Programming Distributed Computing Platforms with COMPSs

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07/02/2023

Winter School, Barcelona

Outline

Agenda

- Presentation of the tutorial presenters
- Introduction to COMPSs (20 min)
- PyCOMPSs: Writing Python applications (1hour)
- Break (15 min)
- Hands-on MN (1 hour)
- PyCOMPSs installation (15 min)
- SLIDES
  - http://compss.bsc.es/releases/tutorials/tutorial-WINTER_SCHOOL_2023/

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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

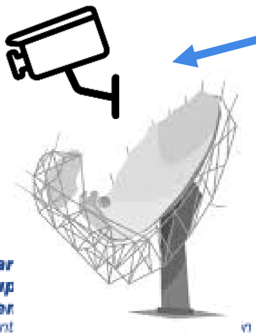
- Resources that appear and disappear
  - How to dynamically add/remove nodes to the infrastructure
- Heterogeneity
  - Different HW characteristics (performance, memory, etc)
  - Different architectures -> compilation issues
- Network
  - Different types of networks
  - Instability
- Trust and Security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

AI everywhere

HPC
Exascale computing
Cloud

Fog devices

Edge devices

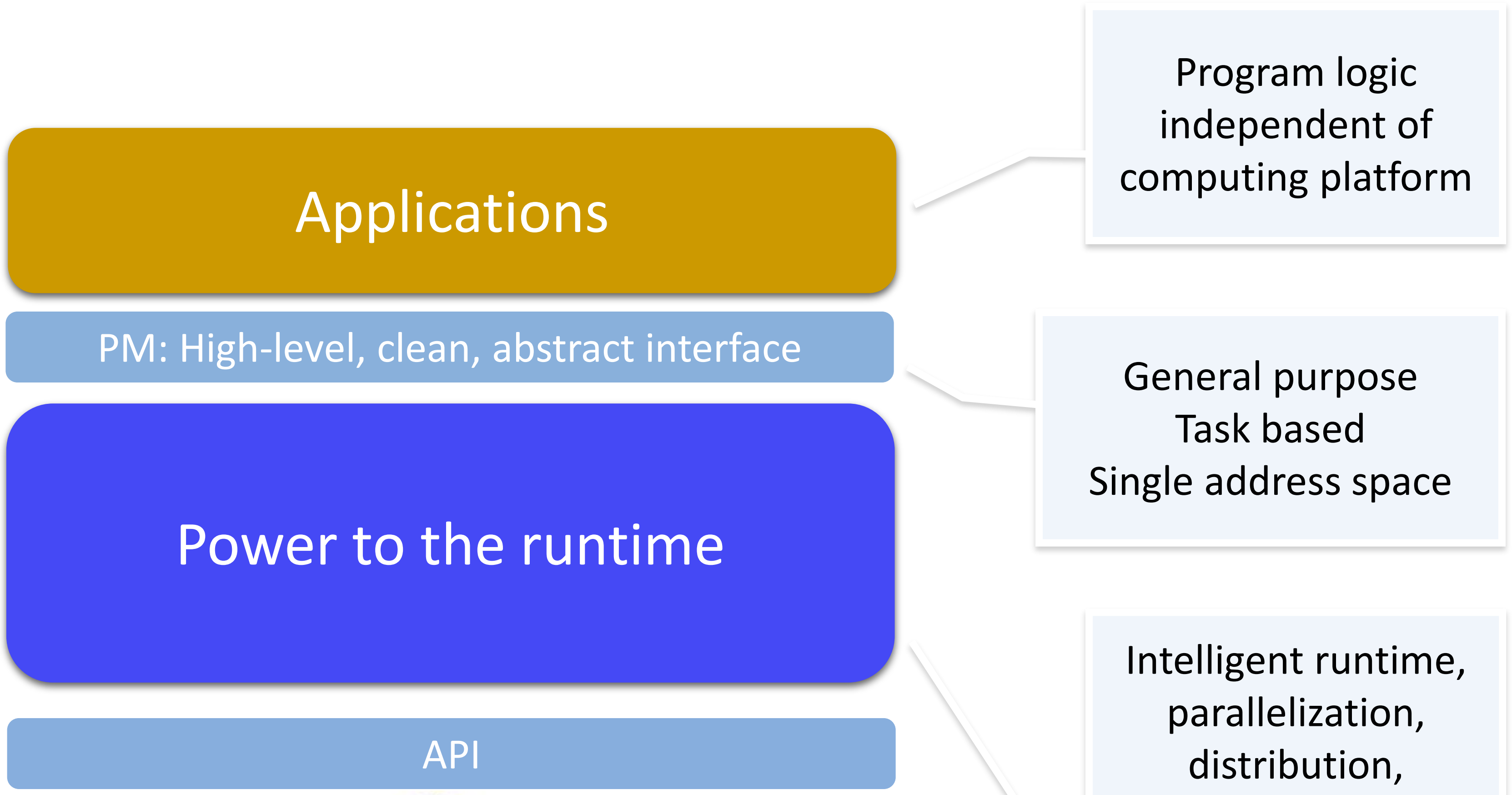


Sensors
Instruments
Actuators

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

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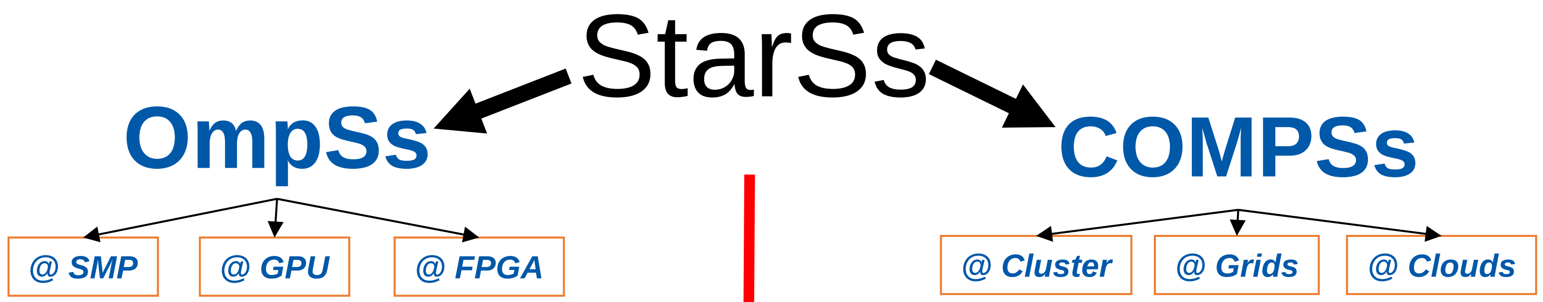
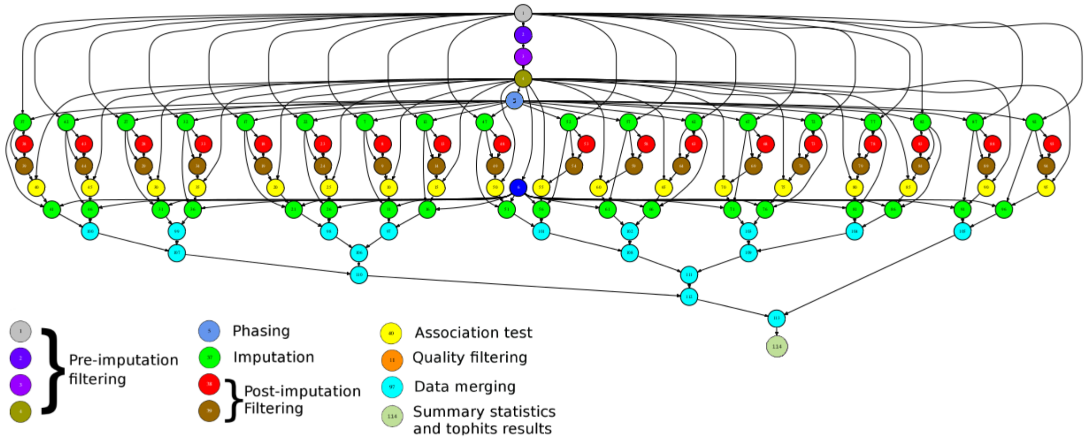
BSC vision on programming models



Average task Granularity: 100 us – 10 ms	10 ms - 1 day
Dependences: Memory address space	Files, Objects
Language bindings: C, C++, FORTRAN	Java, C/C++, Python
Intranode	**Distributed**

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



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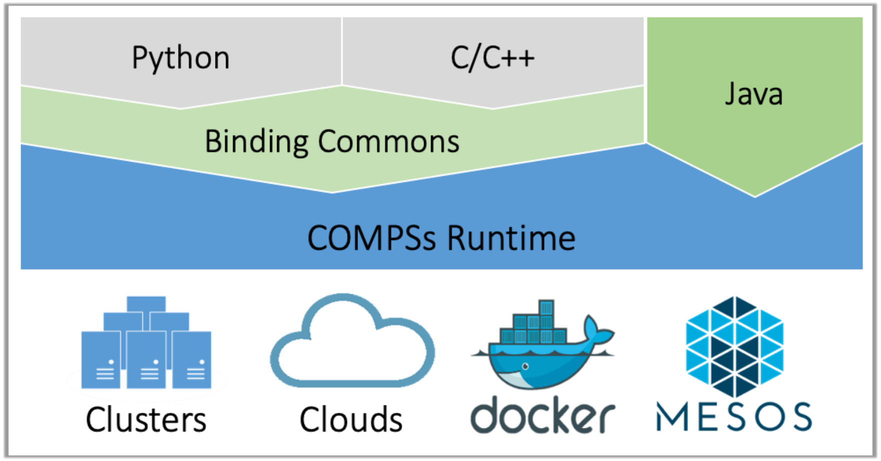
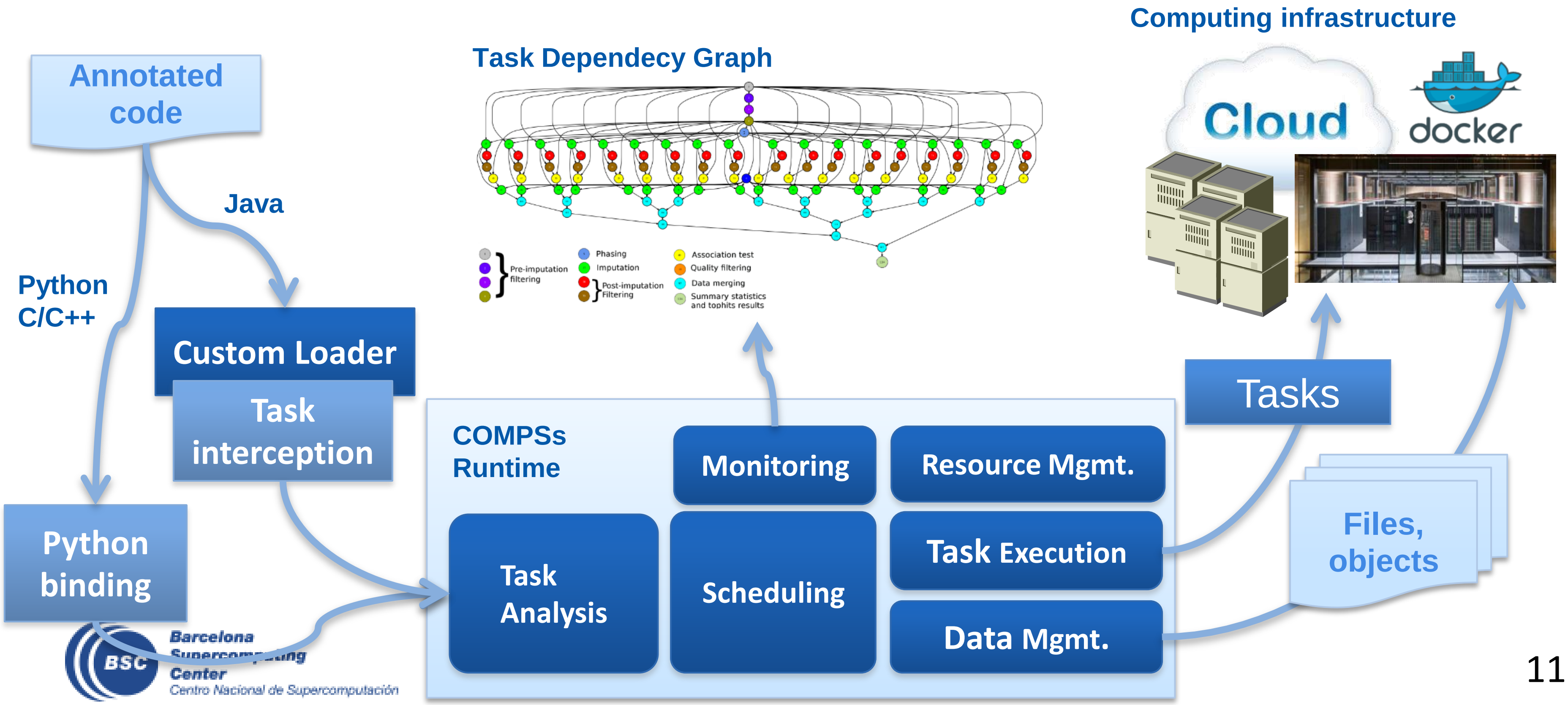
Programming with COMPSs

- 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



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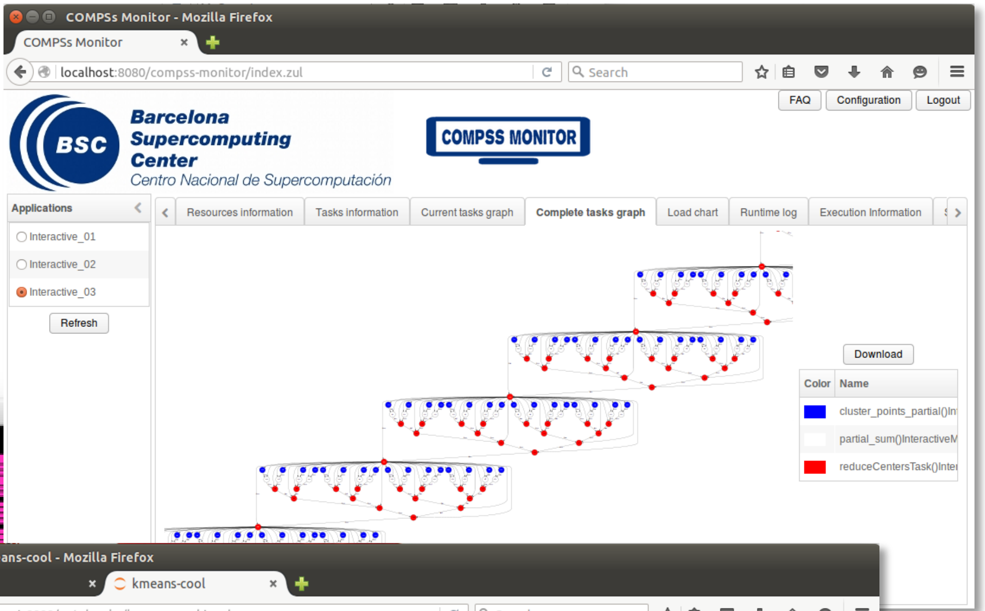
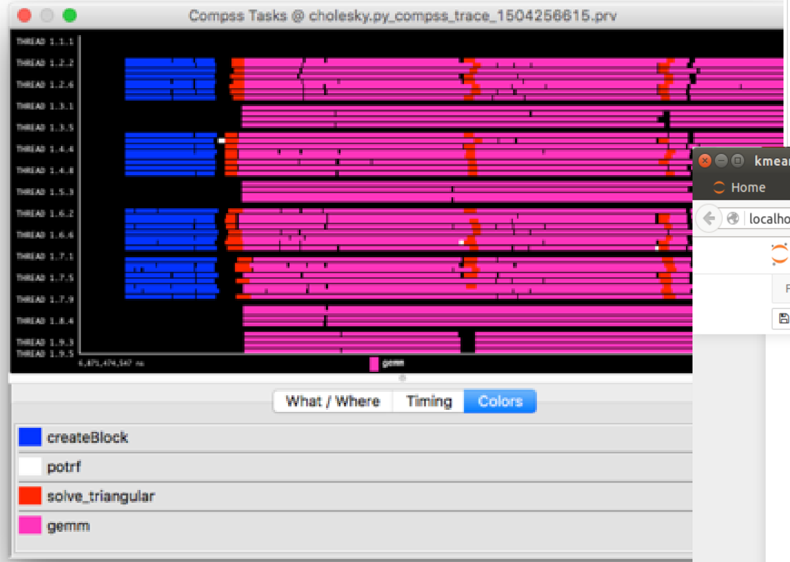
PyCOMPSs development environment

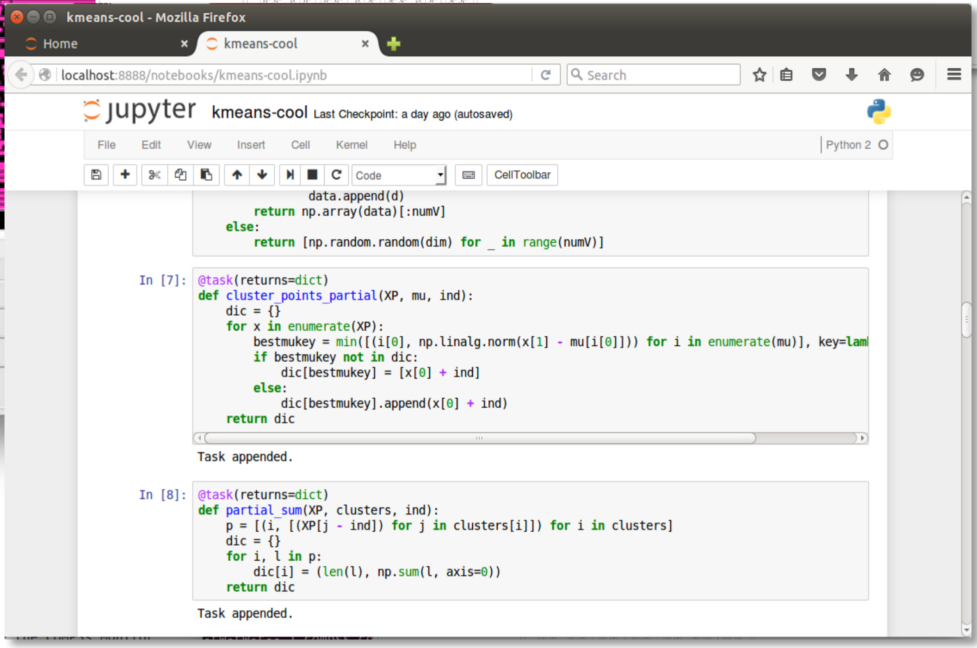
- Runtime monitor
- Paraver traces
- Jupyter-notebooks integration



Color	Name
🟦	cluster_points_partial()In
⬜	partial_sum()InteractiveM
🟥	reduceCentersTask()Inte



🟦	createBlock
⬜	potrf
🟥	solve_triangular
🟪	gemm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Python 2
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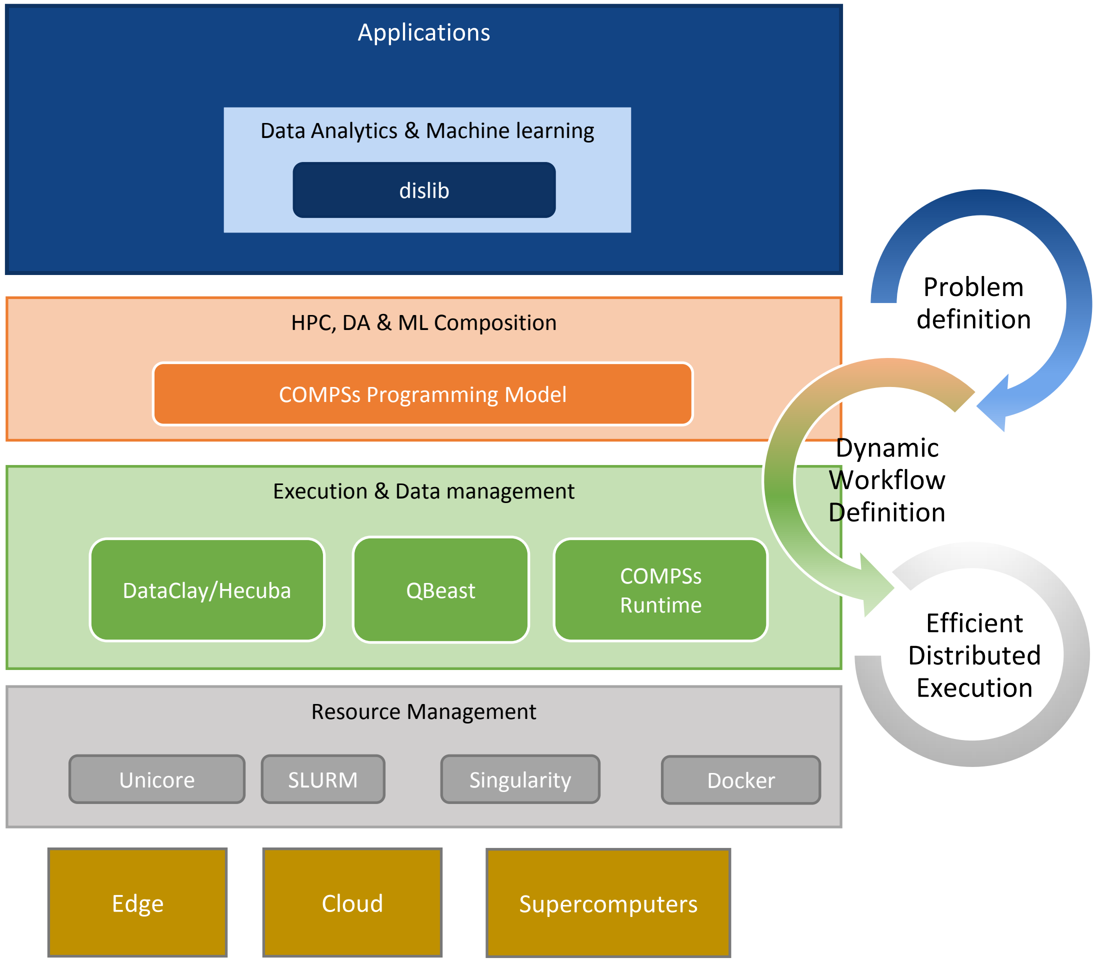
```
            data.append(d)
        return np.array(data)[:numV]
    else:
        return [np.random.random(dim) for _ in range(numV)]
```

```
In [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=lam
                if bestmukey not in dic:
                    dic[bestmukey] = [x[0] + ind]
                else:
                    dic[bestmukey].append(x[0] + ind)
            return dic

        Task appended.
```

```
In [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

        Task appended.
```

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.



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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

Joint Laboratory for Extreme-Scale Computing

Inria NCSA Argonne Barcelona Supercomputing Center JÜLICH RIKEN

BSC Barcelona Supercomputing Center
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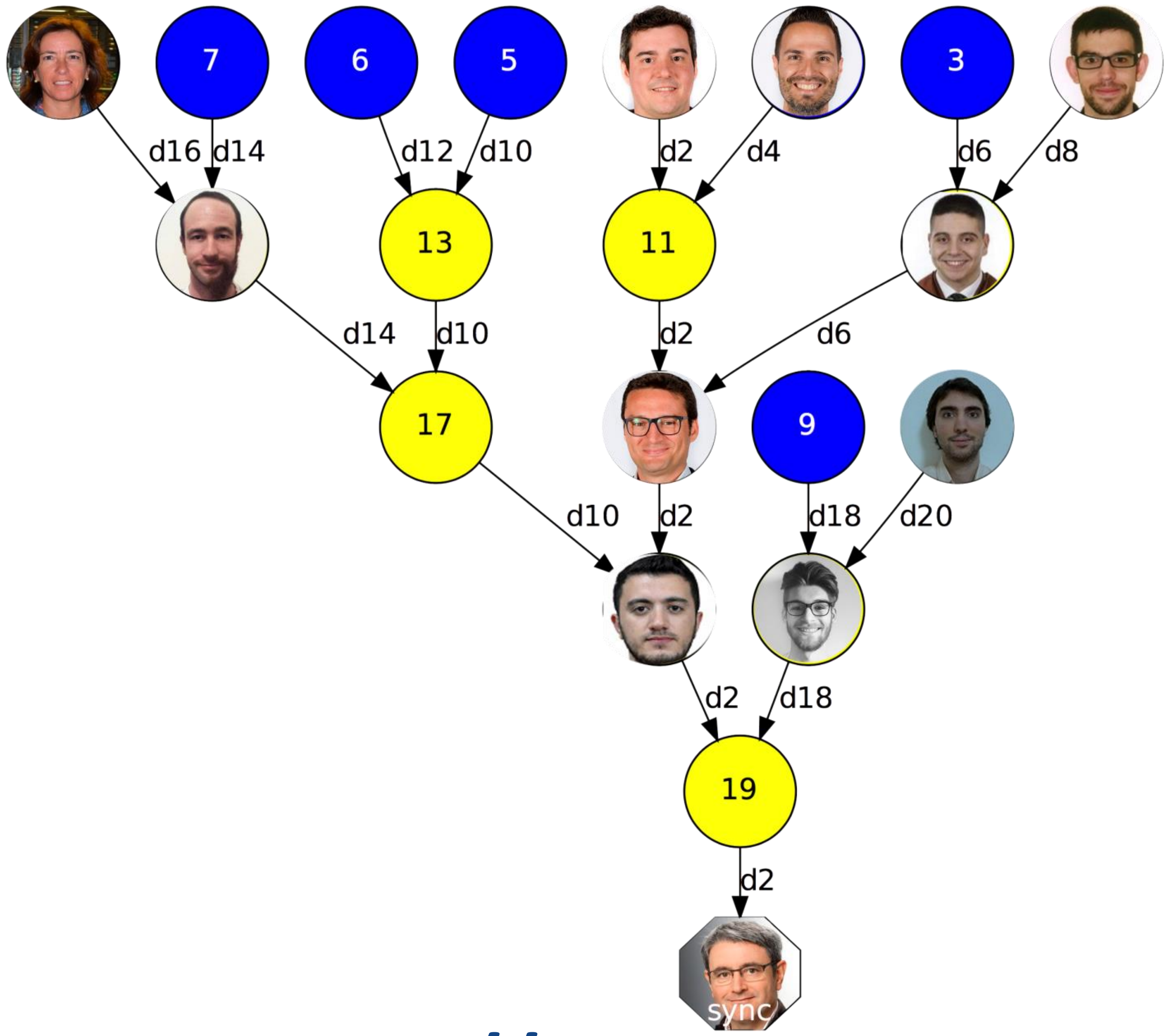
The WDC team



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