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Centro Nacional de Supercomputación

EXCELENCIA SEVERO OCHOA

Programming parallel codes with PyCOMPSs

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28 May 2020

Barcelona, Spain

www.bsc.es

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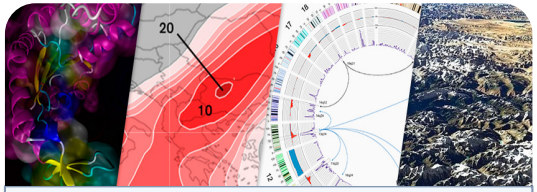
BSC-CNS objectives

Supercomputing services to Spanish and EU researchers



R&D in Computer, Life, Earth and Engineering Sciences

PhD programme, technology transfer, public engagement

BSC-CNS is a consortium that includes

Spanish Government	60%	Gobierno de España · Ministerio de Economía y Competitividad
Catalonian Government	30%	Generalitat de Catalunya · Departament d'Empresa i Coneixement
Univ. Politècnica de Catalunya (UPC)	10%	Universitat Politècnica de Catalunya · BarcelonaTech

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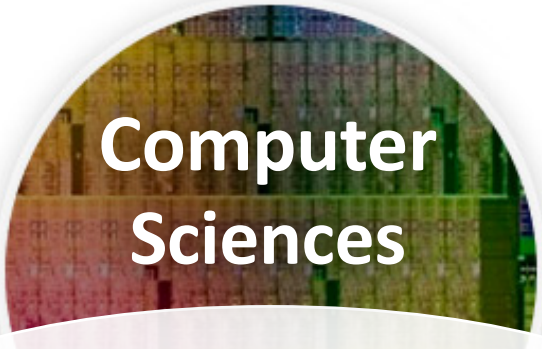
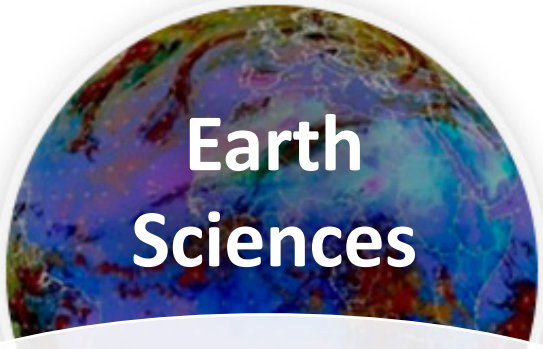
Mission of BSC Scientific Departments



To influence the way machines are built, programmed and used: programming models, performance tools, Big Data, computer architecture, energy efficiency



To develop and implement global and regional state-of-the-art models for short-term air quality forecast and long-term climate applications

To understand living organisms by means of theoretical and computational methods (molecular modeling, genomics, proteomics)

To develop scientific and engineering software to efficiently exploit super-computing capabilities (biomedical, geophysics, atmospheric, energy, social and economic simulations)

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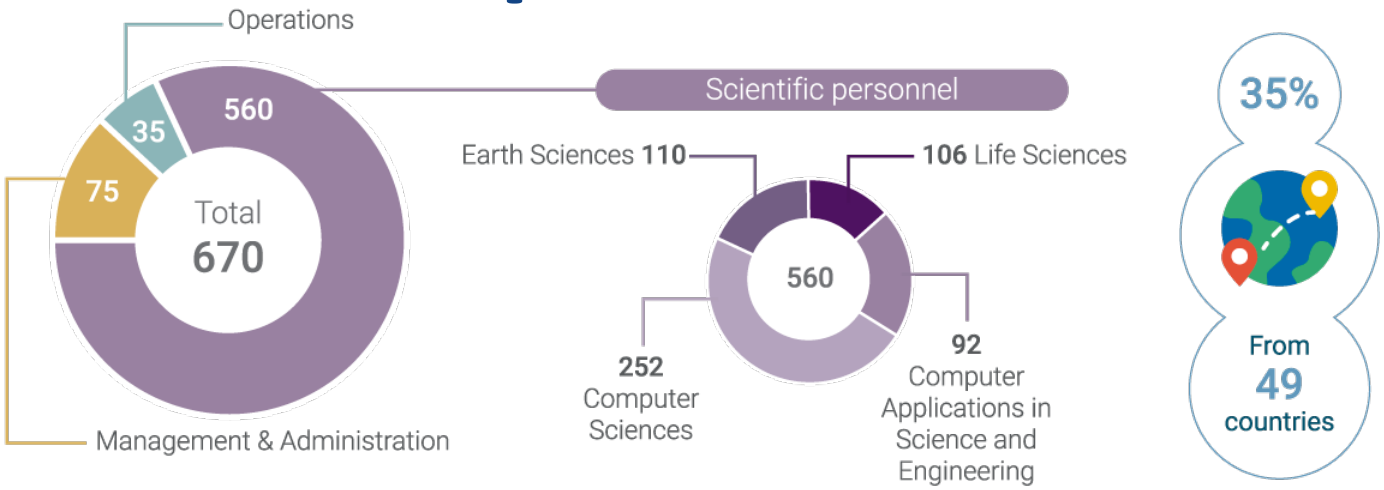
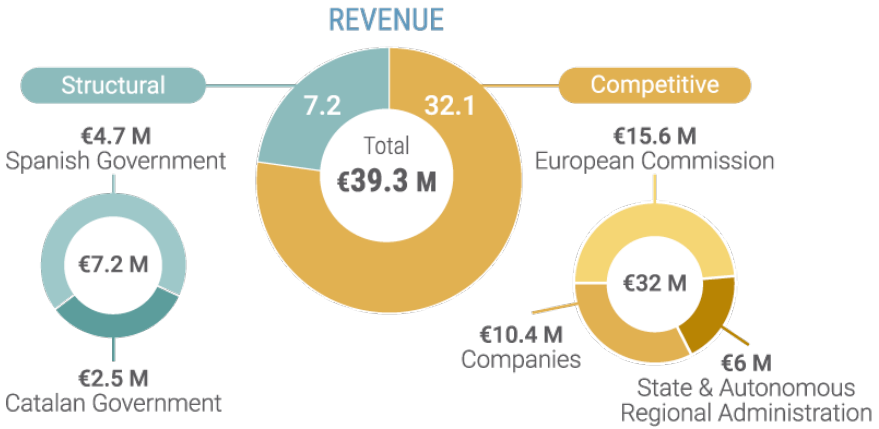
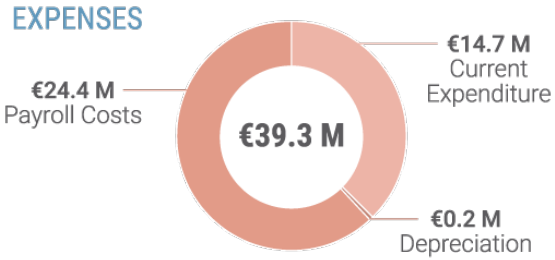
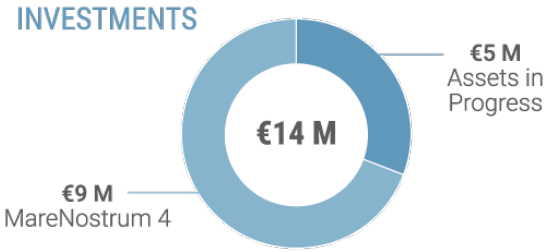
People and resources









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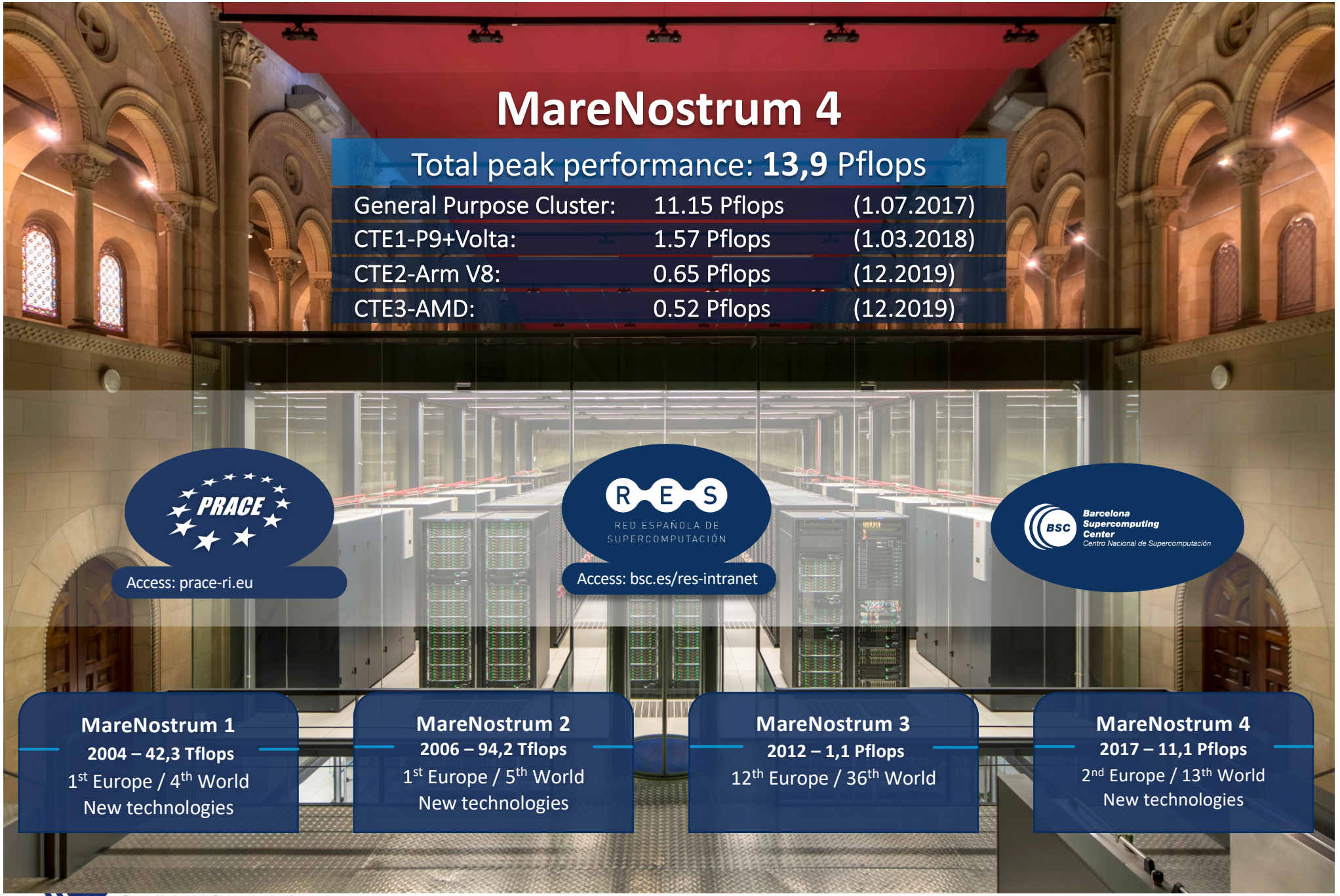
December 31, 2019



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General purpose cluster

Rpeak: 11.15 Pflops
384.75 TB of main memory
3,456 nodes:
- 2x Intel Xeon Platinum 8160
- 216 nodes with 12x32 GB DDR4
- 3240 nodes with 12x8 GB DDR4

Interconnection networks:
- 100Gb Intel Omni-Path Full-Fat Tree
- 10Gb Ethernet

Operating System: SUSE Linux Enterprise Server 12 SP2

MN4 CTE1-P9+Volta

Rpeak: 1.57 Pflops
2 login node and 52 compute nodes:
- 2 x IBM Power9, 20 cores and 4 threads/core, total 160
- 4 x GPU NVIDIA V100 (Volta)
- 512GB of main memory
- 2 x SSD 1.9TB as local storage
- 2 x 3.2TB NVME

GPFS via one fiber link 10 GBit Infiniband interconnection network
The operating system is Red Hat Enterprise Linux Server 7.5 (Maipo).

MN4 CTE AMD (Lenovo)

Rpeak: 0.51 Pflops
34 nodes in 2 racks
- 1xAMD Rome, 64c (estimated 1750 Gflops)
- 2xAMD Radeon Instinct MI500
  - 32GB HMB2 memory each with 6.7 TFlops
- 1024 GB
- 480 GB SSD

34 TB RAM
30 KW*
Mellanox Infiniband HDR100, full non-blocking
DLC-Direct Liquid Cooling

MN4 CTE ARM (Fujitsu)

Rpeak: 0.65 Pflops
Post-FX100
192 nodes in 1/2 rack
- 1xArmv8 + SVE
- 32 GB

6 TB RAM
?? KW*
Tofu Inteconnect & IB EDR
DLC-Direct Liquid Cooling

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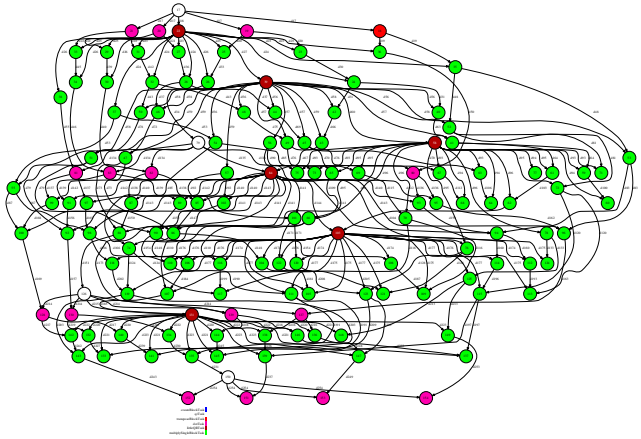
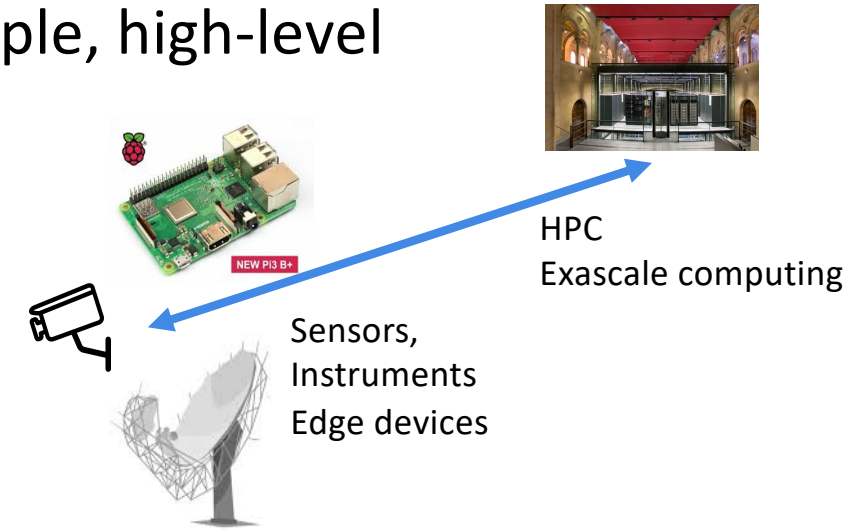
Programming with PyCOMSs/COMPSs

PyCOMPSs/COMPSs ambition



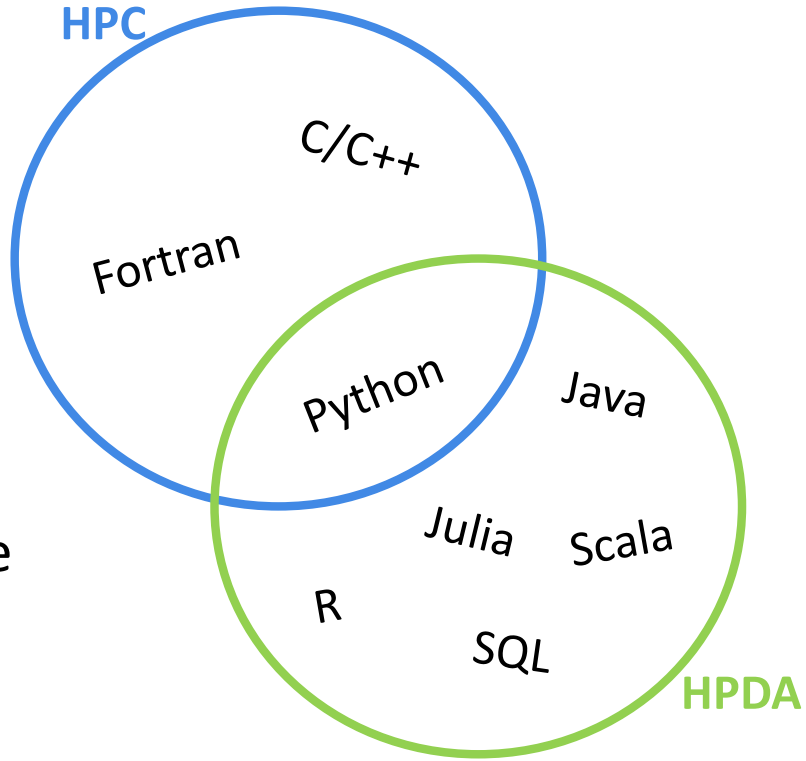
- Complex infrastructures with multiple and heterogeneous components
- Complex applications, composed of multiple components and pieces of software
- How to describe the workflows in such environment?
- Holistic approach where both data and computing are integrated in a single flow built on simple, high-level interfaces
  - Integration of computational workloads, with machine learning and data analytics
  - Intelligent runtime that can make scheduling and allocation, data-transfer, and other decisions



Why Python?

Python is powerful... and fast;
plays well with others;
runs everywhere;
is friendly & easy to learn;
*is Open.**

- Emphasizes code readability, its syntax allows programmers to express concepts in fewer lines of code
- Large community using it, including scientific and numeric
- Large number of software modules available
- Very well integrated with data analytics and machine learning (Tensorflow, PyTorch, dask, scikit-learn, ...)
- Intersection with HPC and data analytics programming languages



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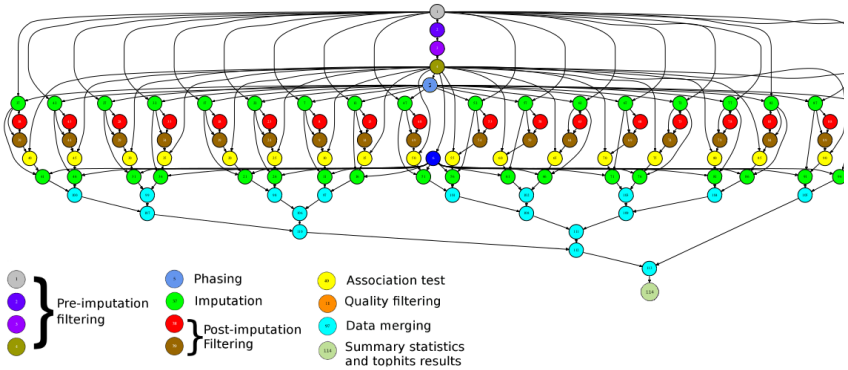
* From python.org

Programming with PyCOMPSs/COMPSs

- Sequential programming, parallel execution
- General purpose programming language + annotations/hints
  - To identify tasks and directionality of data
  - Task based: task is the unit of work
- Builds a task graph at runtime that express potential concurrency
- Exploitation of parallelism
  - … and of parallelism created later on
- Simple linear address space
- Agnostic of computing platform
  - Runtime takes all scheduling and data transfer decisions




```
@task(c=INOUT)
def multiply(a, b, c):
    c += a*b
```

```
initialize_variables()
startMulTime = time.time()
for i in range(MSIZE):
   for j in range(MSIZE):
      for k in range(MSIZE):
         multiply (A[i][k], B[k][j], C[i][
compss_barrier()
mulTime = time.time() - startMulTime
```

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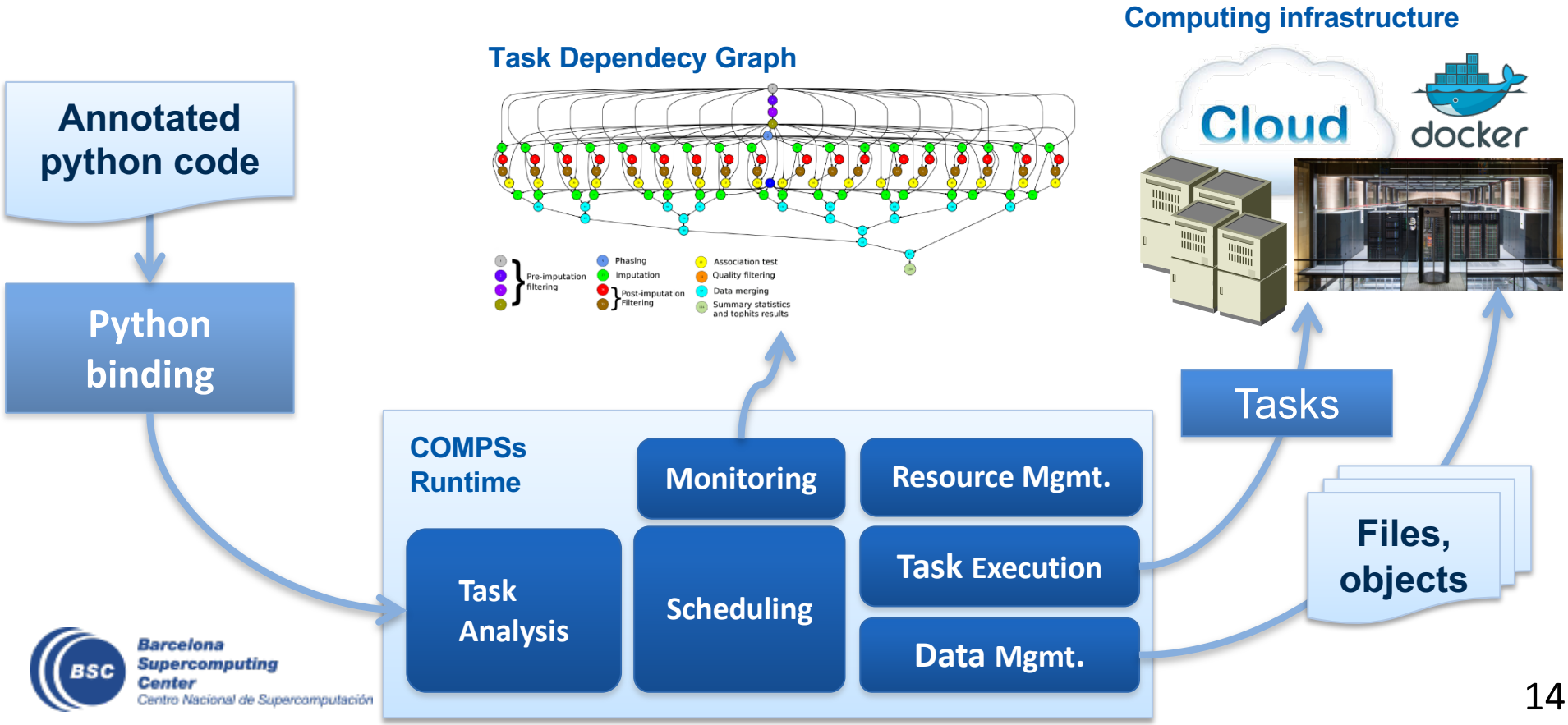
PyCOMPSs/COMPSs runtime

- 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



Other decorators: Tasks' constraints and versions

- Constraints enable to define HW or SW features required to execute a task
  - Runtime performs the match-making between the task and the computing nodes
  - Support for multi-core tasks and for tasks with memory constraints
  - **Support for the heterogeneity of the platform**
- Versions: Mechanism to support multiple implementations of a given behavior (polymorphism)
  - **Runtime selects most appropriate device in the platform to execute each task**

```
@constraint (MemorySize=6.0, ProcessorPerformance="5000")
@task (c=INOUT)
def myfunc(a, b, c):
    ...
```

```
@implement (source class="myclass", method="myfunc")
@constraint (MemorySize=1.0, ProcessorType ="ARM")
@task (c=INOUT)
def myfunc_in_the_edge (a, b, c):
    ...
```

Example use of constraints: Guidance

- Guidance is a tool for Genome-Wide Association Studies (GWAS) (Develop by BSC, with other collaborators)
- This workflow composes multiple external binaries and scripts
- Different tasks, although sequential, have different high memory requirements


```
@constraint (MemorySize=6.0)
@task (gmapFile=FILE_IN, knownHapFile=FILE_IN, ...)
def imputeWithImpute(gmapFile, knownHapFile, theChromo, ...):
...
```

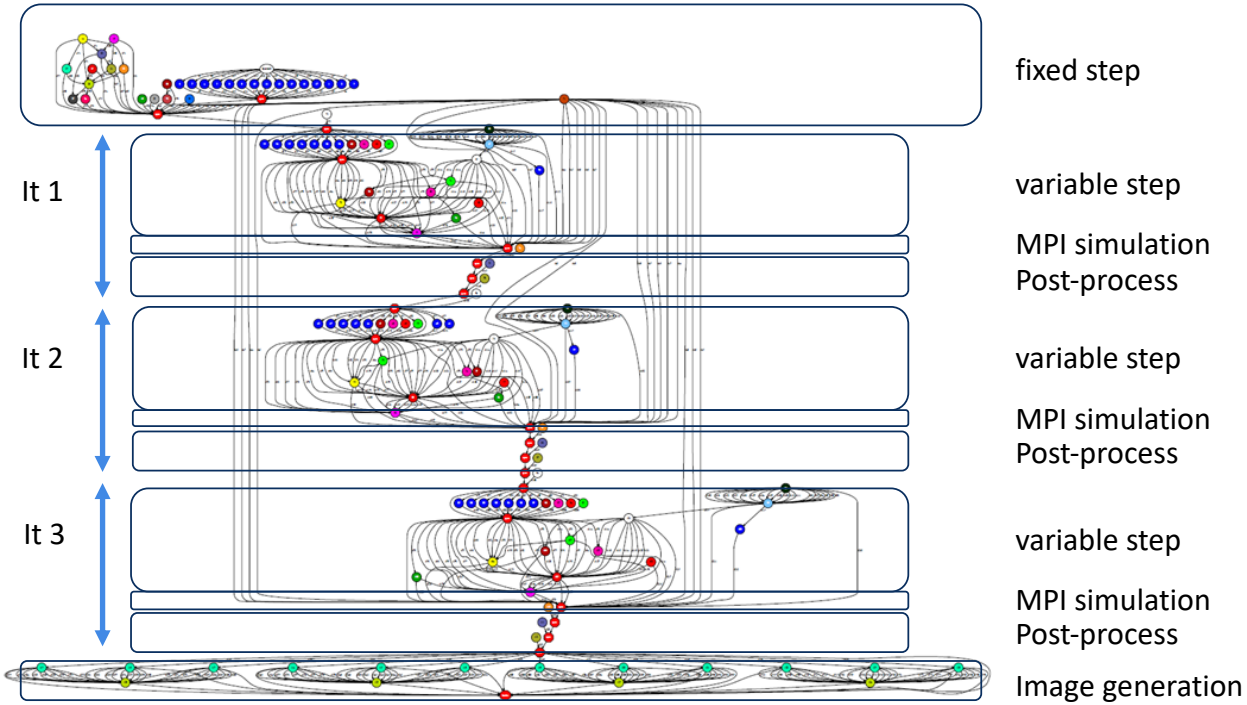
Other decorators: linking with other programming models

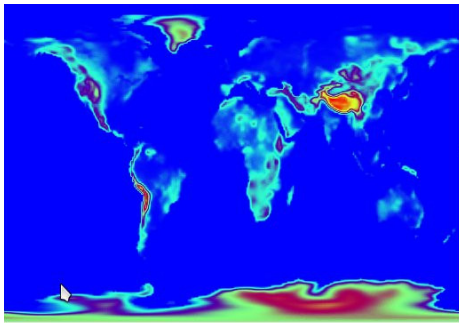
- A task can be more than a sequential function
  - A task in PyCOMPSs can be **sequential, multicore or multi-node**
  - External binary invocation: wrapper function generated automatically
  - Supports for alternative programming models: MPI and OmpSs
- Additional decorators:
  - @binary(binary="app.bin")
  - @ompss(binary="ompssApp.bin")
  - @mpi(binary="mpiApp.bin", runner="mpirun", computingNodes=8)
- Can be combined with the @constraint and @implement decorators

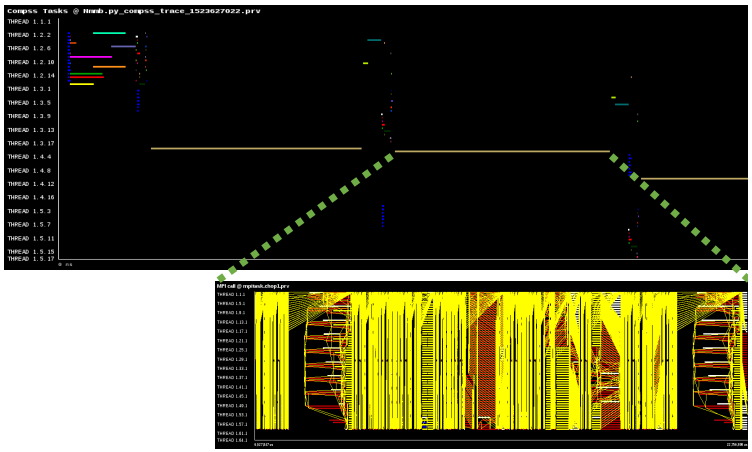
```
@constraint (computingUnits= "248")
@mpi (runner="mpirun", computingNodes= "16", ...)
@task (returns=int, stdOutFile=FILE_OUT_STDOUT, ...)
def nems(stdOutFile, stdErrFile):
    pass
```

NMMB-Monarch: Weather and dust forecast

- Multiscale Online Nonhydrostatic Atmosphere Chemistry model
  - Weather and dust forecast
  - Multiscale: Global to regional (up to 1km) scales allowed
  - Combines multiple scripts with the invocation of an MPI weather simulator







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Failure management and exceptions

- New interface than enables the programmer to give hints about failure management or define timeouts to tasks
  - Options: RETRY, CANCEL_SUCCESSORS, FAIL, IGNORE

```
@task(file_path=FILE_INOUT, on_failure='CANCEL_SUCCESSORS')
def task(file_path):
    ...
    if cond :
        raise Exception()
```

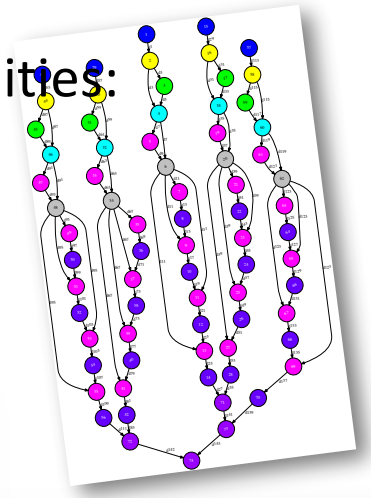
- Task exceptions: enables to cancel a group of tasks on the occurrence of an exception

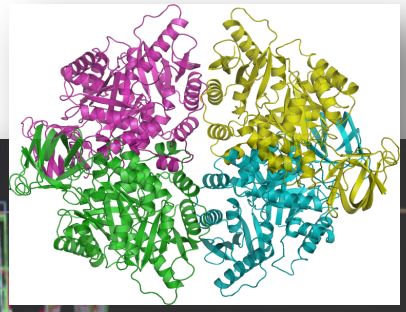
```
@task(file_path=FILE_INOUT)
def comp_task(file_path):
    ...
    raise COMPSsException("Exception")
```

```
def test_cancellation(file_name):
    try:
        with TaskGroup('failedGroup'):
            long_task(file_name)
            long_task(file_name)
            executed_task(file_name)
            comp_task(file_name)
    except COMPSsException:
        print("COMPSsException caught")
        write_two(file_name)
    write_two(file_name)
```

BioExcel Building Blocks (biobb)

- BioBB: Python building blocks that create new layer of compatibility and interoperability over popular bioinformatics tools
- Current version version of BioBB uses PyCOMPSs functionalities:
  - Execution of multi-node tasks
  - Task failure management
  - Task timeouts
- Massive parallel execution with bibobb and PyCOMPSs
  - Pyruvate Kinase protein
  - Simulation of 200 variants
  - ~395.000 atoms MD
  - GROMACS MD runs executed as 4 nodes MPI simulations (192 processes each)
  - Executed with PyCOMPSs, with 800 nodes of MareNostrum 4 (38,400 cores)





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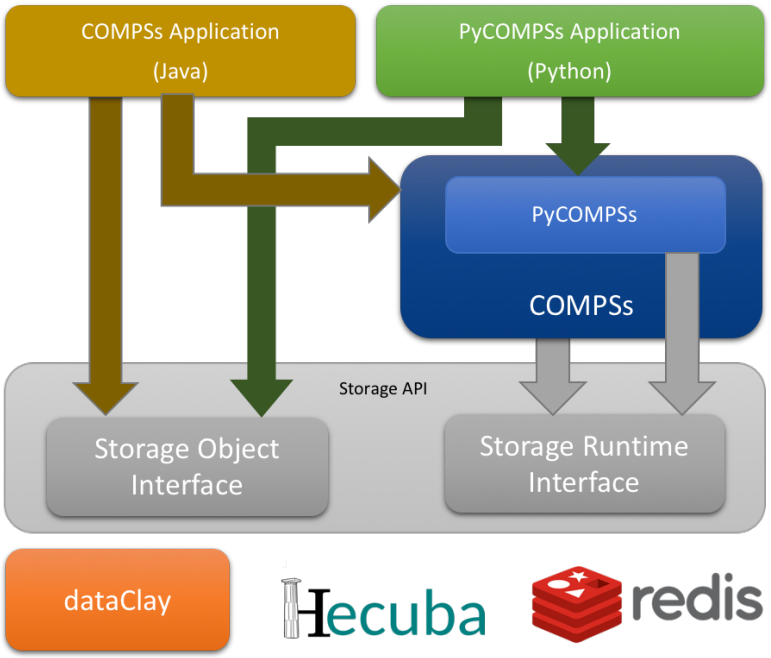
Integration with persistent memory

- Persistent storage layer that offers a shared memory view on a distributed platform
  - Programmer may decide to make persistent specific objects in its code
  - Persistent objects are managed same way as regular objects
  - Tasks can operate with them

```
a = SampleClass ()
a.make_persistent()
Print a.func (3, 4)

a.mytask()
compss_barrier()

o = a.another_object
```



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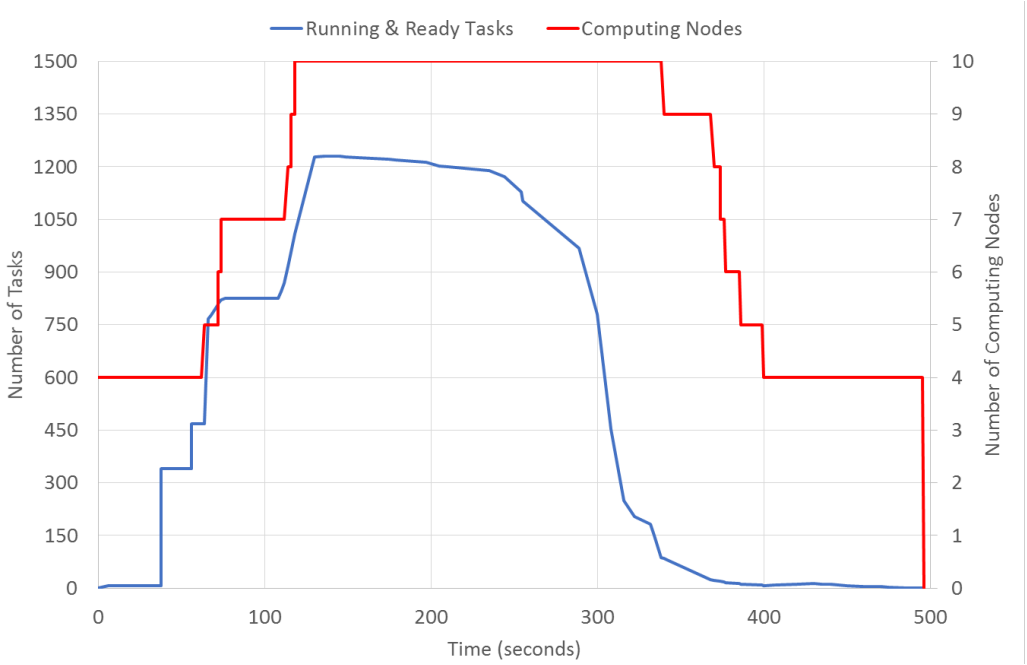
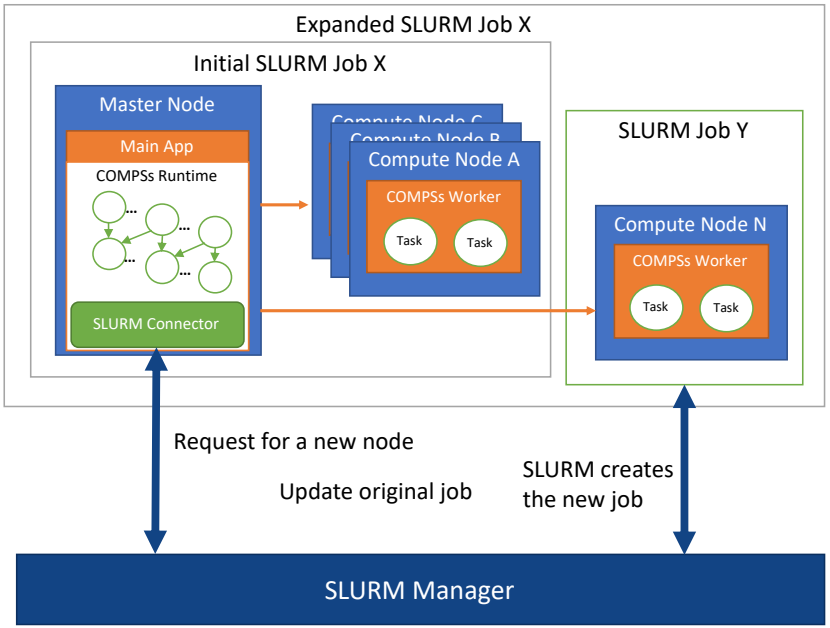
Support for elasticity

- Possibility to adapt the computing infrastructure depending on the actual workload
- Now also for SLURM managed systems
- Feature that contributes to a more effective use of resources





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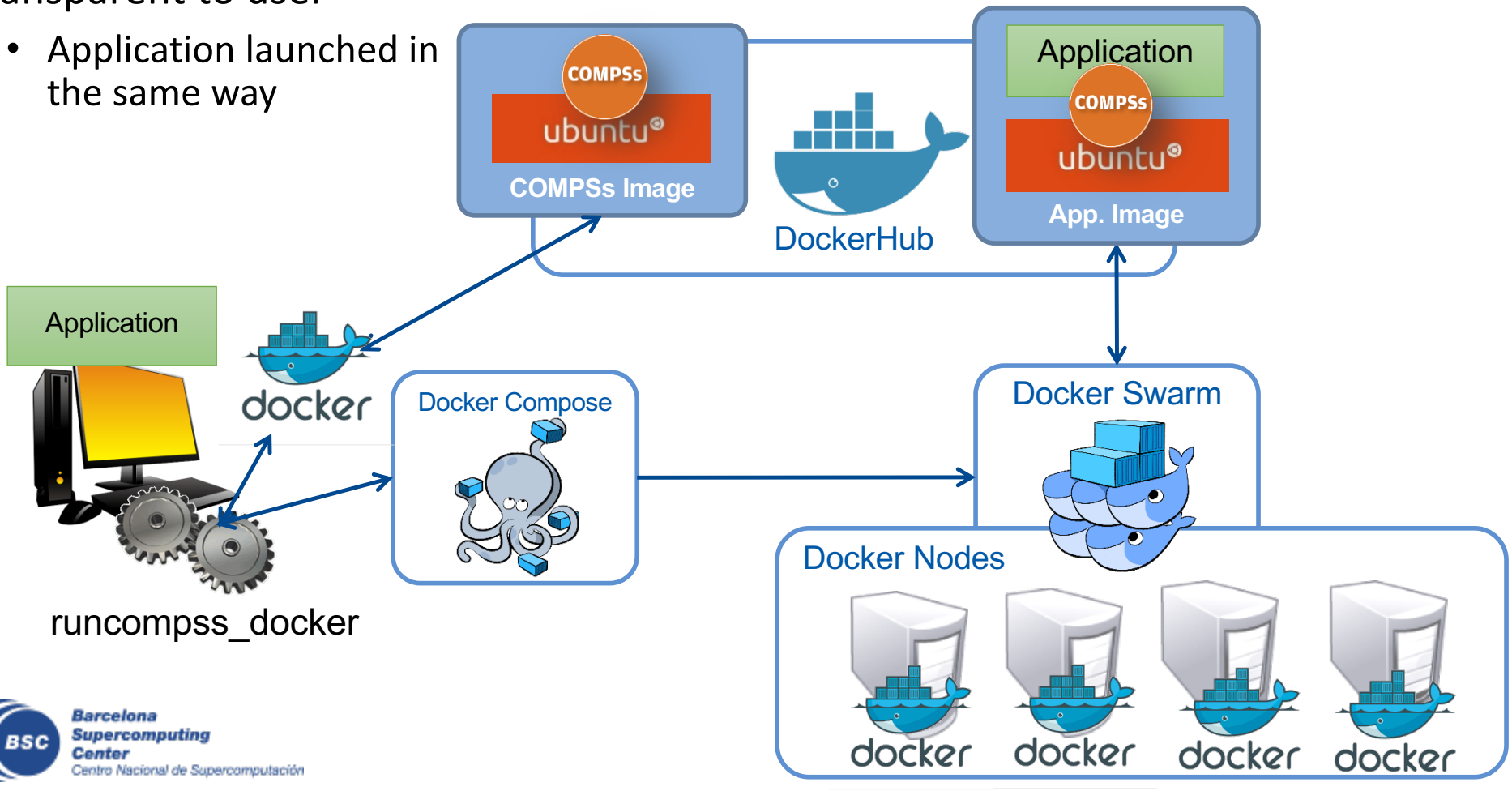
COMPSs runtime: containers

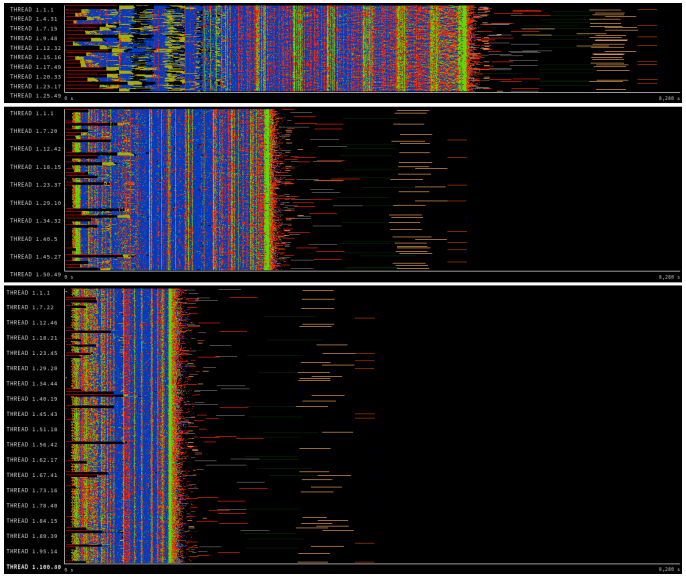
- Applications deployed as a set of docker container
  - Support for Singularity as well
- Support for elasticity
- Transparent to user
  - Application launched in the same way



COMPSs runtime: scalability and robustness

Guidance scalability

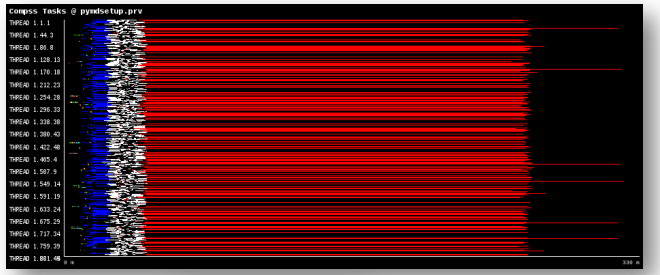
- 300 subjects, 2 genetic DBs, 8 diseases
- 170,152 tasks, around half a million files



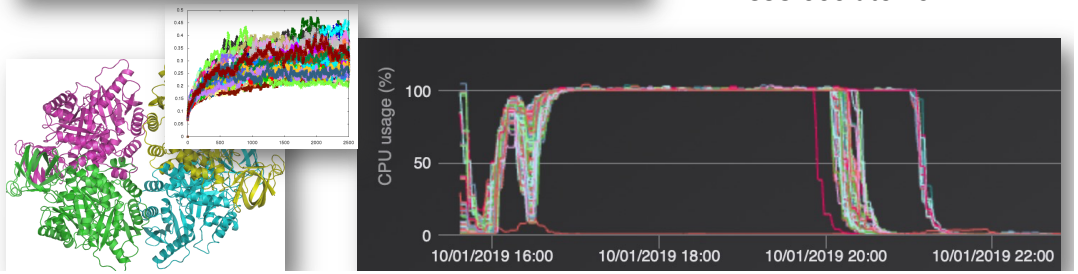
170,152 tasks, half a million files
Up to 100 nodes/4800 cores

BioExcel Building Blocks (biobb)

- Massively parallel execution with BioExcel building blocks and PyCOMPSs



PyMDsetup workflow
Pyruvate Kinase protein
Simulation of 200 variants
~395.000 atoms MD



Workflow execution on 800 MN4 nodes (38400 cores)

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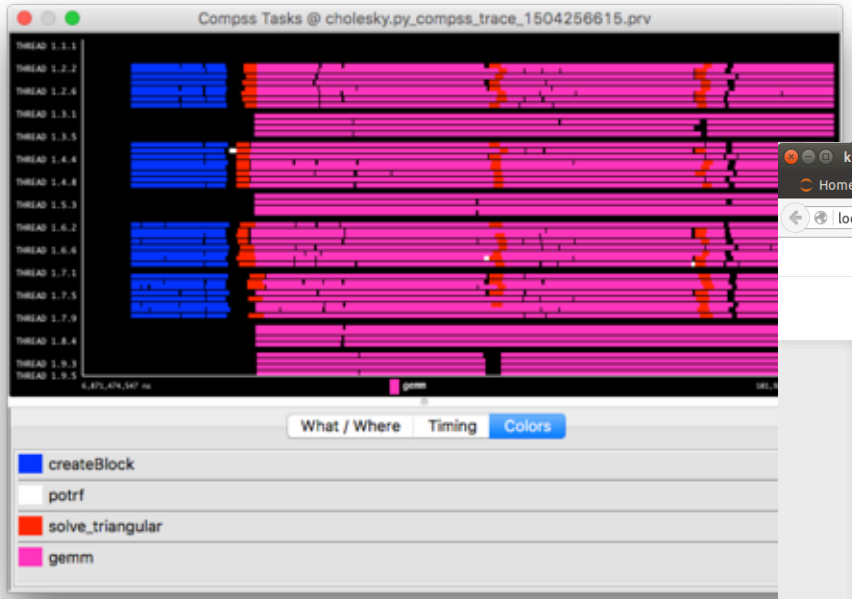
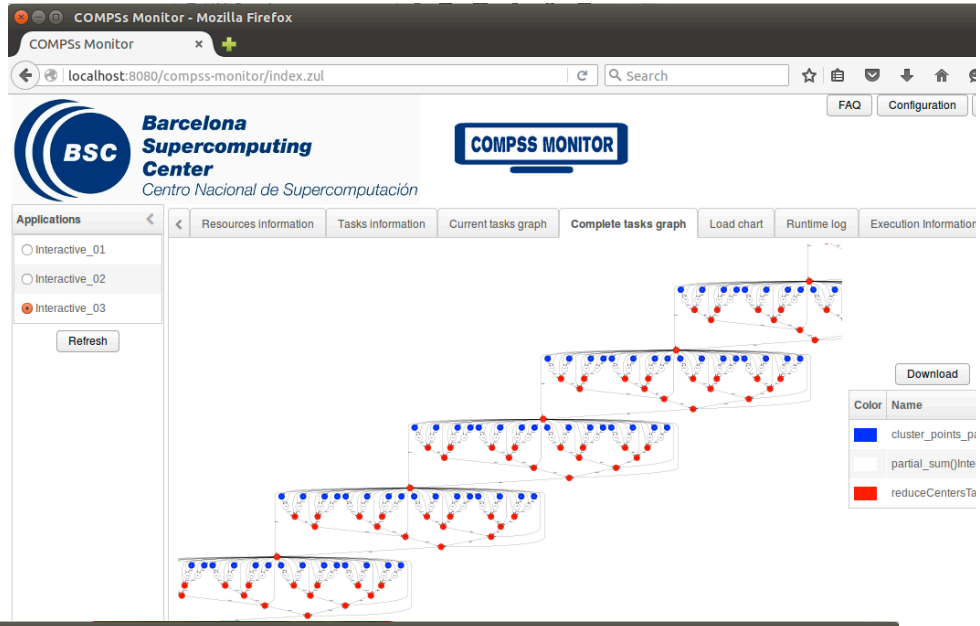
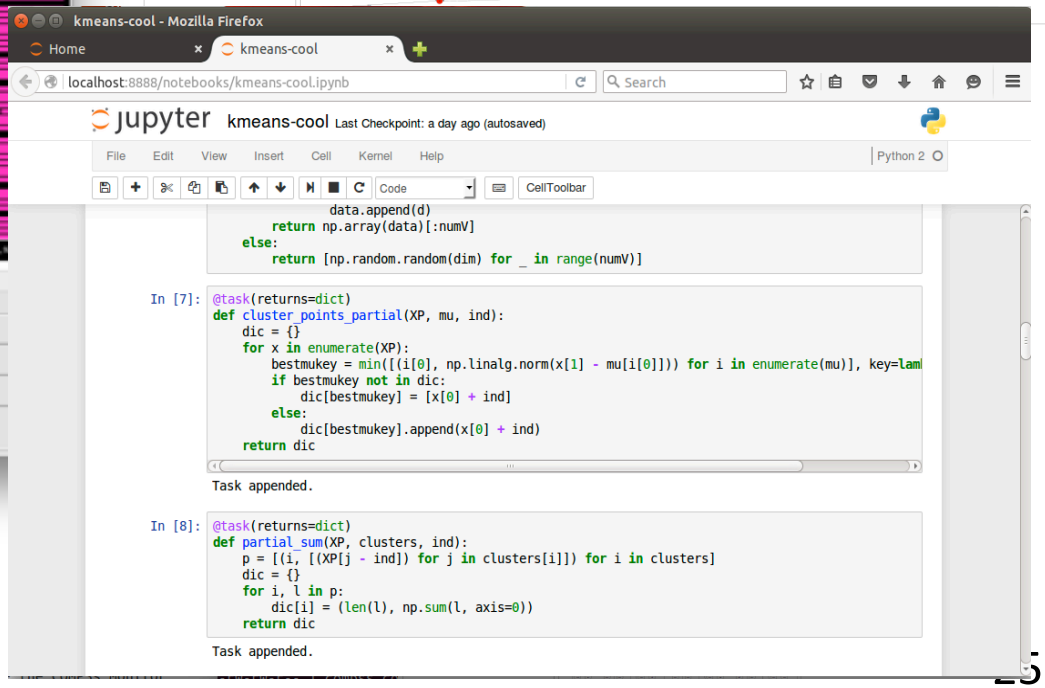
PyCOMPSs development environment

- Runtime monitor
- Paraver traces
- Jupyter-notebooks integration







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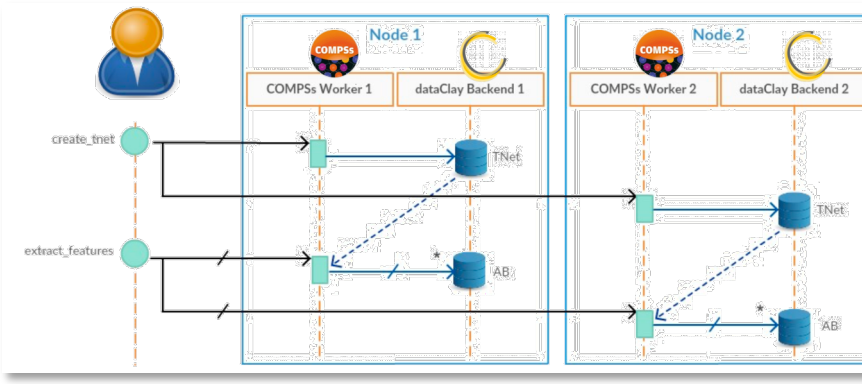
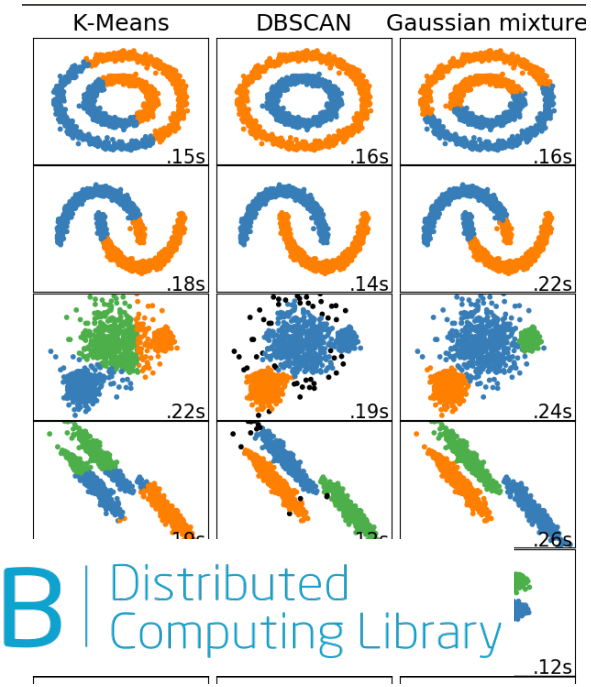
Integration with Machine Learning

- Thanks to the Python interface, the integration with ML packages is smooth:
  - Tensorflow, PyTorch, ...
  - Tiramisu: transfer learning framework Tensorflow + PyCOMPSs + dataClay



- 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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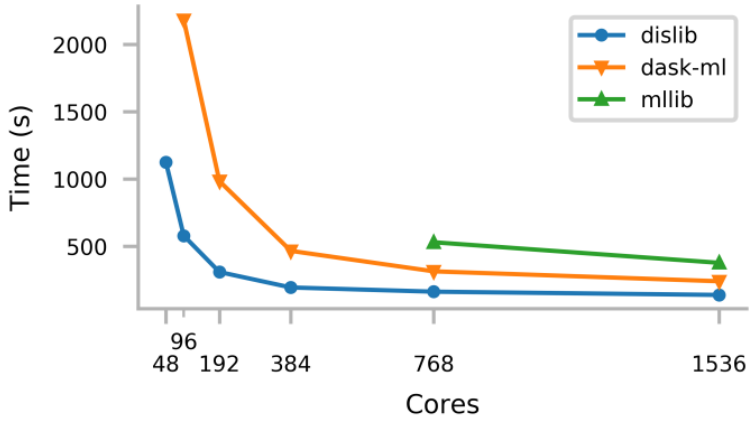
dislib.bsc.es

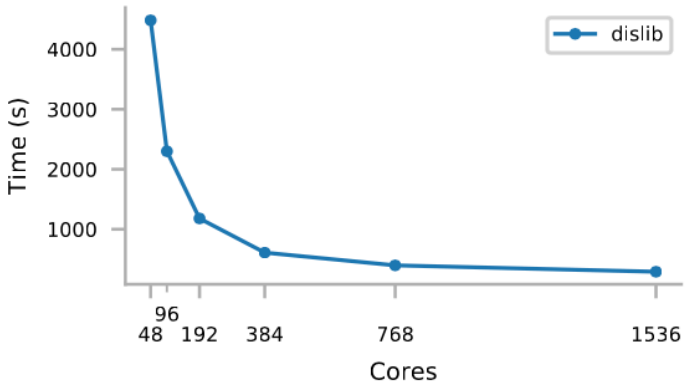
DISLIB | Distributed Computing Library

dislib sample results

- For very large sizes, dislib can obtain results while MLlib and dask fail to finish the execution

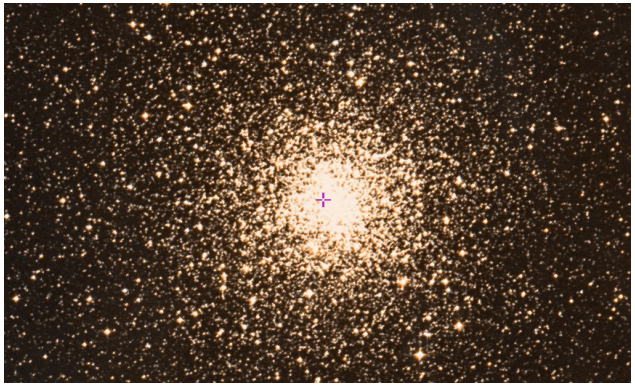


500 million samples
100 features



2 billion samples
100 features

- 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



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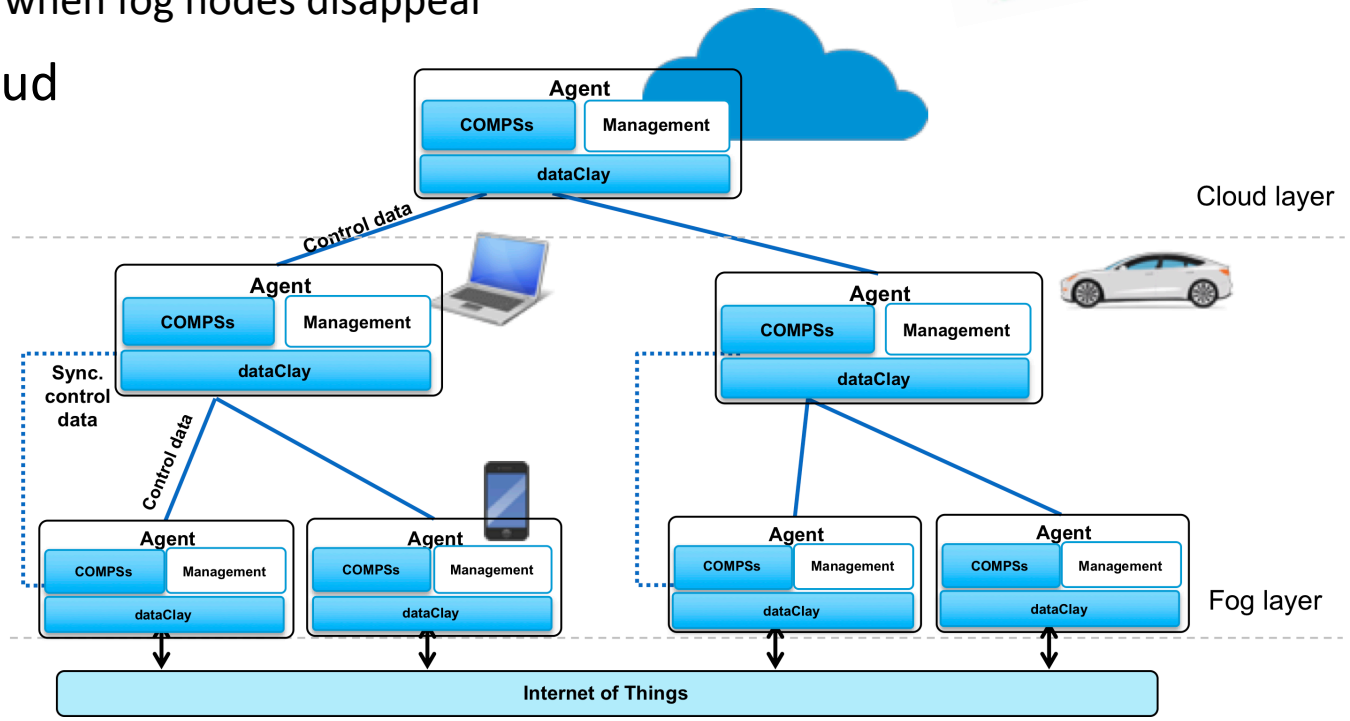
COMPSs in a fog-to-cloud architecture

- **Decentralized** approach to deal with large amounts of data
- New COMPSs runtime handles distribution, parallelism and heterogeneity
- Runtime deployed as a microservice in an agent:
  - Agents are independent, can act as master or worker in an application execution, agents interact between them
  - Hierarchical structure
- Data managed by dataClay, in a federated mode
  - Support for data recovery when fog nodes disappear
- Fog-to-fog and Fog-to-cloud



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Conclusions

Summarizing

- PyCOMPSs/COMPSs is a task-based programming model that offers different user points of view
  - Fine grain Python tasks – linear algebra codes, machine learning algorithms (dislib)
  - Workflows of external binaries or composing large simulations as individual tasks (MPI)
  - Environment for the development of fog-to-cloud applications, based on a new distributed runtime
- The current PyCOMPSs/COMPSs roadmap focuses on its evolution to support the development of workflows in highly distributed computing platforms
- We aim to provide a programming environment able to integrate computational, analytics and machine learning codes

Further Information

- Project page: http://www.bsc.es/compss
  - Documentation
  - Virtual Appliance for testing & sample applications
  - Tutorials
- Source Code

  https://github.com/bsc-wdc/compss
- Docker Image

  https://hub.docker.com/r/compss/compss
- Applications

  https://github.com/bsc-wdc/apps

  https://github.com/bsc-wdc/dislib

Thanks!

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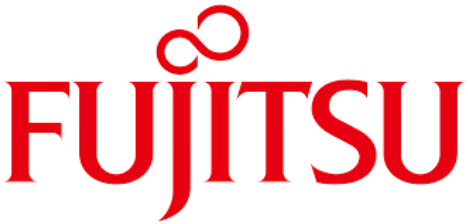
Projects where COMPSs is involved



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EXCELENCIA SEVERO OCHOA

Thanks!

BSC vision on programming models