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EXCELENCIA SEVERO OCHOA

Programming Distributed Computing Platforms with COMPSs

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Workflows & Distributed Computing Group

19/09/2019

13th RES Users Conference

Agenda

14.30 Introduction

14:40 PyCOMPSs syntax

15:20 Overview of COMPSs runtime

15:30 Introduction to dislib

15:40 Break

15:55 Hands-on in MN4:

- PyCOMPSs simple use case in Python
- Use case calling external binaries
- dislib use case

17:00 Closing

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Introduction

BSC vision on programming models

Applications

PM: High-level, clean, abstract interface

Power to the runtime

API

Program logic independent of computing platform

General purpose
Task based
Single address space

Intelligent runtime, parallelization, distribution, interoperability

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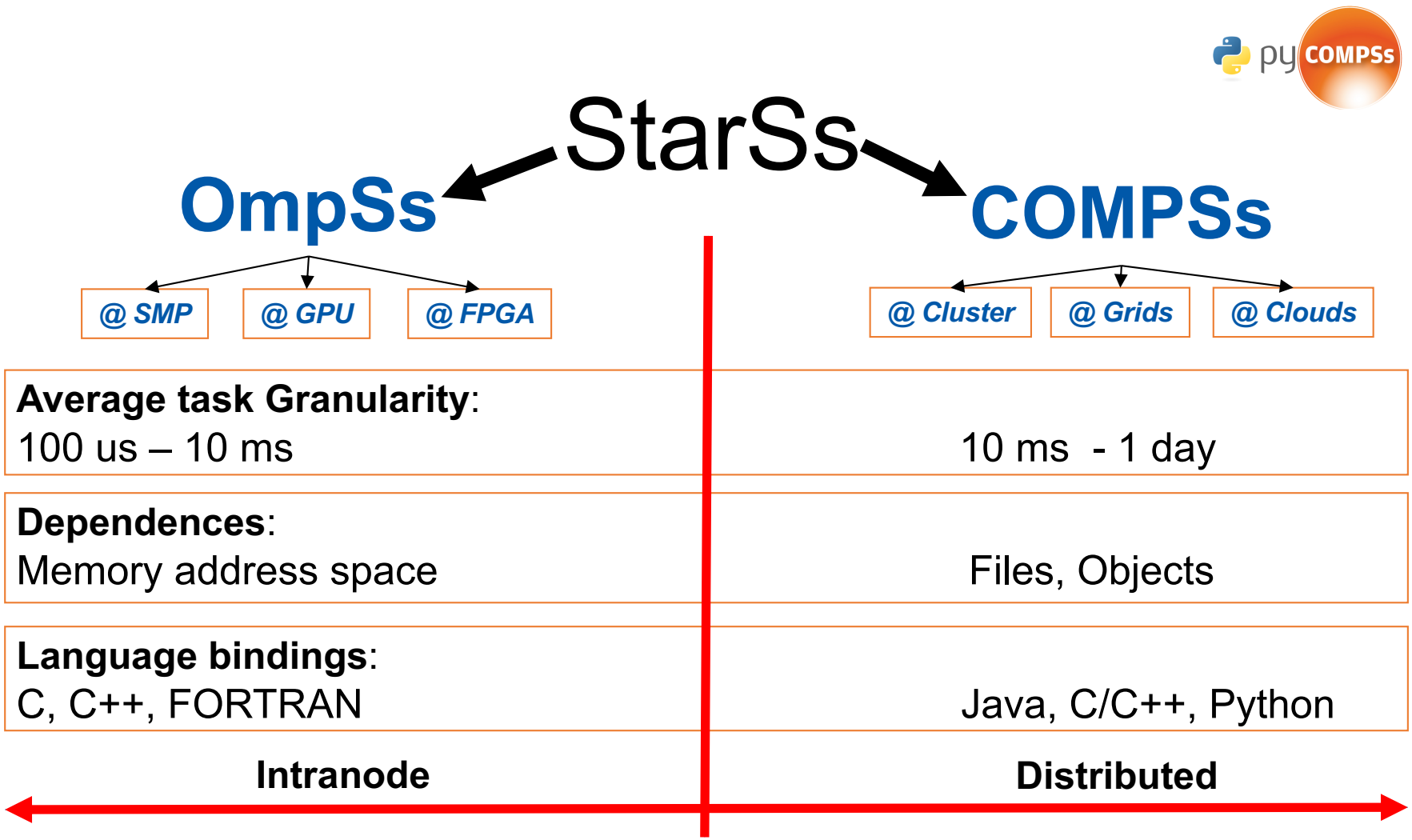
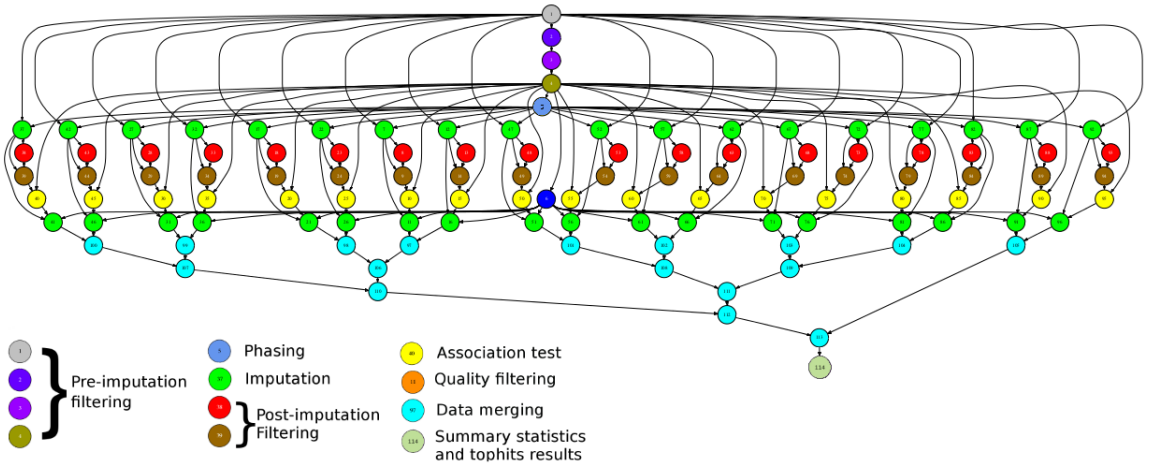
BSC vision on programming models



Programming with PyCOMPSs/COMPSs

- Sequential programming, parallel execution
- General purpose programming language + annotations/hints
  - To identify tasks and directionality of data
- Builds a task graph at runtime that express potential concurrency
- Offers a shared memory illusion to applications in a distributed system
  - The application can address larger data storage space: support for Big Data apps
  - Support for persistent storage
- Agnostic of computing platform
  - Enabled by the runtime for clusters, clouds and container managed clusters
- Available in MN4
  - module load COMPSs



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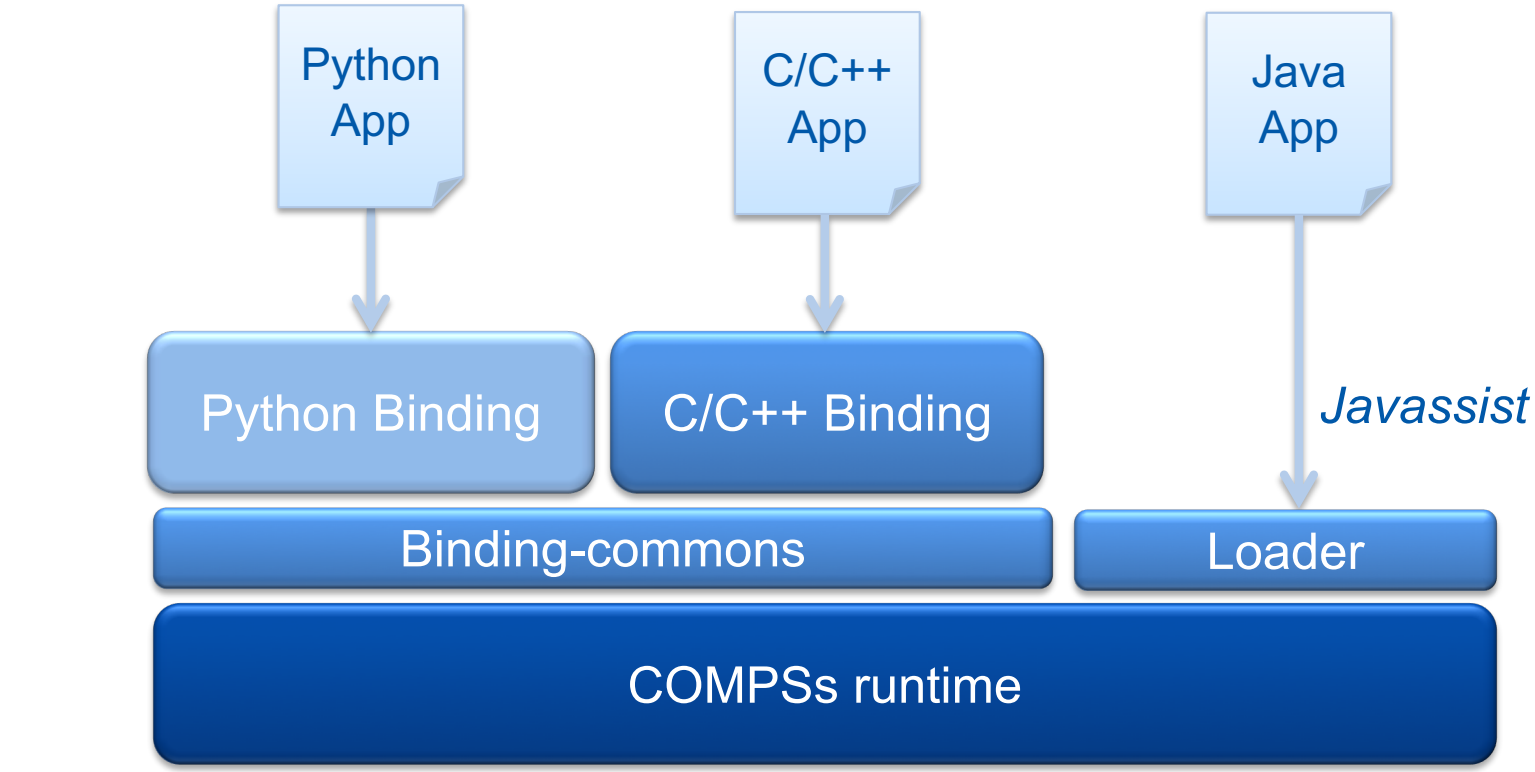
COMPSs Architecture



Grid

Cluster

Cloud

Containers

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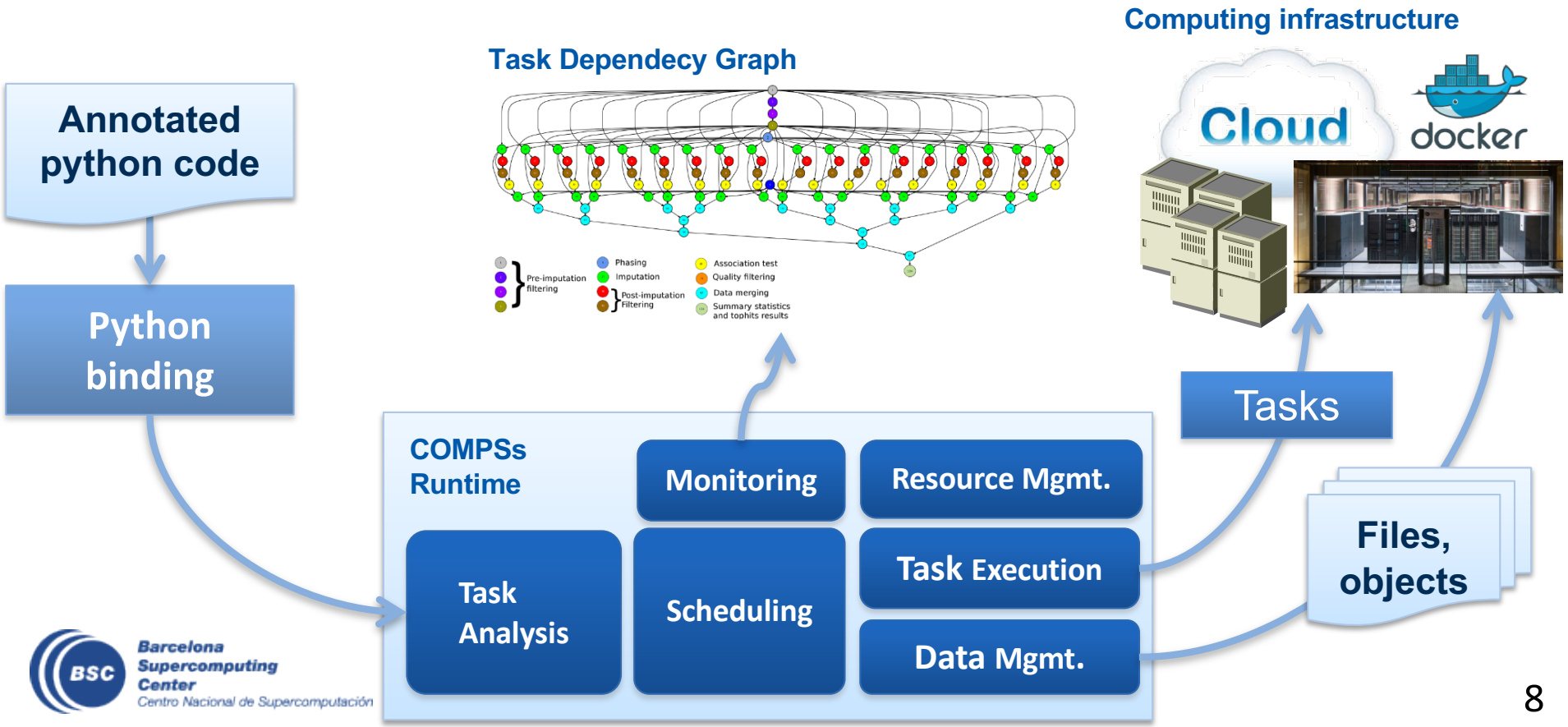
PyCOMPSs/COMPSs runtime

- PyCOMPSs/COMPSs applications executed in distributed mode following the master-worker paradigm
  - Description of computational infrastructure in an XML file
- Sequential execution starts in master node and tasks are offloaded to worker nodes
- All data scheduling decisions and data transfers are performed by the runtime



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Python Syntax (PyCOMPSs)

Tutorial with Jupyter notebooks

- Instructions in:
  - https://github.com/bsc-wdc/notebooks

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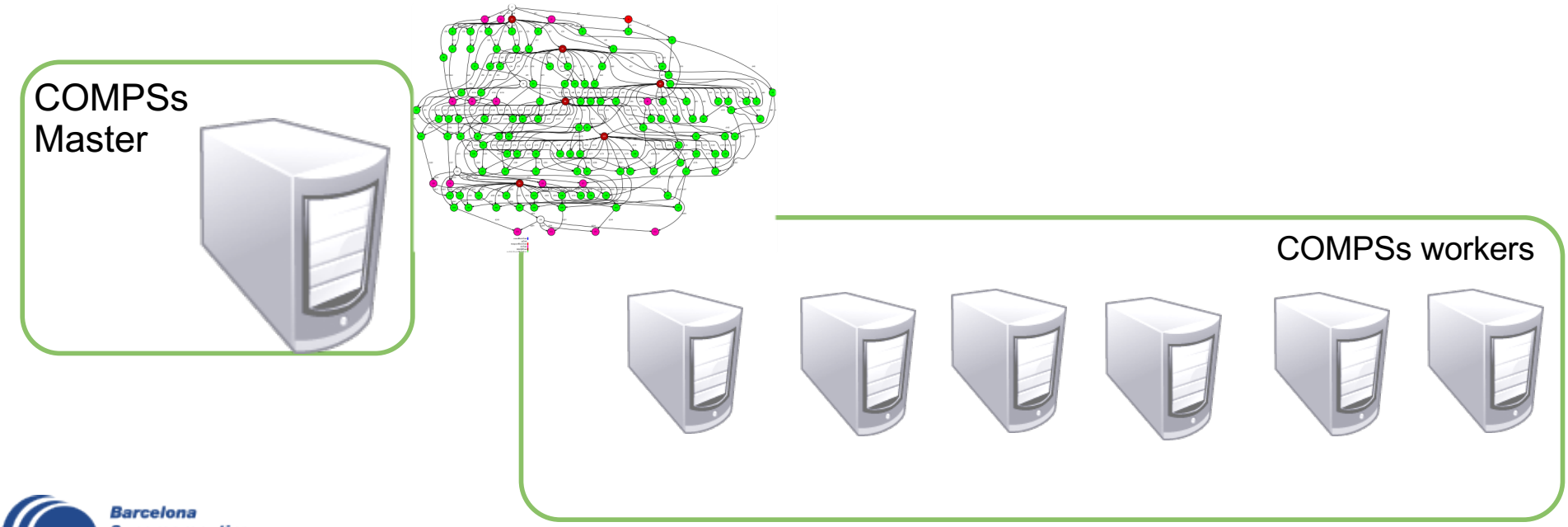
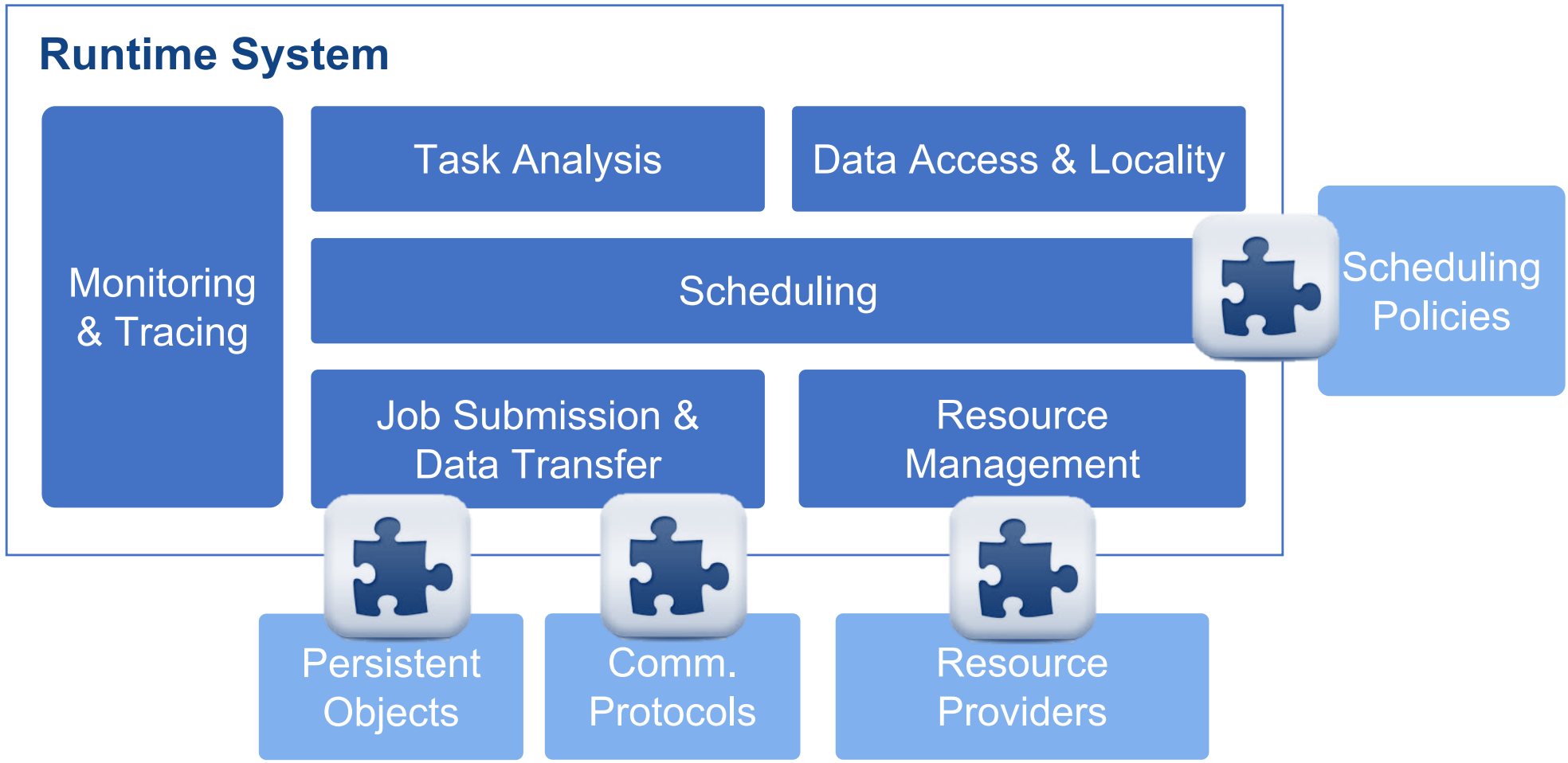
COMPSs runtime and execution environment

Execution environment

- COMPSs runtime is able to execute in distributed computing platforms (clusters, clouds, contained manager clusters)
- Main program + runtime started in master node
  - Takes care of tasks scheduling, data transfers, etc
- Tasks executed in worker nodes



Runtime Architecture

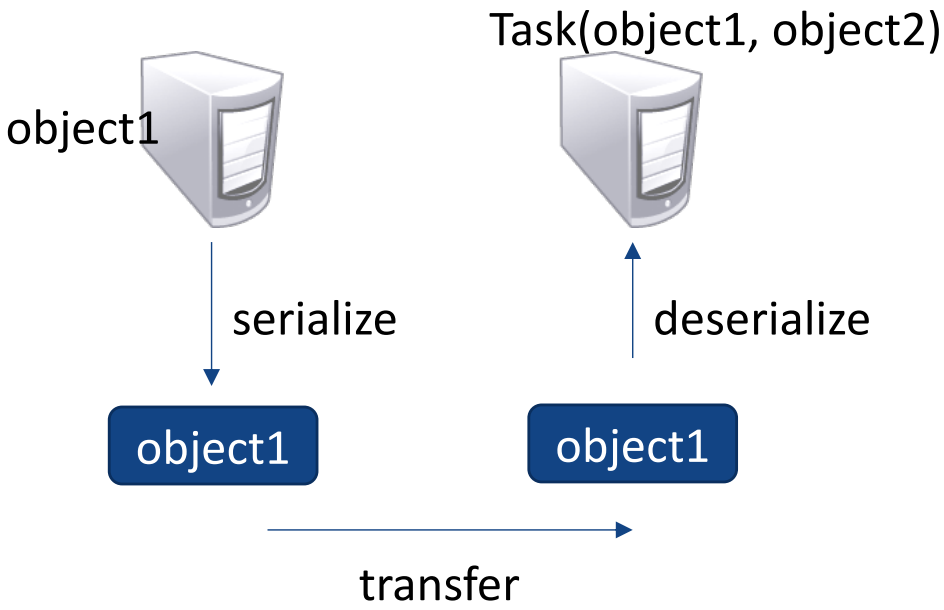


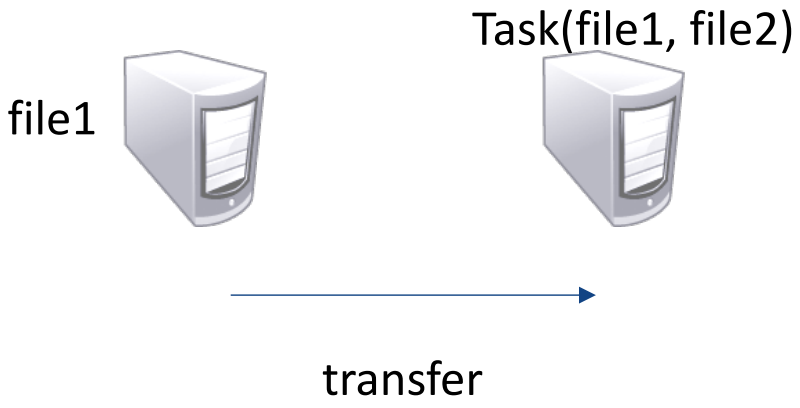
Data management in COMPSs

- COMPSs runtime offers the view of a single memory space and storage system
  - Can address memory spaces much larger than the initial space available in a single node
  - This larger memory space is made available to the application in a transparent way
- Data management
  - Objects can be either created by the main program or tasks
  - When accessed by tasks executed in different worker nodes, the runtime will be in charge of transferring the data between them
  - Files and/or objects can be renamed/versioned
  - Renaming enables further parallelism
  - Versioning reduces the number of required transfers
- Runtime supports shared and distributed filesystems
  - In the first case, no file transfers are required

Data management in COMPSs

- Serialization
  - Due to different address spaces between different nodes, objects in memory need to be transferred
  - Before being transferred are serialized
  - Only for objects, not for files
  - For Python, Pickle or Dill libraries are used





Runtime System

Application

Task Selection Interface

How do I select the execution platform?

Grid

Cluster

Cloud

Execution Environments Configuration

Specifies:
- Resources and Project files
- Scheduler, Comm. Adaptor
- Persistent object storage

runcompss options

Infrastructure Description
- Describe the available resource in the infrastructure
- Describe Cloud Providers: Images and VM Templates

Runtime System

Exec. Mngmt & Data Transfers

Persistent Object Storage: DataClay, Hecuba, Redis

Communication Adaptor: NIO, GAT

Schedulers

Resources

Cloud Connector: jClouds, rOCCI

Slurm, Docker, Mesos

resources.xml

project.xml

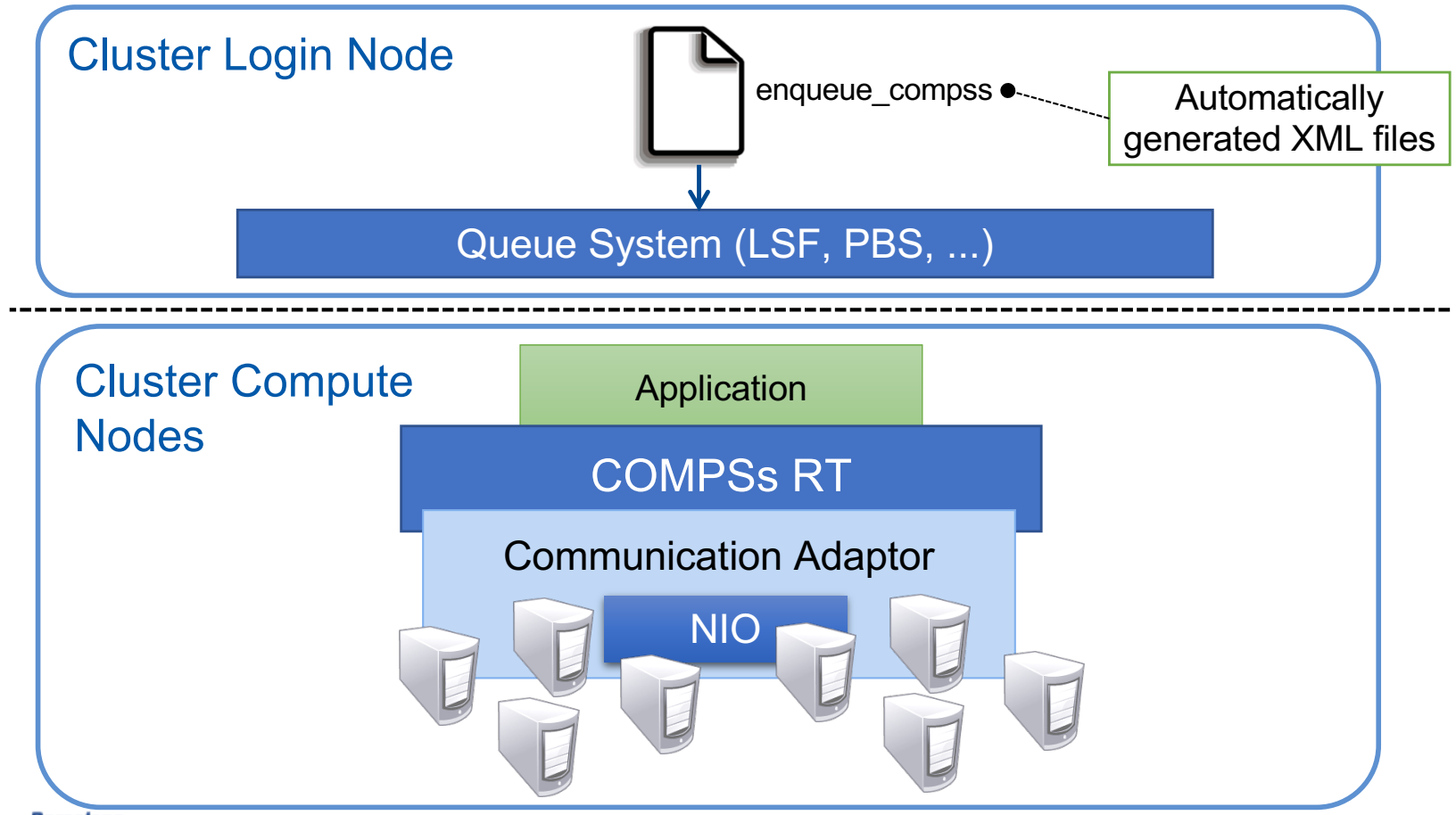
Master-Worker Comm. Mechanism
- GAT: Restrictred environments (only ssh access) and Grid Middleware
- NIO: Efficient Persistent workers implementation in controlled and secured environments

Resource Scalability
- Provide interaction with resource providers to create and destroy new computing resources

Application Exec. Desc.
- Selection of resources
- Application Code Location
- Working directory
- Provided as execution command argument

COMPSs@Cluster

- Execution divided in two phases
  - Launch scripts queue a whole COMPSs app execution
  - Actual execution starts when reservation is obtained



COMPSs in a Cluster

- Use of enqueu_compss command (instead of runcompss)
- Generates project.xml and resources.xml
- Launches application in the allocation

```
enqueue_compss \
  --exec_time=10 \
  --num_nodes=5 \
  --tasks_per_node=16 \
  --master_working_dir=. \
  --worker_working_dir=scratch \
  --lang=python \
  --comm=integratedtoolkit.nio.master.NIOAdaptor \
  --tracing=true \
  --graph=true \
  /home/bsc19/bsc19776/SC16/wordcount/wc_merge.py \
 /gpfs/projects/bsc19/COMPSs_AP PS/wordcount/data/dataset_64f_16mb
```

- Type “enqueue_compss” to see help and options

Configuration with Job scheduler: Resources Specification

```
<?xml version="1.0" encoding="UTF-8" standalone="yes"?>
<ResourcesList>
 <SharedDisk Name="gpfs" />
 <SharedDisk Name="gpfs2" />
 <ComputeNode Name="s12r1b62-ib0">
  <Processor Name="MainProcessor">
   <ComputingUnits>24</ComputingUnits>
   <Architecture>Intel</Architecture>
   <Speed>2.6</Speed>
  </Processor>
  <Memory>
   <Size>92</Size>
  </Memory>
  <OperatingSystem>
   <Type>Linux</Type>
   <Distribution>SMP</Distribution>
   <Version>3.0.101-0.35-default</Version>
  </OperatingSystem>
  <Software>
   <Application>JAVA</Application>
   <Application>PYTHON</Application>
   <Application>EXTRAE</Application>
   <Application>COMPSS</Application>
  </Software>
…
```

Generated automatically by enqueue_compss command in MN4

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```
    ...
 <Adaptors>
      <Adaptor Name="es.bsc.compss.nio.master.NIOAdaptor">
        <SubmissionSystem>
          <Interactive/>
        </SubmissionSystem>
        <Ports>
          <MinPort>43001</MinPort>
          <MaxPort>43002</MaxPort>
          <RemoteExecutionCommand>none</RemoteExecutionCommand>
        </Ports>
      </Adaptor>
      …
    </Adaptors>
    <SharedDisks>
      <AttachedDisk Name="gpfs">
        <MountPoint>/gpfs/</MountPoint>
      </AttachedDisk>
      <AttachedDisk Name="gpfs2">
        <MountPoint>/.statelite/tmpfs/gpfs/</MountPoint>
      </AttachedDisk>
    </SharedDisks>
  </ComputeNode>
  <ComputeNode Name="s12r1b63-ib0">
    <Processor Name="MainProcessor">
      <ComputingUnits>48</ComputingUnits>
      <Architecture>Intel</Architecture>
      <Speed>2.6</Speed>
    </Processor>
    <Memory>
      <Size>92</Size>
    </Memory>
    <OperatingSystem>
      …

</ResourcesList>
```

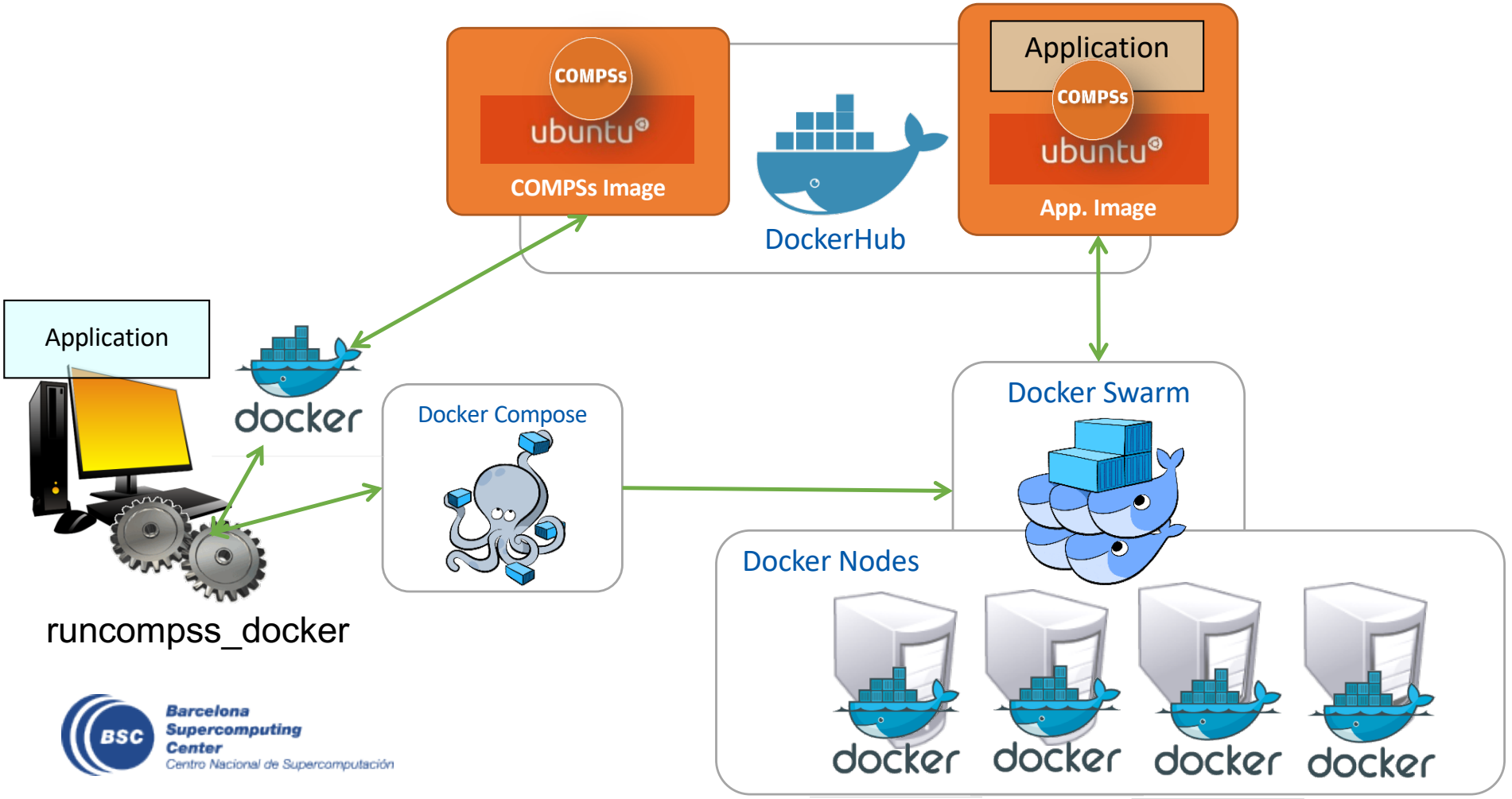
Configuration with Job scheduler: Project Specification

```
<Project>
  <MasterNode>
    <SharedDisks>
      <AttachedDisk Name="gpfs">
        <MountPoint>/gpfs/</MountPoint>
      </AttachedDisk>
      <AttachedDisk Name="gpfs2">
        <MountPoint>/.statelite/tmpfs/gpfs/</MountPoint>
      </AttachedDisk>
    </SharedDisks>
  </MasterNode>

  <ComputeNode Name="s12r1b62-ib0">
    <InstallDir>/apps/COMPSs/2.5</InstallDir>
    <WorkingDir>/home/nct00/nct00002/examples/clustering_comparison/tmp.Ynl9AcAh8D</WorkingDir>
    <Application>
      <LibraryPath>/home/nct00/nct00002/examples/clustering_comparison</LibraryPath>
    </Application>
  </ComputeNode>

 <ComputeNode Name="s12r1b63-ib0">
    <InstallDir>/apps/COMPSs/2.5</InstallDir>
    <WorkingDir>/home/nct00/nct00002/examples/clustering_comparison/tmp.Ynl9AcAh8D</WorkingDir>
    <Application>
      <LibraryPath>/home/nct00/nct00002/examples/clustering_comparison</LibraryPath>
    </Application>
  </ComputeNode>

      ...
</Project>
```

Generated automatically by enqueue_compss command for MN4

COMPSs with Docker

- Keep as transparent for the user as possible
- Same as running a local COMPSs application (runcompss command)
- Deploy applications as a set of docker container



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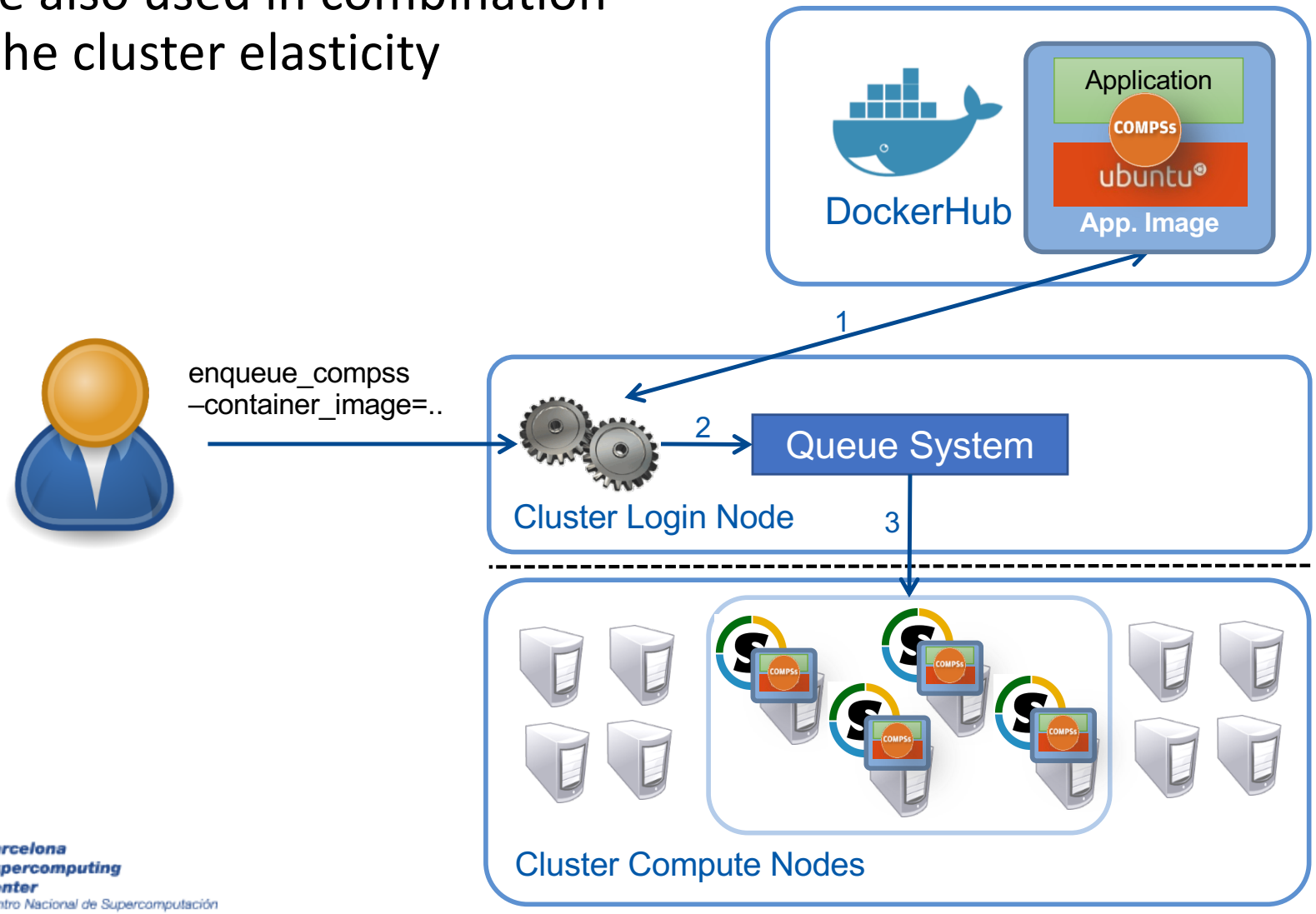
COMPSs@Singularity

- Execute applications from a container image in HPC cluster
- Can be also used in combination with the cluster elasticity



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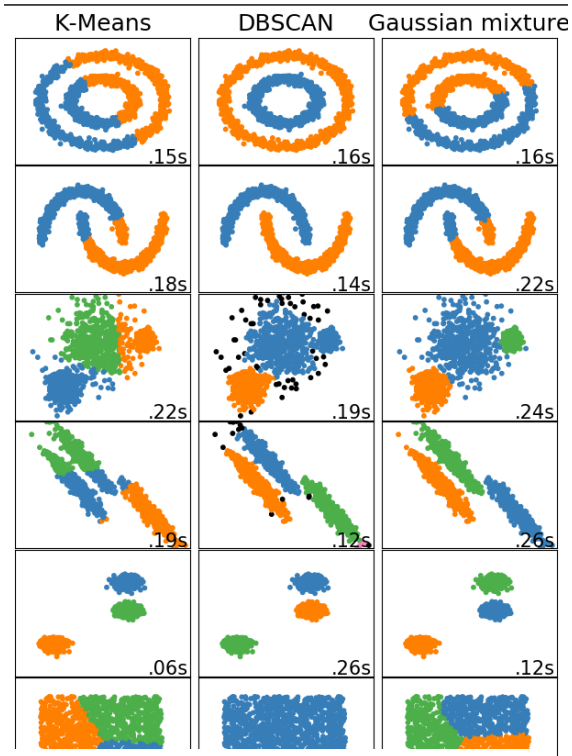
dislib

dislib

- dislib: Collection of machine learning algorithms developed on top of PyCOMPSs
  - Unified interface, inspired in scikit-learn (fit-predict)
  - Unified data acquisition methods and using an independent distributed data representation
  - Parallelism transparent to the user – PyCOMPSs parallelism hidden
  - Open source, available to the community



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FUJITSU

DISLIB | Distributed Computing Library

dislib library

dislib

```
from dislib.cluster import KMeans
from dislib.data import load_txt_file

file_ = "~/my_input_file.csv"

dataset = load_txt_file(file_, 10, 780)

kmeans = KMeans()
kmeans.fit(dataset)
centers = kmeans.centers
```

scikit-learn

```
from sklearn.cluster import KMeans
import numpy as np

file_ = "~/my_input_file.csv"

arr = np.load_txt(file_, delimiter=",")

kmeans = KMeans()
kmeans.fit(arr)
centers = kmeans.centers
```

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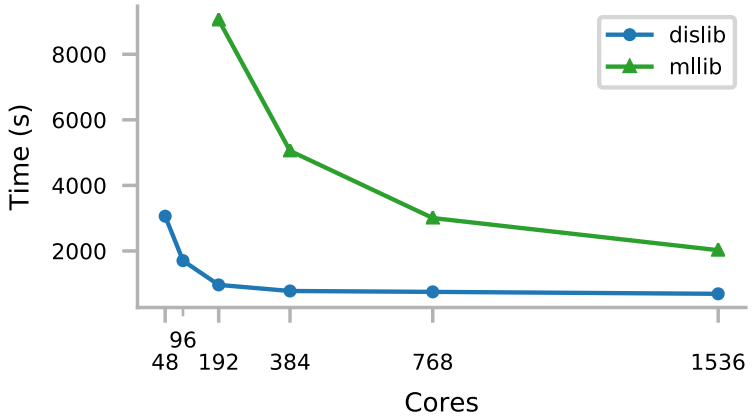
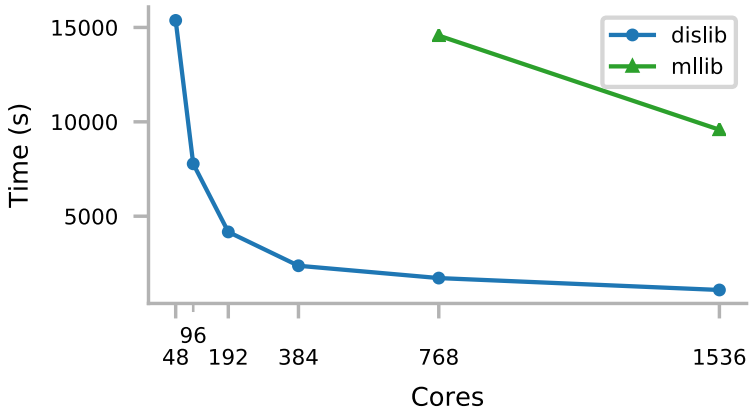
DISLIB | Distributed Computing Library

Comparison with DASK and MLib

- Gaussian mixtures (execution time) – 100 features, 50 components



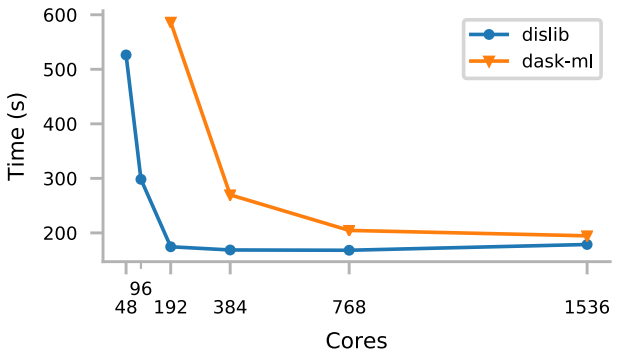
100 million samples



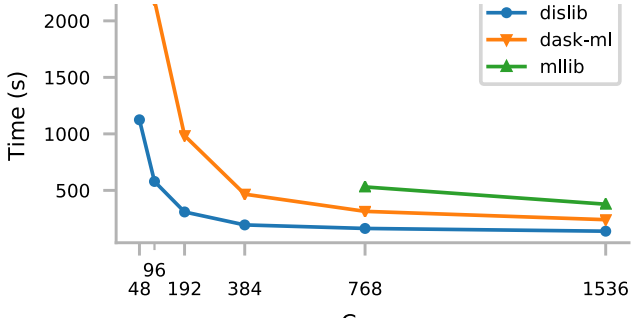
500 million samples

Comparison with DASK and MLib

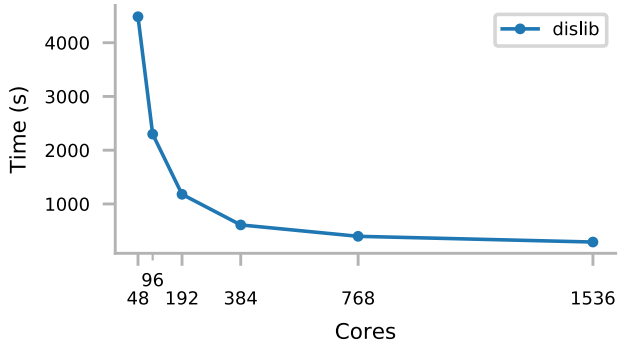
- K-means (execution time) –



1 billion samples with low granularity (50 features and 50 clusters)



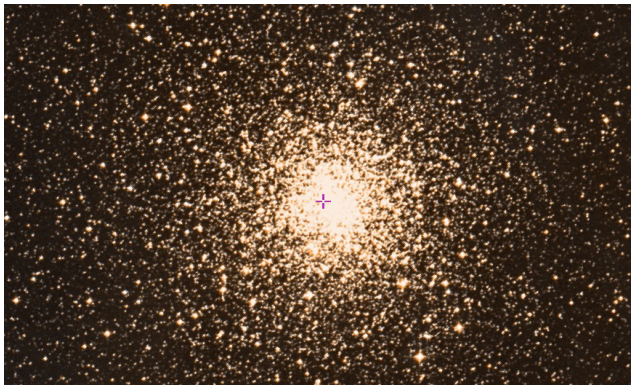
500 million samples with high granularity (100 features and 500 clusters)

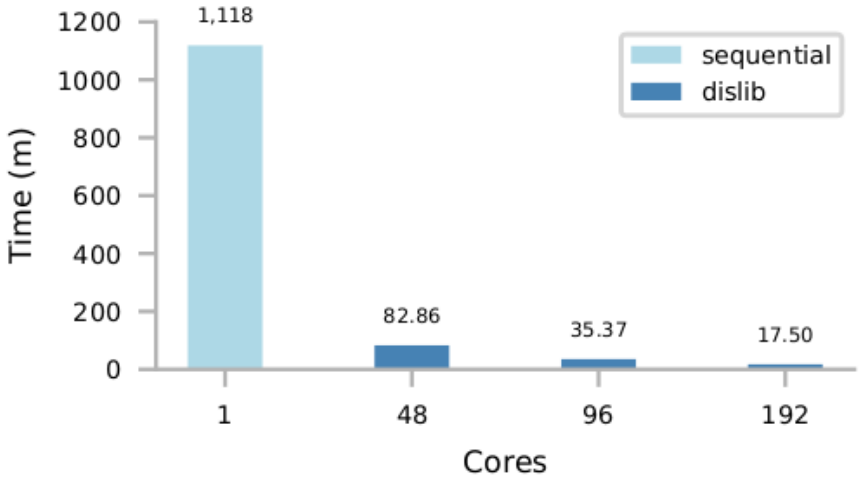


2 billion samples with high granularity (100 features and 500 clusters)

Looking for objects in the sky with dislib

- Gaia satellite data: Sample scientific application:
  - Looking for open clusters in the sky with DBSCAN clustering
  - Subset of astrometric data from 2.5 million stars
    - Total data is 10^9 stars
  - Execution of 6,145 DBSCANs in parallel





Demo dislib

- Jupyter notebook

We are hiring!

COMPSs runtime developer - Junior developer (RE1)

Job Reference	Position	Closing Date
243_19_CS_WDC_RE1	COMPSs runtime developer - Junior developer (RE1)	Sunday, 13 October, 2019

Reference: 243_19_CS_WDC_RE1
Job title: COMPSs runtime developer - Junior developer (RE1)

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