '--num_centres', type=int, default=5,
                        help='Number of centres. Default = 2')
    parser.add_argument('-f', '--fragments', type=int, default=10,
                        help='Number of fragments.' +
                             ' Default = 10. Condition: fragments < points')
    parser.add_argument('-m', '--mode', type=str, default='uniform',
                        choices=['uniform', 'normal'],
                        help='Distribution of points. Default = uniform')
    parser.add_argument('-i', '--iterations', type=int, default=20,
                        help='Maximum number of iterations')
    parser.add_argument('-e', '--epsilon', type=float, default=1e-9,
                        help='Epsilon. Kmeans will stop when: ' +
                             ' |old - new| < epsilon.')
    parser.add_argument('-a', '--arity', type=int, default=50,
                        help='Arity of the reduction carried out during \
                             the computation of the new centroids')
    return parser.parse_args()

from storage_model.fragment import Fragment # this will have to be removed

@task(returns=Fragment)
def generate_fragment(points, dim, mode, seed):
    """
    Generate a random fragment of the specified number of points using the
    specified mode and the specified seed. Note that the generation is
    distributed (the master will never see the actual points).
    :param points: Number of points
    :param dim: Number of dimensions
    :param mode: Dataset generation mode
    :param seed: Random seed
    :return: Dataset fragment
    """
    fragment = Fragment()
    # Make persistent before since it is populated in the task
    fragment.make_persistent()
    fragment.generate_points(points, dim, mode, seed)

def main(seed, numpoints, dimensions, num_centres, fragments, mode, iterations,

```

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```

        epsilon, arity):
    """
    This will be executed if called as main script. Look at the kmeans_frag
    for the KMeans function.
    This code is used for experimental purposes.
    I.e it generates random data from some parameters that determine the size,
    dimensionality and etc and returns the elapsed time.
    :param seed: Random seed
    :param numpoints: Number of points
    :param dimensions: Number of dimensions
    :param num_centres: Number of centres
    :param fragments: Number of fragments
    :param mode: Dataset generation mode
    :param iterations: Number of iterations
    :param epsilon: Epsilon (convergence distance)
    :param arity: Arity
    :return: None
    """
    start_time = time.time()

    # Generate the data
    fragment_list = []
    # Prevent infinite loops in case of not-so-smart users
    points_per_fragment = max(1, numpoints // fragments)

    for l in range(0, numpoints, points_per_fragment):
        # Note that the seed is different for each fragment.
        # This is done to avoid having repeated data.
        r = min(numpoints, l + points_per_fragment)

        fragment_list.append(
            generate_fragment(r - l, dimensions, mode, seed + l)
        )

    compss_barrier()
    print("Generation/Load done")
    initialization_time = time.time()
    print("Starting kmeans")

    # Run kmeans
    centres = kmeans_frag(fragments=fragment_list,
                          dimensions=dimensions,
                          num_centres=num_centres,
                          iterations=iterations,
                          seed=seed,
                          epsilon=epsilon,
                          arity=arity)

    compss_barrier()
    print("Ending kmeans")
    kmeans_time = time.time()

    print("-----")
    print("----- RESULTS -----")
    print("-----")
    print("Initialization time: %f" % (initialization_time - start_time))
    print("Kmeans time: %f" % (kmeans_time - initialization_time))

```

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```

print("Total time: %f" % (kmeans_time - start_time))
print("-----")
centres = compss_wait_on(centres)
print("CENTRES:")
print(centres)
print("-----")

if __name__ == "__main__":
    options = parse_arguments()
    main(**vars(options))

```

Tip: This code can work with Hecuba and Redis if the functions declared in the data model are declared outside the data model, and the kmeans application uses the `points` attribute explicitly.

Since this code is going to be executed with dataClay, it is necessary to declare the `client.properties`, `session.properties` and `storage_props.cfg` files into the `dataClay_confs` with the following contents as example (more configuration options can be found in the dataClay manual):

client.properties

```

HOST=127.0.0.1
TCPPORT=11034

```

session.properties

```

Account=bsc_user
Password=bsc_user
StubsClasspath=./stubs
DataSets=hpc_dataset
DataSetForStore=hpc_dataset
DataClayClientConfig=./client.properties

```

storage_props.cfg

```

BACKENDS_PER_NODE=48

```

An example of the submission script that can be used in MareNostrum IV to launch this kmeans with PyCOMPSs and dataClay is:

```

#!/bin/bash -e

module load gcc/8.1.0
export COMPSS_PYTHON_VERSION=3-ML
module load COMPSs/2.8
module load mkl/2018.1
module load impi/2018.1
module load opencv/4.1.2
module load DATACLAY/2.4.dev

# Retrieve script arguments
job_dependency=${1:-None}
num_nodes=${2:-2}
execution_time=${3:-5}
tracing=${4:-false}
exec_file=${5:-$(pwd)/kmeans.py}

```

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```

# Freeze storage_props into a temporal
# (allow submission of multiple executions with varying parameters)
STORAGE_PROPS=`mktemp -p ~`
cp $(pwd)/dataClay_confs/storage_props.cfg "${STORAGE_PROPS}"

if [[ ! ${tracing} == "false" ]]
then
  extra_tracing_flags="\
    --jvm_workers_opts="-javaagent:/apps/DATACLAY/dependencies/aspectjweaver.jar\" \
    --jvm_master_opts="-javaagent:/apps/DATACLAY/dependencies/aspectjweaver.jar\" \
  "
  echo "Adding DATACLAYSRV_START_CMD to storage properties file"
  echo "\${STORAGE_PROPS}=${STORAGE_PROPS}"
  echo "" >> ${STORAGE_PROPS}
  echo "DATACLAYSRV_START_CMD=\"--tracing\" >> ${STORAGE_PROPS}
fi

# Define script variables
SCRIPT_DIR="$(cd "$(dirname "${BASH_SOURCE[0]}")" && pwd)"
WORK_DIR=${SCRIPT_DIR}/
APP_CLASSPATH=${SCRIPT_DIR}/
APP_PYTHONPATH=${SCRIPT_DIR}/

# Define application variables
graph=$tracing
log_level="off"
qos_flag="--qos=debug"
workers_flag=""
constraints="highmem"

CPUS_PER_NODE=48
WORKER_IN_MASTER=0

shift 5

# Those are evaluated at submit time, not at start time...
COMPSS_VERSION=`module load whatis COMPSS 2>&1 >/dev/null | awk '{print $1 ; exit}'`
DATACLAY_VERSION=`module load whatis DATACLAY 2>&1 >/dev/null | awk '{print $1 ; exit}'`

# Enqueue job
enqueue_compss \
  --job_name=kmeans00_PyCOMPSSs_dataClay \
  --job_dependency="${job_dependency}" \
  --exec_time="${execution_time}" \
  --num_nodes="${num_nodes}" \
  \
  --cpus_per_node="${CPUS_PER_NODE}" \
  --worker_in_master_cpus="${WORKER_IN_MASTER}" \
  --scheduler=es.bsc.compss.scheduler.loadbalancing.LoadBalancingScheduler \
  \
  "${workers_flag}" \
  \
  --worker_working_dir=/gpfs/scratch/user/ \
  \
  --constraints=${constraints} \
  --tracing="${tracing}" \

```

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```

--graph="${graph}" \
--summary \
--log_level="${log_level}" \
"${qos_flag}" \
\
--classpath=${DATACLAY_JAR} \
--pythonpath=${APP_PYTHONPATH}:${PYCLAY_PATH}:${PYTHONPATH} \
--storage_props=${STORAGE_PROPS} \
--storage_home=${COMPSS_STORAGE_HOME} \
--prolog="$DATACLAY_HOME/bin/dataclayprepare,$(pwd)/storage_model/,$(pwd)/,storage_model,
python" \
\
${extra_tracing_flags} \
\
--lang=python \
\
"$exec_file" $@ --use_storage

```

8.2.5 Matmul

The matmul performs the matrix multiplication of two matrices.

```

import time
import numpy as np

from pycompss.api.task import task
from pycompss.api.parameter import INOUT
from pycompss.api.api import compss_barrier
from pycompss.api.api import compss_wait_on

@task(returns=1)
def generate_block(size, num_blocks, seed=0, set_to_zero=False):
    """
    Generate a square block of given size.
    :param size: <Integer> Block size
    :param num_blocks: <Integer> Number of blocks
    :param seed: <Integer> Random seed
    :param set_to_zero: <Boolean> Set block to zeros
    :return: Block
    """
    np.random.seed(seed)
    if not set_to_zero:
        b = np.random.random((size, size))
        # Normalize matrix to ensure more numerical precision
        b /= np.sum(b) * float(num_blocks)
    else:
        b = np.zeros((size, size))
    return b

@task(C=INOUT)
def fused_multiply_add(A, B, C):
    """
    Multiplies two Blocks and accumulates the result in an INOUT Block (FMA).

```

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```

:param A: Block A
:param B: Block B
:param C: Result Block
:return: None
"""
C += np.dot(A, B)

def dot(A, B, C):
    """
    A COMPSs blocked matmul algorithm.
    :param A: Block A
    :param B: Block B
    :param C: Result Block
    :return: None
    """
    n, m = len(A), len(B[0])
    # as many rows as A, as many columns as B
    for i in range(n):
        for j in range(m):
            for k in range(n):
                fused_multiply_add(A[i][k], B[k][j], C[i][j])

def main(num_blocks, elems_per_block, seed):
    """
    Matmul main.
    :param num_blocks: <Integer> Number of blocks
    :param elems_per_block: <Integer> Number of elements per block
    :param seed: <Integer> Random seed
    :return: None
    """
    start_time = time.time()

    # Generate the dataset in a distributed manner
    # i.e: avoid having the master a whole matrix
    A, B, C = [], [], []
    matrix_name = ["A", "B"]
    for i in range(num_blocks):
        for l in [A, B, C]:
            l.append([])
        # Keep track of blockId to initialize with different random seeds
        bid = 0
        for j in range(num_blocks):
            for ix, l in enumerate([A, B]):
                l[-1].append(generate_block(elems_per_block,
                                             num_blocks,
                                             seed=seed + bid))
                bid += 1
            C[-1].append(generate_block(elems_per_block,
                                         num_blocks,
                                         set_to_zero=True))

    compss_barrier()
    initialization_time = time.time()

    # Do matrix multiplication

```

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```

dot(A, B, C)

compss_barrier()
multiplication_time = time.time()

print("-----")
print("----- RESULTS -----")
print("-----")
print("Initialization time: %f" % (initialization_time -
                                start_time))
print("Multiplication time: %f" % (multiplication_time -
                                initialization_time))
print("Total time: %f" % (multiplication_time - start_time))
print("-----")

def parse_args():
    """
    Arguments parser.
    Code for experimental purposes.
    :return: Parsed arguments.
    """
    import argparse
    description = 'COMPSs blocked matmul implementation'
    parser = argparse.ArgumentParser(description=description)
    parser.add_argument('-b', '--num_blocks', type=int, default=1,
                        help='Number of blocks (N in NxN)'
                        )
    parser.add_argument('-e', '--elems_per_block', type=int, default=2,
                        help='Elements per block (N in NxN)'
                        )
    parser.add_argument('--seed', type=int, default=0,
                        help='Pseudo-Random seed'
                        )
    return parser.parse_args()

if __name__ == "__main__":
    opts = parse_args()
    main(**vars(opts))

```

The matrix multiplication application can be executed by invoking the `runcompss` command with the desired parameters (in this case we use `-g` to generate the task dependency graph) and application. The following lines provide an example of its execution considering 4 x 4 Blocks of 1024 x 1024 elements each block, which conforms matrices of 4096 x 4096 elements.

```

compss@bsc:~$ runcompss -g matmul.py -b 4 -e 1024

[ INFO] Inferred PYTHON language
[ INFO] Using default location for project file: /opt/COMPSs/Runtime/configuration/xml/
->projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSs/Runtime/configuration/xml/
->resources/default_resources.xml
[ INFO] Using default execution type: compss

----- Executing matmul.py -----

```

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```

WARNING: COMPSs Properties file is null. Setting default values
[(439)   API] - Starting COMPSs Runtime v2.7 (build 20200519-1005.
↳r6093e5ac94d67250e097a6fad9d3ec00d676fe6c)
-----
----- RESULTS -----
-----
Initialization time: 4.112615
Multiplication time: 2.366103
Total time: 6.478717
-----
[(5609)   API] - Execution Finished
-----

```

Figure 50 depicts the generated task dependency graph. The dataset generation can be identified in the blue tasks, while the white tasks represent the multiplication of a block with another.

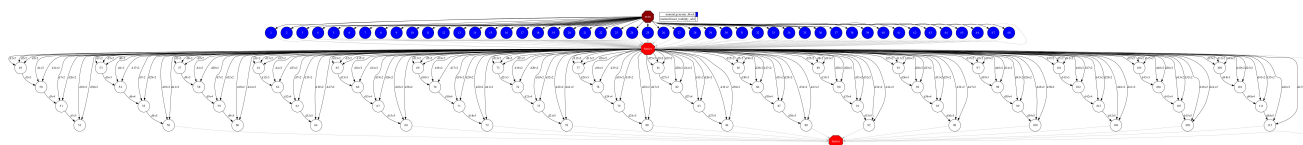


Figure 50: Python matrix multiplication tasks graph

8.2.6 Lysozyme in water

This example will guide a new user through the usage of the `@binary`, `@mpi` and `@constraint` decorators for setting up a simulation system containing a set of proteins (lysozymes) in boxes of water with ions. Each step contains an explanation of input and output, using typical settings for general use.

Extracted from: <http://www.mdtutorials.com/gmx/lysozyme/index.html> Originally done by: Justin A. Lemkul, Ph.D. From: Virginia Tech Department of Biochemistry

Note: This example reaches up to stage 4 (energy minimization).

Important: This application requires **Gromacs** `gmx` and `gmx_mpi`.

```

from os import listdir
from os.path import isfile, join
import sys

from pycompss.api.task import task
from pycompss.api.constraint import constraint
from pycompss.api.binary import binary
from pycompss.api.mpi import mpi
from pycompss.api.parameter import *

# ##### #
# Step 1 tasks #
# ##### #

```

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```

@binary(binary='${GMX_BIN}/gmx')
@task(protein=FILE_IN,
      structure=FILE_OUT,
      topology=FILE_OUT)
def generate_topology(mode='pdb2gmx',
                    protein_flag='-f', protein=None,
                    structure_flag='-o', structure=None,
                    topology_flag='-p', topology=None,
                    flags='-ignh',
                    forcefield_flag='-ff', forcefield='oplsaa',
                    water_flag='-water', water='spce'):
    # Command: gmx pdb2gmx -f protein.pdb -o structure.gro -p topology.top -ignh -ff amber03 -
    ↪water tip3p
    pass

# ##### #
# Step 2 tasks #
# ##### #

@binary(binary='${GMX_BIN}/gmx')
@task(structure=FILE_IN,
      structure_newbox=FILE_OUT)
def define_box(mode='editconf',
              structure_flag='-f', structure=None,
              structure_newbox_flag='-o', structure_newbox=None,
              center_flag='-c',
              distance_flag='-d', distance='1.0',
              boxtype_flag='-bt', boxtype='cubic'):
    # Command: gmx editconf -f structure.gro -o structure_newbox.gro -c -d 1.0 -bt cubic
    pass

# ##### #
# Step 3 tasks #
# ##### #

@binary(binary='${GMX_BIN}/gmx')
@task(structure_newbox=FILE_IN,
      protein_solv=FILE_OUT,
      topology=FILE_IN)
def add_solvate(mode='solvate',
               structure_newbox_flag='-cp', structure_newbox=None,
               configuration_solvent_flag='-cs', configuration_solvent='spc216.gro',
               protein_solv_flag='-o', protein_solv=None,
               topology_flag='-p', topology=None):
    # Command: gmx solvate -cp structure_newbox.gro -cs spc216.gro -o protein_solv.gro -p
    ↪topology.top
    pass

# ##### #
# Step 4 tasks #
# ##### #

@binary(binary='${GMX_BIN}/gmx')
@task(conf=FILE_IN,
      protein_solv=FILE_IN,

```

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```

topology=FILE_IN,
output=FILE_OUT)
def assemble_tpr(mode='grompp',
                 conf_flag='-f', conf=None,
                 protein_solv_flag='-c', protein_solv=None,
                 topology_flag='-p', topology=None,
                 output_flag='-o', output=None):
    # Command: gmx grompp -f ions.mdp -c protein_solv.gro -p topology.top -o ions.tpr
    pass

@binary(binary='${GMX_BIN}/gmx')
@task(ions=FILE_IN,
      output=FILE_OUT,
      topology=FILE_IN,
      group={Type:FILE_IN, StdIOStream:STDIN})
def replace_solvent_with_ions(mode='genion',
                              ions_flag='-s', ions=None,
                              output_flag='-o', output=None,
                              topology_flag='-p', topology=None,
                              pname_flag='-pname', pname='NA',
                              nname_flag='-nname', nname='CL',
                              neutral_flag='-neutral',
                              group=None):
    # Command: gmx genion -s ions.tpr -o 1AKI_solv_ions.gro -p topol.top -pname NA -nname CL -
    ↪neutral < ../config/genion.group
    pass

# ##### #
# Step 5 tasks #
# ##### #

computing_units = "24"
computing_nodes = "1"

@constraint(computing_units=computing_units)
@mpi(runner="mpirun", binary="gmx_mpi", computing_nodes=computing_nodes)
@task(em=FILE_IN,
      em_energy=FILE_OUT)
def energy_minimization(mode='mdrun',
                        verbose_flag='-v',
                        ompthreads_flag='-ntomp', ompthreads='0',
                        em_flag='-s', em=None,
                        em_energy_flag='-e', em_energy=None):
    # Command: gmx mdrun -v -s em.tpr
    pass

# ##### #
# Step 6 tasks #
# ##### #

@binary(binary='${GMX_BIN}/gmx')
@task(em=FILE_IN,
      output=FILE_OUT,
      selection={Type:FILE_IN, StdIOStream:STDIN})
def energy_analysis(mode='energy',
                   em_flag='-f', em=None,

```

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```

        output_flag='-o', output=None,
        selection=None):
    # Command: gmx energy -f em.edr -o output.xvg
    pass

# #####
# MAIN FUNCTION #
# #####

def main(dataset_path, output_path, config_path):
    print("Starting demo")

    protein_names = []
    protein_pdb = []

    # Look for proteins in the dataset folder
    for f in listdir(dataset_path):
        if isfile(join(dataset_path, f)):
            protein_names.append(f.split('.')[0])
            protein_pdb.append(join(dataset_path, f))
    proteins = zip(protein_names, protein_pdb)

    # Iterate over the proteins and process them
    result_image_paths = []
    for name, pdb in proteins:
        # 1st step - Generate topology
        structure = join(output_path, name + '.gro')
        topology = join(output_path, name + '.top')
        generate_topology(protein=pdb,
                        structure=structure,
                        topology=topology)

        # 2nd step - Define box
        structure_newbox = join(output_path, name + '_newbox.gro')
        define_box(structure=structure,
                    structure_newbox=structure_newbox)

        # 3rd step - Add solvate
        protein_solv = join(output_path, name + '_solv.gro')
        add_solvate(structure_newbox=structure_newbox,
                    protein_solv=protein_solv,
                    topology=topology)

        # 4th step - Add ions
        # Assemble with ions.mdp
        ions_conf = join(config_path, 'ions.mdp')
        ions = join(output_path, name + '_ions.tpr')
        assemble_tpr(conf=ions_conf,
                    protein_solv=protein_solv,
                    topology=topology,
                    output=ions)
        protein_solv_ions = join(output_path, name + '_solv_ions.gro')
        group = join(config_path, 'genion.group') # 13 = SOL
        replace_solvent_with_ions(ions=ions,
                                output=protein_solv_ions,
                                topology=topology,
                                group=group)

        # 5th step - Minimize energy

```

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```

# Reassemble with minim.mdp
minim_conf = join(config_path, 'minim.mdp')
em = join(output_path, name + '_em.tpr')
assemble_tpr(conf=minim_conf,
              protein_solv=protein_solv_ions,
              topology=topology,
              output=em)
em_energy = join(output_path, name + '_em_energy.edr')
energy_minimization(em=em,
                    em_energy=em_energy)
# 6th step - Energy analysis (generate xvg image)
energy_result = join(output_path, name + '_potential.xvg')
energy_selection = join(config_path, 'energy.selection') # 10 = potential
energy_analysis(em=em_energy,
                output=energy_result,
                selection=energy_selection)

if __name__=='__main__':
    config_path = sys.argv[1]
    dataset_path = sys.argv[2]
    output_path = sys.argv[3]

    main(dataset_path, output_path, config_path)

```

This application can be executed by invoking the `runcompss` command defining the `config_path`, `dataset_path` and `output_path` where the application inputs and outputs are. For the sake of completeness, we show how to execute this application in a Supercomputer. In this case, the execution will be enqueued in the supercomputer queuing system (e.g. SLURM) through the use of the `enqueue_compss` command, where all parameters used in `runcompss` must appear, as well as some parameters required for the queuing system (e.g. `walltime`).

The following code shows a bash script to submit the execution in MareNostrum IV supercomputer:

```

#!/bin/bash -e

# Define script variables
scriptDir=$(pwd)/$(dirname $0)
execFile=${scriptDir}/src/lysozyme_in_water.py
appClasspath=${scriptDir}/src/
appPythonpath=${scriptDir}/src/

# Retrieve arguments
numNodes=$1
executionTime=$2
tracing=$3

# Leave application args on $@
shift 3

# Load necessary modules
module purge
module load intel/2017.4 impi/2017.4 mkl/2017.4 bsc/1.0
module load COMPSs/2.7
module load gromacs/2016.4 # exposes gmx_mpi binary

export GMX_BIN=/home/user/lysozyme5.1.2/bin # exposes gmx binary

```

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```

# Enqueue the application
enqueue_compss \
--num_nodes=$numNodes \
--exec_time=$executionTime \
--master_working_dir=. \
--worker_working_dir=/gpfs/home/user/lysozyme \
--tracing=$tracing \
--graph=true \
-d \
--classpath=$appClasspath \
--pythonpath=$appPythonpath \
--lang=python \
$execFile $@

#####
# APPLICATION EXECUTION EXAMPLE
# Call:
#      ./launch_md.sh <NUMBER_OF_NODES> <EXECUTION_TIME> <TRACING> <CONFIG_PATH> <DATASET_
→PATH> <OUTPUT_PATH>
#
# Example:
#      ./launch_md.sh 2 10 false $(pwd)/config/ $(pwd)/dataset/ $(pwd)/output/
#
#####

```

Having the 1aki.pdb, 1u3m.pdb and 1xyw.pdb proteins in the dataset folder, the execution of this script produces the submission of the job with the following output:

```

$ ./launch_md.sh 2 10 false $(pwd)/config/ $(pwd)/dataset/ $(pwd)/output/

remove mkl/2017.4 (LD_LIBRARY_PATH)
remove impi/2017.4 (PATH, MANPATH, LD_LIBRARY_PATH)
Set INTEL compilers as MPI wrappers backend
load impi/2017.4 (PATH, MANPATH, LD_LIBRARY_PATH)
load mkl/2017.4 (LD_LIBRARY_PATH)
load java/8u131 (PATH, MANPATH, JAVA_HOME, JAVA_ROOT, JAVA_BINDIR, SDK_HOME, JDK_HOME, JRE_
→HOME)
load papi/5.5.1 (PATH, LD_LIBRARY_PATH, C_INCLUDE_PATH)
Loading default Python 2.7.13.
* For alternative Python versions, please set the COMPSS_PYTHON_VERSION environment variable
→with 2, 3, 2-jupyter or 3-jupyter before loading the COMPSs module.
load PYTHON/2.7.13 (PATH, MANPATH, LD_LIBRARY_PATH, LIBRARY_PATH, PKG_CONFIG_PATH, C_INCLUDE_
→PATH, CPLUS_INCLUDE_PATH, PYTHONHOME)
load lzo/2.10 (LD_LIBRARY_PATH,PKG_CONFIG_PATH,CFLAGS,CXXFLAGS,LDFLAGS)
load boost/1.64.0_py2 (LD_LIBRARY_PATH, LIBRARY_PATH, C_INCLUDE_PATH, CPLUS_INCLUDE_PATH,
→BOOST_ROOT)
load COMPSs/2.7 (PATH, CLASSPATH, MANPATH, GAT_LOCATION, COMPSS_HOME, JAVA_TOOL_OPTIONS,
→LDFLAGS, CPPFLAGS)
load gromacs/2016.4 (PATH, LD_LIBRARY_PATH)
SC Configuration:          default.cfg
JobName:                   COMPSs
Queue:                     default
Reservation:               disabled
Num Nodes:                 2
Num Switches:              0

```

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```

GPUs per node:          0
Job dependency:         None
Exec-Time:             00:10:00
QoS:                   debug
Constraints:            disabled
Storage Home:          null
Storage Properties:
Other:
    --sc_cfg=default.cfg
    --qos=debug
    --master_working_dir=.
    --worker_working_dir=/gpfs/home/user/lysozyme
    --tracing=false
    --graph=true
    --classpath=/home/user/lysozyme/./src/
    --pythonpath=/home/user/lysozyme/./src/
    --lang=python /home/user/lysozyme/./src/lysozyme_in_water.py /home/user/
→ lysozyme/config/ /home/user/lysozyme/dataset/ /home/user/lysozyme/output/

Temp submit script is: /scratch/tmp/tmp.sMHLsaTUUj
Requesting 96 processes
Submitted batch job 10178129

```

Once executed, it produces the `compss-10178129.out` file, containing all the standard output messages flushed during the execution:

```

$ cat compss-10178129.out

----- Launching COMPSs application -----
[ INFO] Using default execution type: compss
[ INFO] Relative Classpath resolved: /home/user/lysozyme/./src/:

----- Executing lysozyme_in_water.py -----
[(590)   API] - Starting COMPSs Runtime v2.7 (build 20200519-1005.
→ r6093e5ac94d67250e097a6fad9d3ec00d676fe6c)
Starting demo

# Here it takes some time to process the dataset

[(290788)  API] - Execution Finished

-----
[LAUNCH_COMPSS] Waiting for application completion

```

Since the execution has been performed with the task dependency graph generation enabled, the result is depicted in [Figure 51](#). It can be identified that PyCOMPSs has been able to analyse the three given proteins in parallel.

The output of the application is a set of files within the output folder. It can be seen that the files decorated with `FILE_OUT` are stored in this folder. In particular, potential (`.xvg`) files represent the final results of the application, which can be visualized with GRACE.

```

user@login:~/lysozyme/output> ls -l
total 79411
-rw-r--r-- 1 user group    8976 may 19 17:06 laki_em_energy.edr
-rw-r--r-- 1 user group 1280044 may 19 17:03 laki_em.tpr
-rw-r--r-- 1 user group   88246 may 19 17:03 laki.gro
-rw-r--r-- 1 user group 1279304 may 19 17:03 laki_ions.tpr

```

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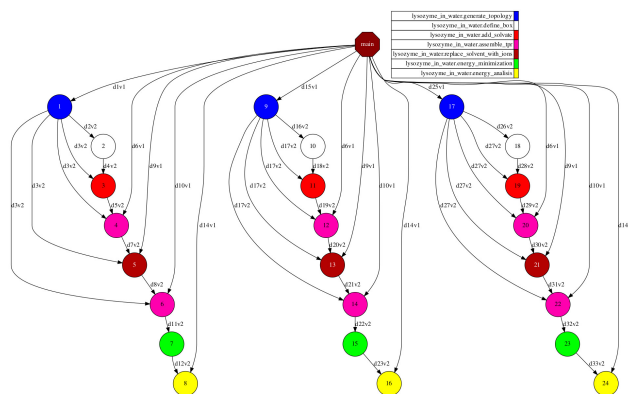


Figure 51: Python Lysozyme in Water tasks graph

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```

-rw-r--r-- 1 user group 88246 may 19 17:03 laki_newbox.gro
-rw-r--r-- 1 user group 2141 may 19 17:06 laki_potential.xvg <-----
-rw-r--r-- 1 user group 1525186 may 19 17:03 laki_solv.gro
-rw-r--r-- 1 user group 1524475 may 19 17:03 laki_solv_ions.gro
-rw-r--r-- 1 user group 577616 may 19 17:03 laki.top
-rw-r--r-- 1 user group 577570 ene 24 16:11 #laki.top.1#
-rw-r--r-- 1 user group 577601 may 19 16:59 #laki.top.10#
-rw-r--r-- 1 user group 577570 may 19 17:03 #laki.top.11#
-rw-r--r-- 1 user group 577601 may 19 17:03 #laki.top.12#
-rw-r--r-- 1 user group 577601 ene 24 16:11 #laki.top.2#
-rw-r--r-- 1 user group 577570 ene 24 16:20 #laki.top.3#
-rw-r--r-- 1 user group 577601 ene 24 16:20 #laki.top.4#
-rw-r--r-- 1 user group 577570 ene 24 16:25 #laki.top.5#
-rw-r--r-- 1 user group 577601 ene 24 16:25 #laki.top.6#
-rw-r--r-- 1 user group 577570 ene 24 16:31 #laki.top.7#
-rw-r--r-- 1 user group 577601 ene 24 16:31 #laki.top.8#
-rw-r--r-- 1 user group 577570 may 19 16:59 #laki.top.9#
-rw-r--r-- 1 user group 8976 may 19 17:08 1u3m_em_energy.edr
-rw-r--r-- 1 user group 1416272 may 19 17:03 1u3m_em.tpr
-rw-r--r-- 1 user group 82046 may 19 17:03 1u3m.gro
-rw-r--r-- 1 user group 1415196 may 19 17:03 1u3m_ions.tpr
-rw-r--r-- 1 user group 82046 may 19 17:03 1u3m_newbox.gro
-rw-r--r-- 1 user group 2151 may 19 17:08 1u3m_potential.xvg <-----
-rw-r--r-- 1 user group 1837046 may 19 17:03 1u3m_solv.gro
-rw-r--r-- 1 user group 1836965 may 19 17:03 1u3m_solv_ions.gro
-rw-r--r-- 1 user group 537950 may 19 17:03 1u3m.top
-rw-r--r-- 1 user group 537904 ene 24 16:11 #1u3m.top.1#
-rw-r--r-- 1 user group 537935 may 19 16:59 #1u3m.top.10#
-rw-r--r-- 1 user group 537904 may 19 17:03 #1u3m.top.11#
-rw-r--r-- 1 user group 537935 may 19 17:03 #1u3m.top.12#
-rw-r--r-- 1 user group 537935 ene 24 16:11 #1u3m.top.2#
-rw-r--r-- 1 user group 537904 ene 24 16:20 #1u3m.top.3#
-rw-r--r-- 1 user group 537935 ene 24 16:20 #1u3m.top.4#
-rw-r--r-- 1 user group 537904 ene 24 16:25 #1u3m.top.5#
-rw-r--r-- 1 user group 537935 ene 24 16:25 #1u3m.top.6#
-rw-r--r-- 1 user group 537904 ene 24 16:31 #1u3m.top.7#
-rw-r--r-- 1 user group 537935 ene 24 16:31 #1u3m.top.8#
-rw-r--r-- 1 user group 537904 may 19 16:59 #1u3m.top.9#
-rw-r--r-- 1 user group 8780 may 19 17:08 1xyw_em_energy.edr

```

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```

-rw-r--r-- 1 user group 1408872 may 19 17:03 lxyw_em.tpr
-rw-r--r-- 1 user group 80112 may 19 17:03 lxyw.gro
-rw-r--r-- 1 user group 1407844 may 19 17:03 lxyw_ions.tpr
-rw-r--r-- 1 user group 80112 may 19 17:03 lxyw_newbox.gro
-rw-r--r-- 1 user group 2141 may 19 17:08 lxyw_potential.xvg <-----
-rw-r--r-- 1 user group 1845237 may 19 17:03 lxyw_solv.gro
-rw-r--r-- 1 user group 1845066 may 19 17:03 lxyw_solv_ions.gro
-rw-r--r-- 1 user group 524026 may 19 17:03 lxyw.top
-rw-r--r-- 1 user group 523980 ene 24 16:11 #lxyw.top.1#
-rw-r--r-- 1 user group 524011 may 19 16:59 #lxyw.top.10#
-rw-r--r-- 1 user group 523980 may 19 17:03 #lxyw.top.11#
-rw-r--r-- 1 user group 524011 may 19 17:03 #lxyw.top.12#
-rw-r--r-- 1 user group 524011 ene 24 16:11 #lxyw.top.2#
-rw-r--r-- 1 user group 523980 ene 24 16:20 #lxyw.top.3#
-rw-r--r-- 1 user group 524011 ene 24 16:20 #lxyw.top.4#
-rw-r--r-- 1 user group 523980 ene 24 16:25 #lxyw.top.5#
-rw-r--r-- 1 user group 524011 ene 24 16:25 #lxyw.top.6#
-rw-r--r-- 1 user group 523980 ene 24 16:31 #lxyw.top.7#
-rw-r--r-- 1 user group 524011 ene 24 16:31 #lxyw.top.8#
-rw-r--r-- 1 user group 523980 may 19 16:59 #lxyw.top.9#

```

Figure 52 depicts the potential results obtained for the lxyw protein.

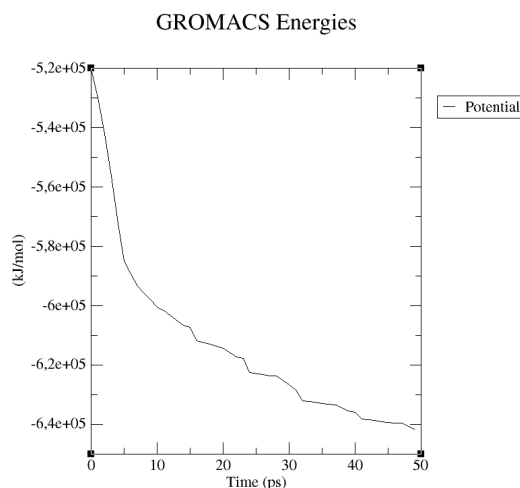


Figure 52: lxyw Potential result (plotted with GRACE)

8.3 C/C++ Sample applications

The first two examples in this section are simple applications developed in COMPSs to easily illustrate how to code, compile and run COMPSs applications. These applications are executed locally and show different ways to take advantage of all the COMPSs features.

The rest of the examples are more elaborated and consider the execution in a cloud platform where the VMs mount a common storage on **/sharedDisk** directory. This is useful in the case of applications that require working with big files, allowing to transfer data only once, at the beginning of the execution, and to enable the application to access the data directly during the rest of the execution.

The Virtual Machine available at our webpage (<http://compss.bsc.es/>) provides a development environment with all the applications listed in the following sections. The codes of all the applications can be found under the `/home/compss/tutorial_apps/c/` folder.

8.3.1 Simple

The Simple application is a C application that increases a counter by means of a task. The counter is stored inside a file that is transferred to the worker when the task is executed. Thus, the tasks interface is defined as follows:

```
// simple.idl
interface simple {
    void increment(inout File filename);
};
```

Next we also provide the invocation of the task from the main code and the increment's method code.

```
// simple.cc

int main(int argc, char *argv[]) {
    // Check and get parameters
    if (argc != 2) {
        usage();
        return -1;
    }
    string initialValue = argv[1];
    file fileName = strdup(FILE_NAME);

    // Init compss
    compss_on();

    // Write file
    ofstream fos (fileName);
    if (fos.is_open()) {
        fos << initialValue << endl;
        fos.close();
    } else {
        cerr << "[ERROR] Unable to open file" << endl;
        return -1;
    }
    cout << "Initial counter value is " << initialValue << endl;

    // Execute increment
    increment(&fileName);

    // Read new value
    string finalValue;
    ifstream fis;
    compss_ifstream(fileName, fis);
    if (fis.is_open()) {
        if (getline(fis, finalValue)) {
            cout << "Final counter value is " << finalValue << endl;
            fis.close();
        } else {
            cerr << "[ERROR] Unable to read final value" << endl;
            fis.close();
            return -1;
        }
    } else {
        cerr << "[ERROR] Unable to open file" << endl;
        return -1;
    }
}
```

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```

// Close COMPSs and end
compss_off();
return 0;
}

```

```

//simple-functions.cc

void increment(file *fileName) {
    cout << "INIT TASK" << endl;
    cout << "Param: " << *fileName << endl;
    // Read value
    char initialValue;
    ifstream fis (*fileName);
    if (fis.is_open()) {
        if (fis >> initialValue) {
            fis.close();
        } else {
            cerr << "[ERROR] Unable to read final value" << endl;
            fis.close();
        }
        fis.close();
    } else {
        cerr << "[ERROR] Unable to open file" << endl;
    }

    // Increment
    cout << "INIT VALUE: " << initialValue << endl;
    int finalValue = ((int)(initialValue) - (int)('0')) + 1;
    cout << "FINAL VALUE: " << finalValue << endl;

    // Write new value
    ofstream fos (*fileName);
    if (fos.is_open()) {
        fos << finalValue << endl;
        fos.close();
    } else {
        cerr << "[ERROR] Unable to open file" << endl;
    }
    cout << "END TASK" << endl;
}

```

Finally, to compile and execute this application users must run the following commands:

```

compss@bsc:~$ cd ~/tutorial_apps/c/simple/
compss@bsc:~/tutorial_apps/c/simple$ compss_build_app simple
compss@bsc:~/tutorial_apps/c/simple$ runcompss --lang=c --project=./xml/project.xml --
resources=./xml/resources.xml ~/tutorial_apps/c/simple/master/simple 1
[ INFO] Using default execution type: compss

----- Executing simple -----

JVM_OPTIONS_FILE: /tmp/tmp.n2eZjgmDGo
COMPSS_HOME: /opt/COMPSS
Args: 1

WARNING: COMPSs Properties file is null. Setting default values

```

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```

[(617)   API] - Starting COMPSs Runtime v<version>
Initial counter value is 1
[  BINDING] - @GS_register - Ref: 0x7fffa35d0f48
[  BINDING] - @GS_register - ENTRY ADDED
[  BINDING] - @GS_register - Entry.type: 9
[  BINDING] - @GS_register - Entry.classname: File
[  BINDING] - @GS_register - Entry.filename: counter
[  BINDING] - @GS_register - setting filename: counter
[  BINDING] - @GS_register - Filename: counter
[  BINDING] - @GS_register - Result is 0
[  BINDING] - @compss_wait_on - Entry.type: 9
[  BINDING] - @compss_wait_on - Entry.classname: File
[  BINDING] - @compss_wait_on - Entry.filename: counter
[  BINDING] - @compss_wait_on - Runtime filename: /home/compss/.COMPSs/simple_01/
→tmpFiles/d1v2_1479141705574.IT
[  BINDING] - @compss_wait_on - File renaming: /home/compss/.COMPSs/simple_01/tmpFiles/
→d1v2_1479141705574.IT to counter
Final counter value is 2
[(3755)   API] - Execution Finished
-----

```

8.3.2 Increment

The Increment application is a C application that increases N times three different counters. Each increase step is developed by a separated task. The purpose of this application is to show parallelism between the three counters.

Next we provide the main code of this application. The code inside the *increment* task is the same than the previous example.

```

// increment.cc

int main(int argc, char *argv[]) {
    // Check and get parameters
    if (argc != 5) {
        usage();
        return -1;
    }
    int N = atoi( argv[1] );
    string counter1 = argv[2];
    string counter2 = argv[3];
    string counter3 = argv[4];

    // Init COMPSs
    compss_on();

    // Initialize counter files
    file fileName1 = strdup(FILE_NAME1);
    file fileName2 = strdup(FILE_NAME2);
    file fileName3 = strdup(FILE_NAME3);
    initializeCounters(counter1, counter2, counter3, fileName1, fileName2, fileName3);

    // Print initial counters state
    cout << "Initial counter values: " << endl;
    printCounterValues(fileName1, fileName2, fileName3);
}

```

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```

// Execute increment tasks
for (int i = 0; i < N; ++i) {
    increment(&fileName1);
    increment(&fileName2);
    increment(&fileName3);
}

// Print final state
cout << "Final counter values: " << endl;
printCounterValues(fileName1, fileName2, fileName3);

// Stop COMPSs
compss_off();

return 0;
}

```

As shown in the main code, this application has 4 parameters that stand for:

1. **N**: Number of times to increase a counter
2. **counter1**: Initial value for counter 1
3. **counter2**: Initial value for counter 2
4. **counter3**: Initial value for counter 3

Next we will compile and run the Increment application with the `-g` option to be able to generate the final graph at the end of the execution.

```

compss@bsc:~$ cd ~/tutorial_apps/c/increment/
compss@bsc:~/tutorial_apps/c/increment$ compss_build_app increment
compss@bsc:~/tutorial_apps/c/increment$ runcompss --lang=c -g --project=./xml/project.xml --
resources=./xml/resources.xml ~/tutorial_apps/c/increment/master/increment 10 1 2 3
[ INFO] Using default execution type: compss

----- Executing increment -----

JVM_OPTIONS_FILE: /tmp/tmp.mgCheFd3kL
COMPSS_HOME: /opt/COMPSSs
Args: 10 1 2 3

WARNING: COMPSs Properties file is null. Setting default values
[(655)   API] - Starting COMPSs Runtime v<version>
Initial counter values:
- Counter1 value is 1
- Counter2 value is 2
- Counter3 value is 3
[ BINDING] - @GS_register - Ref: 0x7ffea17719f0
[ BINDING] - @GS_register - ENTRY ADDED
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file1.txt
[ BINDING] - @GS_register - setting filename: file1.txt
[ BINDING] - @GS_register - Filename: file1.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea17719f8
[ BINDING] - @GS_register - ENTRY ADDED
[ BINDING] - @GS_register - Entry.type: 9

```

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```

[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file2.txt
[ BINDING] - @GS_register - setting filename: file2.txt
[ BINDING] - @GS_register - Filename: file2.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea1771a00
[ BINDING] - @GS_register - ENTRY ADDED
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file3.txt
[ BINDING] - @GS_register - setting filename: file3.txt
[ BINDING] - @GS_register - Filename: file3.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea17719f0
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file1.txt
[ BINDING] - @GS_register - setting filename: file1.txt
[ BINDING] - @GS_register - Filename: file1.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea17719f8
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file2.txt
[ BINDING] - @GS_register - setting filename: file2.txt
[ BINDING] - @GS_register - Filename: file2.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea1771a00
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file3.txt
[ BINDING] - @GS_register - setting filename: file3.txt
[ BINDING] - @GS_register - Filename: file3.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea17719f0
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file1.txt
[ BINDING] - @GS_register - setting filename: file1.txt
[ BINDING] - @GS_register - Filename: file1.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea17719f8
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file2.txt
[ BINDING] - @GS_register - setting filename: file2.txt
[ BINDING] - @GS_register - Filename: file2.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea1771a00
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9

```

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```

[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file3.txt
[ BINDING] - @GS_register - setting filename: file3.txt
[ BINDING] - @GS_register - Filename: file3.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea17719f0
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file1.txt
[ BINDING] - @GS_register - setting filename: file1.txt
[ BINDING] - @GS_register - Filename: file1.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea17719f8
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file2.txt
[ BINDING] - @GS_register - setting filename: file2.txt
[ BINDING] - @GS_register - Filename: file2.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea1771a00
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file3.txt
[ BINDING] - @GS_register - setting filename: file3.txt
[ BINDING] - @GS_register - Filename: file3.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea17719f0
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file1.txt
[ BINDING] - @GS_register - setting filename: file1.txt
[ BINDING] - @GS_register - Filename: file1.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea17719f8
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file2.txt
[ BINDING] - @GS_register - setting filename: file2.txt
[ BINDING] - @GS_register - Filename: file2.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea1771a00
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file3.txt
[ BINDING] - @GS_register - setting filename: file3.txt
[ BINDING] - @GS_register - Filename: file3.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea17719f0
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9

```

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```

[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file1.txt
[ BINDING] - @GS_register - setting filename: file1.txt
[ BINDING] - @GS_register - Filename: file1.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea17719f8
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file2.txt
[ BINDING] - @GS_register - setting filename: file2.txt
[ BINDING] - @GS_register - Filename: file2.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea1771a00
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file3.txt
[ BINDING] - @GS_register - setting filename: file3.txt
[ BINDING] - @GS_register - Filename: file3.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea17719f0
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file1.txt
[ BINDING] - @GS_register - setting filename: file1.txt
[ BINDING] - @GS_register - Filename: file1.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea17719f8
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file2.txt
[ BINDING] - @GS_register - setting filename: file2.txt
[ BINDING] - @GS_register - Filename: file2.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea1771a00
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file3.txt
[ BINDING] - @GS_register - setting filename: file3.txt
[ BINDING] - @GS_register - Filename: file3.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea17719f0
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file1.txt
[ BINDING] - @GS_register - setting filename: file1.txt
[ BINDING] - @GS_register - Filename: file1.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea17719f8
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9

```

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```

[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file2.txt
[ BINDING] - @GS_register - setting filename: file2.txt
[ BINDING] - @GS_register - Filename: file2.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea1771a00
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file3.txt
[ BINDING] - @GS_register - setting filename: file3.txt
[ BINDING] - @GS_register - Filename: file3.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea17719f0
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file1.txt
[ BINDING] - @GS_register - setting filename: file1.txt
[ BINDING] - @GS_register - Filename: file1.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea17719f8
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file2.txt
[ BINDING] - @GS_register - setting filename: file2.txt
[ BINDING] - @GS_register - Filename: file2.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea1771a00
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file3.txt
[ BINDING] - @GS_register - setting filename: file3.txt
[ BINDING] - @GS_register - Filename: file3.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea17719f0
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file1.txt
[ BINDING] - @GS_register - setting filename: file1.txt
[ BINDING] - @GS_register - Filename: file1.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea17719f8
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9
[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file2.txt
[ BINDING] - @GS_register - setting filename: file2.txt
[ BINDING] - @GS_register - Filename: file2.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @GS_register - Ref: 0x7ffea1771a00
[ BINDING] - @GS_register - ENTRY FOUND
[ BINDING] - @GS_register - Entry.type: 9

```

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```

[ BINDING] - @GS_register - Entry.classname: File
[ BINDING] - @GS_register - Entry.filename: file3.txt
[ BINDING] - @GS_register - setting filename: file3.txt
[ BINDING] - @GS_register - Filename: file3.txt
[ BINDING] - @GS_register - Result is 0
[ BINDING] - @compss_wait_on - Entry.type: 9
[ BINDING] - @compss_wait_on - Entry.classname: File
[ BINDING] - @compss_wait_on - Entry.filename: file1.txt
[ BINDING] - @compss_wait_on - Runtime filename: /home/compss/.COMPSs/increment_01/
→tmpFiles/d1v11_1479142004112.IT
[ BINDING] - @compss_wait_on - File renaming: /home/compss/.COMPSs/increment_01/
→tmpFiles/d1v11_1479142004112.IT to file1.txt
[ BINDING] - @compss_wait_on - Entry.type: 9
[ BINDING] - @compss_wait_on - Entry.classname: File
[ BINDING] - @compss_wait_on - Entry.filename: file2.txt
[ BINDING] - @compss_wait_on - Runtime filename: /home/compss/.COMPSs/increment_01/
→tmpFiles/d2v11_1479142004112.IT
[ BINDING] - @compss_wait_on - File renaming: /home/compss/.COMPSs/increment_01/
→tmpFiles/d2v11_1479142004112.IT to file2.txt
[ BINDING] - @compss_wait_on - Entry.type: 9
[ BINDING] - @compss_wait_on - Entry.classname: File
[ BINDING] - @compss_wait_on - Entry.filename: file3.txt
[ BINDING] - @compss_wait_on - Runtime filename: /home/compss/.COMPSs/increment_01/
→tmpFiles/d3v11_1479142004112.IT
[ BINDING] - @compss_wait_on - File renaming: /home/compss/.COMPSs/increment_01/
→tmpFiles/d3v11_1479142004112.IT to file3.txt
Final counter values:
- Counter1 value is 2
- Counter2 value is 3
- Counter3 value is 4
[(4288)  API] - Execution Finished
-----

```

By running the *compss_gengraph* command users can obtain the task graph of the above execution. Next we provide the set of commands to obtain the graph show in [Figure 53](#).

```

compss@bsc:~$ cd ~/.COMPSs/increment_01/monitor/
compss@bsc:~/.COMPSs/increment_01/monitor$ compss_gengraph complete_graph.dot
compss@bsc:~/.COMPSs/increment_01/monitor$ evince complete_graph.pdf

```

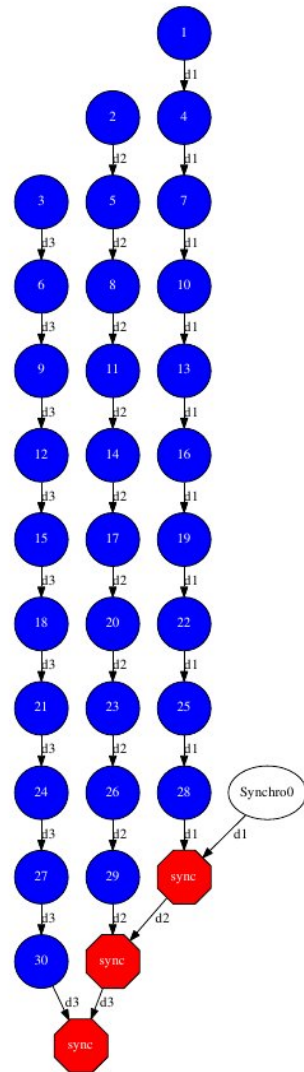


Figure 53: C increment tasks graph

Chapter 9

PyCOMPSs Player

The PyCOMPSs player (`pycompss-player`) provides a tool to use PyCOMPSs within local machines interactively through docker containers. This tool has been implemented on top of the [PyCOMPSs programming model](#), and it is being developed by the [Workflows and Distributed Computing group](#) of the [Barcelona Supercomputing Center](#), and can be easily downloaded and installed from the Pypi repository.

9.1 Requirements and Installation

9.1.1 Requirements

- Python 3
- [docker](#) `>= 17.12.0-ce`
- [docker](#) for python

9.1.2 Installation

1. Install Docker (continue with step 2 if already installed):

- 1.1. Suggested Docker installation instructions:

- [Docker for Mac](#). Or, if you prefer to use [Homebrew](#).
- [Docker for Ubuntu](#).
- [Docker for Arch Linux](#).

Be aware that for some distributions the Docker package has been renamed from `docker` to `docker-ce`. Make sure you install the new package.

- 1.2. Add user to docker group to run the containers as a non-root user:

- [Instructions](#)

- 1.3. Check that docker is correctly installed:

```
$ docker --version
$ docker ps # this should be empty as no docker processes are yet running.
```

2. Install [docker](#) for python (continue with step 3 if already installed):

```
$ python3 -m pip install docker
```

3. Install [pycompss-player](#):

Since the PyCOMPSs playerpackage is available in Pypi, it can be easily installed with `pip` as follows:

```
$ python3 -m pip install pycompss-player
```

4. Check the [pycompss-player](#) installation:

In order to check that it is correctly installed, check that the `pycompss-player` executables (`pycompss`, `compss` and `dislib`, which can be used indifferently) are available from your command line.

```
$ pycompss
[PyCOMPSs player options will be shown]
```

Tip: Some Linux distributions do not include the `$HOME/.local/bin` folder in the `PATH` environment variable, preventing to access to the `pycompss-player` commands (and any other Python packages installed in the user `HOME`).

If you experience that the `pycompss|compss|dislib` command is not available after the installation, you may need to include the following line into your `.bashrc` and execute it in your current session:

```
$ export PATH=${HOME}/.local/bin:${PATH}
```

9.2 Usage

`pycompss-player` provides the `pycompss` command line tool (`compss` and `dislib` are also alternatives to `pycompss`).

This command line tool enables to deal with docker in order to deploy a COMPSs infrastructure in containers.

The supported flags are:

```
$ pycompss
PyCOMPSs|COMPSS Player:

Usage: pycompss COMMAND | compss COMMAND | dislib COMMAND

Available commands:
  init -w [WORK_DIR] -i [IMAGE]: initializes COMPSs in the current working dir or in WORK_
  →DIR if -w is set.
  →i (it can also be
  →variable).
  kill: stops and kills all instances of the COMPSs.
  update: updates the COMPSs docker image (use only when installing
  →master branch).
  exec CMD: executes the CMD command inside the COMPSs master
  →container.
  run [OPTIONS] FILE [PARAMS]: runs FILE with COMPSs, where OPTIONS are COMPSs options
  →and PARAMS are application parameters.
  monitor [start|stop]: starts or stops the COMPSs monitoring.
  jupyter [PATH|FILE]: starts jupyter-notebook in the given PATH or FILE.
  gengraph [FILE.dot]: converts the .dot graph into .pdf
  components list: lists COMPSs actives components.
  components add RESOURCE: adds the RESOURCE to the pool of workers of the COMPSs.
  Example given: pycompss components add worker 2 # to add 2 local workers.
  Example given: pycompss components add worker <IP>:<CORES> # to add a remote worker
  Note: compss and dislib can be used instead of pycompss in both examples.
  components remove RESOURCE: removes the RESOURCE to the pool of workers of the COMPSs.
  Example given: pycompss components remove worker 2 # to remove 2 local workers.
  Example given: pycompss components remove worker <IP>:<CORES> # to remove a remote
  →worker
  Note: compss and dislib can be used instead of pycompss in both examples.
```

9.2.1 Start COMPSs infrastructure in your development directory

Initialize the COMPSs infrastructure where your source code will be (you can re-init anytime). This will allow docker to access your local code and run it inside the container.

```
$ pycompss init # operates on the current directory as working directory.
```

Note: The first time needs to download the docker image from the repository, and it may take a while.

Alternatively, you can specify the working directory, the COMPSs docker image to use, or both at the same time:

```
$ # You can also provide a path
$ pycompss init -w /home/user/replace/path/
$
$ # Or the COMPSs docker image to use
$ pycompss init -i compss/compss-tutorial:2.7
$
$ # Or both
$ pycompss init -w /home/user/replace/path/ -i compss/compss-tutorial:2.7
```

9.2.2 Running applications

In order to show how to run an application, clone the PyCOMPSs' tutorial apps repository:

```
$ git clone https://github.com/bsc-wdc/tutorial_apps.git
```

Init the COMPSs environment in the root of the repository. The source files path are resolved from the init directory which sometimes can be confusing. As a rule of thumb, initialize the library in a current directory and check the paths are correct running the file with `python3 path_to/file.py` (in this case `python3 python/simple/src/simple.py`).

```
$ cd tutorial_apps
$ pycompss init
```

Now we can run the `simple.py` application:

```
$ pycompss run python/simple/src/simple.py 1
```

The log files of the execution can be found at `$HOME/.COMPSs`.

You can also init the COMPSs environment inside the examples folder. This will mount the examples directory inside the container so you can execute it without adding the path:

```
$ cd python/simple/src
$ pycompss init
$ pycompss run simple.py 1
```

9.2.3 Running the COMPSs monitor

The COMPSs monitor can be started using the `pycompss monitor start` command. This will start the COMPSs monitoring facility which enables to check the application status while running. Once started, it will show the url to open the monitor in your web browser (i.e. <http://127.0.0.1:8080/compss-monitor>)

Important: Include the `--monitor=<REFRESH_RATE_MS>` flag in the execution before the binary to be executed.

```
$ cd python/simple/src
$ pycompss init
$ pycompss monitor start
$ pycompss run --monitor=1000 -g simple.py 1
$ # During the execution, go to the URL in your web browser
$ pycompss monitor stop
```

If running a notebook, just add the monitoring parameter into the COMPSs runtime start call.

Once finished, it is possible to stop the monitoring facility by using the `pycompss monitor stop` command.

9.2.4 Running Jupyter notebooks

Notebooks can be run using the `pycompss jupyter` command. Run the following snippet from the root of the project:

```
$ cd tutorial_apps/python
$ pycompss init
$ pycompss jupyter ./notebooks
```

An alternative and more flexible way of starting jupyter is using the `pycompss run` command in the following way:

```
$ pycompss run jupyter-notebook ./notebooks --ip=0.0.0.0 --NotebookApp.token='' --allow-root
```

And access interactively to your notebook by opening following the <http://127.0.0.1:8888/> URL in your web browser.

Caution: If the notebook process is not properly closed, you might get the following warning when trying to start jupyter notebooks again:

The port 8888 is already in use, trying another port.

To fix it, just restart the container with `pycompss init`.

9.2.5 Generating the task graph

COMPSs is able to produce the task graph showing the dependencies that have been respected. In order to produce it, include the `--graph` flag in the execution command:

```
$ cd python/simple/src
$ pycompss init
$ pycompss run --graph simple.py 1
```

Once the application finishes, the graph will be stored into the `~\.COMPSs\app_name_XX\monitor\complete_graph.dot` file. This dot file can be converted to pdf for easier visualization through the use of the `gengraph` parameter:

```
$ pycompss gengraph .COMPSs/simple.py_01/monitor/complete_graph.dot
```

The resulting pdf file will be stored into the `~\.COMPSs\app_name_XX\monitor\complete_graph.pdf` file, that is, the same folder where the dot file is.

9.2.6 Tracing applications or notebooks

COMPSs is able to produce tracing profiles of the application execution through the use of EXTRAE. In order to enable it, include the `--tracing` flag in the execution command:

```
$ cd python/simple/src
$ pycompss init
$ pycompss run --tracing simple.py 1
```

If running a notebook, just add the tracing parameter into the COMPSs runtime start call.

Once the application finishes, the trace will be stored into the `~\.COMPSs\app_name_XX\trace` folder. It can then be analysed with Paraver.

9.2.7 Adding more nodes

Note: Adding more nodes is still in beta phase. Please report issues, suggestions, or feature requests on [Github](#).

To add more computing nodes, you can either let docker create more workers for you or manually create and config a custom node.

For docker just issue the desired number of workers to be added. For example, to add 2 docker workers:

```
$ pycompss components add worker 2
```

You can check that both new computing nodes are up with:

```
$ pycompss components list
```

If you want to add a custom node it needs to be reachable through ssh without user. Moreover, pycompss will try to copy the `working_dir` there, so it needs write permissions for the scp.

For example, to add the local machine as a worker node:

```
$ pycompss components add worker '127.0.0.1:6'
```

- '127.0.0.1': is the IP used for ssh (can also be a hostname like 'localhost' as long as it can be resolved).
- '6': desired number of available computing units for the new node.

Important: Please be aware** that `pycompss components` will not list your custom nodes because they are not docker processes and thus it can't be verified if they are up and running.

9.2.8 Removing existing nodes

Note: Removing nodes is still in beta phase. Please report issues, suggestions, or feature requests on [Github](#).

For docker just issue the desired number of workers to be removed. For example, to remove 2 docker workers:

```
$ pycompss components remove worker 2
```

You can check that the workers have been removed with:

```
$ pycompss components list
```

If you want to remove a custom node, you just need to specify its IP and number of computing units used when defined.

```
$ pycompss components remove worker '127.0.0.1:6'
```

9.2.9 Stop pycompss

The infrastructure deployed can be easily stopped and the docker instances closed with the following command:

```
$ pycompss kill
```

Chapter 10

PyCOMPSs Notebooks

This section contains all PyCOMPSs related tutorial notebooks (sources available in <https://github.com/bsc-wdc/notebooks>).

It is divided into three main folders:

1. **Syntax:** Contains the main tutorial notebooks. They cover the syntax and main functionalities of PyCOMPSs.
2. **Hands-On:** Contains example applications and hands-on exercises.
3. **Demos:** Contains demonstration notebooks.

10.1 Syntax

Here you will find the syntax notebooks used in the tutorials.

10.1.1 Basics of programming with PyCOMPSs

In this example we will see basics of programming with PyCOMPSs: - Runtime start - Task definition - Task invocation - Runtime stop

10.1.1.1 Let's get started with a simple example

First step

- Import the PyCOMPSs library

```
[1]: import pycompss.interactive as ipycompss
```

Second step

- Initialize COMPSs runtime. Parameters indicates if the execution will generate task graph, tracefile, monitor interval and debug information.

```
[2]: import os
if 'BINDER_SERVICE_HOST' in os.environ:
    ipycompss.start(graph=True,
                    project_xml='../xml/project.xml',
                    resources_xml='../xml/resources.xml')
```

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```

else:
    ipycompss.start(graph=True, monitor=1000) # debug=True, trace=True

*****
***** PyCOMPSS Interactive *****
*****
*
*      .~-.~-.      |-----|      |-----|      *
*      :              |-----|      |-----|      *
*      ~ ~ -. \      /.- ~ ~ .      |-----|      | (---) |      *
*      >      .      '      <      /---/      \---/      /      *
*      (      .~-.~-.      )      | |-----|      -      /      /      *
*      '-_-~-'      ~-.--'      |-----|      | |      /---/      *
*      (      :      )      |-----|      | |      /---/      *
*      ~--      :      ~--      .~-.~-.~-      }      *
*      ~-.-~-.~-      \      .~-.~-.~-      *
*      \      \      \      \      \      \      *
*      \      \      \      \      \      \      *
*      \      \      \      \      \      \      *
*      . - ~ ~ - \      \      \      \      *
*      .~-.~-      } ~ ~ ~-.-      *
*      . ' .~-.~-      .~-.~-      :/~-.~-.~-      *
*      /~-.~-      ~-      ~-.-.-      *
*      ~-.-.-      *
*****
* - Starting COMPSS runtime...      *
* - Log path : /home/javier/.COMPSS/InteractiveMode_01/      *
* - PyCOMPSS Runtime started... Have fun!      *
*****

```

Third step

- Import task module before annotating functions or methods

```
[3]: from pycompss.api.task import task
```

Fourth step

- Declare functions and decorate with `@task` those that should be tasks

```
[4]: @task(returns=int)
def square(val1):
    return val1 * val1
```

```
[5]: @task(returns=int)
def add(val2, val3):
    return val2 + val3
```

```
[6]: @task(returns=int)
def multiply(val1, val2):
    return val1 * val2
```


Fifth step

- Invoke tasks

```
[7]: a = square(2)
Found task: square
```

```
[8]: b = add(a, 4)
Found task: add
```

```
[9]: c = multiply(b, 5)
Found task: multiply
```

Sixth step (last)

- Stop COMPSs runtime. All data can be synchronized in the main program .

```
[10]: ipycompss.stop(sync=True)

*****
***** STOPPING PyCOMPSs *****
*****
Checking if any issue happened.
Synchronizing all future objects left on the user scope.
Found a future object: a
Found a future object: b
Found a future object: c
*****
```

```
[11]: print("Results after stopping PyCOMPSs: ")
print("a: %d" % a)
print("b: %d" % b)
print("c: %d" % c)

Results after stopping PyCOMPSs:
a: 4
b: 8
c: 40
```

10.1.2 PyCOMPSs: Synchronization

In this example we will see how to synchronize with PyCOMPSs.

10.1.2.1 Import the PyCOMPSs library

```
[1]: import pycompss.interactive as ipycompss
```

10.1.2.2 Start the runtime

Initialize COMPSs runtime Parameters indicates if the execution will generate task graph, tracefile, monitor interval and debug information.

```
[2]: import os
    if 'BINDER_SERVICE_HOST' in os.environ:
        ipycompss.start(graph=True, debug=False,
                        project_xml='../xml/project.xml',
                        resources_xml='../xml/resources.xml')
    else:
        ipycompss.start(graph=True, monitor=1000, trace=False)
```

```

*****
***** PyCOMPSs Interactive *****
*****
*
*      .~-._-..
*      :      )      |-----\      /-----\
*      :      |-----\      /-----\
*      .~ ~ -. \      /.- ~ ~ .
*      >      \      '      <      /-----/      \-----/
*      (      .- .-      )      | |----- -      /      /
*      \_-_-~ \_-_-! \_-_-!      |-----| |      /--/
*      (      :      )      -_-.-:-
*      ~--.      :      .-~      .-~      .-~      }
*      ~-_-_-_-~ \_-      .~      .-~      .-~
*      \ \      \ \      \ \      \ \      \ \      \ \
*      \ \      \ \      \ \      \ \      \ \      \ \
*      .- ~ ~-_-_- \ \      \ \      \ \      \ \
*      .-~      .- ~      }~ ~ ~-_-_-
*      .-~      .-~      :/~-.-~-.:/
*      /~_-_- .- ~      ~-.-~-_-
*      ~-.-<
*
*****
* - Starting COMPSs runtime...
* - Log path : /home/javier/.COMPSs/InteractiveMode_02/
* - PyCOMPSs Runtime started... Have fun!
*****

```

Importing task and parameter modules

Import task module before annotating functions or methods

```
[3]: from pycompss.api.task import task
      from pycompss.api.parameter import *
      from pycompss.api.api import compss_wait_on
```

10.1.2.3 Declaring tasks

Declare functions and decorate with `@task` those that should be tasks

```
[4]: @task(returns=int)
def square(val1):
    return val1 * val1
```

```
[5]: @task(returns=int)
def add(val2, val3):
    return val2 + val3
```

```
[6]: @task(returns=int)
def multiply(val1, val2):
    return val1 * val2
```

10.1.2.4 Invoking tasks

```
[7]: a = square(2)
Found task: square
```

```
[8]: b = add(a, 4)
Found task: add
```

```
[9]: c = multiply (b, 5)
Found task: multiply
```

Accessing data outside tasks requires synchronization

```
[10]: c = compss_wait_on(c)
```

```
[11]: c = c + 1
```

```
[12]: print("a: %s" % a)
print("b: %s" % b)
print("c: %d" % c)

a: <pycompss.runtime.management.classes.Future object at 0x7f2340f4e040>
b: <pycompss.runtime.management.classes.Future object at 0x7f2315523a30>
c: 41
```

```
[13]: a = compss_wait_on(a)
```

```
[14]: print("a: %d" % a)

a: 4
```

10.1.2.5 Stop the runtime

```
[15]: ipycompss.stop(sync=True)

*****
***** STOPPING PyCOMPSs *****
*****
Checking if any issue happened.
Synchronizing all future objects left on the user scope.
Found a future object: b
*****
```

```
[16]: print("Results after stopping PyCOMPSs: ")
print("a: %d" % a)
print("b: %d" % b)
print("c: %d" % c)
```

```
Results after stopping PyCOMPSs:
a: 4
b: 8
c: 41
```

10.1.3 PyCOMPSs: Using objects, lists, and synchronization

In this example we will see how classes and objects can be used from PyCOMPSs, and that class methods can become tasks.

10.1.3.1 Import the PyCOMPSs library

```
[1]: import pycompss.interactive as ipycompss
```

10.1.3.2 Start the runtime

Initialize COMPSs runtime Parameters indicates if the execution will generate task graph, tracefile, monitor interval and debug information.

```
[2]: import os
if 'BINDER_SERVICE_HOST' in os.environ:
    ipycompss.start(graph=True, debug=True,
                    project_xml='../xml/project.xml',
                    resources_xml='../xml/resources.xml')
else:
    ipycompss.start(graph=True, monitor=1000, debug=True)
```

```
*****
***** PyCOMPSs Interactive *****
*****
*      .-~-.--.      |      |      |      *
*      :          )    |____ \    / ____ \  *
*  .~ ~ -. \      /.- ~ ~ .    ____ ) |    | (____ ) | *
*  >      \ . . '      <    / ____/    \____ /    *
*  (      .- -.      )    | |____ _    / ____/    *
*  \ - .-~ \ - -' ~ - -' |_____| |    / __/      *
*  (      :          )      _ _ .-:      *
*  ~-- . :      .--~      .-~ .-~ }      *
```

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[illegible]

10.1.3.3 Importing task and arguments directionality modules

Import task module before annotating functions or methods

```
[3]: from pycompss.api.api import compss_barrier
      from pycompss.api.api import compss_wait_on
```

10.1.3.4 Declaring a class

```
[4]: %%writefile my_shaper.py

from pycompss.api.task import task
from pycompss.api.parameter import IN

class Shape(object):
    def __init__(self,x,y):
        self.x = x
        self.y = y

    @task(returns=int)
    def area(self):
        return self.x * self.y

    @task(returns=int)
    def perimeter(self):
        return 2 * self.x + 2 * self.y

    def describe(self,text):
        self.description = text

    @task()
    def scaleSize(self,scale):
        self.x = self.x * scale
        self.y = self.y * scale

    @task(target_direction=IN)
    def infoShape(self):
        print('Shape x=', self.x, 'y= ', self.y)
```

Overwriting my_shaper.py

10.1.3.5 Invoking tasks

```
[5]: from my_shaper import Shape

[6]: my_shapes = []
     my_shapes.append(Shape(100,45))
     my_shapes.append(Shape(50,50))

[7]: all_areas = []

[8]: for this_shape in my_shapes:
     all_areas.append(this_shape.area())

[9]: # Need it if we want to synchronize nested objects
     all_areas = compss_wait_on(all_areas)
     print(all_areas)

[4500, 2500]

[10]: rectangle = Shape(200,25)
      rectangle.scaleSize(5)
      area_rectangle = rectangle.area()
      rectangle = compss_wait_on(rectangle)
      print('X = %d' % rectangle.x)
      area_rectangle = compss_wait_on(area_rectangle)
      print('Area = %d' % area_rectangle)

X = 1000
Area = 125000

[11]: all_perimeters=[]
      my_shapes.append(rectangle)
      for this_shape in my_shapes:
          this_shape.infoShape()
          all_perimeters.append(this_shape.perimeter())

[12]: all_perimeters = compss_wait_on(all_perimeters)
      print(all_perimeters)

[290, 200, 2250]
```

10.1.3.6 Stop the runtime

```
[13]: ipycompss.stop(sync=True)

*****
***** STOPPING PyCOMPSs *****
*****
Checking if any issue happened.
Synchronizing all future objects left on the user scope.
Found a list to synchronize: my_shapes
Found a list to synchronize: all_areas
Found a list to synchronize: all_perimeters
*****
```

10.1.4 PyCOMPSs: Using objects, lists, and synchronization

In this example we will see how classes and objects can be used from PyCOMPSs, and that class methods can become tasks.

10.1.4.1 Import the PyCOMPSs library

```
[1]: import pycompss.interactive as ipycompss
```

10.1.4.2 Start the runtime

Initialize COMPSs runtime Parameters indicates if the execution will generate task graph, tracefile, monitor interval and debug information.

```
[2]: import os
if 'BINDER_SERVICE_HOST' in os.environ:
    ipycompss.start(graph=True, debug=True,
                    project_xml='../xml/project.xml',
                    resources_xml='../xml/resources.xml')
else:
    ipycompss.start(graph=True, monitor=1000, debug=True, trace=False)
```

[illegible]

10.1.4.3 Importing task and arguments directionality modules

Import task module before annotating functions or methods

```
[3]: from pycompss.api.api import compss_barrier
from pycompss.api.api import compss_wait_on
from pycompss.api.task import task
```

10.1.4.4 Declaring a class

```
[4]: %%writefile my_shaper.py

from pycompss.api.task import task
from pycompss.api.parameter import IN

class Shape(object):
    def __init__(self,x,y):
        self.x = x
        self.y = y
        description = "This shape has not been described yet"

    @task(returns=int)
    def area(self):
        return self.x * self.y

    @task(returns=int)
    def perimeter(self):
        return 2 * self.x + 2 * self.y

    def describe(self,text):
        self.description = text

    @task()
    def scaleSize(self,scale):
        self.x = self.x * scale
        self.y = self.y * scale

    @task(target_direction=IN)
    def infoShape(self):
        print('Shape x=', self.x, 'y= ', self.y)
```

Overwriting my_shaper.py

```
[5]: @task(returns=int)
def addAll(*mylist):
    sum = 0
    for ll in mylist:
        sum = sum + ll
    return sum
```


10.1.4.5 Invoking tasks

```
[6]: from my_shaper import Shape

[7]: my_shapes = []
    my_shapes.append(Shape(100,45))
    my_shapes.append(Shape(50,50))
    my_shapes.append(Shape(10,100))
    my_shapes.append(Shape(20,30))

[8]: all_areas = []

[9]: for this_shape in my_shapes:
    all_areas.append(this_shape.area())

[10]: # Need it if we want to synchronize nested objects
    all_areas = compss_wait_on(all_areas)
    print(all_areas)

    [4500, 2500, 1000, 600]

[11]: rectangle = Shape(200,25)
    rectangle.scaleSize(5)
    area_rectangle = rectangle.area()
    rectangle = compss_wait_on(rectangle)
    print('X = %d' % rectangle.x)
    area_rectangle = compss_wait_on(area_rectangle)
    print('Area = %d' % area_rectangle)

    X = 1000
    Area = 125000

[12]: all_perimeters=[]
    my_shapes.append(rectangle)
    for this_shape in my_shapes:
        this_shape.infoShape()
        all_perimeters.append(this_shape.perimeter())

[13]: # all_perimeters = compss_wait_on(all_perimeters)
    # print all_perimeters

[14]: mysum = addAll(*all_perimeters)
    mysum = compss_wait_on(mysum)
    print(mysum)

    Task definition detected.
    Found task: addAll
    3060
```

10.1.4.6 Stop the runtime

```
[15]: ipycomps.stop(sync=True)

*****
***** STOPPING PyCOMPSs *****
*****
Checking if any issue happened.
Synchronizing all future objects left on the user scope.
Found a list to synchronize: my_shapes
Found a list to synchronize: all_areas
Found a list to synchronize: all_perimeters
*****
```

10.1.5 PyCOMPSs: Using objects, lists, and synchronization. Using collections.

In this example we will see how classes and objects can be used from PyCOMPSs, and that class methods can become tasks. The example also illustrates the use of collections

10.1.5.1 Import the PyCOMPSs library

```
[1]: import pycompss.interactive as ipycompss
```

10.1.5.2 Start the runtime

Initialize COMPSs runtime Parameters indicates if the execution will generate task graph, tracefile, monitor interval and debug information.

```
[2]: import os
    if 'BINDER_SERVICE_HOST' in os.environ:
        ipycompss.start(graph=True, debug=True,
                        project_xml='../xml/project.xml',
                        resources_xml='../xml/resources.xml')
    else:
        ipycompss.start(graph=True, monitor=1000, debug=True, trace=False)
```

[illegible]

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```
*****
* - Starting COMPSs runtime...                               *
* - Log path : /home/javier/.COMPSs/InteractiveMode_05/      *
* - PyCOMPSs Runtime started... Have fun!                    *
*****
```

10.1.5.3 Importing task and arguments directionality modules

Import task module before annotating functions or methods

```
[3]: from pycompss.api.api import compss_barrier
      from pycompss.api.api import compss_wait_on
      from pycompss.api.task import task
      from pycompss.api.parameter import *
```

10.1.5.4 Declaring a class

```
[4]: %%writefile my_shaper.py

from pycompss.api.task import task
from pycompss.api.parameter import IN

class Shape(object):
    def __init__(self,x,y):
        self.x = x
        self.y = y
        description = "This shape has not been described yet"

    @task(returns=int, target_direction=IN)
    def area(self):
        import time
        time.sleep(4)
        return self.x * self.y

    @task()
    def scaleSize(self,scale):
        import time
        time.sleep(4)
        self.x = self.x * scale
        self.y = self.y * scale

    @task(returns=int, target_direction=IN)
    def perimeter(self):
        import time
        time.sleep(4)
        return 2 * self.x + 2 * self.y

    def describe(self,text):
        self.description = text

    @task(target_direction=IN)
    def infoShape(self):
        import time
```

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```
time.sleep(1)
print('Shape x=', self.x, 'y= ', self.y)
```

Overwriting my_shaper.py

[5]: *#Operations with collections: previous to release 2.5*

```
@task(returns=1)
def addAll(*mylist):
    import time
    time.sleep(1)
    sum = 0
    for ll in mylist:
        sum = sum + ll
    return sum
```

[6]: @task(returns=int, mylist=COLLECTION_IN)

```
def addAll_C(mylist):
    import time
    time.sleep(4)
    sum = 0
    for ll in mylist:
        sum = sum + ll
    return sum
```

[7]: @task(returns=2, mylist=COLLECTION_IN, my_otherlist=COLLECTION_IN)

```
def addAll_C2(mylist, my_otherlist):
    import time
    time.sleep(4)
    sum = 0
    sum2 = 0
    for ll in mylist:
        sum = sum + ll
    for jj in my_otherlist:
        sum2 = sum2 + jj
    return sum, sum2
```

[8]: @task(mylist=COLLECTION_INOUT)

```
def scale_all(mylist, scale):
    import time
    time.sleep(4)
    for ll in mylist:
        ll.x = ll.x * scale
        ll.y = ll.y * scale
```

10.1.5.5 Invoking tasks

[9]: `from my_shaper import Shape`

[10]: `my_shapes = []`
`my_shapes.append(Shape(100,45))`
`my_shapes.append(Shape(50,50))`
`my_shapes.append(Shape(10,100))`
`my_shapes.append(Shape(20,30))`

```
[11]: all_areas = []
```

```
[12]: for this_shape in my_shapes:
      all_areas.append(this_shape.area())
```

10.1.5.6 Synchronizing results from tasks

```
[13]: all_areas = compss_wait_on(all_areas)
      print(all_areas)

[4500, 2500, 1000, 600]
```

```
[14]: rectangle = Shape(200,25)
      rectangle.scaleSize(5)
      area_rectangle = rectangle.area()
      rectangle = compss_wait_on(rectangle)
      print('X =', rectangle.x)
      area_rectangle = compss_wait_on(area_rectangle)
      print('Area =', area_rectangle)

X = 1000
Area = 125000
```

10.1.5.7 Accessing data in collections

```
[15]: all_perimeters = []
      my_shapes.append(rectangle)
      for this_shape in my_shapes:
          all_perimeters.append(this_shape.perimeter())
```

```
[16]: mysum = addAll_C(all_perimeters)
      mysum = compss_wait_on(mysum)
      print(mysum)

Task definition detected.
Found task: addAll_C
3060
```

```
[17]: # Previous version without collections
      # mysum = addAll(*all_perimeters)
      # mysum = compss_wait_on(mysum)
      # print(mysum)
```

10.1.5.8 Accessing two collections

```
[18]: all_perimeters = []
      all_areas = []
      for this_shape in my_shapes:
          all_perimeters.append(this_shape.perimeter())
          all_areas.append(this_shape.area())
```

```
[19]: [my_per, my_area] = addAll_C2(all_perimeters, all_areas)
      [my_per, my_area] = compss_wait_on([my_per, my_area])
      print([my_per, my_area])
```

```
Task definition detected.
Found task: addAll_C2
[3060, 133600]
```

10.1.5.9 Scattering data from a collection

```
[20]: scale_all(my_shapes,2)
      scaled_areas=[]
      for this_shape in my_shapes:
          scaled_areas.append(this_shape.area())

      scaled_areas = compss_wait_on(scaled_areas)
      print(scaled_areas)
```

```
Task definition detected.
Found task: scale_all
[18000, 10000, 4000, 2400, 500000]
```

10.1.5.10 Stop the runtime

```
[21]: ipycompss.stop(sync=True)

*****
***** STOPPING PyCOMPSs *****
*****
Checking if any issue happened.
Synchronizing all future objects left on the user scope.
Found a list to synchronize: my_shapes
Found a list to synchronize: all_areas
Found a list to synchronize: all_perimeters
Found a list to synchronize: scaled_areas
*****
```

10.1.6 PyCOMPSs: Using objects, lists, and synchronization. Using dictionary.

In this example we will see how classes and objects can be used from PyCOMPSs, and that class methods can become tasks. The example also illustrates the use of dictionary

10.1.6.1 Import the PyCOMPSs library

```
[1]: import pycompss.interactive as ipycompss
```


10.1.6.4 Declaring a class

```
[4]: %%writefile my_shaper.py

from pycompss.api.task import task
from pycompss.api.parameter import IN

class Shape(object):
    def __init__(self,x,y):
        self.x = x
        self.y = y
        description = "This shape has not been described yet"

    @task(returns=int, target_direction=IN)
    def area(self):
        import time
        time.sleep(4)
        return self.x * self.y

    @task()
    def scaleSize(self,scale):
        import time
        time.sleep(4)
        self.x = self.x * scale
        self.y = self.y * scale

    @task(returns=int, target_direction=IN)
    def perimeter(self):
        import time
        time.sleep(4)
        return 2 * self.x + 2 * self.y

    def describe(self,text):
        self.description = text

    @task(target_direction=IN)
    def infoShape(self):
        import time
        time.sleep(1)
        print('Shape x=', self.x, 'y= ', self.y)
```

Overwriting my_shaper.py

```
[5]: @task(returns=int, mydict = DICTIONARY_IN)
def addAll(mydict):
    import time
    time.sleep(4)
    sum = 0
    for key, value in mydict.items():
        sum = sum + value
    return sum

[6]: @task(returns=2, mydict=DICTIONARY_IN, my_otherdict=DICTIONARY_IN)
def addAll_2(mydict, my_otherdict):
    import time
    time.sleep(4)
    sum = 0
```

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```

sum2 = 0
for key, value in mydict.items():
    sum = sum + value
for key2, value2 in my_otherdict.items():
    sum2 = sum2 + value2
return sum, sum2

```

```

[7]: @task(mydict=DICTIONARY_INOUT)
def scale_all(mydict, scale):
    import time
    time.sleep(4)
    for key, value in mydict.items():
        mydict[key].x = value.x * scale
        mydict[key].y = value.y * scale

```

10.1.6.5 Invoking tasks

```

[8]: from my_shaper import Shape

```

```

[9]: my_shapes = {}
my_shapes["rectangle"] = Shape(100,45)
my_shapes["square"] = Shape(50,50)
my_shapes["long_rectangle"] = Shape(10,100)
my_shapes["small_rectangle"] = Shape(20,30)

```

```

[10]: all_areas = {}

```

```

[11]: for key, value in my_shapes.items():
    all_areas[key] = value.area()

```

10.1.6.6 Synchronizing results from tasks

```

[12]: all_areas = compss_wait_on(all_areas)
print(all_areas)

{'rectangle': 4500, 'square': 2500, 'long_rectangle': 1000, 'small_rectangle': 600}

```

```

[13]: rectangle = Shape(200,25)
rectangle.scaleSize(5)
area_rectangle = rectangle.area()
rectangle = compss_wait_on(rectangle)
print('X =', rectangle.x)
area_rectangle = compss_wait_on(area_rectangle)
print('Area =', area_rectangle)

X = 1000
Area = 125000

```

10.1.6.7 Accessing data in collections

```
[14]: all_perimeters = {}  
my_shapes["new_shape"] = rectangle  
for key, value in my_shapes.items():  
    all_perimeters[key] = value.perimeter()
```

```
[15]: mysum = addAll(all_perimeters)  
mysum = compss_wait_on(mysum)  
print(mysum)
```

```
Task definition detected.  
Found task: addAll  
3060
```

10.1.6.8 Accessing two collections

```
[16]: all_perimeters = {}  
all_areas = {}  
for key, value in my_shapes.items():  
    all_perimeters[key] = value.perimeter()  
    all_areas[key] = value.area()
```

```
[17]: [my_per, my_area] = addAll_2(all_perimeters, all_areas)  
[my_per, my_area] = compss_wait_on([my_per, my_area])  
print([my_per, my_area])
```

```
Task definition detected.  
Found task: addAll_2  
[3060, 133600]
```

10.1.6.9 Scattering data from a collection

```
[18]: scale_all(my_shapes, 2)  
scaled_areas = {}  
for key, value in my_shapes.items():  
    scaled_areas[key] = value.area()  
  
scaled_areas = compss_wait_on(scaled_areas)  
print(scaled_areas)
```

```
Task definition detected.  
Found task: scale_all  
{'rectangle': 18000, 'square': 10000, 'long_rectangle': 4000, 'small_rectangle': 2400, 'new_  
↪shape': 500000}
```

10.1.6.10 Stop the runtime

```
[19]: ipycompss.stop(sync=True)

*****
***** STOPPING PyCOMPSs *****
*****
Checking if any issue happened.
Synchronizing all future objects left on the user scope.
*****
```

10.1.7 PyCOMPSs: Using objects, lists, and synchronization. Managing fault-tolerance.

In this example we will see how classes and objects can be used from PyCOMPSs, and that class methods can become tasks. The example also illustrates the current fault-tolerance management provided by the runtime.

10.1.7.1 Import the PyCOMPSs library

```
[1]: import ipycompss.interactive as ipycompss
```

10.1.7.2 Start the runtime

Initialize COMPSs runtime Parameters indicates if the execution will generate task graph, tracefile, monitor interval and debug information.

```
[2]: import os
if 'BINDER_SERVICE_HOST' in os.environ:
    ipycompss.start(graph=True, debug=False,
                    project_xml='../xml/project.xml',
                    resources_xml='../xml/resources.xml')
else:
    ipycompss.start(graph=True, monitor=1000, trace=False, debug=False)

*****
***** PyCOMPSs Interactive *****
*****
*      .-~~-.-.-.      |____\      /____\      *
*      :          )    |____\      /____\      *
*      .~ ~-.-.\      /.- ~ ~ .    |____|      | (____) |      *
*      >        \      /      <    /____/      \_____/      *
*      (         .-.-.      )    |____|      /____/      *
*      '-.-.-~ -.-.-' ~.-.-' |____|      /____/      *
*      (         :         )    |____|      /____/      *
*      ~-.-. :         .-.-~      .-.-~      }      *
*      ~-.-.-.-~ \      .~ .-.-~      *
*      \      \      \      \      *
*      \      \      \      \      *
*      .- ~ ~-.-.-\      \      *
*      .- ~ ~-.-.-} ~ ~-.-.-      *
*      /~ .-.-.      .-~      :/~-.-.-./:      *
*      /~ -.-.- ~      ~-.-.-      *
*      ~-.-.-      *
*****
```

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```
* - Starting COMPSs runtime... *
* - Log path : /home/javier/.COMPSs/InteractiveMode_07/
* - PyCOMPSs Runtime started... Have fun! *
*****
```

10.1.7.3 Importing task and arguments directionality modules

Import task module before annotating functions or methods

```
[3]: from pycompss.api.api import compss_barrier
from pycompss.api.api import compss_wait_on
from pycompss.api.task import task
from pycompss.api.parameter import *
```

10.1.7.4 Declaring a class

```
[4]: %%writefile my_shaper.py

from pycompss.api.task import task
from pycompss.api.parameter import IN
import sys

class Shape(object):
    def __init__(self,x,y):
        self.x = x
        self.y = y
        description = "This shape has not been described yet"

    @task(returns=int, target_direction=IN)
    def area(self):
        return self.x * self.y

    @task()
    def scaleSize(self,scale):
        self.x = self.x * scale
        self.y = self.y * scale

    # on_failure= 'IGNORE', on_failure= 'RETRY', on_failure= 'FAIL', 'CANCEL_SUCCESORS'
    @task(on_failure= 'CANCEL_SUCCESORS')
    def downScale(self,scale):
        if (scale <= 0):
            sys.exit(1)
        else:
            self.x = self.x/scale
            self.y = self.y/scale

    @task(returns=int, target_direction=IN)
    def perimeter(self):
        return 2 * self.x + 2 * self.y

    def describe(self,text):
        self.description = text
```

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```
@task(target_direction=IN)
def infoShape(self):
    print('Shape x=', self.x, 'y= ', self.y)
```

Overwriting my_shaper.py

10.1.7.5 Invoking tasks

```
[5]: from my_shaper import Shape
```

```
[6]: my_shapes = []
my_shapes.append(Shape(100,45))
my_shapes.append(Shape(50,50))
my_shapes.append(Shape(10,100))
my_shapes.append(Shape(20,30))
my_shapes.append(Shape(200,25))
```

```
[7]: all_perimeters = []
```

```
[8]: i=4
for this_shape in my_shapes:
    this_shape.scaleSize(2)
    this_shape.area()
    i = i - 1
    this_shape.downScale(i)
    all_perimeters.append(this_shape.perimeter())
```

10.1.7.6 Synchronizing results from tasks

```
[9]: # all_perimeters = compss_wait_on(all_perimeters)
# print all_perimeters
```

10.1.7.7 Stop the runtime

```
[10]: ipycompss.stop(sync=False)
```

```
*****
***** STOPPING PyCOMPSs *****
*****
Checking if any issue happened.
```

```
[ERRMGR] - WARNING: Job 15, running Task 15 on worker localhost, has failed.
[ERRMGR] - WARNING: Notifying task 15 failure
[ERRMGR] - WARNING: Task 'my_shaper.Shape.downScale' TOTALLY FAILED.
[ERRMGR] - WARNING: Task 16(Action: 16) with name my_shaper.Shape.perimeter has been
→cancelled.
[ERRMGR] - WARNING: Task failed: [[Task id: 15], [Status: FAILED], [Core id: 2], [Priority:
→false], [NumNodes: 1], [MustReplicate: false], [MustDistribute: false], [my_shaper.Shape.
→downScale(INT_T)]]
[ERRMGR] - WARNING: Task canceled: [[Task id: 16], [Status: CANCELED], [Core id: 3],
→[Priority: false], [NumNodes: 1], [MustReplicate: false], [MustDistribute: false], [my_
→shaper.Shape.perimeter()]]
```

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```
[ERRMGR] - WARNING: Job 18, running Task 19 on worker localhost, has failed.
[ERRMGR] - WARNING: Notifying task 19 failure
[ERRMGR] - WARNING: Task 'my_shaper.Shape.downScale' TOTALLY FAILED.
[ERRMGR] - WARNING: Task 20(Action: 20) with name my_shaper.Shape.perimeter has been↵
↵cancelled.
[ERRMGR] - WARNING: Task failed: [[Task id: 19], [Status: FAILED], [Core id: 2], [Priority:↵
↵false], [NumNodes: 1], [MustReplicate: false], [MustDistribute: false], [my_shaper.Shape.
↵downScale(INT_T)]]
[ERRMGR] - WARNING: Task canceled: [[Task id: 20], [Status: CANCELED], [Core id: 3],↵
↵[Priority: false], [NumNodes: 1], [MustReplicate: false], [MustDistribute: false], [my_
↵shaper.Shape.perimeter()]]
```

Warning: some of the variables used with PyCOMPSs may have not been brought to the master.

10.1.8 PyCOMPSs: Using files

In this example we will how files can be used with PyCOMPSs.

10.1.8.1 Import the PyCOMPSs library

```
[1]: import pycompss.interactive as ipycompss
```

10.1.8.2 Start the runtime

Initialize COMPSs runtime Parameters indicates if the execution will generate task graph, tracefile, monitor interval and debug information.

```
[2]: import os
if 'BINDER_SERVICE_HOST' in os.environ:
    ipycompss.start(graph=True, debug=False,
                    project_xml='../xml/project.xml',
                    resources_xml='../xml/resources.xml')
else:
    ipycompss.start(graph=True, monitor=1000, trace=False, debug=False)
```

[illegible]

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```

*      /_~_ _ . - ~      ~-.~-.~_      *
*      ~-.<      *
*****
* - Starting COMPSs runtime...      *
* - Log path : /home/javier/.COMPSs/InteractiveMode_08/
* - PyCOMPSs Runtime started... Have fun!      *
*****

```

10.1.8.3 Importing task and parameter modules

Import task module before annotating functions or methods

```

[3]: from pycompss.api.task import task
      from pycompss.api.parameter import FILE_IN, FILE_OUT, FILE_INOUT
      from pycompss.api.api import compss_wait_on, compss_open

```

10.1.8.4 Declaring tasks

Declare functions and decorate with @task those that should be tasks

```

[4]: @task(fout=FILE_OUT)
      def write(fout, content):
          with open(fout, 'w') as fout_d:
              fout_d.write(content)

[5]: @task(finout=FILE_INOUT)
      def append(finout):
          finout_d = open(finout, 'a')
          finout_d.write("\n====> INOUT FILE ADDED CONTENT")
          finout_d.close()

[6]: @task(fin=FILE_IN, returns=str)
      def readFile(fin):
          fin_d = open(fin, 'r')
          content = fin_d.read()
          fin_d.close()
          return content

```

10.1.8.5 Invoking tasks

```

[7]: f = "myFile.txt"
      content = "OUT FILE CONTENT"
      write(f, content)

      Found task: write

```

```

[8]: append(f)

      Found task: append

```

```

[9]: readed = readFile(f)

```

```
Found task: readFile
```

```
[10]: append(f)
```

Accessing data outside tasks requires synchronization

```
[11]: readed = compss_wait_on(readed)
print(readed)
```

```
OUT FILE CONTENT
==> INOUT FILE ADDED CONTENT
```

```
[12]: with compss_open(f) as fd:
        f_content = fd.read()
print(f_content)
```

```
OUT FILE CONTENT
==> INOUT FILE ADDED CONTENT
==> INOUT FILE ADDED CONTENT
```

10.1.8.6 Stop the runtime

```
[13]: ipycompss.stop(sync=True)
```

```
*****
***** STOPPING PyCOMPSs *****
*****
Checking if any issue happened.
Synchronizing all future objects left on the user scope.
*****
```

10.1.9 PyCOMPSs: Using constraints

In this example we will how to define task constraints with PyCOMPSs.

10.1.9.1 Import the PyCOMPSs library

```
[1]: import pycompss.interactive as ipycompss
```

10.1.9.2 Starting runtime

Initialize COMPSs runtime Parameters indicates if the execution will generate task graph, tracefile, monitor interval and debug information.

```
[2]: import os
if 'BINDER_SERVICE_HOST' in os.environ:
    ipycompss.start(graph=True, debug=False,
                    project_xml='../xml/project.xml',
                    resources_xml='../xml/resources.xml')
else:
    ipycompss.start(graph=True, monitor=1000, trace=True, debug=False)
```


[illegible]

10.1.9.3 Importing task and arguments directionality modules

Import task module before annotating functions or methods

```
[3]: from pycompss.api.task import task
from pycompss.api.parameter import *
from pycompss.api.api import compss_barrier
from pycompss.api.constraint import constraint
from pycompss.api.implement import implement
```

10.1.9.4 Declaring tasks

Declare functions and decorate with `@task` those that should be tasks

```
[4]: @constraint(computing_units="2")
    @task(returns=int)
    def square(val1):
        return val1 * val1
```

```
[5]: @constraint(computing_units="1")
    @task(returns=int)
    def add(val2, val3):
        return val2 + val3
```

```
[6]: @constraint(computing_units="4")
    @task(returns=int)
    def multiply(val1, val2):
        return val1 * val2
```

10.1.9.5 Invoking tasks

```
[7]: for i in range(20):
      r1 = square(i)
      r2 = add(r1,i)
      r3 = multiply(r2,r1)

      compss_barrier()

Found task: square
Found task: add
Found task: multiply
```

10.1.9.6 Stop the runtime

```
[8]: ipycompss.stop(sync=True)

*****
***** STOPPING PyCOMPSs *****
*****
Checking if any issue happened.
Synchronizing all future objects left on the user scope.
Found a future object: r1
Found a future object: r2
Found a future object: r3
*****
```

```
[9]: print(r1)
      print(r2)
      print(r3)

361
380
137180
```

10.1.10 PyCOMPSs: Polymorphism

In this example we will how to use polimorphism with PyCOMPSs.

10.1.10.1 Import the PyCOMPSs library

```
[1]: import pycompss.interactive as ipycompss
```

10.1.10.2 Start the runtime

Initialize COMPSs runtime Parameters indicates if the execution will generate task graph, tracefile, monitor interval and debug information.

```
[2]: import os
      if 'BINDER_SERVICE_HOST' in os.environ:
          ipycompss.start(graph=True, debug=False,
                          project_xml='../xml/project.xml',
                          resources_xml='../xml/resources.xml')
```

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```
else:
    ipycompss.start(graph=True, monitor=1000, trace=False, debug=False)
```

```
*****
***** PyCOMPSs Interactive *****
*****
*
*      .-~~-.-.
*      :      )      |____ \      /____ \
*      .~ ~-.\      /.- ~ ~ .      ____ ) |      | (____ ) |
*      >      \      . '      <      /____/      \_____/
*      (      .-.-.      )      | |____ _      /      /
*      \-.-~ \-.-' ~-.-' |____| |      /____/
*      (      :      )      -.-.-:
*      ~-.-. :      .-.-~      .-.-.-~ }
*      ~-.-.-~ \      .~ .-.-~
*      \      \      \      \      \
*      \      \      \      \      \
*      . - ~ ~-.- \      \      \
*      .-.-~ . - ~ ~} ~ ~-.-.
*      . ' .-.- .-.- :/~-.-./:
*      /-.- . - ~      ~-.-.-
*      ~-.-<
*****
* - Starting COMPSs runtime...
* - Log path : /home/javier/.COMPSs/InteractiveMode_10/
* - PyCOMPSs Runtime started... Have fun!
*****
```

10.1.10.3 Create a file to define the tasks

Importing task, implement and constraint modules

```
[3]: %%writefile module.py

from pycompss.api.task import task
from pycompss.api.implement import implement
from pycompss.api.constraint import constraint

Writing module.py
```

10.1.10.4 Declaring tasks into the file

Declare functions and decorate with @task those that should be tasks

```
[4]: %%writefile -a module.py

@constraint(computing_units='1')
@task(returns=list)
def addtwovectors(list1, list2):
    for i in range(len(list1)):
        list1[i] += list2[i]
    return list1

Appending to module.py
```

```
[5]: %%writefile -a module.py

@implement(source_class="module", method="addtwovectors")
@constraint(computing_units='4')
@task(returns=list)
def addtwovectorsWithNumpy(list1, list2):
    import numpy as np
    x = np.array(list1)
    y = np.array(list2)
    z = x + y
    return z.tolist()
```

Appending to module.py

10.1.10.5 Invoking tasks

```
[6]: from pycompss.api.api import compss_wait_on
from module import addtwovectors # Just import and use addtwovectors
from random import random

vectors = 100
vector_length = 5000
vectors_a = [[random() for i in range(vector_length)] for i in range(vectors)]
vectors_b = [[random() for i in range(vector_length)] for i in range(vectors)]

results = []
for i in range(vectors):
    results.append(addtwovectors(vectors_a[i], vectors_b[i]))
```

Accessing data outside tasks requires synchronization

```
[7]: results = compss_wait_on(results)
print(len(results))
print(results[0])

100
[1.1342111850577536, 0.5278806345422292, 1.7941518439053241, 0.477653194894226, 1.
→643013525597227, 0.6045875820938854, 1.3846094340234631, 1.0876896292407676, 0.
→8244129257491345, 1.4043757995506223, 0.3056240277168034, 0.9201439479275588, 1.
→246609587866201, 1.2687853546889625, 1.4683707828223982, 0.8593918066098046, 1.
→4914222265622252, 1.9175226487486383, 1.397593438527184, 0.799869415930711, 1.
→7839321841565448, 1.655664412093415, 0.706206155776546, 1.0514874173801259, 1.
→1741535712194424, 0.7816711714346283, 0.3709620768909637, 1.2421283483285572, 1.
→0898514081809914, 1.7119215417673588, 1.43035279168674, 0.31335527355349213, 1.
→2130943648505186, 0.8609455786135065, 0.970040083675359, 0.9493184902133436, 0.
→7455981142716729, 1.4261010705365287, 1.3006884738220161, 0.794818426368219, 1.
→6078648432243612, 1.8146416498733728, 1.6262307529486548, 1.1076894390611458, 1.
→188617847835821, 0.565889835111468, 0.3765595525929517, 1.144012272635464, 1.
→1269479981959045, 1.5779476598395945, 0.5310416609319845, 1.2137146824340994, 1.
→3115412433664884, 1.3302391252758574, 1.092595718830884, 0.5971210231687093, 1.
→1248315975536989, 0.23336156073497716, 1.2986094731417164, 0.8567830336155204, 1.
→0204230133832413, 1.0426277660329069, 1.7457395348340272, 1.4979604887008002, 0.
→8999443968466122, 1.4610993201757707, 1.0434640443395091, 0.6804818160272217, 1.
→4371220774959597, 0.968686692289904, 1.1876358267837062, 1.291750511582375, 0.
→27877854842348593, 0.8217107391322082, 0.7850745749977232, 0.8523202575880965, 1.
→3886142437375102, 0.6232592725501601, 0.7998842122724923, 1.7132197658739705,
→0330350895263634, 0.3117934109281717, 0.5185430494930532, 0.9387478919316365, 0.
→7454802352345299, 1.6802344758730607, 0.7644442608577788, 0.7564584668865939, 1.
→922484237126712, 1.1568822733714978, 0.6158415795264056, 1.4257938142255737, 1.
→1458452771762542, 1.0372175606985587, 1.4077745052139004, 1.3703714582458701, 1.
→3879941521630865, 1.9010169842232587, 0.5109223444345973, 1.25749671734493, 1.
→5782547444429478, 1.6479874937676084, 0.40217473662961434, 1.119986901274799, 1.
```

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10.1.10.6 Stop the runtime

```
[8]: ipycompss.stop(sync=True)

*****
***** STOPPING PyCOMPSs *****
*****
Checking if any issue happened.
Synchronizing all future objects left on the user scope.
Found a list to synchronize: vectors_a
Found a list to synchronize: vectors_b
Found a list to synchronize: results
*****
```

10.1.11 PyCOMPSs: Other decorators - *Binary*

In this example we will how to invoke binaries as tasks with PyCOMPSs.

10.1.11.1 Import the PyCOMPSs library

```
[1]: import pycompss.interactive as ipycompss
```

10.1.11.2 Start the runtime

Initialize COMPSs runtime Parameters indicates if the execution will generate task graph, tracefile, monitor interval and debug information.

```
[2]: import os
if 'BINDER_SERVICE_HOST' in os.environ:
    ipycompss.start(debug=False,
                    project_xml='../xml/project.xml',
                    resources_xml='../xml/resources.xml')
else:
    ipycompss.start(graph=True, monitor=1000, trace=True, debug=True)
```

```
*****
***** PyCOMPSs Interactive *****
*****
*          .-~-.--.          *
*          :          )      |____ \      /____ \      *
*          .~ ~ -. \      /.- ~ ~ .      ____ ) |      | (____ ) | *
*          >          \      /      <      /____/      \_____/      *
*          (          .- -.      )      | |____ _      /      /      *
*          \ - -. ~ \ - -.      | ____ | |      /____/      *
*          (          :          )      - - - - -      *
*          ~ - -.      :          .-~-.--.      }      *
*          ~ - -. ~ - -. \      .~ .-~-.~ - ~      *
*          \ - -. ~ - -. \ \      \ \      - ~      *
*          \ \      \ \      //      //      *
*          . - ~ ~ - -. \ \      //      *
*          .-~ . - ~ ~ } ~ ~ - -.~ - .      *
```

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```

*      .! .-~      .-~      :/~-.~-./:      *
*      /_~_ _ . - ~      ~-.~-. _      *
*      ~-.<      *
*****
* - Starting COMPSs runtime...      *
* - Log path : /home/javier/.COMPSs/InteractiveMode_11/      *
* - PyCOMPSs Runtime started... Have fun!      *
*****

```

10.1.11.3 Importing task and binary modules

Import task module before annotating functions or methods

```
[3]: from pycompss.api.task import task
from pycompss.api.binary import binary
from pycompss.api.parameter import *
```

10.1.11.4 Declaring tasks

Declare functions and decorate with @task those that should be tasks and with @binary the ones that execute a binary file

```
[4]: @binary(binary="sed")
@task(file=FILE_INOUT)
def sed(flag, expression, file):
    # Equivalent to: $ sed flag expression file
    pass
```

```
[5]: @binary(binary="grep")
@task(infile={Type:FILE_IN, StdIOStream:STDIN}, result={Type:FILE_OUT, StdIOStream:STDOUT})
def grep(keyword, infile, result):
    # Equivalent to: $ grep keyword < infile > result
    pass
```

10.1.11.5 Invoking tasks

```
[6]: from pycompss.api.api import compss_open

finout = "inoutfile.txt"
with open(finout, 'w') as finout_d:
    finout_d.write("Hi, this a simple test!")
    finout_d.write("\nHow are you?")

sed('-i', 's/Hi/Hello/g', finout)
fout = "outfile.txt"
grep("Hello", finout, fout)

Task definition detected.
Found task: sed
Task definition detected.
Found task: grep
```

Accessing data outside tasks requires synchronization

```
[7]: # Check the result of 'sed'
with compss_open(finout, "r") as finout_r:
    sedresult = finout_r.read()
print(sedresult)
```

Hello, this a simple test!
How are you?

```
[8]: # Check the result of 'grep'
with compss_open(fout, "r") as fout_r:
    grepresult = fout_r.read()
print(grepresult)
```

Hello, this a simple test!

10.1.11.6 Stop the runtime

```
[9]: ipycompss.stop(sync=True)

*****
***** STOPPING PyCOMPSs *****
*****
Checking if any issue happened.
Synchronizing all future objects left on the user scope.
[ERRMGR] - WARNING: Error while trying to merge files
*****
```

10.1.12 PyCOMPSs: Integration with Numba

In this example we will how to use Numba with PyCOMPSs.

10.1.12.1 Import the PyCOMPSs library

```
[1]: import pycompss.interactive as ipycompss
```

10.1.12.2 Starting runtime

Initialize COMPSs runtime Parameters indicates if the execution will generate task graph, tracefile, monitor interval and debug information.

```
[2]: import os
if 'BINDER_SERVICE_HOST' in os.environ:
    ipycompss.start(graph=True, debug=False,
                    project_xml='../xml/project.xml',
                    resources_xml='../xml/resources.xml')
else:
    ipycompss.start(graph=True, monitor=1000, trace=True, debug=False)

*****
***** PyCOMPSs Interactive *****
```

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```

*****
*                               *
*      .~..-.-.                |-----| |-----| *
*      :      )                |-----| |-----| *
*      .~..-.-. \      /.- ~.  |-----| |-----| *
*      >      \      /      <  |-----| |-----| *
*      (      .~..-.-. )      |-----| |-----| *
*      \      /      /      \  |-----| |-----| *
*      (      :      )      .~..-.-. *
*      ~..-.-. :      .~..-.-. } *
*      ~..-.-. \      /      .~..-.-. *
*      \      /      /      \  // *
*      .~..-.-. \      /      .~..-.-. *
*      .~..-.-. } ~..-.-. *
*      .~..-.-. :/~..-.-./: *
*      /~..-.-. ~..-.-. *
*      ~..-.-. < *
*****
* - Starting COMPSs runtime... *
* - Log path : /home/javier/.COMPSs/InteractiveMode_12/ *
* - PyCOMPSs Runtime started... Have fun! *
*****

```

10.1.12.3 Importing task and arguments directionality modules

Import task module before annotating functions or methods

```
[3]: from pycompss.api.task import task
      from pycompss.api.parameter import *
      from pycompss.api.api import compss_barrier
      from pycompss.api.api import compss_wait_on
```

10.1.12.4 Importing other modules

Import the time and numpy modules

```
[4]: import time
      import numpy as np
```

10.1.12.5 Declaring tasks

Declare functions and decorate with @task those that should be tasks – Note that they are exactly the same but the “numba” parameter in the @task decorator

```
[5]: @task(returns=1, numba=False) # Default: numba=False
      def ident_loops(x):
          r = np.empty_like(x)
          n = len(x)
          for i in range(n):
              r[i] = np.cos(x[i]) ** 2 + np.sin(x[i]) ** 2
          return r
```



```
[6]: @task(returns=1, numba=True)
def ident_loops_jit(x):
    r = np.empty_like(x)
    n = len(x)
    for i in range(n):
        r[i] = np.cos(x[i]) ** 2 + np.sin(x[i]) ** 2
    return r
```

10.1.12.6 Invoking tasks

```
[7]: size = 1000000
ntasks = 8

# Run some tasks without numba jit
start = time.time()
for i in range(ntasks):
    out = ident_loops(np.arange(size))
compss_barrier()
end = time.time()

# Run some tasks with numba jit
start_jit = time.time()
for i in range(ntasks):
    out_jit = ident_loops_jit(np.arange(size))
compss_barrier()
end_jit = time.time()

# Get the last result of each run to compare that the results are ok
out = compss_wait_on(out)
out_jit = compss_wait_on(out_jit)

print("TIMING RESULTS:")
print("* ident_loops      : %s seconds" % str(end - start))
print("* ident_loops_jit   : %s seconds" % str(end_jit - start_jit))
if len(out) == len(out_jit) and list(out) == list(out_jit):
    print("* SUCCESS: Results match.")
else:
    print("* FAILURE: Results are different!!!")

Found task: ident_loops
Found task: ident_loops_jit
TIMING RESULTS:
* ident_loops      : 0.06554532051086426 seconds
* ident_loops_jit   : 0.05343270301818848 seconds
* SUCCESS: Results match.
```

10.1.12.7 Stop the runtime

```
[8]: ipycompss.stop(sync=False)

*****
***** STOPPING PyCOMPSs *****
*****
Checking if any issue happened.
Warning: some of the variables used with PyCOMPSs may
        have not been brought to the master.
*****
```

10.1.13 Dislib tutorial

This tutorial will show the basics of using [dislib](#).

10.1.13.1 Setup

First, we need to start an interactive PyCOMPSs session:

[illegible]

Next, we import `dislib` and we are all set to start working!

```
[2]: import dislib as ds
```

10.1.13.2 Distributed arrays

The main data structure in dislib is the distributed array (or ds-array). These arrays are a distributed representation of a 2-dimensional array that can be operated as a regular Python object. Usually, rows in the array represent samples, while columns represent features.

To create a random array we can run the following NumPy-like command:

```
[3]: x = ds.random_array(shape=(500, 500), block_size=(100, 100))
      print(x.shape)
      x
(500, 500)
[3]: ds-array(blocks=(...), top_left_shape=(100, 100), reg_shape=(100, 100), shape=(500, 500),
      ↪sparse=False)
```

Now `x` is a 500x500 ds-array of random numbers stored in blocks of 100x100 elements. Note that `x` is not stored in memory. Instead, `random_array` generates the contents of the array in tasks that are usually executed remotely. This allows the creation of really big arrays.

The content of `x` is a list of `Futures` that represent the actual data (wherever it is stored).

To see this, we can access the `_blocks` field of `x`:

```
[4]: x._blocks[0][0]
[4]: <pycompss.runtime.management.classes.Future at 0x7fb7a58ca8b0>
```

`block_size` is useful to control the granularity of dislib algorithms.

To retrieve the actual contents of `x`, we use `collect`, which synchronizes the data and returns the equivalent NumPy array:

```
[5]: x.collect()
[5]: array([[0.48604732, 0.68571232, 0.98557605, ..., 0.51530027, 0.39511585,
            0.42942001],
          [0.03398195, 0.40964073, 0.5437061 , ..., 0.16162333, 0.79046618,
            0.71677277],
          [0.82399233, 0.80869154, 0.16965568, ..., 0.79380114, 0.31004525,
            0.51511589],
          ...,
          [0.57630698, 0.72028925, 0.11842501, ..., 0.92236462, 0.5837854 ,
            0.92114111],
          [0.84521256, 0.17909749, 0.42140394, ..., 0.95331429, 0.01587735,
            0.58532187],
          [0.81065273, 0.5666422 , 0.65635218, ..., 0.58820423, 0.42493203,
            0.84351429]])
```

Another way of creating ds-arrays is using array-like structures like NumPy arrays or lists:

```
[6]: x1 = ds.array([[1, 2, 3], [4, 5, 6]], block_size=(1, 3))
      x1
[6]: ds-array(blocks=(...), top_left_shape=(1, 3), reg_shape=(1, 3), shape=(2, 3), sparse=False)
```

Distributed arrays can also store sparse data in CSR format:

```
[7]: from scipy.sparse import csr_matrix

sp = csr_matrix([[0, 0, 1], [1, 0, 1]])
x_sp = ds.array(sp, block_size=(1, 3))
x_sp

[7]: ds-array(blocks=(...), top_left_shape=(1, 3), reg_shape=(1, 3), shape=(2, 3), sparse=True)
```

In this case, `collect` returns a CSR matrix as well:

```
[8]: x_sp.collect()

[8]: <2x3 sparse matrix of type '<class 'numpy.int64'>'
      with 3 stored elements in Compressed Sparse Row format>
```

Loading data

A typical way of creating ds-arrays is to load data from disk. Dislib currently supports reading data in CSV and SVMLight formats like this:

```
[9]: x, y = ds.load_svmlight_file("./files/libsvm/1", block_size=(20, 100), n_features=780, store_
      ↪sparse=True)

print(x)

csv = ds.load_txt_file("./files/csv/1", block_size=(500, 122))

print(csv)

ds-array(blocks=(...), top_left_shape=(20, 100), reg_shape=(20, 100), shape=(61, 780), ↪
      ↪sparse=True)
ds-array(blocks=(...), top_left_shape=(500, 122), reg_shape=(500, 122), shape=(4235, 122), ↪
      ↪sparse=False)
```

Slicing

Similar to NumPy, ds-arrays support the following types of slicing:

(Note that slicing a ds-array creates a new ds-array)

```
[10]: x = ds.random_array((50, 50), (10, 10))
```

Get a single row:

```
[11]: x[4]

[11]: ds-array(blocks=(...), top_left_shape=(1, 10), reg_shape=(10, 10), shape=(1, 50), ↪
      ↪sparse=False)
```

Get a single element:

```
[12]: x[2, 3]

[12]: ds-array(blocks=(...), top_left_shape=(1, 1), reg_shape=(1, 1), shape=(1, 1), sparse=False)
```

Get a set of rows or a set of columns:

```
[13]: # Consecutive rows
print(x[10:20])

# Consecutive columns
print(x[:, 10:20])

# Non consecutive rows
print(x[[3, 7, 22]])

# Non consecutive columns
print(x[:, [5, 9, 48]])

ds-array(blocks=(...), top_left_shape=(10, 10), reg_shape=(10, 10), shape=(10, 50),
→sparse=False)
ds-array(blocks=(...), top_left_shape=(10, 10), reg_shape=(10, 10), shape=(50, 10),
→sparse=False)
ds-array(blocks=(...), top_left_shape=(3, 10), reg_shape=(10, 10), shape=(3, 50),
→sparse=False)
ds-array(blocks=(...), top_left_shape=(10, 3), reg_shape=(10, 10), shape=(50, 3),
→sparse=False)
```

Get any set of elements:

```
[14]: x[0:5, 40:45]

[14]: ds-array(blocks=(...), top_left_shape=(5, 5), reg_shape=(10, 10), shape=(5, 5), sparse=False)
```

Other functions

Apart from this, ds-arrays also provide other useful operations like `transpose` and `mean`:

```
[15]: x.mean(axis=0).collect()

[15]: array([0.51352356, 0.49396794, 0.4661033 , 0.48026991, 0.50136143,
0.49323405, 0.51248831, 0.51658519, 0.4904544 , 0.47166468,
0.50245676, 0.49936659, 0.47499634, 0.52566765, 0.53676456,
0.59127036, 0.50947458, 0.47320677, 0.42695456, 0.54335201,
0.51780756, 0.49855486, 0.53845333, 0.37299501, 0.51229418,
0.43110043, 0.47262688, 0.41698864, 0.54994596, 0.46676007,
0.46070067, 0.48861301, 0.45868291, 0.53380687, 0.50555055,
0.53453463, 0.43711111, 0.52115681, 0.48152436, 0.49215593,
0.41552034, 0.47669533, 0.5610678 , 0.43511911, 0.49611885,
0.44116871, 0.42241364, 0.48626255, 0.51636529, 0.44251849])

[16]: x.transpose().collect()

[16]: array([[0.02733543, 0.65891797, 0.36654465, ..., 0.52109164, 0.86395718,
0.93593907],
[0.41462264, 0.97419918, 0.14124931, ..., 0.15893453, 0.49486474,
0.14138483],
[0.91312707, 0.53860404, 0.96686988, ..., 0.78763956, 0.18268972,
0.20551984],
...,
[0.19468602, 0.62184611, 0.81007025, ..., 0.88719987, 0.55132466,
0.32694948],
[0.19221646, 0.64678511, 0.98416872, ..., 0.18736269, 0.51392039,
0.59614856],
```

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```
[0.49591758, 0.17913008, 0.11419029, ..., 0.02701779, 0.22316829,  
0.78426262]])
```

10.1.13.3 Machine learning with dislib

Dislib provides an estimator-based API very similar to [scikit-learn](#). To run an algorithm, we first create an estimator. For example, a K-means estimator:

```
[17]: from dislib.cluster import KMeans  
  
km = KMeans(n_clusters=3)
```

Now, we create a ds-array with some blob data, and fit the estimator:

```
[18]: from sklearn.datasets import make_blobs  
  
# create ds-array  
x, y = make_blobs(n_samples=1500)  
x_ds = ds.array(x, block_size=(500, 2))  
  
km.fit(x_ds)
```

```
[18]: KMeans(n_clusters=3, random_state=RandomState(MT19937) at 0x7FB7D4FFB240)
```

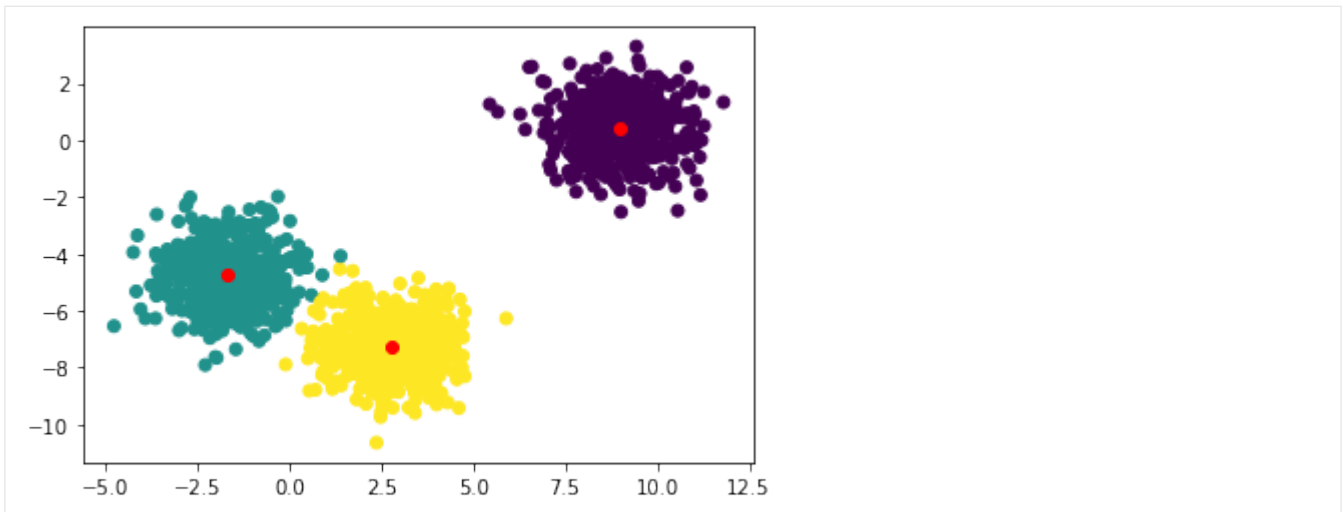
Finally, we can make predictions on new (or the same) data:

```
[19]: y_pred = km.predict(x_ds)  
y_pred  
  
[19]: ds-array(blocks=(...), top_left_shape=(500, 1), reg_shape=(500, 1), shape=(1500, 1),  
→sparse=False)
```

`y_pred` is a ds-array of predicted labels for `x_ds`

Let's plot the results

```
[20]: %matplotlib inline  
import matplotlib.pyplot as plt  
  
centers = km.centers  
  
# set the color of each sample to the predicted label  
plt.scatter(x[:, 0], x[:, 1], c=y_pred.collect())  
  
# plot the computed centers in red  
plt.scatter(centers[:, 0], centers[:, 1], c='red')  
  
[20]: <matplotlib.collections.PathCollection at 0x7fb7a137d640>
```



Note that we need to call `y_pred.collect()` to retrieve the actual labels and plot them. The rest is the same as if we were using `scikit-learn`.

Now let's try a more complex example that uses some preprocessing tools.

First, we load a classification data set from `scikit-learn` into `ds-arrays`.

Note that this step is only necessary for demonstration purposes. Ideally, your data should be already loaded in `ds-arrays`.

```
[21]: from sklearn.datasets import load_breast_cancer
from sklearn.model_selection import train_test_split

x, y = load_breast_cancer(return_X_y=True)

x_train, x_test, y_train, y_test = train_test_split(x, y)

x_train = ds.array(x_train, block_size=(100, 10))
y_train = ds.array(y_train.reshape(-1, 1), block_size=(100, 1))

x_test = ds.array(x_test, block_size=(100, 10))
y_test = ds.array(y_test.reshape(-1, 1), block_size=(100, 1))
```

Next, we can see how support vector machines perform in classifying the data. We first fit the model (ignore any warnings in this step):

```
[22]: from dislib.classification import CascadeSVM

csvm = CascadeSVM()

csvm.fit(x_train, y_train)

/home/javier/.local/lib/python3.8/site-packages/dislib/classification/csvm/base.py:374:
↳RuntimeWarning: overflow encountered in exp
    k = np.exp(k)
/home/javier/.local/lib/python3.8/site-packages/dislib/classification/csvm/base.py:342:
↳RuntimeWarning: invalid value encountered in double_scalars
    delta = np.abs((w - self._last_w) / self._last_w)
```

```
[22]: CascadeSVM()
```

and now we can make predictions on new data using `csvm.predict()`, or we can get the model accuracy on the test set with:

```
[23]: score = csvm.score(x_test, y_test)
```

`score` represents the classifier accuracy, however, it is returned as a `Future`. We need to synchronize to get the actual value:

```
[24]: from pycompss.api.api import compss_wait_on

print(compss_wait_on(score))

0.6503496503496503
```

The accuracy should be around 0.6, which is not very good. We can scale the data before classification to improve accuracy. This can be achieved using `dislib`'s `StandardScaler`.

The `StandardScaler` provides the same API as other estimators. In this case, however, instead of making predictions on new data, we transform it:

```
[25]: from dislib.preprocessing import StandardScaler

sc = StandardScaler()

# fit the scaler with train data and transform it
scaled_train = sc.fit_transform(x_train)

# transform test data
scaled_test = sc.transform(x_test)
```

Now `scaled_train` and `scaled_test` are the scaled samples. Let's see how SVM performs now.

```
[26]: csvm.fit(scaled_train, y_train)
score = csvm.score(scaled_test, y_test)
print(compss_wait_on(score))

0.972027972027972
```

The new accuracy should be around 0.9, which is a great improvement!

Close the session

To finish the session, we need to stop PyCOMPSs:

```
[27]: ipycompss.stop()

*****
***** STOPPING PyCOMPSs *****
*****
Checking if any issue happened.
Warning: some of the variables used with PyCOMPSs may
        have not been brought to the master.
*****
```



```
[5]: (60000, 1)
```

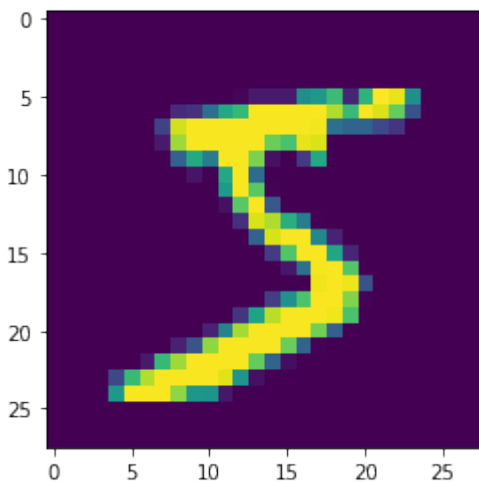
```
[6]: y_array = y.collect()  
y_array
```

```
[6]: array([5., 0., 4., ..., 5., 6., 8.])
```

```
[7]: img = x[0].collect().reshape(28,28)
```

```
[8]: %matplotlib inline  
import matplotlib.pyplot as plt  
plt.imshow(img)
```

```
[8]: <matplotlib.image.AxesImage at 0x7fcdade69e48>
```



```
[9]: int(y[0].collect())
```

```
[9]: 5
```

10.1.14.3 dislib algorithms

Preprocessing

```
[10]: from dislib.preprocessing import StandardScaler  
from dislib.decomposition import PCA
```

Clustering

```
[11]: from dislib.cluster import KMeans  
from dislib.cluster import DBSCAN  
from dislib.cluster import GaussianMixture
```

Classification

```
[12]: from dislib.classification import CascadeSVM
      from dislib.classification import RandomForestClassifier
```

Recommendation

```
[13]: from dislib.recommendation import ALS
```

Model selection

```
[14]: from dislib.model_selection import GridSearchCV
```

Others

```
[15]: from dislib.regression import LinearRegression
      from dislib.neighbors import NearestNeighbors
```

10.1.14.4 Examples

KMeans

```
[16]: kmeans = KMeans(n_clusters=10)
      pred_clusters = kmeans.fit_predict(x).collect()
```

Get the number of images of each class in the cluster 0:

```
[17]: from collections import Counter
      Counter(y_array[pred_clusters==0])
```

```
[17]: Counter({3.0: 4064,
              8.0: 1942,
              9.0: 110,
              2.0: 381,
              1.0: 10,
              5.0: 1910,
              0.0: 187,
              6.0: 29,
              7.0: 6,
              4.0: 1})
```

GaussianMixture

Fit the GaussianMixture with the painted pixels of a single image:

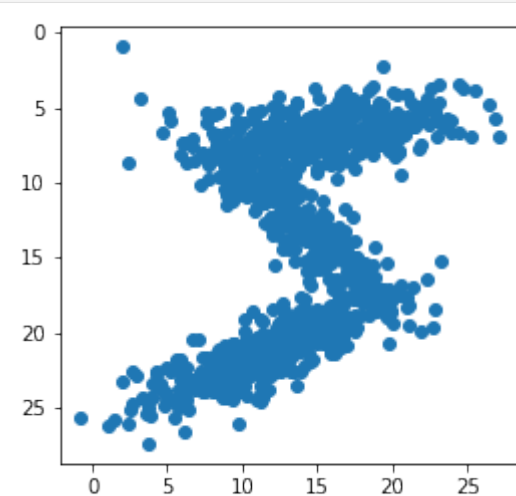
```
[18]: import numpy as np
img_filtered_pixels = np.stack([np.array([i, j]) for i in range(28) for j in range(28) if
    img[i,j] > 10])
img_pixels = ds.array(img_filtered_pixels, block_size=(50,2))
gm = GaussianMixture(n_components=7, random_state=0)
gm.fit(img_pixels)
```

Get the parameters that define the Gaussian components:

```
[19]: from pycompss.api import compss_wait_on
means = compss_wait_on(gm.means_)
covariances = compss_wait_on(gm.covariances_)
weights = compss_wait_on(gm.weights_)
```

Use the Gaussian mixture model to sample random pixels replicating the original distribution:

```
[20]: samples = np.concatenate([np.random.multivariate_normal(means[i], covariances[i],
    int(weights[i]*1000))
    for i in range(7)])
plt.scatter(samples[:,1], samples[:,0])
plt.gca().set_aspect('equal', adjustable='box')
plt.gca().invert_yaxis()
plt.draw()
```



PCA

```
[21]: pca = PCA()
pca.fit(x)
```

```
[21]: PCA(arity=50, n_components=None)
```

Calculate the explained variance of the 10 first eigenvectors:

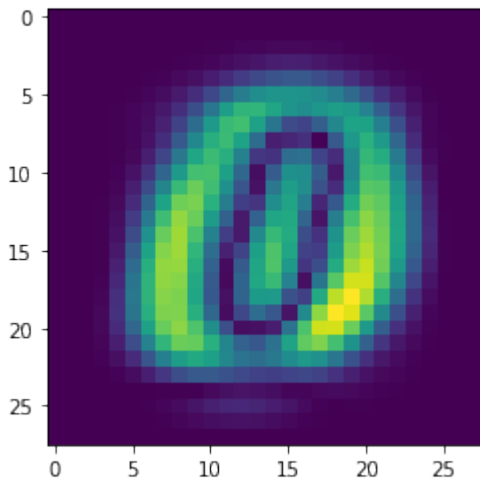
```
[22]: sum(pca.explained_variance_[0:10])/sum(pca.explained_variance_)
```

```
[22]: 0.4881498035493399
```

Show the weights of the first eigenvector:

```
[23]: plt.imshow(np.abs(pca.components_[0]).reshape(28,28))
```

```
[23]: <matplotlib.image.AxesImage at 0x7fcd9ea5c550>
```



RandomForestClassifier

```
[24]: rf = RandomForestClassifier(n_estimators=5, max_depth=3)
      rf.fit(x, y)
```

```
[24]: RandomForestClassifier(distr_depth='auto', hard_vote=False, max_depth=3,
                             n_estimators=5, random_state=None,
                             sklearn_max=100000000.0, try_features='sqrt')
```

Use the test dataset to get an accuracy score:

```
[25]: x_test, y_test = ds.load_svmlight_file('/tmp/mnist/mnist.test', block_size=(10000, 784), n_
      ↪ features=784, store_sparse=False)
      score = rf.score(x_test, y_test)
      print(compss_wait_on(score))
0.5965
```

Close the session

To finish the session, we need to stop PyCOMPSs:

```
[26]: ipycompss.stop()

*****
***** STOPPING PyCOMPSs *****
*****
Warning: some of the variables used with PyCOMPSs may
        have not been brought to the master.
*****
```

10.2 Hands-on

Here you will find the hands on notebooks used in the tutorials.

10.2.1 Sort by Key

Algorithm that sorts the elements of a set of files and merges the partial results respecting the order.

10.2.1.1 First of all - Create a dataset

This step can be avoided if the dataset already exists.

If not, this code snippet creates a set of files with dictionary on each one generated randomly. Uses pickle.

```
[1]: def datasetGenerator(directory, numFiles, numPairs):
      import random
      import pickle
      import os
      if os.path.exists(directory):
          print("Dataset directory already exists... Removing")
          import shutil
          shutil.rmtree(directory)
      os.makedirs(directory)
      for f in range(numFiles):
          fragment = {}
          while len(fragment) < numPairs:
              fragment[random.random()] = random.randint(0, 1000)
          filename = 'file_' + str(f) + '.data'
          with open(directory + '/' + filename, 'wb') as fd:
              pickle.dump(fragment, fd)
          print('File ' + filename + ' has been created.')
```

```
[2]: numFiles = 2
      numPairs = 10
      directoryName = 'mydataset'
      datasetGenerator(directoryName, numFiles, numPairs)
```

```
Dataset directory already exists... Removing
File file_0.data has been created.
File file_1.data has been created.
```

```
[3]: # Show the files that have been created
      %ls -l $directoryName
```

```
total 8
-rw-r--r-- 1 javier users 133 may 18 16:29 file_0.data
-rw-r--r-- 1 javier users 134 may 18 16:29 file_1.data
```

10.2.1.2 Algorithm definition

```
[4]: import pycompss.interactive as ipycompss
```

```
[5]: import os
if 'BINDER_SERVICE_HOST' in os.environ:
    ipycompss.start(graph=True,
                    project_xml='../xml/project.xml',
                    resources_xml='../xml/resources.xml')
else:
    ipycompss.start(graph=True, monitor=1000)
```

```
*****
***** PyCOMPSs Interactive *****
*****
*
*      .-~~-.-..
*      :      )      |____ \      /____ \
*      .~ ~-.\      /.- ~ ~ .      ____ ) |      | (____ ) |
*      >      \      '      <      /____/      \_____/
*      (      .-.-.      )      | |____ |      /      /
*      \-.-.-~ \-.-.-~ \-.-.-~ |_____| |      /____/
*      (      :      )      - - -.-:
*      ~-.-.      :      .-.-~      .-.-~ }
*      ~-.-.-.-~ \      .~ .-.-~
*      \      \      \      //
*      . - ~ ~-.-.\      .-.-.//
*      .-.-~      .-.-~ } ~ ~-.-.-.
*      .'.-.-~      .-.-~      :/~-.-.-./:
*      /-.-.-.-~      .-.-~      ~-.-.-.
*      ~-.-.-.
*
*****
* - Starting COMPSs runtime...
* - Log path : /home/javier/.COMPSs/InteractiveMode_17/
* - PyCOMPSs Runtime started... Have fun!
*****
```

```
[6]: from pycompss.api.task import task
from pycompss.api.parameter import FILE_IN
```

```
[7]: @task(returns=list, dataFile=FILE_IN)
def sortPartition(dataFile):
    """
    Reads the dataFile and sorts its content which is assumed to be a dictionary {K: V}
    :param path: file that contains the data
    :return: a list of (K, V) pairs sorted.
    """
    import pickle
    import operator
    with open(dataFile, 'rb') as f:
        data = pickle.load(f)
    # res = sorted(data, key=lambda (k, v): k, reverse=not ascending)
    partition_result = sorted(data.items(), key=operator.itemgetter(0), reverse=False)
    return partition_result
```

```
[8]: @task(returns=list, priority=True)
```

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```
def reducetask(a, b):
    '''
    Merges two partial results (lists of (K, V) pairs) respecting the order
    :param a: Partial result a
    :param b: Partial result b
    :return: The merging result sorted
    '''
    partial_result = []
    i = 0
    j = 0
    while i < len(a) and j < len(b):
        if a[i] < b[j]:
            partial_result.append(a[i])
            i += 1
        else:
            partial_result.append(b[j])
            j += 1
    if i < len(a):
        partial_result + a[i:]
    elif j < len(b):
        partial_result + b[j:]
    return partial_result
```

```
[9]: def merge_reduce(function, data):
    import sys
    if sys.version_info[0] >= 3:
        import queue as Queue
    else:
        import Queue
    q = Queue.Queue()
    for i in data:
        q.put(i)
    while not q.empty():
        x = q.get()
        if not q.empty():
            y = q.get()
            q.put(function(x, y))
        else:
            return x
```

MAIN

Parameters (that can be configured in the following cell): * datasetPath: The path where the dataset is (default: the same as created previously).

```
[10]: import os
import time
from pycompss.api.api import compss_wait_on

datasetPath = directoryName # Where the dataset is
files = []
for f in os.listdir(datasetPath):
    files.append(datasetPath + '/' + f)
```

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```

startTime = time.time()

partialSorted = []
for f in files:
    partialSorted.append(sortPartition(f))
result = merge_reduce(reducetask, partialSorted)

result = compss_wait_on(result)

print("Elapsed Time(s)")
print(time.time() - startTime)
import pprint
pprint.pprint(result)

```

```

Found task: sortPartition
Found task: reducetask
Elapsed Time(s)
3.6193034648895264
[(0.027312894275046573, 993),
 (0.07138432853012677, 426),
 (0.10308291658301261, 252),
 (0.10421523358827744, 356),
 (0.10743720335209561, 614),
 (0.19426330574322814, 89),
 (0.2120037521887378, 4),
 (0.21274769665858428, 680),
 (0.27702759534915444, 393),
 (0.29308205906959617, 789),
 (0.31724024656512495, 669),
 (0.42922792366256235, 700),
 (0.4319642313815307, 756),
 (0.46956964955534164, 707),
 (0.6944486231937671, 841),
 (0.708700562554975, 720),
 (0.7478662969947636, 874),
 (0.9589965652687729, 304),
 (0.9687167493887274, 12)]

```

```
[11]: ipycompss.stop()
```

```

*****
***** STOPPING PyCOMPSs *****
*****
Checking if any issue happened.
Warning: some of the variables used with PyCOMPSs may
        have not been brought to the master.
*****

```

10.2.2 KMeans

KMeans is machine-learning algorithm (NP-hard), popularly employed for cluster analysis in data mining, and interesting for benchmarking and performance evaluation.

The objective of the Kmeans algorithm is to group a set of multidimensional points into a predefined number of clusters, in which each point belongs to the closest cluster (with the nearest mean distance), in an iterative process.

```
[1]: import pycompss.interactive as ipycompss
```

```
[2]: import os  
if 'BINDER_SERVICE_HOST' in os.environ:  
    ipycompss.start(graph=True,                                     # trace=True  
                    project_xml='../xml/project.xml',  
                    resources_xml='../xml/resources.xml')  
else:  
    ipycompss.start(graph=True, monitor=1000) # trace=True  
  
*****  
***** PyCOMPSs Interactive *****  
*****  
*                               *  
*      :           )          |--- \   /----- \   *  
*     .~ ~ -. \       /. - ~ ~ .   ---) |   | (---) |   *  
*    >         \     .'         <   /---/   \----- /   *  
*   (      _.-.-.      )    | |---| _   / /   *  
*   '-_-.-~   '-_-.'   ~-.-.-'   |-----| | |   /--/   *  
*   (            )          -_-.-:-:   *  
*   ~--:        _.-~-   .-.~   .-~ .-~}   *  
*   ~-.-.-.-\   .-~   .-~   .-~   *  
*              \|     \|     \|     *  
*               \|     \|     //     *  
*             .- ~ ~-.-.-\.\.-//     *  
*             .- ~ ~-.-.-}~ ~ ~-.-.- *  
*             .' .-~   .-~   :/~-.~-.:/:   *  
*           /_~--.-.- ~         ~-.-.-.- *  
*                                           ~-.-.<   *  
*****  
* - Starting COMPSs runtime... *  
* - Log path : /home/javier/.COMPSs/InteractiveMode_15/ *  
* - PyCOMPSs Runtime started... Have fun! *  
*****
```

```
[3]: from pycompss.api.task import task
```

```
[4]: import numpy as np
```

```
[5]: def init_random(numV, dim, seed):
    np.random.seed(seed)
    c = [np.random.uniform(-3.5, 3.5, dim)]
    while len(c) < numV:
        p = np.random.uniform(-3.5, 3.5, dim)
        distance = [np.linalg.norm(p-i) for i in c]
        if min(distance) > 2:
            c.append(p)
    return c
```

```
[6]: #@task(returns=list) # Not a task for plotting
def genFragment(numV, K, c, dim, mode='gauss'):
    if mode == "gauss":
        n = int(float(numV) / K)
        r = numV % K
        data = []
        for k in range(K):
            s = np.random.uniform(0.05, 0.75)
            for i in range(n+r):
                d = np.array([np.random.normal(c[k][j], s) for j in range(dim)])
                data.append(d)
        return np.array(data)[:numV]
    else:
        return [np.random.random(dim) for _ in range(numV)]

[7]: @task(returns=dict)
def cluster_points_partial(XP, mu, ind):
    dic = {}
    for x in enumerate(XP):
        bestmukey = min([(i[0], np.linalg.norm(x[1] - mu[i[0]])) for i in enumerate(mu)],
            ↪key=lambda t: t[1])[0]
        if bestmukey not in dic:
            dic[bestmukey] = [x[0] + ind]
        else:
            dic[bestmukey].append(x[0] + ind)
    return dic

[8]: @task(returns=dict)
def partial_sum(XP, clusters, ind):
    p = [(i, [(XP[j] - ind) for j in clusters[i]]) for i in clusters]
    dic = {}
    for i, l in p:
        dic[i] = (len(l), np.sum(l, axis=0))
    return dic

[9]: @task(returns=dict, priority=True)
def reduceCentersTask(a, b):
    for key in b:
        if key not in a:
            a[key] = b[key]
        else:
            a[key] = (a[key][0] + b[key][0], a[key][1] + b[key][1])
    return a

[10]: def mergeReduce(function, data):
    from collections import deque
    q = deque(list(range(len(data))))
    while len(q):
        x = q.popleft()
        if len(q):
            y = q.popleft()
            data[x] = function(data[x], data[y])
            q.append(x)
        else:
            return data[x]
```

```
[11]: def has_converged(mu, oldmu, epsilon, iter, maxIterations):
    print("iter: " + str(iter))
    print("maxIterations: " + str(maxIterations))
    if oldmu != []:
        if iter < maxIterations:
            aux = [np.linalg.norm(oldmu[i] - mu[i]) for i in range(len(mu))]
            distancia = sum(aux)
            if distancia < epsilon * epsilon:
                print("Distance_T: " + str(distancia))
                return True
            else:
                print("Distance_F: " + str(distancia))
                return False
        else:
            # Reached the max amount of iterations
            return True

[12]: def plotKMEANS(dim, mu, clusters, data):
    import pylab as plt
    colors = ['b', 'g', 'r', 'c', 'm', 'y', 'k']
    if dim == 2 and len(mu) <= len(colors):
        from matplotlib.patches import Circle
        from matplotlib.collections import PatchCollection
        fig, ax = plt.subplots(figsize=(10,10))
        patches = []
        pcolors = []
        for i in range(len(clusters)):
            for key in clusters[i].keys():
                d = clusters[i][key]
                for j in d:
                    j = j - i * len(data[0])
                    C = Circle((data[i][j][0], data[i][j][1]), .05)
                    pcolors.append(colors[key])
                    patches.append(C)
        collection = PatchCollection(patches)
        collection.set_facecolor(pcolors)
        ax.add_collection(collection)
        x, y = zip(*mu)
        plt.plot(x, y, '*', c='y', markersize=20)
        plt.autoscale(enable=True, axis='both', tight=False)
        plt.show()
    elif dim == 3 and len(mu) <= len(colors):
        from mpl_toolkits.mplot3d import Axes3D
        fig = plt.figure()
        ax = fig.add_subplot(111, projection='3d')
        for i in range(len(clusters)):
            for key in clusters[i].keys():
                d = clusters[i][key]
                for j in d:
                    j = j - i * len(data[0])
                    ax.scatter(data[i][j][0], data[i][j][1], data[i][j][2], 'o',
                                c=colors[key])
        x, y, z = zip(*mu)
        for i in range(len(mu)):
            ax.scatter(x[i], y[i], z[i], s=80, c='y', marker='D')
        plt.show()
```

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```

else:
    print("No representable dim or not enough colours")

```

10.2.2.1 MAIN

Parameters (that can be configured in the following cell): * numV: number of vectors (default: 10.000)
 * dim: dimension of the points (default: 2) * k: number of centers (default: 4) * numFrag: number of fragments (default: 16) * epsilon: convergence condition (default: 1e-10) * maxIterations: Maximum number of iterations (default: 20)

```

[13]: %matplotlib inline
import ipywidgets as widgets
from pycompss.api.api import compss_wait_on

w_numV = widgets.IntText(value=10000)          # Number of Vectors - with 1000 it is feasible_
↳to see the evolution across iterations
w_dim = widgets.IntText(value=2)               # Number of Dimensions
w_k = widgets.IntText(value=4)                 # Centers
w_numFrag = widgets.IntText(value=16)          # Fragments
w_epsilon = widgets.FloatText(value=1e-10)     # Convergence condition
w_maxIterations = widgets.IntText(value=20)     # Max number of iterations
w_seed = widgets.IntText(value=8)              # Random seed

def kmeans(numV, dim, k, numFrag, epsilon, maxIterations, seed):
    size = int(numV / numFrag)
    cloudCenters = init_random(k, dim, seed) # centers to create data groups
    X = [genFragment(size, k, cloudCenters, dim, mode='gauss') for _ in range(numFrag)]
    mu = init_random(k, dim, seed - 1)        # First centers
    oldmu = []
    n = 0
    while not has_converged(mu, oldmu, epsilon, n, maxIterations):
        oldmu = mu
        clusters = [cluster_points_partial(X[f], mu, f * size) for f in range(numFrag)]
        partialResult = [partial_sum(X[f], clusters[f], f * size) for f in range(numFrag)]
        mu = mergeReduce(reduceCentersTask, partialResult)
        mu = compss_wait_on(mu)
        mu = [mu[c][1] / mu[c][0] for c in mu]
        while len(mu) < k:
            # Add new random center if one of the centers has no points.
            indP = np.random.randint(0, size)
            indF = np.random.randint(0, numFrag)
            mu.append(X[indF][indP])
        n += 1
    clusters = compss_wait_on(clusters)
    plotKMEANS(dim, mu, clusters, X)
    print("-----")
    print("Result:")
    print("Iterations: ", n)
    print("Centers: ", mu)
    print("-----")

widgets.interact_manual(kmeans, numV=w_numV, dim=w_dim, k=w_k, numFrag=w_numFrag, epsilon=w_
↳epsilon, maxIterations=w_maxIterations, seed=w_seed)

```

```
interactive(children=(IntText(value=10000, description='numV'), IntText(value=2, description=
→ 'dim'), IntText(v...
```

```
[13]: <function __main__.kmeans(numV, dim, k, numFrag, epsilon, maxIterations, seed)>
```

```
[14]: ipycompss.stop()
```

```
*****
***** STOPPING PyCOMPSs *****
*****
Checking if any issue happened.
Warning: some of the variables used with PyCOMPSs may
        have not been brought to the master.
*****
```

10.2.3 KMeans with Reduce

KMeans is machine-learning algorithm (NP-hard), popularly employed for cluster analysis in data mining, and interesting for benchmarking and performance evaluation.

The objective of the Kmeans algorithm to group a set of multidimensional points into a predefined number of clusters, in which each point belongs to the closest cluster (with the nearest mean distance), in an iterative process.

```
[1]: import pycompss.interactive as ipycompss
```

```
[2]: import os
if 'BINDER_SERVICE_HOST' in os.environ:
    ipycompss.start(graph=True,                # trace=True
                    project_xml='../xml/project.xml',
                    resources_xml='../xml/resources.xml')
else:
    ipycompss.start(graph=True, monitor=1000) # trace=True
```

```
*****
***** PyCOMPSs Interactive *****
*****
*      .-~~-.---.      |-----|      |-----|      *
*      :          )      |_____\      /_____\      *
*      .~ ~ -. \      /.- ~ ~ .      |_____) |      | (_____) | *
*      >          \      <      /____/      \_____/      *
*      (          .- .- .      ) | |____|      /____/      *
*      \-.-.-~ \-.-.-~ \-.-.-~ |_____| |_____| /____/      *
*      (          :          )      - - .-:      *
*      ~-.-.      :      .-.-~      .-~ .-~ }      *
*      ~-.-.-~-.-~ \      .~ .-~ .-~      *
*      \      \      \      \      \      *
*      \      \      \      \      \      *
*      . - ~ ~ -.-.- \      \      \      *
*      .-~ .-~ }~ ~ ~-.-.-      *
*      .-~ .-~      :/~-.-~-./:      *
*      /-~ - - . - ~      ~-.-~-_-      *
*      ~-.-<      *
*****
* - Starting COMPSs runtime...      *
* - Log path : /home/javier/.COMPSs/InteractiveMode_16/      *
* - PyCOMPSs Runtime started... Have fun!      *
*****
```

```
[3]: from pycompss.api.task import task
```

```
[4]: import numpy as np
```

```
[5]: def init_random(numV, dim, seed):
    np.random.seed(seed)
    c = [np.random.uniform(-3.5, 3.5, dim)]
    while len(c) < numV:
        p = np.random.uniform(-3.5, 3.5, dim)
        distance = [np.linalg.norm(p-i) for i in c]
        if min(distance) > 2:
            c.append(p)
    return c
```

```
[6]: #@task(returns=list) # Not a task for plotting
def genFragment(numV, K, c, dim, mode='gauss'):
    if mode == "gauss":
        n = int(float(numV) / K)
        r = numV % K
        data = []
        for k in range(K):
            s = np.random.uniform(0.05, 0.75)
            for i in range(n+r):
                d = np.array([np.random.normal(c[k][j], s) for j in range(dim)])
                data.append(d)
        return np.array(data)[:numV]
    else:
        return [np.random.random(dim) for _ in range(numV)]
```

```
[7]: @task(returns=dict)
def cluster_points_partial(XP, mu, ind):
    dic = {}
    for x in enumerate(XP):
        bestmukey = min([(i[0], np.linalg.norm(x[1] - mu[i[0]])) for i in enumerate(mu)],
            ↪key=lambda t: t[1])[0]
        if bestmukey not in dic:
            dic[bestmukey] = [x[0] + ind]
        else:
            dic[bestmukey].append(x[0] + ind)
    return dic
```

```
[8]: @task(returns=dict)
def partial_sum(XP, clusters, ind):
    p = [(i, [(XP[j] - ind) for j in clusters[i]]) for i in clusters]
    dic = {}
    for i, l in p:
        dic[i] = (len(l), np.sum(l, axis=0))
    return dic
```

```
[9]: def reduceCenters(a, b):
    """
    Reduce method to sum the result of two partial_sum methods
    :param a: partial_sum {cluster_ind: (#points_a, sum(points_a))}
    :param b: partial_sum {cluster_ind: (#points_b, sum(points_b))}
    :return: {cluster_ind: (#points_a+#points_b, sum(points_a+points_b))}
```

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```

"""
for key in b:
    if key not in a:
        a[key] = b[key]
    else:
        a[key] = (a[key][0] + b[key][0], a[key][1] + b[key][1])
return a

```

```

[10]: @task(returns=dict)
def reduceCentersTask(*data):
    reduce_value = data[0]
    for i in range(1, len(data)):
        reduce_value = reduceCenters(reduce_value, data[i])
    return reduce_value

```

```

[11]: def mergeReduce(function, data, chunk=50):
    """ Apply function cumulatively to the items of data,
        from left to right in binary tree structure, so as to
        reduce the data to a single value.
    :param function: function to apply to reduce data
    :param data: List of items to be reduced
    :return: result of reduce the data to a single value
    """
    while(len(data)) > 1:
        dataToReduce = data[:chunk]
        data = data[chunk:]
        data.append(function(*dataToReduce))
    return data[0]

```

```

[12]: def has_converged(mu, oldmu, epsilon, iter, maxIterations):
    print("iter: " + str(iter))
    print("maxIterations: " + str(maxIterations))
    if oldmu != []:
        if iter < maxIterations:
            aux = [np.linalg.norm(oldmu[i] - mu[i]) for i in range(len(mu))]
            distancia = sum(aux)
            if distancia < epsilon * epsilon:
                print("Distance_T: " + str(distancia))
                return True
            else:
                print("Distance_F: " + str(distancia))
                return False
        else:
            # Reached the max amount of iterations
            return True

```

```

[13]: def plotKMEANS(dim, mu, clusters, data):
    import pylab as plt
    colors = ['b', 'g', 'r', 'c', 'm', 'y', 'k']
    if dim == 2 and len(mu) <= len(colors):
        from matplotlib.patches import Circle
        from matplotlib.collections import PatchCollection
        fig, ax = plt.subplots(figsize=(10,10))
        patches = []
        pcolors = []

```

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```

for i in range(len(clusters)):
    for key in clusters[i].keys():
        d = clusters[i][key]
        for j in d:
            j = j - i * len(data[0])
            C = Circle((data[i][j][0], data[i][j][1]), .05)
            pcolors.append(colors[key])
            patches.append(C)
collection = PatchCollection(patches)
collection.set_facecolor(pcolors)
ax.add_collection(collection)
x, y = zip(*mu)
plt.plot(x, y, '*', c='y', markersize=20)
plt.autoscale(enable=True, axis='both', tight=False)
plt.show()
elif dim == 3 and len(mu) <= len(colors):
    from mpl_toolkits.mplot3d import Axes3D
    fig = plt.figure()
    ax = fig.add_subplot(111, projection='3d')
    for i in range(len(clusters)):
        for key in clusters[i].keys():
            d = clusters[i][key]
            for j in d:
                j = j - i * len(data[0])
                ax.scatter(data[i][j][0], data[i][j][1], data[i][j][2], 'o',
→c=colors[key])
            x, y, z = zip(*mu)
            for i in range(len(mu)):
                ax.scatter(x[i], y[i], z[i], s=80, c='y', marker='D')
    plt.show()
else:
    print("No representable dim or not enough colours")

```

10.2.3.1 MAIN

Parameters (that can be configured in the following cell): * numV: number of vectors (default: 10.000)

* dim: dimension of the points (default: 2) * k: number of centers (default: 4) * numFrag: number of fragments (default: 16) * epsilon: convergence condition (default: 1e-10) * maxIterations: Maximum number of iterations (default: 20)

```

[14]: %matplotlib inline
import ipywidgets as widgets
from pycompss.api.api import compss_wait_on

w_numV = widgets.IntText(value=10000)           # Number of Vectors - with 1000 it is feasible
→to see the evolution across iterations
w_dim = widgets.IntText(value=2)                # Number of Dimensions
w_k = widgets.IntText(value=4)                  # Centers
w_numFrag = widgets.IntText(value=16)           # Fragments
w_epsilon = widgets.FloatText(value=1e-10)      # Convergence condition
w_maxIterations = widgets.IntText(value=20)     # Max number of iterations
w_seed = widgets.IntText(value=8)               # Random seed

```

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```

def kmeans(numV, dim, k, numFrag, epsilon, maxIterations, seed):
    size = int(numV / numFrag)
    cloudCenters = init_random(k, dim, seed) # centers to create data groups
    X = [genFragment(size, k, cloudCenters, dim, mode='gauss') for _ in range(numFrag)]
    mu = init_random(k, dim, seed - 1)      # First centers
    oldmu = []
    n = 0
    while not has_converged(mu, oldmu, epsilon, n, maxIterations):
        oldmu = mu
        clusters = [cluster_points_partial(X[f], mu, f * size) for f in range(numFrag)]
        partialResult = [partial_sum(X[f], clusters[f], f * size) for f in range(numFrag)]
        mu = mergeReduce(reduceCentersTask, partialResult, chunk=4)
        mu = compss_wait_on(mu)
        mu = [mu[c][1] / mu[c][0] for c in mu]
        while len(mu) < k:
            # Add new random center if one of the centers has no points.
            indP = np.random.randint(0, size)
            indF = np.random.randint(0, numFrag)
            mu.append(X[indF][indP])
        n += 1
        clusters = compss_wait_on(clusters)
        plotKMEANS(dim, mu, clusters, X)
        print("-----")
        print("Result:")
        print("Iterations: ", n)
        print("Centers: ", mu)
        print("-----")

widgets.interact_manual(kmeans, numV=w_numV, dim=w_dim, k=w_k, numFrag=w_numFrag, epsilon=w_
→epsilon, maxIterations=w_maxIterations, seed=w_seed)

interactive(children=(IntText(value=10000, description='numV'), IntText(value=2, description=
→'dim'), IntText(v...

```

```
[14]: <function __main__.kmeans(numV, dim, k, numFrag, epsilon, maxIterations, seed)>
```

```
[15]: ipycompss.stop()
```

```

*****
***** STOPPING PyCOMPSs *****
*****
Checking if any issue happened.
Warning: some of the variables used with PyCOMPSs may
        have not been brought to the master.
*****

```

10.2.4 Cholesky Decomposition/Factorization

Given a symmetric positive definite matrix A , the Cholesky decomposition is an upper triangular matrix U (with strictly positive diagonal entries) such that:

$$A = U^T U$$

```
[1]: import pycompss.interactive as ipycompss
```


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```

from scipy.linalg.lapack import dpotrf
import os
os.environ['MKL_NUM_THREADS']=str(MKLProc)
A = dpotrf(A, lower=True)[0]
return A

@task(returns=np.ndarray)
def solve_triangular(A, B, MKLProc):
    from scipy.linalg import solve_triangular
    from numpy import transpose
    import os
    os.environ['MKL_NUM_THREADS']=str(MKLProc)
    B = transpose(B)
    B = solve_triangular(A, B, lower=True) # , trans='T'
    B = transpose(B)
    return B

@task(returns=np.ndarray)
def gemm(alpha, A, B, C, beta, MKLProc):
    from scipy.linalg.blas import dgemm
    from numpy import transpose
    import os
    os.environ['MKL_NUM_THREADS']=str(MKLProc)
    B = transpose(B)
    C = dgemm(alpha, A, B, c=C, beta=beta)
    return C

```

10.2.4.2 Auxiliar functions

```

[5]: def genMatrix(MSIZE, BSIZE, MKLProc, A):
    for i in range(MSIZE):
        A.append([])
        for j in range(MSIZE):
            A[i].append([])
    for i in range(MSIZE):
        mb = createBlock(BSIZE, MKLProc, True)
        A[i][i]=mb
        for j in range(i+1,MSIZE):
            mb = createBlock(BSIZE, MKLProc, False)
            A[i][j]=mb
            A[j][i]=mb

[6]: def cholesky_blocked(MSIZE, BSIZE, mkl_threads, A):
    import os
    for k in range(MSIZE):
        # Diagonal block factorization
        A[k][k] = potrf(A[k][k], mkl_threads)
        # Triangular systems
        for i in range(k+1, MSIZE):
            A[i][k] = solve_triangular(A[k][k], A[i][k], mkl_threads)
            A[k][i] = np.zeros((BSIZE,BSIZE))
        # update trailing matrix
        for i in range(k+1, MSIZE):
            for j in range(i, MSIZE):

```

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```

    A[j][i] = gemm(-1.0, A[j][k], A[i][k], A[j][i], 1.0, mkl_threads)
return A

```

MAIN Code

Parameters (that can be configured in the following cell): * MSIZE: Matrix size (default: 8) * BSIZE: Block size (default: 1024) * mkl_threads: Number of MKL threads (default: 1)

```

[7]: import ipywidgets as widgets
from pycompss.api.api import compss_barrier
import time

w_MSIZE = widgets.IntText(value=8)
w_BSIZE = widgets.IntText(value=1024)
w_mkl_threads = widgets.IntText(value=1)

def cholesky(MSIZE, BSIZE, mkl_threads):
    # Generate de matrix
    startTime = time.time()

    # Generate supermatrix
    A = []
    res = []
    genMatrix(MSIZE, BSIZE, mkl_threads, A)
    compss_barrier()

    initTime = time.time() - startTime
    startDecompTime = time.time()
    res = cholesky_blocked(MSIZE, BSIZE, mkl_threads, A)
    compss_barrier()

    decompTime = time.time() - startDecompTime
    totalTime = decompTime + initTime

    print("----- Elapsed Times -----")
    print("initT:{}".format(initTime))
    print("decompT:{}".format(decompTime))
    print("totalTime:{}".format(totalTime))
    print("-----")

widgets.interact_manual(cholesky, MSIZE=w_MSIZE, BSIZE=w_BSIZE, mkl_threads=w_mkl_threads)
interactive(children=(IntText(value=8, description='MSIZE'), IntText(value=1024, description=
↪ 'BSIZE'), IntText...

[7]: <function __main__.cholesky(MSIZE, BSIZE, mkl_threads)>

```

```

[8]: ipycompss.stop()

*****
***** STOPPING PyCOMPSs *****
*****
Checking if any issue happened.
Warning: some of the variables used with PyCOMPSs may
        have not been brought to the master.
*****

```

10.2.5 Wordcount Exercise

10.2.5.1 Sequential version

```
[1]: import os

[2]: def read_file(file_path):
    """ Read a file and return a list of words.
    :param file_path: file's path
    :return: list of words
    """
    data = []
    with open(file_path, 'r') as f:
        for line in f:
            data += line.split()
    return data

[3]: def wordCount(data):
    """ Construct a frequency word dictionary from a list of words.
    :param data: a list of words
    :return: a dictionary where key=word and value=#appearances
    """
    partialResult = {}
    for entry in data:
        if entry in partialResult:
            partialResult[entry] += 1
        else:
            partialResult[entry] = 1
    return partialResult

[4]: def merge_two_dicts(dic1, dic2):
    """ Update a dictionary with another dictionary.
    :param dic1: first dictionary
    :param dic2: second dictionary
    :return: dic1+=dic2
    """
    for k in dic2:
        if k in dic1:
            dic1[k] += dic2[k]
        else:
            dic1[k] = dic2[k]
    return dic1

[5]: # Get the dataset path
pathDataset = os.getcwd() + '/dataset'

# Read file's content execute a wordcount on each of them
partialResult = []
for fileName in os.listdir(pathDataset):
    file_path = os.path.join(pathDataset, fileName)
    data = read_file(file_path)
    partialResult.append(wordCount(data))

# Accumulate the partial results to get the final result.
result = {}
for partial in partialResult:
```

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```
result = merge_two_dicts(result, partial)
```

```
[6]: print("Result:")
from pprint import pprint
pprint(result)
print("Words: {}".format(sum(result.values())))
```

```
Result:
{'Adipisci': 227,
 'Aliquam': 233,
 'Amet': 207,
 'Consectetur': 201,
 'Dolor': 198,
 'Dolore': 236,
 'Dolorem': 232,
 'Eius': 251,
 'Est': 197,
 'Etincidunt': 232,
 'Ipsum': 228,
 'Labore': 229,
 'Magnum': 195,
 'Modi': 201,
 'Neque': 205,
 'Non': 226,
 'Numquam': 253,
 'Porro': 205,
 'Quaerat': 217,
 'Quiquia': 212,
 'Quisquam': 214,
 'Sed': 225,
 'Sit': 220,
 'Tempora': 189,
 'Ut': 217,
 'Velit': 218,
 'Voluptatem': 235,
 'adipisci': 1078,
 'aliquam': 1107,
 'amet': 1044,
 'consectetur': 1073,
 'dolor': 1120,
 'dolore': 1065,
 'dolorem': 1107,
 'eius': 1048,
 'est': 1101,
 'etincidunt': 1114,
 'ipsum': 1061,
 'labore': 1070,
 'magnum': 1096,
 'modi': 1127,
 'neque': 1093,
 'non': 1099,
 'numquam': 1094,
 'porro': 1101,
 'quaerat': 1086,
 'quiquia': 1079,
 'quisquam': 1144,
```

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```
'sed': 1109,
'sit': 1130,
'tempora': 1064,
'ut': 1070,
'velit': 1105,
'voluptatem': 1121}
Words: 35409
```

10.2.6 Wordcount Solution

10.2.6.1 Complete version

```
[1]: import os

[2]: import pycompss.interactive as ipycompss

[3]: from pycompss.api.task import task

[4]: from pycompss.api.parameter import *

[5]: if 'BINDER_SERVICE_HOST' in os.environ:
    ipycompss.start(graph=True, trace=True, debug=False,
                    project_xml='../xml/project.xml',
                    resources_xml='../xml/resources.xml')
else:
    ipycompss.start(graph=True, monitor=1000, trace=True, debug=False)

*****
***** PyCOMPSs Interactive *****
*****
*      .-~~-.-.-.      |____|      |____|      *
*      :      )      |____| \      /____| \      *
*      .~ ~ -.- \      /.- ~ ~ .      |____| | (____) | *
*      >      \      /      <      /____/      \____/ *
*      (      .-.-.      )      |____|      /____/ *
*      '-.-.-~ -.-.-' ~.-.-' |____| |____| /____/ *
*      (      :      )      |____|      |____| *
*      ~.-.-. :      .-.-~      .-.-~ } *
*      ~.-.-.-.-~ \      .~ .-.-~ *
*      \      \      \      \      \ *
*      \      \      \      \      \ *
*      . - ~ ~ -.- \      \      // *
*      .-.-. . - ~ ~ } ~ ~ -.-.-. *
*      /      .-.-.      :/~-.-.-./: *
*      /_~ -.-. - ~      ~.-.-.-. *
*      ~.-.-< *
*****
* - Starting COMPSs runtime... *
* - Log path : /home/javier/.COMPSs/InteractiveMode_19/ *
* - PyCOMPSs Runtime started... Have fun! *
*****
```



```
[6]: @task(returns=list)
def read_file(file_path):
    """ Read a file and return a list of words.
    :param file_path: file's path
    :return: list of words
    """
    data = []
    with open(file_path, 'r') as f:
        for line in f:
            data += line.split()
    return data

[7]: @task(returns=dict)
def wordCount(data):
    """ Construct a frequency word dictionary from a list of words.
    :param data: a list of words
    :return: a dictionary where key=word and value=#appearances
    """
    partialResult = {}
    for entry in data:
        if entry in partialResult:
            partialResult[entry] += 1
        else:
            partialResult[entry] = 1
    return partialResult

[8]: @task(returns=dict, priority=True)
def merge_two_dicts(dic1, dic2):
    """ Update a dictionary with another dictionary.
    :param dic1: first dictionary
    :param dic2: second dictionary
    :return: dic1+=dic2
    """
    for k in dic2:
        if k in dic1:
            dic1[k] += dic2[k]
        else:
            dic1[k] = dic2[k]
    return dic1

[9]: from pycompss.api.api import compss_wait_on

# Get the dataset path
pathDataset = os.getcwd() + '/dataset'

# Read file's content execute a wordcount on each of them
partialResult = []
for fileName in os.listdir(pathDataset):
    file_path = os.path.join(pathDataset, fileName)
    data = read_file(file_path)
    partialResult.append(wordCount(data))

# Accumulate the partial results to get the final result.
result = {}
for partial in partialResult:
    result = merge_two_dicts(result, partial)
```

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```
# Wait for result
result = compss_wait_on(result)

Found task: read_file
Found task: wordCount
Found task: merge_two_dicts
```

```
[10]: print("Result:")
      from pprint import pprint
      pprint(result)
      print("Words: {}".format(sum(result.values())))
```

```
Result:
{'Adipisci': 227,
 'Aliquam': 233,
 'Amet': 207,
 'Consectetur': 201,
 'Dolor': 198,
 'Dolore': 236,
 'Dolorem': 232,
 'Eius': 251,
 'Est': 197,
 'Etincidunt': 232,
 'Ipsum': 228,
 'Labore': 229,
 'Magnum': 195,
 'Modi': 201,
 'Neque': 205,
 'Non': 226,
 'Numquam': 253,
 'Porro': 205,
 'Quaerat': 217,
 'Quia': 212,
 'Quisquam': 214,
 'Sed': 225,
 'Sit': 220,
 'Tempora': 189,
 'Ut': 217,
 'Velit': 218,
 'Voluptatem': 235,
 'adipisci': 1078,
 'aliquam': 1107,
 'amet': 1044,
 'consectetur': 1073,
 'dolor': 1120,
 'dolore': 1065,
 'dolorem': 1107,
 'eius': 1048,
 'est': 1101,
 'etincidunt': 1114,
 'ipsum': 1061,
 'labore': 1070,
 'magnum': 1096,
 'modi': 1127,
 'neque': 1093,
 'non': 1099,
```

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```
'numquam': 1094,
'porro': 1101,
'quaerat': 1086,
'quiquia': 1079,
'quisquam': 1144,
'sed': 1109,
'sit': 1130,
'tempora': 1064,
'ut': 1070,
'velit': 1105,
'voluptatem': 1121}
Words: 35409
```

```
[11]: ipycompss.stop()
```

```
*****
***** STOPPING PyCOMPSs *****
*****
Checking if any issue happened.
Warning: some of the variables used with PyCOMPSs may
        have not been brought to the master.
*****
```

10.2.7 Wordcount Solution (With reduce)

10.2.7.1 Complete version

```
[1]: import os
```

```
[2]: import pycompss.interactive as ipycompss
```

```
[3]: from pycompss.api.task import task
```

```
[4]: from pycompss.api.parameter import *
```

```
[5]: if 'BINDER_SERVICE_HOST' in os.environ:
    ipycompss.start(graph=True, trace=True, debug=False,
                    project_xml='../xml/project.xml',
                    resources_xml='../xml/resources.xml')
else:
    ipycompss.start(graph=True, monitor=1000, trace=True, debug=False)
```

```
*****
***** PyCOMPSs Interactive *****
*****
*          .-~-.--.          |____| |____| *
*          :          )      |____| \  /____| \ *
*  .~ ~ -. \          /.- ~ ~ .  |____| |  |____| | *
*  >      \ .      . ' <      /____| \____| / *
*  (      .- -.      )  | |____| _  /____| / *
*  \ - -.~ \ - -' ~ - -' |____| | |  /____| / *
*  (      :          )      - - .-: *
*  ~ - - :      .-~ *
*  ~ - - ^ - - \_ .~ .-~ *
*          .~ .-~ .~
```

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```

*          \ \ '      \ ' _ _ ~          *
*          \ \ \ .    //          *
*      . - ~ ~ _ _ \ \ \ _ _ //          *
*      . ~ . - ~ } ~ ~ _ _ _ .          *
*      . ' . ~ . - ~ : / ~ _ _ _ . / :          *
*      / _ _ _ . - ~      ~ _ _ _ _          *
*          ~ _ . <          *
*****
* - Starting COMPSs runtime...          *
* - Log path : /home/javier/.COMPSs/InteractiveMode_20/          *
* - PyCOMPSs Runtime started... Have fun!          *
*****

```

```

[6]: @task(returns=list)
def read_file(file_path):
    """ Read a file and return a list of words.
    :param file_path: file's path
    :return: list of words
    """
    data = []
    with open(file_path, 'r') as f:
        for line in f:
            data += line.split()
    return data

[7]: @task(returns=dict)
def wordCount(data):
    """ Construct a frequency word dictionary from a list of words.
    :param data: a list of words
    :return: a dictionary where key=word and value=#appearances
    """
    partialResult = {}
    for entry in data:
        if entry in partialResult:
            partialResult[entry] += 1
        else:
            partialResult[entry] = 1
    return partialResult

[8]: @task(returns=dict, priority=True)
def merge_dicts(*dictionaries):
    import queue
    q = queue.Queue()
    for i in dictionaries:
        q.put(i)
    while not q.empty():
        x = q.get()
        if not q.empty():
            y = q.get()
            for k in y:
                if k in x:
                    x[k] += y[k]
                else:
                    x[k] = y[k]
            q.put(x)

```

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```
return(x)
```

```
[9]: from pycompss.api.api import compss_wait_on

# Get the dataset path
pathDataset = os.getcwd() + '/dataset'

# Construct a list with the file's paths from the dataset
partialResult = []
for fileName in os.listdir(pathDataset):
    p = os.path.join(pathDataset, fileName)
    data=read_file(p)
    partialResult.append(wordCount(data))

# Accumulate the partial results to get the final result.
result=merge_dicts(*partialResult)

# Wait for result
result = compss_wait_on(result)

Found task: read_file
Found task: wordCount
Found task: merge_dicts
```

```
[10]: print("Result:")
from pprint import pprint
pprint(result)
print("Words: {}".format(sum(result.values())))
```

```
Result:
{'Adipisci': 227,
 'Aliquam': 233,
 'Amet': 207,
 'Consectetur': 201,
 'Dolor': 198,
 'Dolore': 236,
 'Dolorem': 232,
 'Eius': 251,
 'Est': 197,
 'Etincidunt': 232,
 'Ipsum': 228,
 'Labore': 229,
 'Magna': 195,
 'Modi': 201,
 'Neque': 205,
 'Non': 226,
 'Numquam': 253,
 'Porro': 205,
 'Quaerat': 217,
 'Quia': 212,
 'Quisquam': 214,
 'Sed': 225,
 'Sit': 220,
 'Tempora': 189,
 'Ut': 217,
 'Velit': 218,
```

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```
'Voluptatem': 235,  
'adipisci': 1078,  
'aliquam': 1107,  
'amet': 1044,  
'consectetur': 1073,  
'dolor': 1120,  
'dolore': 1065,  
'dolorem': 1107,  
'eius': 1048,  
'est': 1101,  
'etincidunt': 1114,  
'ipsum': 1061,  
'labore': 1070,  
'magnam': 1096,  
'modi': 1127,  
'neque': 1093,  
'non': 1099,  
'numquam': 1094,  
'porro': 1101,  
'quaerat': 1086,  
'quiquia': 1079,  
'quisquam': 1144,  
'sed': 1109,  
'sit': 1130,  
'tempora': 1064,  
'ut': 1070,  
'velit': 1105,  
'voluptatem': 1121}  
Words: 35409
```

```
[11]: ipycompss.stop()
```

```
*****  
***** STOPPING PyCOMPSs *****  
*****  
Checking if any issue happened.  
Warning: some of the variables used with PyCOMPSs may  
         have not been brought to the master.  
*****
```

10.3 Demos

Here you will find the demonstration notebooks used in the tutorials.

10.3.1 Accelerating parallel code with PyCOMPSs and Numba

10.3.1.1 Demo Supercomputing 2019

What is mandelbrot?

The mandelbrot set is a fractal, which is plotted on the complex plane. It shows how intricate can be formed from a simple equation.

It is generated using the algorithm:

$$Z_{n+1} = z_n^2 + A \quad (1)$$

(2)

Where Z and A are complex numbers, and n represents the number of iterations.

First, import time to measure the elapsed execution times and create an ordered dictionary to keep all measures -> we are going to measure and plot the performance with different conditions!

```
[1]: import time
from collections import OrderedDict
times = OrderedDict()
```

And then, all required imports

```
[2]: from numpy import NaN, arange, abs, array
```

Mandelbrot set implementation:

```
[3]: def mandelbrot(a, max_iter):
    z = 0
    for n in range(1, max_iter):
        z = z**2 + a
        if abs(z) > 2:
            return n
    return NaN
```

```
[4]: def mandelbrot_set(y, X, max_iter):
    Z = [0 for _ in range(len(X))]
    for ix, x in enumerate(X):
        Z[ix] = mandelbrot(x + 1j * y, max_iter)
    return Z
```

Main function to generate the mandelbrot set. It splits the space in vertical chunks, and calculates the mandelbrot set of each one, generating the result Z .

```
[5]: def run_mandelbrot(X, Y, max_iter):
    st = time.time()
    Z = [[] for _ in range(len(Y))]
    for iy, y in enumerate(Y):
        Z[iy] = mandelbrot_set(y, X, max_iter)
    elapsed = time.time() - st
    print("Elapsed time (s): {}".format(elapsed))
    return Z, elapsed
```

The following function plots the fractal inline (the coerced parameter `**` is used to set *NaN* in coerced elements within Z).

```
[6]: %matplotlib inline
def plot_fractal(Z, coerced):
    if coerced:
        Z = [[NaN if c == -2**63 else c for c in row] for row in Z]
    import matplotlib.pyplot as plt
    Z = array(Z)
    plt.imshow(Z, cmap='plasma')
    plt.show()
```

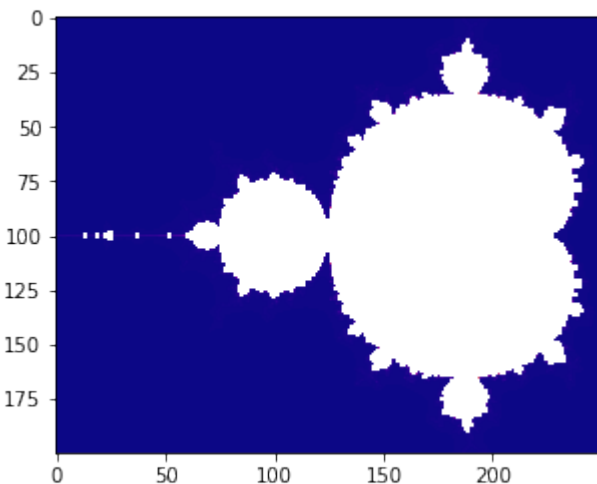
Define a benchmarking function:

```
[7]: def generate_fractal(coerced=False):
    X = arange(-2, .5, .01)
    Y = arange(-1.0, 1.0, .01)
    max_iterations = 2000
    Z, elapsed = run_mandelbrot(X, Y, max_iterations)
    plot_fractal(Z, coerced)
    return elapsed
```

Run the previous code **sequentially**:

```
[8]: times['Sequential'] = generate_fractal()
```

Elapsed time (s): 53.43384051322937

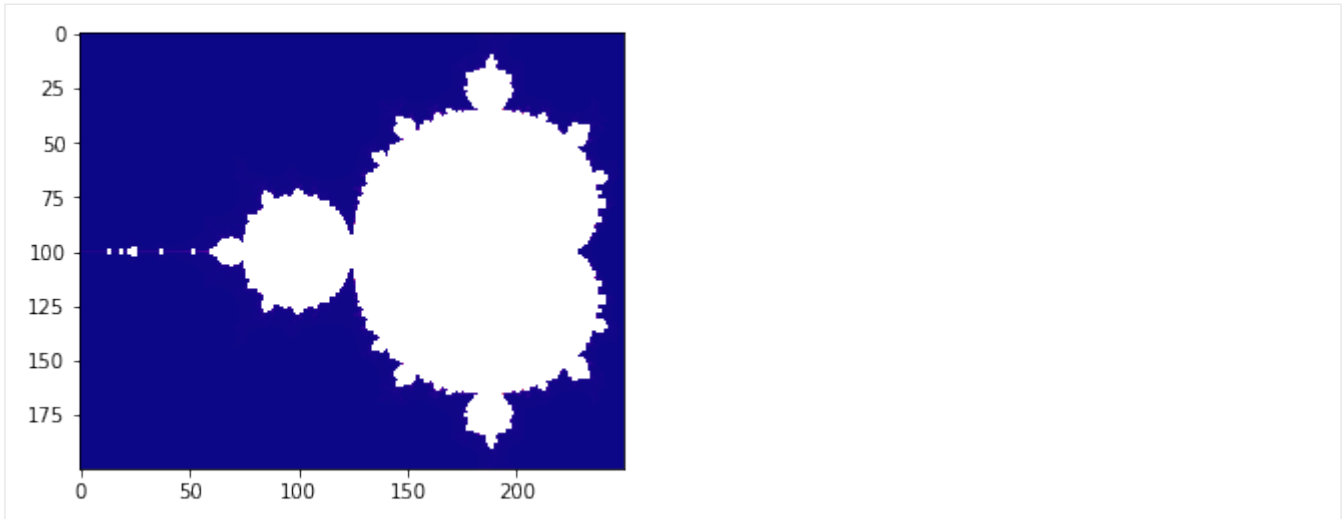


10.3.1.2 Parallelization with PyCOMPSs

After analysing the code, each mandelbrot set can be considered as a task, requiring only to decorate the `mandelbrot_set` function. It is interesting to observe that all sets are independent among them, so they can be computed completely independently, enabling to exploit multiple resources concurrently.

In order to run this code with we need first to start the **COMPSs** runtime:

```
[9]: import os
import pycompss.interactive as ipycompss
if 'BINDER_SERVICE_HOST' in os.environ:
    ipycompss.start(project_xml='../xml/project.xml',
                    resources_xml='../xml/resources.xml')
else:
    ipycompss.start(graph=False, trace=True, monitor=1000)
```

10.3.1.3 Accelerating the tasks with Numba

To this end, it is necessary to either use: 1. the Numba's `@jit` decorator under the PyCOMPSs `@task` decorator 2. or define the `numba=True` within the `@task` decorator.

First, we decorate the inner function (`mandelbrot`) with `@jit` since it is also a target function to be optimized with Numba.

```
[15]: from numba import jit

@jit
def mandelbrot(a, max_iter):
    z = 0
    for n in range(1, max_iter):
        z = z**2 + a
        if abs(z) > 2:
            return n
    return NaN # NaN is coerced by Numba
```

Option 1 - Add the `@jit` decorator explicitly under `@task` decorator

```
@task(returns=list) @jit def mandelbrot_set(y, X, max_iter): Z = [0 for _ in range(len(X))] for ix, x in enumerate(X): Z[ix] = mandelbrot(x + 1j * y, max_iter) return Z
```

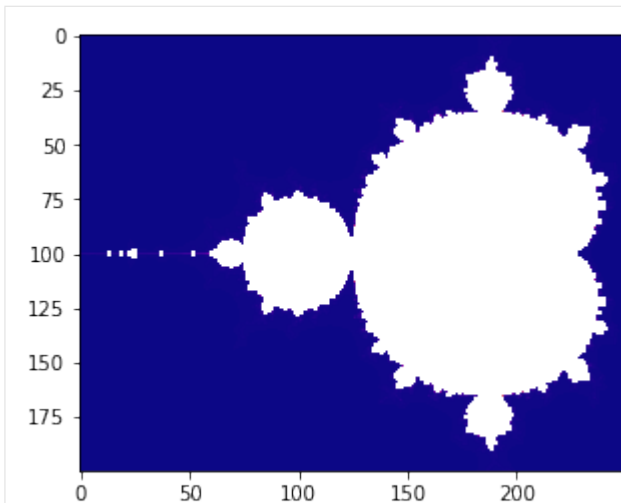
Option 2 - Add the `numba=True` flag within `@task` decorator

```
[16]: @task(returns=list, numba=True)
def mandelbrot_set(y, X, max_iter):
    Z = [0 for _ in range(len(X))]
    for ix, x in enumerate(X):
        Z[ix] = mandelbrot(x + 1j * y, max_iter)
    return Z
```

Run the benchmark with **Numba**:

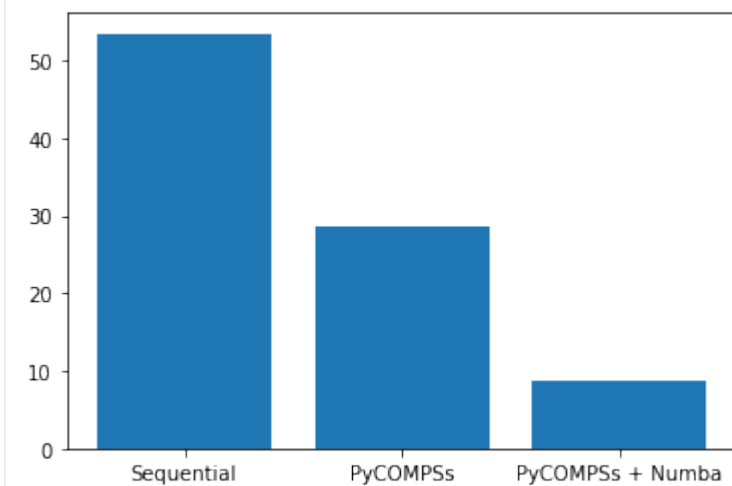
```
[17]: times['PyCOMPSs + Numba'] = generate_fractal(coerced=True)

Found task: mandelbrot_set
Elapsed time (s): 8.703550577163696
```



Plot the times:

```
[18]: import matplotlib.pyplot as plt
plt.bar(*zip(*times.items()))
plt.show()
```



Stop COMPSs runtime

```
[19]: ipycompss.stop()

*****
***** STOPPING PyCOMPSs *****
*****
Checking if any issue happened.
Warning: some of the variables used with PyCOMPSs may
        have not been brought to the master.
*****
```

Hint: These notebooks can be used within **MyBinder**, with the **PyCOMPSs Player**, within **Docker**, within **Virtual Machine** (recommended for Windows) provided by BSC, or locally.

Prerequisites

- Using *MyBinder*:

– Open  [launch binder](#)

Caution: Sometimes it may take a while to deploy the COMPSs infrastructure.

- Using **PyCOMPSs Player**:
 - `pycompss-player` (see [Requirements and Installation](#))
- Using **Docker**:
 - Docker
 - Git
- Using **Virtual Machine**:
 - VirtualBox
- For **local** execution:
 - Python 2 or 3
 - Install COMPSs requirements described in [Dependencies](#).
 - Install COMPSs (See [Building from sources](#))
 - Jupyter (with the desired ipykernel)
 - ipywidgets (only for some hands-on notebooks)
 - numpy (only for some notebooks)
 - dislib (only for some notebooks)
 - numba (only for some notebooks)
 - Git

Instructions

- Using **MyBinder**:

Just explore the folders and run the examples (they have the same structure as this documentation).
- Using `pycompss-player`:

Check the `pycompss-player` usage instructions (see [Usage](#))
Get the notebooks:

```
$ git clone https://github.com/bsc-wdc/notebooks.git
```

- Using **Docker**:

Run in your machine:

```
$ git clone https://github.com/bsc-wdc/notebooks.git
$ docker pull compss/compss:2.7
$ # Update the path to the notebooks path in the next command before running
↪ it
$ docker run --name mycompss -p 8888:8888 -p 8080:8080 -v /PATH/TO/notebooks:/
↪ home/notebooks -itd compss/compss:2.7
$ docker exec -it mycompss /bin/bash
```

Now that docker is running and you are connected:

```
$ cd /home/notebooks
$ /etc/init.d/compss-monitor start
$ jupyter-notebook --no-browser --allow-root --ip=172.17.0.2 --NotebookApp.
↪ token=
```

From local web browser:

```
Open COMPSs monitor: http://localhost:8080/compss-monitor/index.zul
Open Jupyter notebook interface: http://localhost:8888/
```

- Using **Virtual Machine**:
 - Download the OVA from: <https://www.bsc.es/research-and-development/software-and-apps/software-list/comp-superscalar/downloads> (Look for *Virtual Appliances* section)
 - Import the OVA from VirtualBox
 - Start the Virtual Machine
 - * User: **compss**
 - * Password: **compss2019**
 - Open a console and run:

```
$ git clone https://github.com/bsc-wdc/notebooks.git
$ cd notebooks
$ /etc/init.d/compss-monitor start
$ jupyter-notebook
```

- Open the web browser:

```
* Open COMPSs monitor: http://localhost:8080/compss-monitor/index.zul
* Open Jupyter notebook interface: http://localhost:8888/
```

- Using local installation
 - Get the notebooks and start jupyter

```
$ git clone https://github.com/bsc-wdc/notebooks.git
$ cd notebooks
$ /etc/init.d/compss-monitor start
$ jupyter-notebook
```

- Then

```
* Open COMPSs monitor: http://localhost:8080/compss-monitor/index.zul
* Open Jupyter notebook interface: http://localhost:8888/
* Look for the application.ipynb of interest.
```

Important: It is necessary to **RESTART** the python kernel from Jupyter after the execution of any notebook.

Troubleshooting

- ISSUE 1: Cannot connect using docker pull.
REASON: *The docker service is not running:*

```
$ # Error message:
$ Cannot connect to the Docker daemon at unix:///var/run/docker.sock. Is the
→docker daemon running?
$ # SOLUTION: Restart the docker service:
$ sudo service docker start
```

- ISSUE 2: The notebooks folder is empty or contains other data using docker.
REASON: *The notebooks path in the docker run command is wrong.*

```
$ # Remove the docker instance and reinstantiate with the appropriate
→notebooks path
$ exit
$ docker stop mycompss
$ docker rm mycompss
$ # Pay attention and UPDATE: /PATH/TO in the next command
$ docker run --name mycompss -p 8888:8888 -p 8080:8080 -v /PATH/TO/notebooks:/
→home/notebooks -itd compss/compss-tutorial:2.7
$ # Continue as normal
```

- ISSUE 3: COMPSs does not start in Jupyter.
REASON: *The python kernel has not been restarted between COMPSs start, or some processes from previous failed execution may exist.*

```
$ # SOLUTION: Restart the python kernel from Jupyter and check that there are
→no COMPSs' python/java processes running.
```

- ISSUE 4: Numba is not working with the VM or Docker.
REASON: *Numba is not installed in the VM or docker*

```
$ # SOLUTION: Install Numba in the VM/Docker
$ #           Open a console in the VM/Docker and follow the next steps.
$ # For Python 2:
$ sudo python2 -m pip install numba
$ # For Python 3:
$ sudo python3 -m pip install numba
```

- ISSUE 5: Matplotlib is not working with the VM or Docker.
REASON: *Matplotlib is not installed in the VM or docker*

```
$ # SOLUTION: Install Matplotlib in the VM/Docker
$ #           Open a console in the VM/Docker and follow the next steps.
$ # For Python 2:
$ sudo python2 -m pip install matplotlib
$ # For Python 3:
$ sudo python3 -m pip install matplotlib
```

Contact support-compss@bsc.es

Chapter 11

Troubleshooting

This section provides answers for the most common issues of the execution of COMPSs applications and its known limitations.

For specific issues not covered in this section, please do not hesitate to contact us at: support-compss@bsc.es.

11.1 How to debug

When an error/exception happens during the execution of an application, the first thing that users must do is to check the application output:

- Using `runcompss` the output is shown in the console.
- Using `enqueue_compss` the output is in the `compss-<JOB_ID>.out` and `compss-<JOB_ID>.err`

If the error happens within a task, it will not appear in these files. Users must check the log folder in order to find what has failed. The log folder is by default in:

- Using `runcompss`: `$HOME/.COMPSs/<APP_NAME>_XX` (where XX is a number between 00 and 99, and increases on each run).
- Using `enqueue_compss`: `$HOME/.COMPSs/<JOB_ID>`

This log folder contains the `jobs` folder, where all output/errors of the tasks are stored. In particular, each task produces a `JOB<TASK_NUMBER>_NEW.out` and `JOB<TASK_NUMBER>_NEW.err` files when a task fails.

Tip: If the user enables the **debug mode** by including the `-d` flag into `runcompss` or `enqueue_compss` command, more information will be stored in the log folder of each run easing the error detection. In particular, all output and error output of all tasks will appear within the `jobs` folder.

In addition, some more log files will appear:

- `runtime.log`
- `pycompss.log` (only if using the Python binding).
- `pycompss.err` (only if using the Python binding and an error in the binding happens.)
- `resources.log`
- `workers` folder. This folder will contain four files per worker node:
 - `worker_<MACHINE_NAME>.out`
 - `worker_<MACHINE_NAME>.err`
 - `binding_worker_<MACHINE_NAME>.out`
 - `binding_worker_<MACHINE_NAME>.err`

As a suggestion, users should check the last lines of the `runtime.log`. If the file-transfers or the tasks are failing an error message will appear in this file. If the file-transfers are successfully and the jobs are submitted, users should check the `jobs` folder and look at the error messages produced inside each job. Users should notice that if there are **RESUBMITTED** files something inside the job is failing.

If the `workers` folder is empty, means that the execution failed and the COMPSs runtime was not able to retrieve the workers logs. In this case, users must connect to the workers and look directly into the worker logs. Alternatively, if the user is running with a shared disk (e.g. in a supercomputer), the user can define a shared folder in the `--worker_working_directory=/shared/folder` where a `tmp_XXXXXX` folder will be created on the application execution and all worker logs will be stored.

Tip: When debug is enabled, the workers also produce log files which are transferred to the master when the application finishes. These log files are always removed from the workers (even if there is a failure to avoid abandoning files). Consequently, it is possible **to disable the removal of the log files produced by the workers**, so that users can still check them in the worker nodes if something fails and these logs are not transferred to the master node. To this end, include the following flag into `runcompss` or `enqueue_compss`:

```
--keep_workingdir
```

Please, note that the workers will store the log files into the folder defined by the `--worker_working_directory`, that can be a shared or local folder.

Tip: If segmentation fault occurs, the core dump file can be generated by setting the following flag into `runcompss` or `enqueue_compss`:

```
--gen_coredump
```

The following subsections show debugging examples depending on the choosen flavour (Java, Python or C/C++).

11.1.1 Java examples

11.1.1.1 Exception in the main code

TODO

Missing subsection

11.1.1.2 Exception in a task

TODO

Missing subsection

11.1.2 Python examples

11.1.2.1 Exception in the main code

Consider the following code where an intended error in the main code has been introduced to show how it can be debugged.

```
from pycompss.api.task import task

@task(returns=1)
```

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```
def increment(value):
    return value + 1

def main():
    initial_value = 1
    result = increment(initial_value)

    result = result + 1 # Try to use result without synchronizing it: Error

    print("Result: " + str(result))

if __name__ == '__main__':
    main()
```

When executed, it produces the following output:

```
$ runcompss error_in_main.py

[ INFO] Inferred PYTHON language
[ INFO] Using default location for project file: /opt/COMPSs//Runtime/configuration/xml/
→projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSs//Runtime/configuration/xml/
→resources/default_resources.xml
[ INFO] Using default execution type: compss

----- Executing error_in_main.py -----

WARNING: COMPSs Properties file is null. Setting default values
[(377)   API] - Starting COMPSs Runtime v2.7 (build 20200519-1005.
→r6093e5ac94d67250e097a6fad9d3ec00d676fe6c)
[ ERROR ]: An exception occurred: unsupported operand type(s) for +: 'Future' and 'int'
Traceback (most recent call last):
  File "/opt/COMPSs//Bindings/python/2/pycompss/runtime/launch.py", line 204, in compss_main
    execfile(APP_PATH, globals()) # MAIN EXECUTION
  File "error_in_main.py", line 16, in <module>
    main()
  File "error_in_main.py", line 11, in main
    result = result + 1 # Try to use result without synchronizing it: Error
TypeError: unsupported operand type(s) for +: 'Future' and 'int'
[ERRMGR] - WARNING: Task 1(Action: 1) with name error_in_main.increment has been cancelled.
[ERRMGR] - WARNING: Task canceled: [[Task id: 1], [Status: CANCELED], [Core id: 0],
→[Priority: false], [NumNodes: 1], [MustReplicate: false], [MustDistribute: false], [error_
→in_main.increment(INT_T)]]
[(3609)   API] - Execution Finished

Error running application
```

It can be identified the complete traceback pointing where the error is, and the reason. In this example, the reason is `TypeError: unsupported operand type(s) for +: 'Future' and 'int'` since we are trying to use an object that has not been synchronized.

Tip: Any exception raised from the main code will appear in the same way, showing the traceback helping to identify the line which produced the exception and its reason.

11.1.2.2 Exception in a task

Consider the following code where an intended error in a task code has been introduced to show how it can be debugged.

```
from pycompss.api.task import task
from pycompss.api.api import compss_wait_on

@task(returns=1)
def increment(value):
    return value + 1 # value is an string, can not add an int: Error

def main():
    initial_value = "1" # the initial value is a string instead of an integer
    result = increment(initial_value)
    result = compss_wait_on(result)
    print("Result: " + str(result))

if __name__=='__main__':
    main()
```

When executed, it produces the following output:

```
$ runcompss error_in_task.py

[ INFO] Inferred PYTHON language
[ INFO] Using default location for project file: /opt/COMPSs/Runtime/configuration/xml/
→projects/default_project.xml
[ INFO] Using default location for resources file: /opt/COMPSs/Runtime/configuration/xml/
→resources/default_resources.xml
[ INFO] Using default execution type: compss

----- Executing error_in_task.py -----

WARNING: COMPSs Properties file is null. Setting default values
[(570)  API] - Starting COMPSs Runtime v2.7 (build 20200519-1005.
→r6093e5ac94d67250e097a6fad9d3ec00d676fe6c)
[ERRMGR] - WARNING: Job 1 for running task 1 on worker localhost has failed; resubmitting
→task to the same worker.
[ERRMGR] - WARNING: Task 1 execution on worker localhost has failed; rescheduling task
→execution. (changing worker)
[ERRMGR] - WARNING: Job 2 for running task 1 on worker localhost has failed; resubmitting
→task to the same worker.
[ERRMGR] - WARNING: Task 1 has already been rescheduled; notifying task failure.
[ERRMGR] - WARNING: Task 'error_in_task.increment' TOTALLY FAILED.
           Possible causes:
               -Exception thrown by task 'error_in_task.increment'.
               -Expected output files not generated by task 'error_in_task.
→increment'.
               -Could not provide nor retrieve needed data between master and
→worker.

           Check files '/home/user/.COMPSs/error_in_task.py_01/jobs/job[1|2]' to
→find out the error.

[ERRMGR] - ERROR: Task failed: [[Task id: 1], [Status: FAILED], [Core id: 0], [Priority:
→false], [NumNodes: 1], [MustReplicate: false], [MustDistribute: false], [error_in_task.
→increment(String_T)]]
```

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```
[ERRMGR] - Shutting down COMPSs...
[(4711)  API] - Execution Finished
Shutting down the running process
```

```
Error running application
```

The output describes that there has been an issue with the task number 1. Since the default behaviour of the runtime is to resubmit the failed task, task 2 also fails.

In this case, the runtime suggests to check the log files of the tasks: `/home/user/.COMPSs/error_in_task.py_01/jobs/job[1|2]`

Looking into the logs folder, it can be seen that the jobs folder contains the logs of the failed tasks:

```
$HOME/.COMPSs
├── error_in_task.py_01
│   └── jobs
│       ├── job1_NEW.err
│       ├── job1_NEW.out
│       ├── job1_RESUBMITTED.err
│       ├── job1_RESUBMITTED.out
│       ├── job2_NEW.err
│       ├── job2_NEW.out
│       ├── job2_RESUBMITTED.err
│       └── job2_RESUBMITTED.out
├── resources.log
├── runtime.log
├── tmpFiles
└── workers
```

And the `job1_NEW.err` contains the complete traceback of the exception that has been raised (`TypeError: cannot concatenate 'str' and 'int' objects as consequence of using a string for the task input which tries to add 1`):

```
[EXECUTOR] executeTask - Error in task execution
es.bsc.compss.types.execution.exceptions.JobExecutionException: Job 1 exit with value 1
  at es.bsc.compss.invokers.external.piped.PipedInvoker.invokeMethod(PipedInvoker.java:78)
  at es.bsc.compss.invokers.Invoker.invoke(Invoker.java:352)
  at es.bsc.compss.invokers.Invoker.processTask(Invoker.java:287)
  at es.bsc.compss.executor.Executor.executeTask(Executor.java:486)
  at es.bsc.compss.executor.Executor.executeTaskWrapper(Executor.java:322)
  at es.bsc.compss.executor.Executor.execute(Executor.java:229)
  at es.bsc.compss.executor.Executor.processRequests(Executor.java:198)
  at es.bsc.compss.executor.Executor.run(Executor.java:153)
  at es.bsc.compss.executor.utils.ExecutionPlatform$2.run(ExecutionPlatform.java:178)
  at java.lang.Thread.run(Thread.java:748)
Traceback (most recent call last):
  File "/opt/COMPSs/Bindings/python/2/pycompss/worker/commons/worker.py", line 265, in task_
→ execution
    **compss_kwargs)
  File "/opt/COMPSs/Bindings/python/2/pycompss/api/task.py", line 267, in task_decorator
    return self.worker_call(*args, **kwargs)
  File "/opt/COMPSs/Bindings/python/2/pycompss/api/task.py", line 1523, in worker_call
    **user_kwargs)
  File "/home/user/temp/Bugs/documentation/error_in_task.py", line 6, in increment
    return value + 1
TypeError: cannot concatenate 'str' and 'int' objects
```

Tip: Any exception raised from the task code will appear in the same way, showing the traceback helping to identify the line which produced the exception and its reason.

11.1.3 C/C++ examples

11.1.3.1 Exception in the main code

TODO

Missing subsection

11.1.3.2 Exception in a task

TODO

Missing subsection

11.2 Common Issues

11.2.1 Tasks are not executed

If the tasks remain in **Blocked** state probably there are no existing resources matching the specific task constraints. This error can be potentially caused by two facts: the resources are not correctly loaded into the runtime, or the task constraints do not match with any resource.

In the first case, users should take a look at the `resources.log` and check that all the resources defined in the `project.xml` file are available to the runtime. In the second case users should re-define the task constraints taking into account the resources capabilities defined into the `resources.xml` and `project.xml` files.

11.2.2 Jobs fail

If all the application's tasks fail because all the submitted jobs fail, it is probably due to the fact that there is a resource miss-configuration. In most of the cases, the resource that the application is trying to access has no passwordless access through the configured user. This can be checked by:

- Open the `project.xml`. (The default file is stored under `/opt/COMPSs/ Runtime/configuration/xml/projects/project.xml`)
- For each resource annotate its name and the value inside the `User` tag. Remember that if there is no `User` tag COMPSs will try to connect this resource with the same username than the one that launches the main application.
- For each annotated resourceName - user please try `ssh user@resourceName`. If the connection asks for a password then there is an error in the configuration of the ssh access in the resource.

The problem can be solved running the following commands:

```
compss@bsc:~$ scp ~/.ssh/id_rsa.pub user@resourceName:./myRSA.pub
compss@bsc:~$ ssh user@resourceName "cat myRSA.pub >> ~/.ssh/authorized_keys; rm ./myRSA.pub"
```

These commands are a quick solution, for further details please check the [Additional Configuration](#) Section.

11.2.3 Exceptions when starting the Worker processes

When the COMPSs master is not able to communicate with one of the COMPSs workers described in the *project.xml* and *resources.xml* files, different exceptions can be raised and logged on the *runtime.log* of the application. All of them are raised during the worker start up and contain the *[WorkerStarter]* prefix. Next we provide a list with the common exceptions:

InitNodeException Exception raised when the remote SSH process to start the worker has failed.

UnstartedNodeException Exception raised when the worker process has aborted.

Connection refused Exception raised when the master cannot communicate with the worker process (NIO).

All these exceptions encapsulate an error when starting the worker process. This means that **the worker machine is not properly configured** and thus, you need to check the environment of the failing worker. Further information about the specific error can be found on the worker log, available at the working directory path in the remote worker machine (the worker working directory specified in the *project.xml* file).

Next, we list the most common errors and their solutions:

java command not found Invalid path to the java binary. Check the *JAVA_HOME* definition at the remote worker machine.

Cannot create WD Invalid working directory. Check the rw permissions of the worker's working directory.

No exception The worker process has started normally and there is no exception. In this case the issue is normally due to the firewall configuration preventing the communication between the COMPSs master and worker. Please check that the worker firewall has in and out permissions for TCP and UDP in the adaptor ports (the adaptor ports are specified in the *resources.xml* file. By default the port rank is 43000-44000.

11.2.4 Compilation error: @Method not found

When trying to compile Java applications users can get some of the following compilation errors:

```
error: package es.bsc.compss.types.annotations does not exist
import es.bsc.compss.types.annotations.Constraints;
~

error: package es.bsc.compss.types.annotations.task does not exist
import es.bsc.compss.types.annotations.task.Method;
~

error: package es.bsc.compss.types.annotations does not exist
import es.bsc.compss.types.annotations.Parameter;
~

error: package es.bsc.compss.types.annotations.Parameter does not exist
import es.bsc.compss.types.annotations.parameter.Direction;
~

error: package es.bsc.compss.types.annotations.Parameter does not exist
import es.bsc.compss.types.annotations.parameter.Type;
~

error: cannot find symbol
@Parameter(type = Type.FILE, direction = Direction.INOUT)
~
    symbol:   class Parameter
    location: interface APPLICATION_Itf

error: cannot find symbol
@Constraints(computingUnits = "2")
~
    symbol:   class Constraints
    location: interface APPLICATION_Itf

error: cannot find symbol
@Method(declaringClass = "application.ApplicationImpl")
```

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```

^
symbol:    class Method
location:  interface APPLICATION_Itf

```

All these errors are raised because the `compss-engine.jar` is not listed in the CLASSPATH. The default COMPSs installation automatically inserts this package into the CLASSPATH but it may have been overwritten or deleted. Please check that your environment variable CLASSPATH contains the `compss-engine.jar` location by running the following command:

```
$ echo $CLASSPATH | grep compss-engine
```

If the result of the previous command is empty it means that you are missing the `compss-engine.jar` package in your classpath.

The easiest solution is to manually export the CLASSPATH variable into the user session:

```
$ export CLASSPATH=$CLASSPATH:/opt/COMPSs/Runtime/compss-engine.jar
```

However, you will need to remember to export this variable every time you log out and back in again. Consequently, we recommend to add this export to the `.bashrc` file:

```
$ echo "# COMPSs variables for Java compilation" >> ~/.bashrc
$ echo "export CLASSPATH=$CLASSPATH:/opt/COMPSs/Runtime/compss-engine.jar" >> ~/.bashrc
```

Warning: The `compss-engine.jar` is installed inside the COMPSs installation directory. If you have performed a custom installation, the path of the package may be different.

11.2.5 Jobs failed on method reflection

When executing an application the main code gets stuck executing a task. Taking a look at the `runtime.log` users can check that the job associated to the task has failed (and all its resubmissions too). Then, opening the `jobX_NEW.out` or the `jobX_NEW.err` files users find the following error:

```

[ERROR|es.bsc.compss.Worker|Executor] Can not get method by reflection
es.bsc.compss.nio.worker.executors.Executor$JobExecutionException: Can not get method by reflection
    at es.bsc.compss.nio.worker.executors.JavaExecutor.executeTask(JavaExecutor.java:142)
    at es.bsc.compss.nio.worker.executors.Executor.execute(Executor.java:42)
    at es.bsc.compss.nio.worker.JobLauncher.executeTask(JobLauncher.java:46)
    at es.bsc.compss.nio.worker.JobLauncher.processRequests(JobLauncher.java:34)
    at es.bsc.compss.util.RequestDispatcher.run(RequestDispatcher.java:46)
    at java.lang.Thread.run(Thread.java:745)
Caused by: java.lang.NoSuchMethodException: simple.Simple.increment(java.lang.String)
    at java.lang.Class.getMethod(Class.java:1678)
    at es.bsc.compss.nio.worker.executors.JavaExecutor.executeTask(JavaExecutor.java:140)
    ... 5 more

```

This error is due to the fact that COMPSs cannot find one of the tasks declared in the Java Interface. Commonly this is triggered by one of the following errors:

- The *declaringClass* of the tasks in the Java Interface has not been correctly defined.
- The parameters of the tasks in the Java Interface do not match the task call.
- The tasks have not been defined as *public*.

11.2.6 Jobs failed on reflect target invocation null pointer

When executing an application the main code gets stuck executing a task. Taking a look at the `runtime.log` users can check that the job associated to the task has failed (and all its resubmissions too). Then, opening the `jobX_NEW.out` or the `jobX_NEW.err` files users find the following error:

```
[ERROR|es.bsc.compss.Worker|Executor]
java.lang.reflect.InvocationTargetException
    at sun.reflect.NativeMethodAccessorImpl.invoke0(Native Method)
    at sun.reflect.NativeMethodAccessorImpl.invoke(NativeMethodAccessorImpl.java:57)
    at sun.reflect.DelegatingMethodAccessorImpl.invoke(DelegatingMethodAccessorImpl.java:
↪43)
    at java.lang.reflect.Method.invoke(Method.java:606)
    at es.bsc.compss.nio.worker.executors.JavaExecutor.executeTask(JavaExecutor.java:154)
    at es.bsc.compss.nio.worker.executors.Executor.execute(Executor.java:42)
    at es.bsc.compss.nio.worker.JobLauncher.executeTask(JobLauncher.java:46)
    at es.bsc.compss.nio.worker.JobLauncher.processRequests(JobLauncher.java:34)
    at es.bsc.compss.util.RequestDispatcher.run(RequestDispatcher.java:46)
    at java.lang.Thread.run(Thread.java:745)
Caused by: java.lang.NullPointerException
    at simple.Ll.printY(Ll.java:25)
    at simple.Simple.task(Simple.java:72)
    ... 10 more
```

This cause of this error is that the Java object accessed by the task has not been correctly transferred and one or more of its fields is null. The transfer failure is normally caused because the transferred object is not serializable.

Users should check that all the object parameters in the task are either implementing the serializable interface or following the *java beans* model (by implementing an empty constructor and getters and setters for each attribute).

11.2.7 Tracing merge failed: too many open files

When too many nodes and threads are instrumented, the tracing merge can fail due to an OS limitation, namely: the maximum open files. This problem usually happens when using advanced mode due to the larger number of threads instrumented. To overcome this issue users have two choices. **First option**, use *Extræ* parallel MPI merger. This merger is automatically used if COMPSs was installed with MPI support. In Ubuntu you can install the following packets to get MPI support:

```
$ sudo apt-get install libcr-dev mpich2 mpich2-doc
```

Please note that *extrae* is never compiled with MPI support when building it locally (with `buildlocal` command).

To check if COMPSs was deployed with MPI support, you can check the installation log and look for the following *Extræ* configuration output:

```
Package configuration for Extræe VERSION based on extrae/trunk rev. 3966:
-----
Installation prefix: /gpfs/apps/MN3/COMPSs/Trunk/Dependencies/extrae
Cross compilation: no
CC: gcc
CXX: g++
Binary type: 64 bits

MPI instrumentation: yes
  MPI home: /apps/OPENMPI/1.8.1-mellanox
  MPI launcher: /apps/OPENMPI/1.8.1-mellanox/bin/mpirun
```

On the other hand, if you already installed COMPSs, you can check *Extræ* configuration executing the script `/opt/COMPSs/Dependencies/extrae/etc/configured.sh`. Users should check that flags `--with-mpi=/usr` and

--enable-parallel-merge are present and that MPI path is correct and exists. Sample output:

```
EXTRAЕ_HOME is not set. Guessing from the script invoked that Extrae was installed in /opt/
↳COMPSs/Dependencies/extrae
The directory exists .. OK
Loaded specs for Extrae from /opt/COMPSs/Dependencies/extrae/etc/extrae-vars.sh

Extrae SVN branch extrae/trunk at revision 3966

Extrae was configured with:
$ ./configure --enable-gettimeofday-clock --without-mpi --without-unwind --without-dyninst --
↳without-binutils --with-mpi=/usr --enable-parallel-merge --with-papi=/usr --with-java-jdk=/
↳usr/lib/jvm/java-7-openjdk-amd64/ --disable-openmp --disable-nanos --disable-smpss --
↳prefix=/opt/COMPSs/Dependencies/extrae --with-mpi=/usr --enable-parallel-merge --libdir=/
↳opt/COMPSs/Dependencies/extrae/lib

CC was gcc
CFLAGS was -g -O2 -fno-optimize-sibling-calls -Wall -W
CXX was g++
CXXFLAGS was -g -O2 -fno-optimize-sibling-calls -Wall -W

MPI_HOME points to /usr and the directory exists .. OK
LIBXML2_HOME points to /usr and the directory exists .. OK
PAPI_HOME points to /usr and the directory exists .. OK
DYNINST support seems to be disabled
UNWINDing support seems to be disabled (or not needed)
Translating addresses into source code references seems to be disabled (or not needed)

Please, report bugs to tools@bsc.es
```

Important: Disclaimer: the parallel merge with MPI will not bypass the system's maximum number of open files, just distribute the files among the resources. If all resources belong to the same machine, the merge will fail anyways.

The **second option** is to increase the OS maximum number of open files. For instance, in Ubuntu add `` ulimit -n 40000 `` just before the start-stop-daemon line in the do_start section.

11.2.8 Performance issues

11.2.8.1 Different work directories

Having different work directories (for master and workers) may lead to performance issues. In particular, if the work directories belong to different mount points and with different performance, where the copy of files may be required. For example, using folders that are shared across nodes in a supercomputer but with different performance (e.g. `scratch` and `projects` in MareNostrum 4) for the master and worker workspaces.

11.3 Memory Profiling

COMPSs also provides a mechanism to show the memory usage over time when running Python applications. This is particularly useful when memory issues happen (e.g. memory exhausted – causing the application crash), or performance analysis (e.g. problem size scalability).

To this end, the `runcompss` and `enqueue_compss` commands provide the `--python_memory_profile` flag, which provides a set of files (one per node used in the application execution) where the memory used during the execution is recorded at the end of the application. They are generated in the same folder where the execution has been launched.

Important: The `memory-profiler` package is mandatory in order to use the `--python_memory_profile` flag.

It can be easily installed with pip:

```
$ python -m pip install memory-profiler --user
```

Tip: If you want to store from the memory profiler in a different folder, export the `COMPSS_WORKER_PROFILE_PATH` with the destination path:

```
$ export COMPSS_WORKER_PROFILE_PATH=/path/to/destination
```

When `--python_memory_profile` is included, a file with name `mprofile_<DATE_TIME>.dat` is generated for the master memory profiling, while for the workers they are named `<WORKER_NODE_NAME>.dat`. These files can be displayed with the `mprof` tool:

```
$ mprof plot <FILE>.dat
```

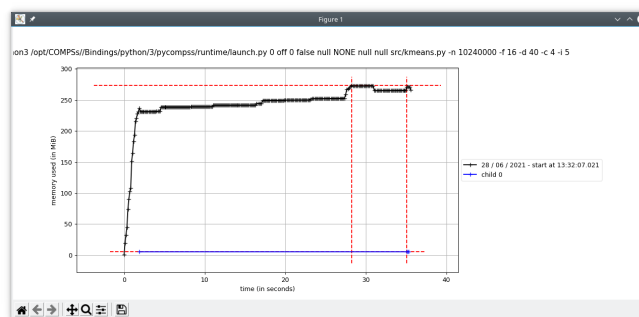


Figure 54: mprof plot example

11.3.1 Advanced profiling

For a more fine grained memory profiling and analysing the **workers** memory usage, PyCOMPSs provides the `@profile` decorator. This decorator is able to display the memory usage per line of the code. It can be imported from the PyCOMPSs functions module:

```
from pycompss.functions.profile import profile
```

This decorator can be placed over any function:

Over the `@task` decorator (or over the decorator stack of a task) This will display the memory usage in the master (through standard output).

Under the @task decorator: This will display the memory used by the actual task in the worker. The memory usage will be shown through standard output, so it is mandatory to enable debug (`--log_level=debug`) and check the job output file from `.COMPSs/<app_folder>/jobs/`.

Over a non task function: Will display the memory usage of the function in the master (through standard output).

11.4 Known Limitations

The current COMPSs version has the following limitations:

11.4.1 Global

Exceptions The current COMPSs version is not able to propagate exceptions raised from a task to the master. However, the runtime catches any exception and sets the task as failed.

Use of file paths The persistent workers implementation has a unique *Working Directory* per worker. That means that tasks should not use hardcoded file names to avoid file collisions and tasks misbehaviours. We recommend to use files declared as task parameters, or to manually create a sandbox inside each task execution and/or to generate temporary random file names.

11.4.2 With Java Applications

Java tasks Java tasks **must** be declared as **public**. Despite the fact that tasks can be defined in the main class or in other ones, we recommend to define the tasks in a separated class from the main method to force its public declaration.

Java objects Objects used by tasks must follow the *java beans* model (implementing an empty constructor and getters and setters for each attribute) or implement the *serializable* interface. This is due to the fact that objects will be transferred to remote machines to execute the tasks.

Java object aliasing If a task has an object parameter and returns an object, the returned value must be a new object (or a cloned one) to prevent any aliasing with the task parameters.

```
// @Method(declaringClass = "...")
// DummyObject incorrectTask (
//     @Parameter(type = Type.OBJECT, direction = Direction.IN) DummyObject a,
//     @Parameter(type = Type.OBJECT, direction = Direction.IN) DummyObject b
// );
public DummyObject incorrectTask (DummyObject a, DummyObject b) {
    if (a.getValue() > b.getValue()) {
        return a;
    }
    return b;
}

// @Method(declaringClass = "...")
// DummyObject correctTask (
//     @Parameter(type = Type.OBJECT, direction = Direction.IN) DummyObject a,
//     @Parameter(type = Type.OBJECT, direction = Direction.IN) DummyObject b
// );
public DummyObject correctTask (DummyObject a, DummyObject b) {
    if (a.getValue() > b.getValue()) {
        return a.clone();
    }
    return b.clone();
}
```

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```

public static void main() {
    DummyObject a1 = new DummyObject();
    DummyObject b1 = new DummyObject();
    DummyObject c1 = new DummyObject();
    c1 = incorrectTask(a1, b1);
    System.out.println("Initial value: " + c1.getValue());
    a1.modify();
    b1.modify();
    System.out.println("Aliased value: " + c1.getValue());

    DummyObject a2 = new DummyObject();
    DummyObject b2 = new DummyObject();
    DummyObject c2 = new DummyObject();
    c2 = incorrectTask(a2, b2);
    System.out.println("Initial value: " + c2.getValue());
    a2.modify();
    b2.modify();
    System.out.println("Non-aliased value: " + c2.getValue());
}

```

11.4.3 With Python Applications

Python constraints in the cloud When using python applications with constraints in the cloud the minimum number of VMs must be set to 0 because the initial VM creation does not respect the tasks constraints. Notice that if no constraints are defined the initial VMs are still usable.

Intermediate files Some applications may generate intermediate files that are only used among tasks and are never needed inside the master's code. However, COMPSs will transfer back these files to the master node at the end of the execution. Currently, the only way to avoid transferring these intermediate files is to manually erase them at the end of the master's code. Users must take into account that this only applies for files declared as task parameters and **not** for files created and/or erased inside a task.

User defined classes in Python User defined classes in Python **must not be declared in the same file that contains the main method** (if `__name__ == '__main__'`) to avoid serialization problems of the objects.

Python object hierarchy dependency detection Dependencies are detected only on the objects that are task parameters or outputs. Consider the following code:

```

# a.py
class A:
    def __init__(self, b):
        self.b = b

# main.py
from a import A
from pycompss.api.task import task
from pycompss.api.parameter import *
from pycompss.api.api import compss_wait_on

@task(obj = IN, returns = int)
def get_b(obj):
    return obj.b

@task(obj = INOUT)
def inc(obj):
    obj += [1]

```

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```
def main():
    my_a = A([5])
    inc(my_a.b)
    obj = get_b(my_a)
    obj = compss_wait_on(obj)
    print obj

if __name__ == '__main__':
    main()
```

Note that there should exist a dependency between `A` and `A.b`. However, PyCOMPSs is not capable to detect dependencies of that kind. These dependencies must be handled (and avoided) manually.

Python modules with global states Some modules (for example `logging`) have internal variables apart from functions. These modules are not guaranteed to work in PyCOMPSs due to the fact that master and worker code are executed in different interpreters. For instance, if a `logging` configuration is set on some worker, it will not be visible from the master interpreter instance.

Python global variables This issue is very similar to the previous one. PyCOMPSs does not guarantee that applications that create or modify global variables while worker code is executed will work. In particular, this issue (and the previous one) is due to Python's Global Interpreter Lock (GIL).

Python application directory as a module If the Python application root folder is a python module (i.e: it contains an `__init__.py` file) then `runcompss` must be called from the parent folder. For example, if the Python application is in a folder with an `__init__.py` file named `my_folder` then PyCOMPSs will resolve all functions, classes and variables as `my_folder.object_name` instead of `object_name`. For example, consider the following file tree:

```
my_apps/
├── kmeans/
│   ├── __init__.py
│   └── kmeans.py
```

Then the correct command to call this app is `runcompss kmeans/kmeans.py` from the `my_apps` directory.

Python early program exit All intentional, premature exit operations must be done with `sys.exit`. PyCOMPSs needs to perform some cleanup tasks before exiting and, if an early exit is performed with `sys.exit`, the event will be captured, allowing PyCOMPSs to perform these tasks. If the exit operation is done in a different way then there is no guarantee that the application will end properly.

Python with numpy and MKL Tasks that invoke numpy and MKL may experience issues if tasks use a different number of MKL threads. This is due to the fact that MKL reuses threads along different calls and it does not change the number of threads from one call to another.

11.4.4 With Services

Services types The current COMPSs version only supports SOAP based services that implement the WS interoperability standard. REST services are not supported.