Barcelona Supercomputing Center
Centro Nacional de Supercomputación

EXCELENCIA SEVERO OCHOA

Programming Distributed Computing Platforms with COMPSs

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Workflows & Distributed Computing Group

24-25/01/2023

Barcelona

Outline

Day 1

- Roundtable (9:30 – 09:45): Presentation of the tutorial and speakers
- Session 1 (09:45 – 10:15): Introduction to COMPSs
- Session 2 (10:15-11:15): PyCOMPSs: Writing Python applications
- Coffee break (11:15 – 11:45)
- Session 3 (11:45 a 13.00) Python Hands-on using Jupyter notebooks
- Lunch break (13:00-14:30)
- Session 4 (14:30 - 15:00) Machine learning with dislib
- Session 5 (15:00 -16:30): Hands-on with dislib
- SLIDES
  - http://compss.bsc.es/releases/tutorials/tutorial-PATC_2023/

Outline

Day 2

- Session 6 (9:30-11:00): Java & C++Writing Java applications
  - Java Hands-on + debug
  - C++ Syntax
- Coffee break (11:00 – 11:30)
- Session 7 (11:30-13:00): COMPSs Advanced Features
  - Using binaries and MPI code, Fault Tolerance and Exception management, Numba
  - COMPSs execution environments
  - Provenance and checkpointing
- Lunch break (13:00 – 14:30)
- Session 8 (14:30-16:30): Cluster Hands-on (MareNostrum)
- Session 9 (16:30-16:45) COMPSs Installation & Final Notes

INTRODUCTION

Motivation

- New complex architectures constantly emerging
  - With their own way of programming them
    - Fine grain: e.g. Programming models and APIs to run with GPUs, NVMs (Non-Volatile Memories)
    - Coarse grain: e.g. APIs to deploy in Clouds
  - **Difficult** for programmers
    - Higher learning curve / Time To Market (TTM)
    - What about non computer scientists???
  - **Difficult** to understand what is going on during execution
    - Was it fast? Could it be even faster? Am I paying more than I should? (**Efficiency**)
  - Tune your application for each architecture (or cluster)
    - E.g. partitioning data among nodes

Motivation

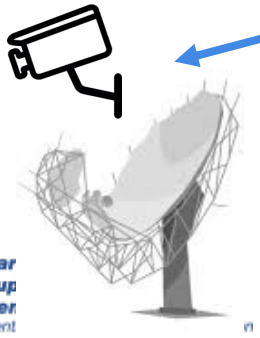
- Resources that appear and disappear
  - How to dynamically add/remove nodes to the infrastructure
- Heterogeneity
  - Different HW characteristics (performance, memory, etc)
  - Different architectures -> compilation issues
- Network
  - Different types of networks
  - Instability
- Trust and Security
- Power constraints from the devices in the edge
- Data & Storage

AI everywhere

HPC
Exascale computing
Cloud

Fog devices

Edge devices



Sensors
Instruments
Actuators

Motivation

- Create tools that make developers' life **easier**
  - Allow developers to focus on their problem
  - Intermediate layer: let the difficult parts to those tools
    - Act on behalf of the user
    - Distribute the work through resources
    - Deal with architecture specifics
    - Automatically improve performance
  - Tools for visualization
    - Monitoring
    - Performance analysis
  - Integration of computational workloads, with machine learning and data analytics

BSC vision on programming models

Applications

PM: High-level, clean, abstract interface

Power to the runtime

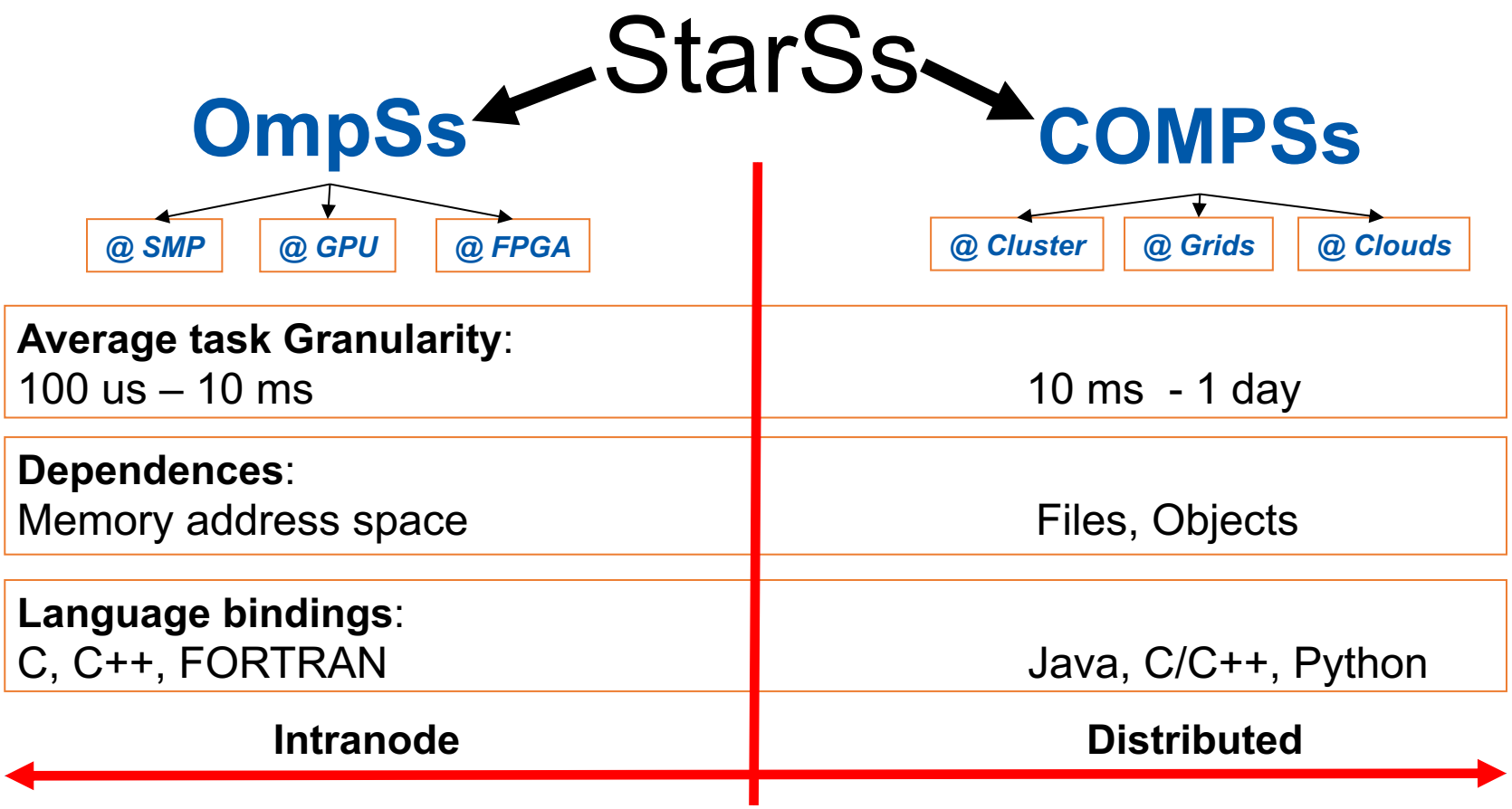
API

Program logic independent of computing platform

General purpose
Task based
Single address space

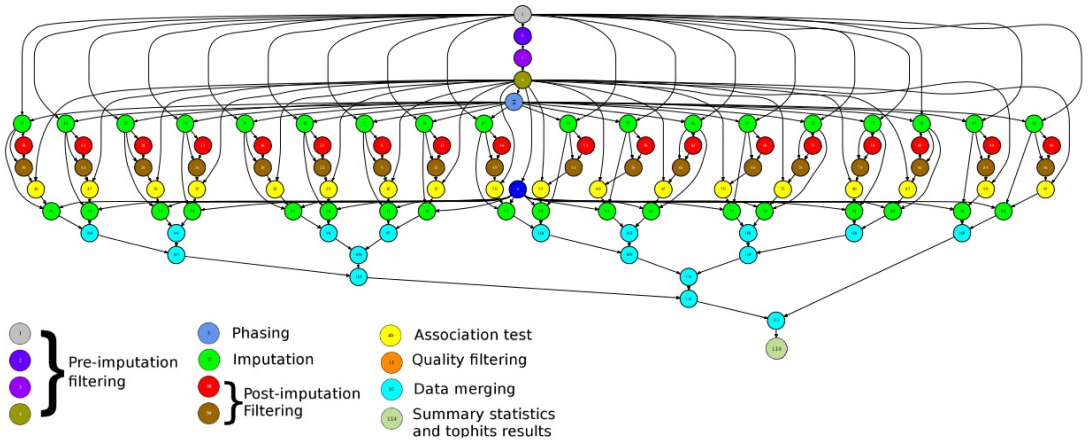
Intelligent runtime, parallelization, distribution, interoperability

BSC vision on programming models



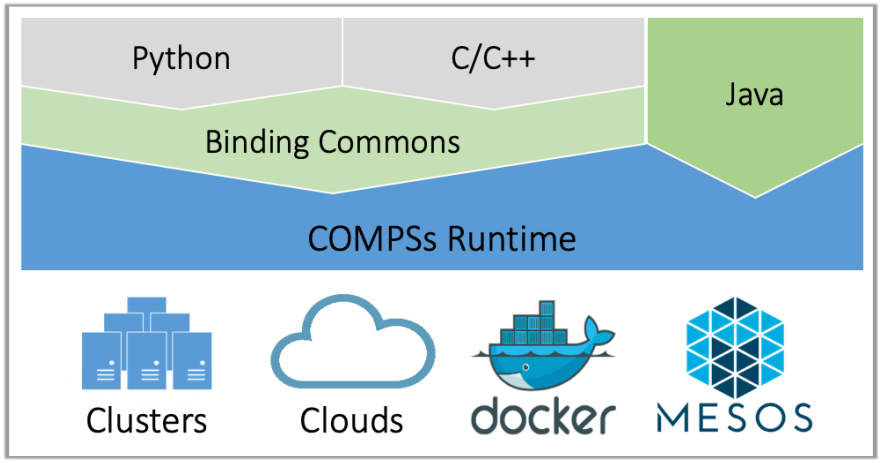
Programming with COMPSs

- Sequential programming
- General purpose programming language + annotations/hints
  - To identify tasks and directionality of data
- Task based: task is the unit of work
- Simple linear address space
- Builds a task graph at runtime that express potential concurrency
  - Implicit workflow
- Exploitation of parallelism
  - … and of distant parallelism
- Agnostic of computing platform
  - Enabled by the runtime for clusters, clouds and grids



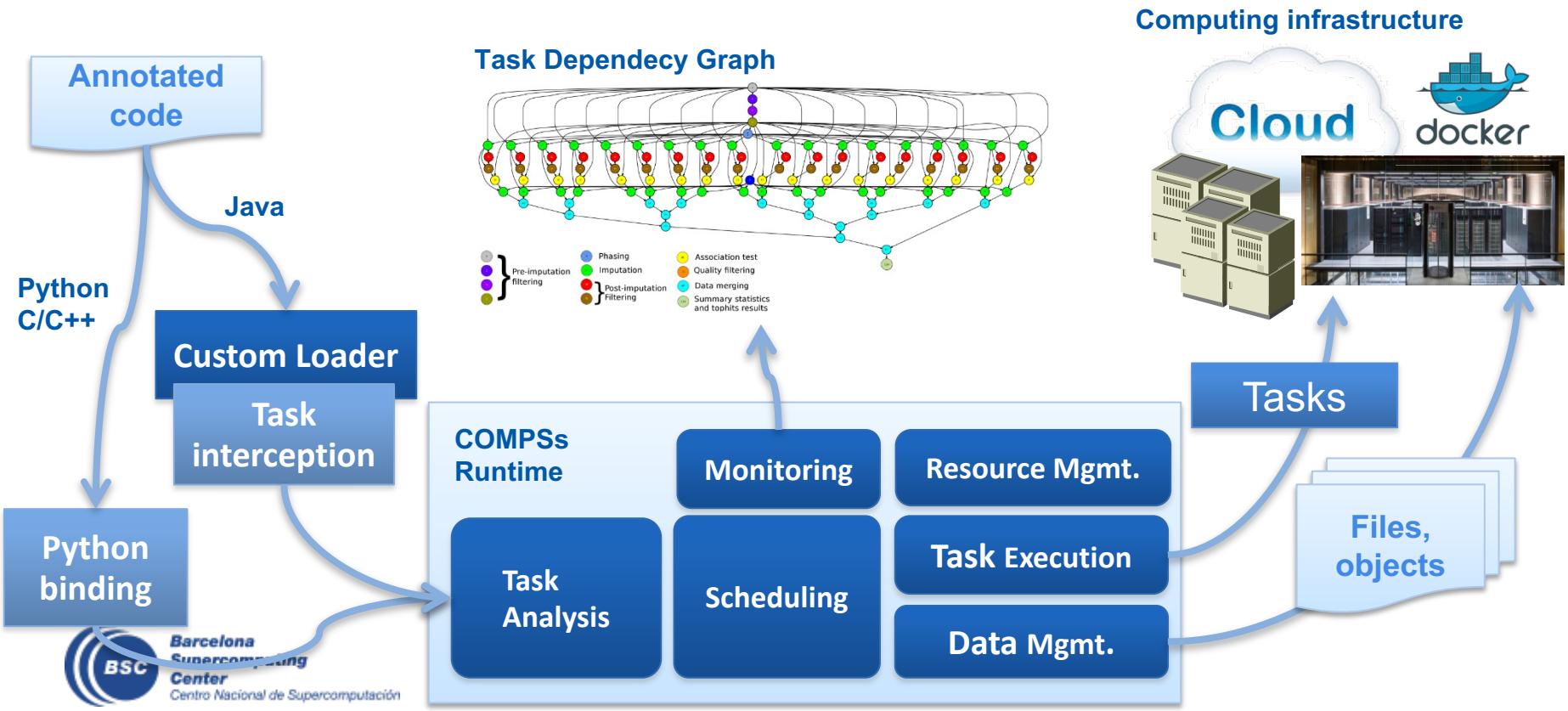
Programming with COMPSs

- Support for other types of parallelism
  - Threaded tasks (I.e., MKL kernels)
  - MPI applications -> tasks that involve several nodes
  - Integration with BSC OmpSs
  - Streaming tasks for data flow executions
- Support to Failure Management
- Parallel Machine Learning with dislib
- Available in MareNostrum and other supercomputers in Europe, in the EGI Federated Cloud and in Chameleon Cloud



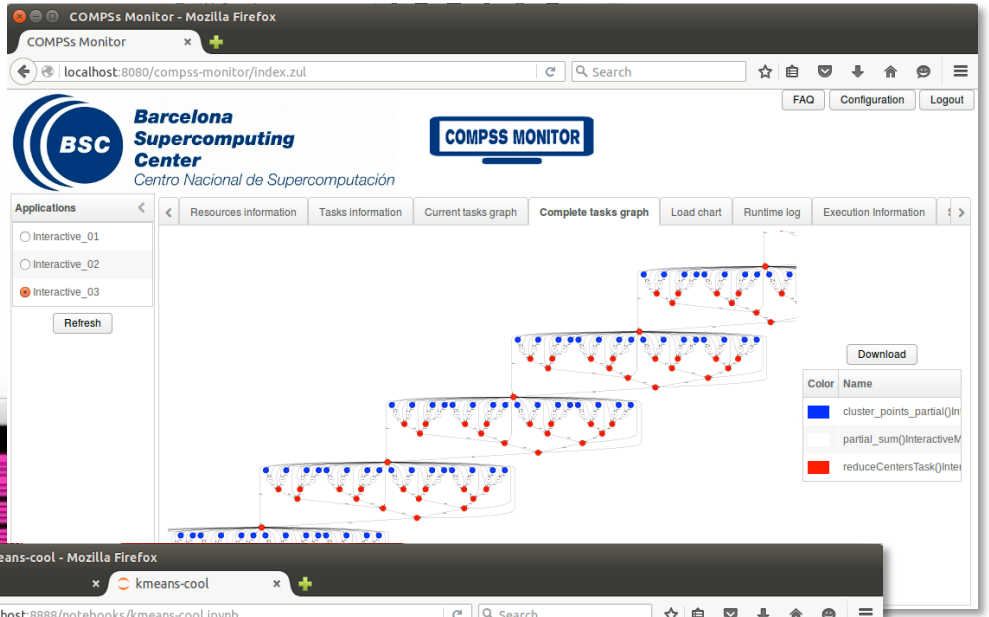
COMPSs runtime

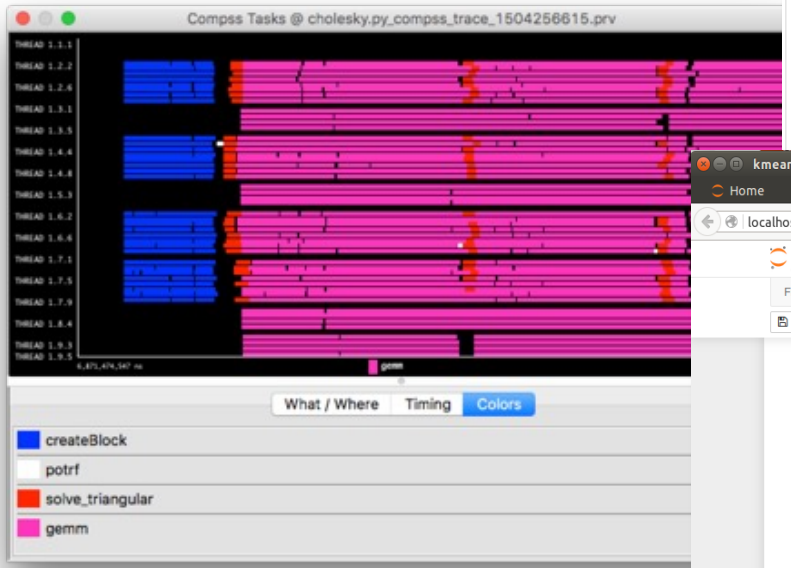
- PyCOMPSs/COMPSs applications executed in distributed mode following the master-worker paradigm
- Sequential execution starts in master node
- Tasks are offloaded to worker nodes
- All data scheduling decisions and data transfers are performed by the runtime

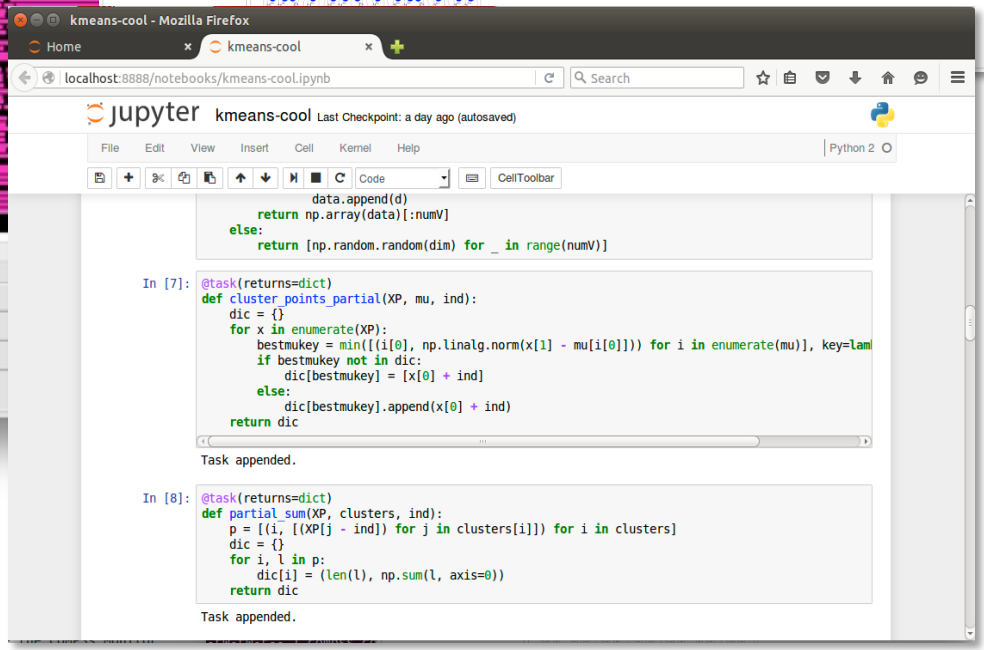


PyCOMPSs development environment

- Runtime monitor
- Paraver traces
- Jupyter-notebooks integration







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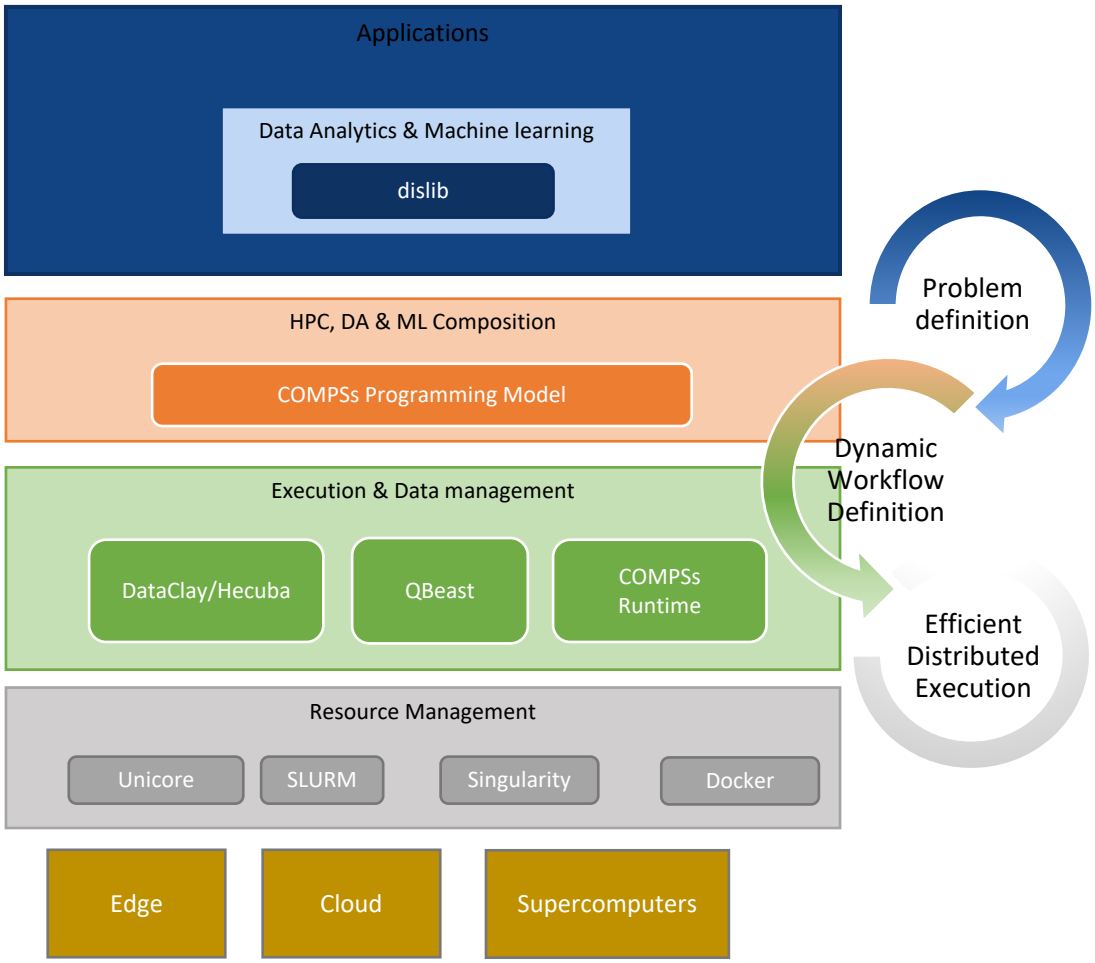
Conclusions

- COMPSs provides a workflow environment that enables the integration of HPC simulation and modelling with big data analytics and machine learning
- Support for dynamic workflows that can change their behaviour during the execution
- Support for dynamic resource management depending on the actual workload needs
- Support for data-streaming enabling the combination of task-flow and data-flow in the same workflow
- Support for persistent storage beyond traditional file systems.



Projects where COMPSs is used/developed

AI SPRINT
AI IN SECURE PRIVACY-PRESERVING COMPUTING CONTINUUM

CAELESTIS

ICOS

DT-GEO

Per Med CoE

HPC/Exascale Centre of Excellence in Personalised Medicine

MEEP
MareNostrum Experimental Exascale Platform

eFlows4HPC

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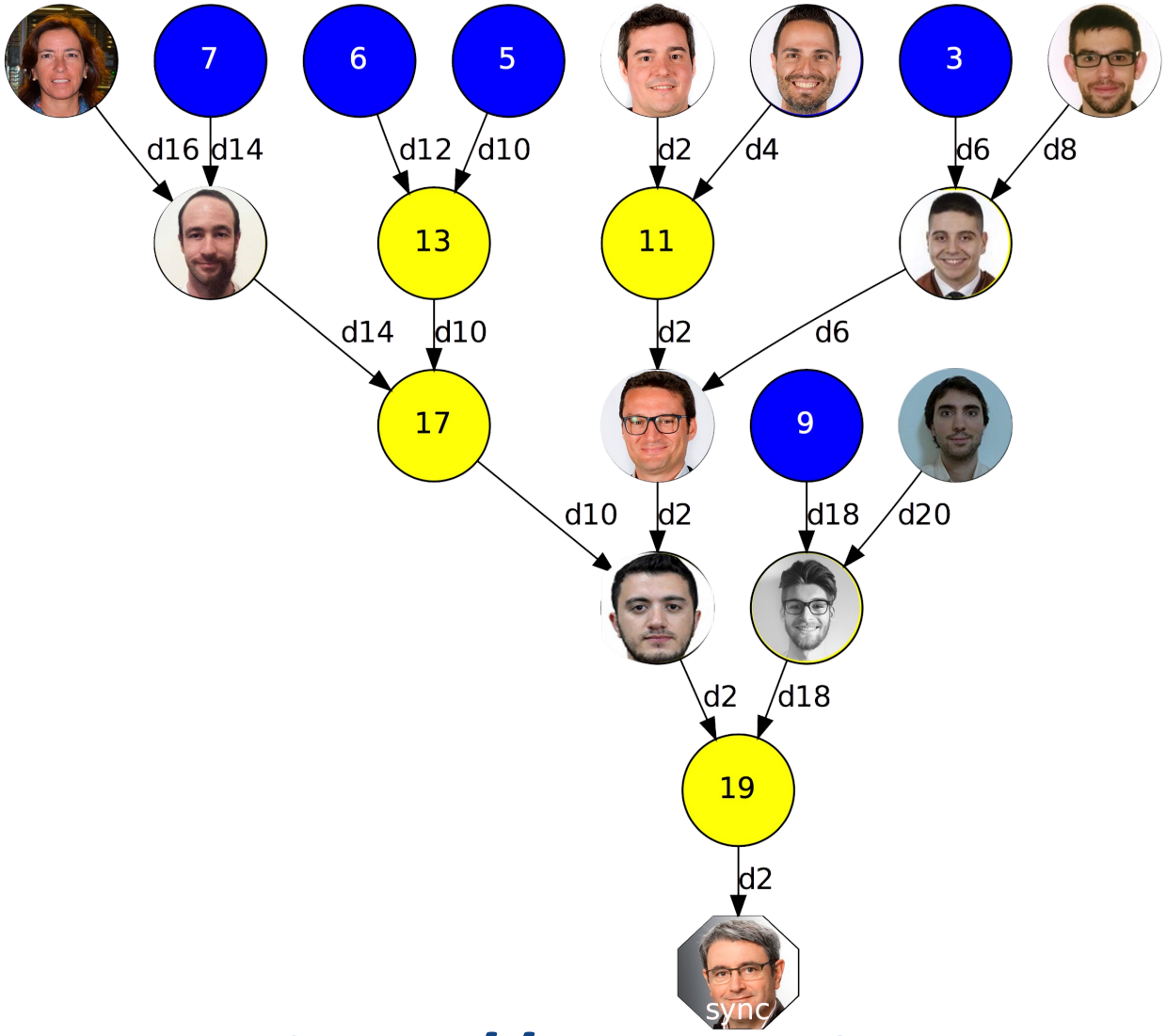
Joint Laboratory for Extreme-Scale Computing
Argonne NATIONAL LABORATORY · Inria · NCSA · JÜLICH · RIKEN

The WDC team



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