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EXCELENCIA SEVERO OCHOA

Programming dynamic workflows in the Exascale Era

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Workflows and Distributed Computing Group

ESiWACE2 Workshop on Emerging Technologies for Weather and Climate Modelling

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Challenges in highly distributed infrastructures

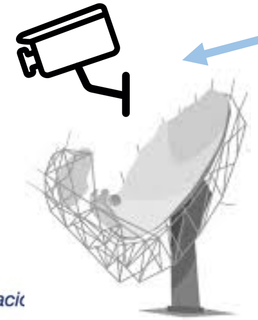
- Resources that appear and disappear
  - How to dynamically add/remove nodes to the infrastructure
- Heterogeneity
  - Different HW characteristics (performance, memory, etc)
  - Different architectures -> compilation issues
- Network
  - Different types of networks
  - Instability
- Trust and Security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

HPC
Exascale computing
Cloud

AI everywhere

Fog devices

Edge devices



Sensors
Instruments
Actuators

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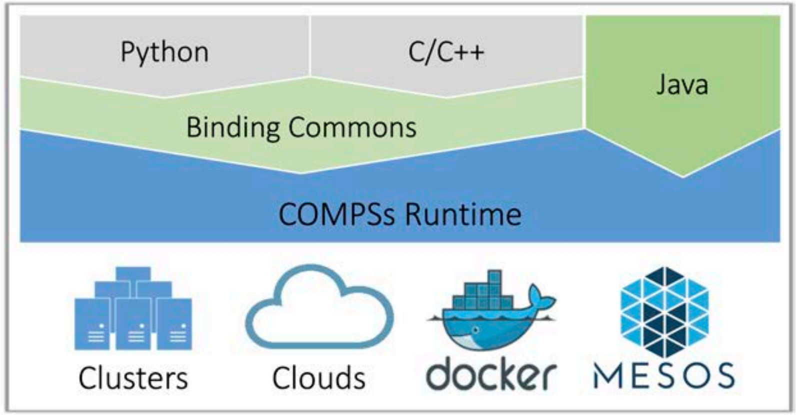
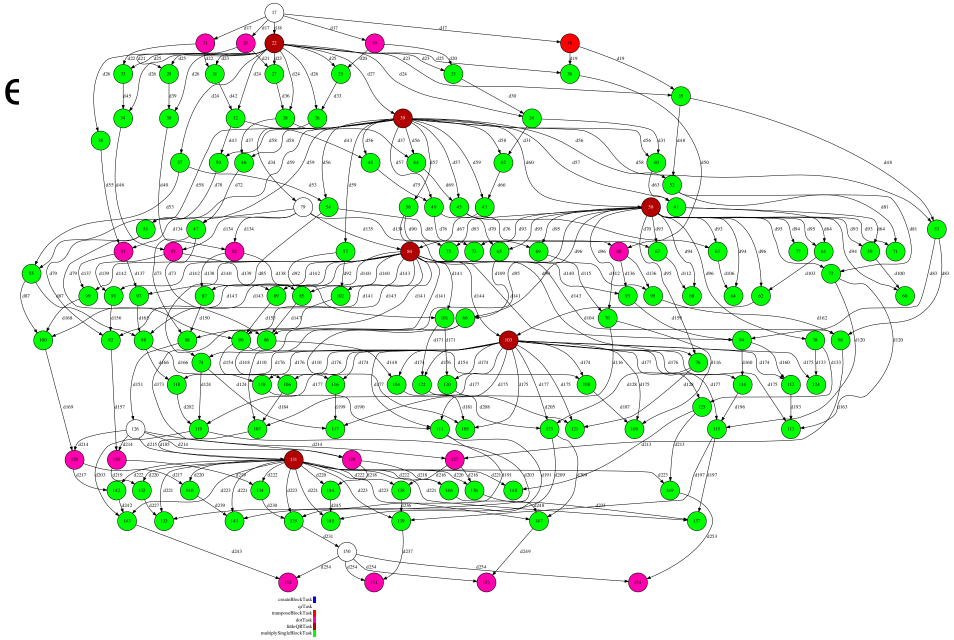
Data and storage challenge

- Sensors and instruments as sources of large amounts of heterogeneous data
  - Control of edge devices and remote access to sensor data
  - Edge devices typically have SDcards, much slower than SSD
- Compute and store close to the sensors
  - To avoid data transfers
  - For privacy/security aspects
- New data storage abstractions that enable access from the different devices
  - Object store versus file system?
  - Data reduction/lossy compression
- Task flow versus data flow:
  data streaming
- Metadata and traceability

Orchestration challenges

- How to describe the workflows in such environment? Which is the right interface?
- Focus:
  - Integration of computational workloads, with machine learning and data analytics
- Intelligent runtime that can make scheduling and allocation, data-transfer, and other decisions
- PyCOMPSs is a parallel task-based programming model for distributed computing platforms. Based on a sequential interface, at execution time the COMPSs runtime is able to exploit the inherent parallelism of applications at task level.





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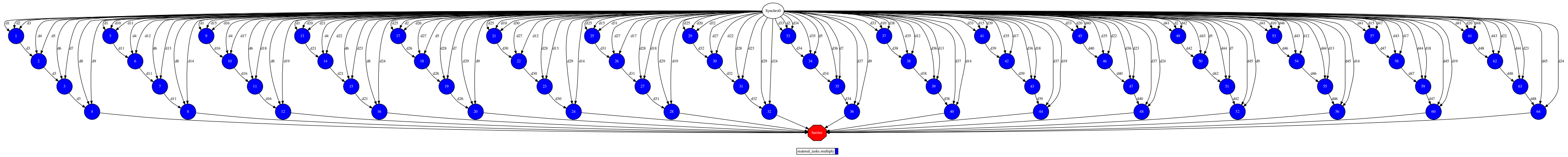
PyCOMPSs Syntax

- Use of **decorators** to annotate tasks and to indicate arguments directionality
- Small API for data synchronization



Tasks definition

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

Main Program

```
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][j])
compss_barrier()
mulTime = time.time() - startMulTime
```

Other decorators: Tasks’ constraints

- 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 heterogeneity on the devices in the platform**
- Versions: Mechanism to support multiple implementations of a given behavior (polymorphism)
  - **Runtime selects to execute the task in the most appropriate device in the platform**

```
@constraint (MemorySize=6.0, ProcessorPerformance=“5000”, ComputingUnits=“8”)
@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_other(a, b, c):
    ...
```

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Failure Management

- Interface than enables the programmer to give hints about failure management

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

- Options: RETRY, CANCEL_SUCCESSORS, FAIL, IGNORE
- Implications on file management:
  - I.e, on IGNORE, output files: are generated empty
- **Possibility of ignoring part of the execution of the workflow, for example if a task fails in an unstable device**
- **Opens the possibility of dynamic workflow behaviour depending on the actual outcome of the tasks**

Task Nesting

- Tasks that internally invoke new tasks

```
@compss(app_name="csvm-driver.py",
        computingNodes=”2”, …)
@constraint(ComputingUnits= “48”)
@task(returns=int)
def run_csvm(iflag="-i", i=1, cflag="-c", ...
    pass
```

- Why is task nesting relevant?
  - Support for structured programming
  - Reduces bottlenecks in scheduling and other runtime features
  - Better support for heterogeneous computing platforms

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Integration of HPC, ML and data analytics

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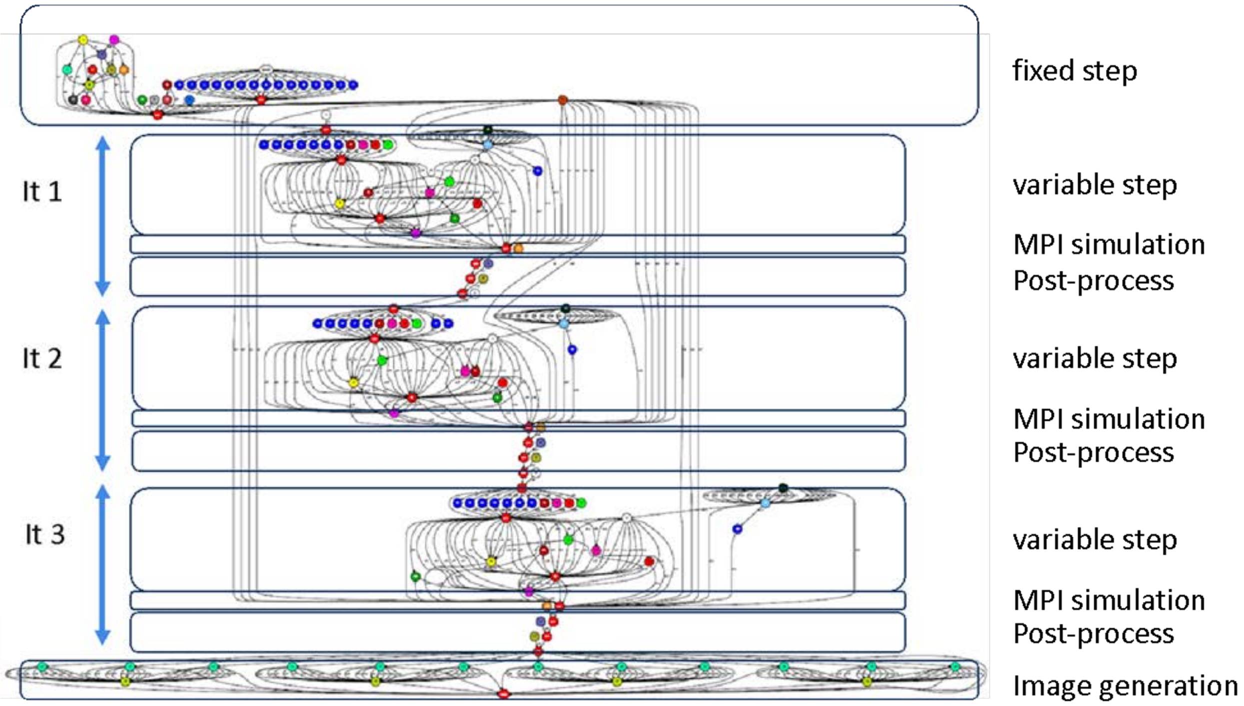
Other decorators: linking with other programming models

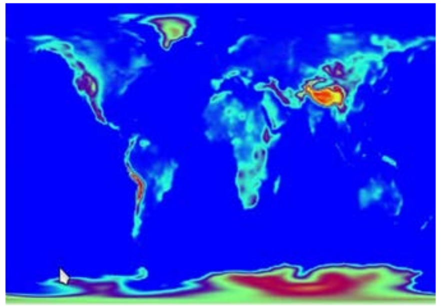
- A task can be more than a sequential function
  - A task in PyCOMPSs can be sequential, multicore or multi-node
  - External binary invocation: wrapper function generated automatically
  - Supports for alternative programming models: MPI and OmpSs
- Additional decorators:
  - @binary(binary="app.bin")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

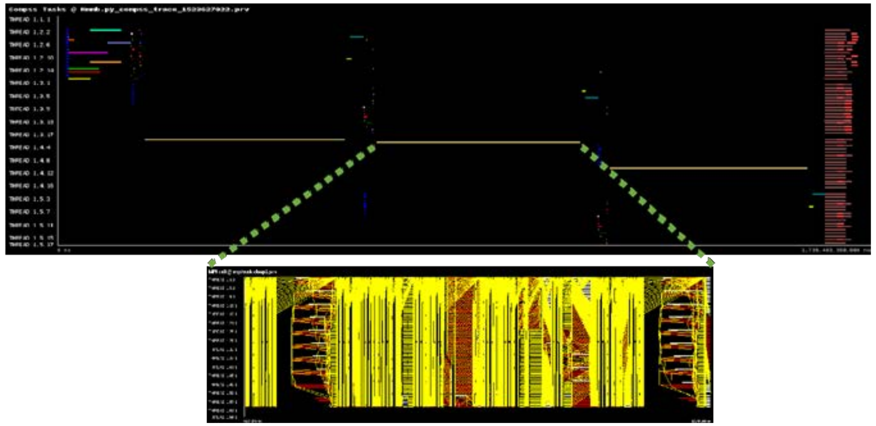
```
@constraint (computingUnits= "248")
@mpi (runner="mpirun", computingNodes= ”16”, ...)
@task (returns=int, stdOutFile=FILE_OUT_STDOUT, ...)
def nems(stdOutFile, stdErrFile):
    pass
```

NMMB-Monarch: Weather and dust forecast

- An example of usage of this idea is the application Multiscale Online Nonhydrostatic Atmosphere Chemistry model (NMMB-Monarch) aims at providing short to medium range weather and gas-phase chemistry forecasts from regional to global scales that performs weather and dust forecast. NMMB-Monarch is used as an operational tool to provide information services at BSC.
- The application combines multiple sequential scripts and MPI simulations. PyCOMPSs enables the smooth orchestration of all them as a single workflow.







Integration with persistent memory

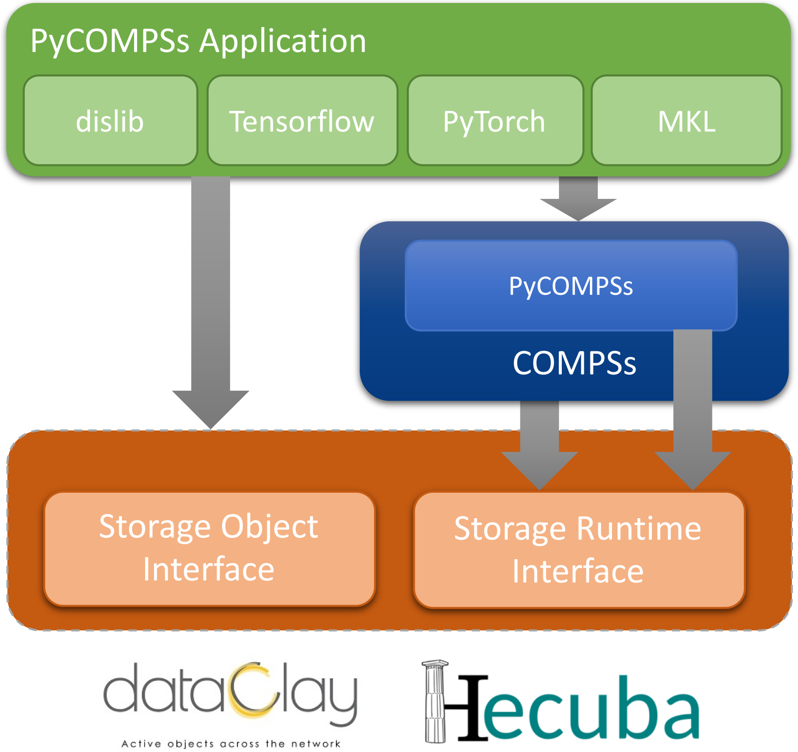
- Programmer may decide to make persistent specific objects in its code
- Persistent objects are managed same way as regular objects
- Tasks can operate with them

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

a.mytask()
compss_barrier()

o = a.another_object
```

- **Objects can be accessed/shared transparently in a distributed computing platform**



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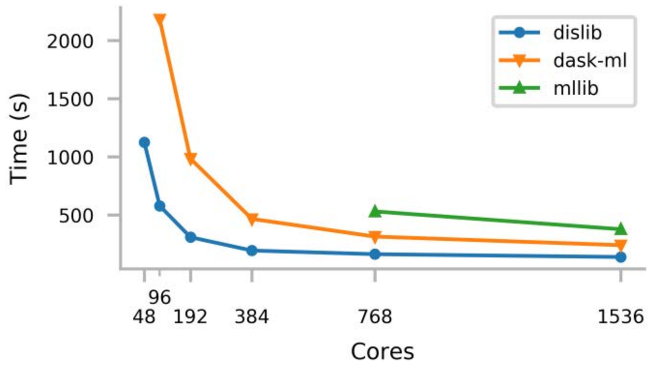
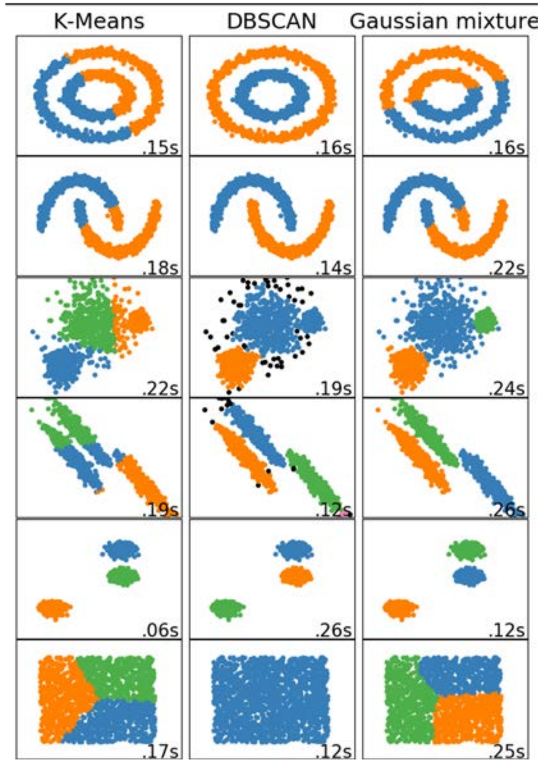
Dislib: parallel machine learning

- Dislib, a distributed machine learning library parallelized with PyCOMPSs that enables large-scale data analytics on HPC infrastructures.
- Inspired by scikit-learn, dislib provides an estimator-based interface that improves productivity by making algorithms easy to use and interchangeable. This interface also makes programming with dislib very easy to scientists already familiar with scikit-learn.
- Dislib also provides a distributed data structure that can be operated as a regular Python object. The combination of this data structure and the estimator-based interface makes dislib a distributed version of scikit-learn, where communications, data transfers, and parallelism are automatically handled behind the scene

- 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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FUJITSU

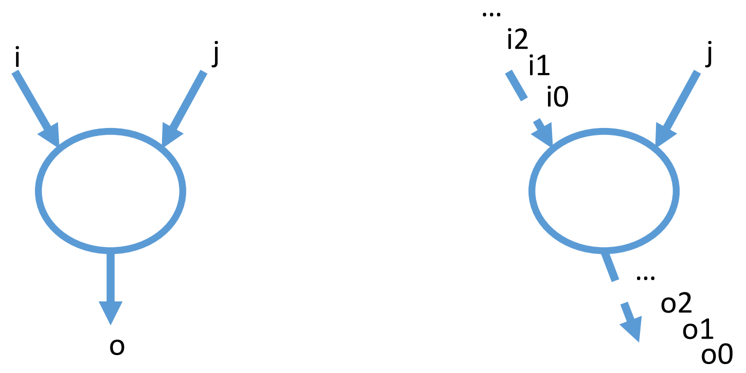
DISLIB Distributed Computing Library

Support for data streams: Task-flow versus data-flow

- New interface to support streaming data in tasks
- Task-flow and data-flow tasks live together in PyCOMPSs/COMPSs workflows
- Data-flow tasks persist while streams are not closed
  - Parameters can be one/multiple streams and non-streamed
- Runtime implementation based on Kafka

```
@task(fds=STREAM_OUT)
def sensor(fds):
        ...
    while not end():
        data = get_data_from_sensor()
        f.write(data)
    fds.close()
```

Task-flow task   Data-flow task



Task-flow task

- Receives data once
- Generates data once
- Does not persist in time
- Stateless tasks

Data-flow task

- Receives data multiple times
- Generates data multiple times
- Tasks persists in time
- Stateful tasks

```
@task(fds_sensor=STREAM_IN, filtered=OUT)
def filter(fds_sensor, filtered):
        ...
    while not fds_sensor.is_closed():
        get_and_filter(fds_sensor, filtered)
```

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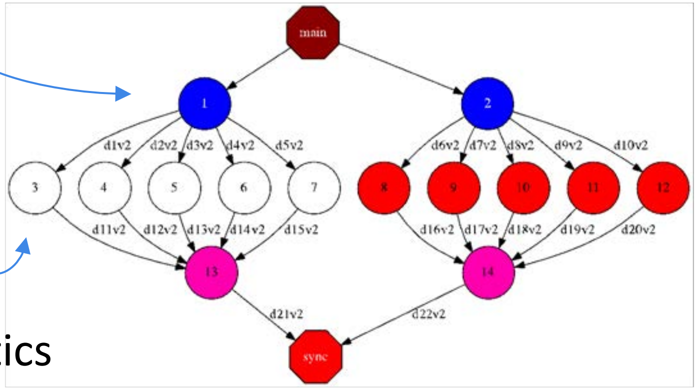
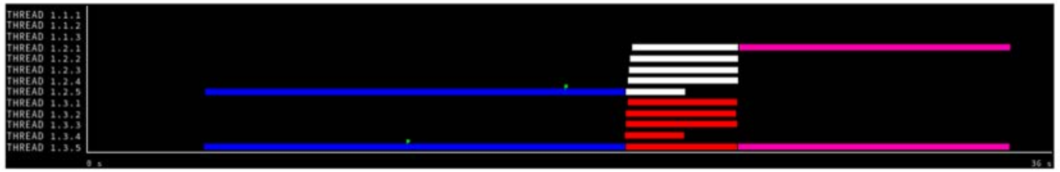
Use case: MPI simulations, analytics and streaming

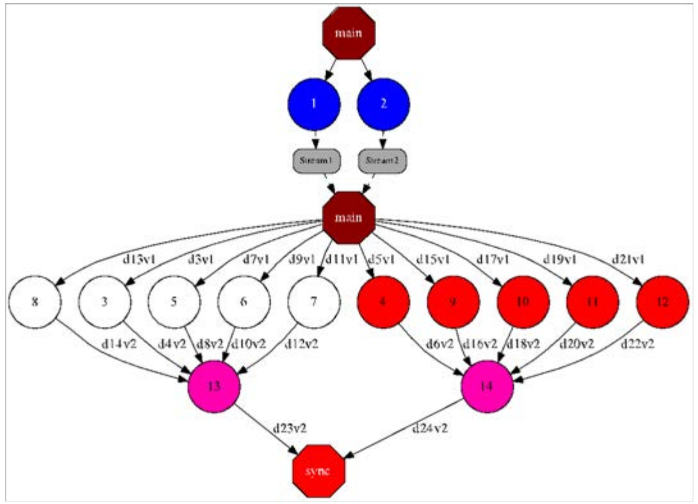
- Sample case: MPI simulations generating at given steps data to be processed by some analytics

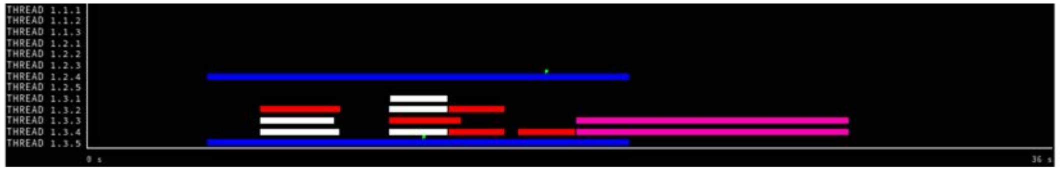
MPI



Analytics







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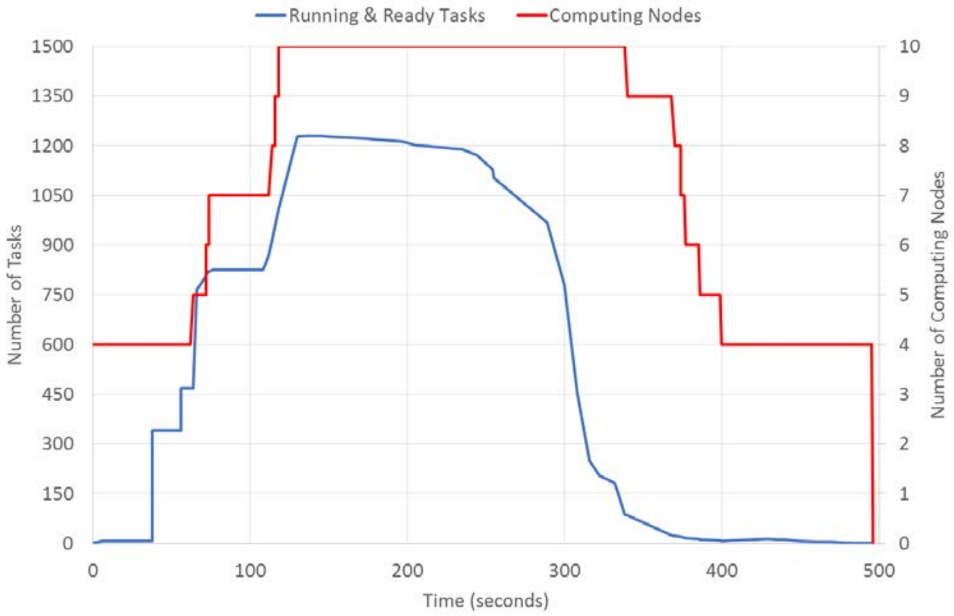
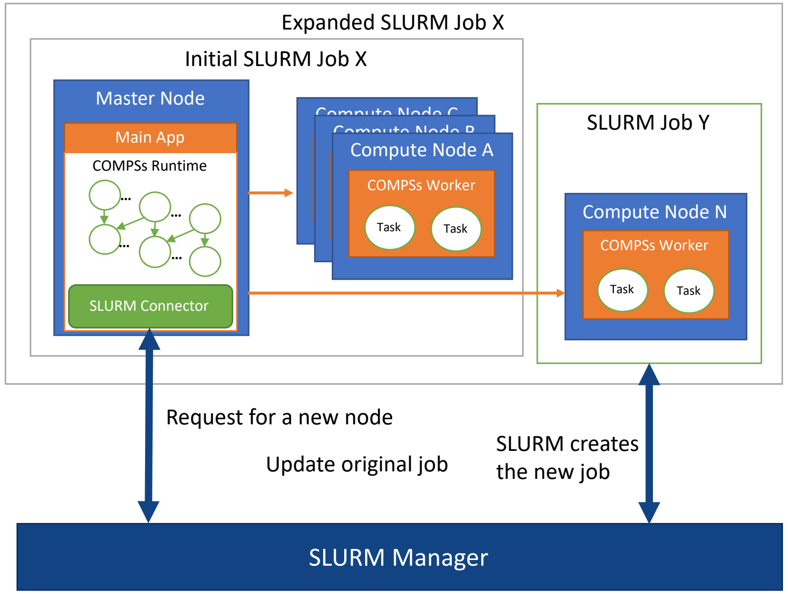
COMPSs runtime: support for elasticity

- Possibility to adapt the computing infrastructure depending on the actual workload
- Typical for cloud, now also SLURM managed systems
- Feature that contributes to a more effective use of resources
- Is **very relevant in the edge**, where power is a constraint





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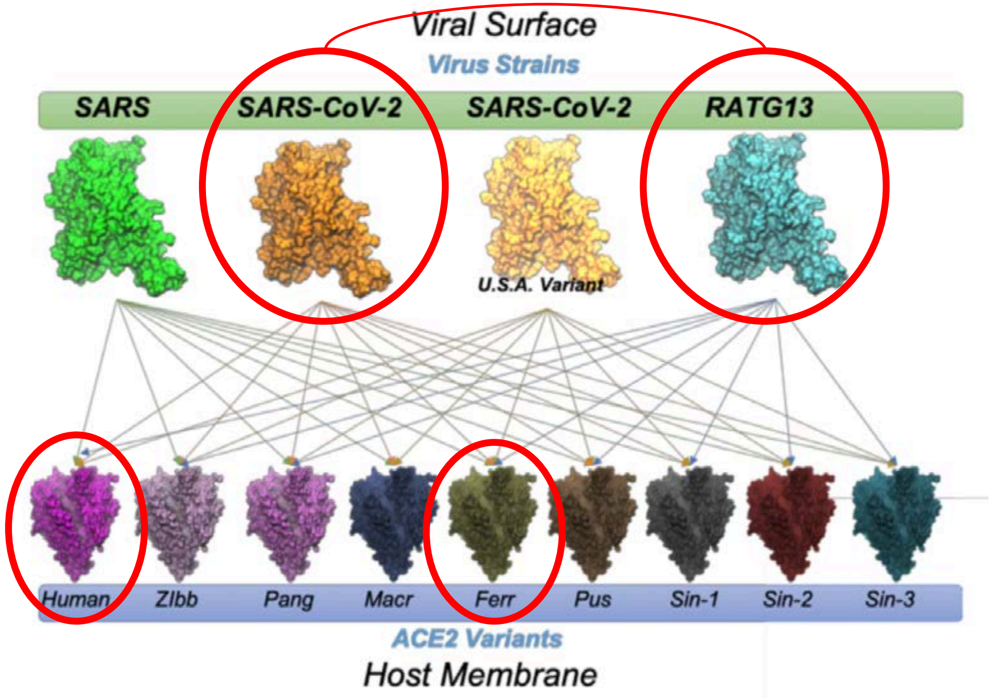
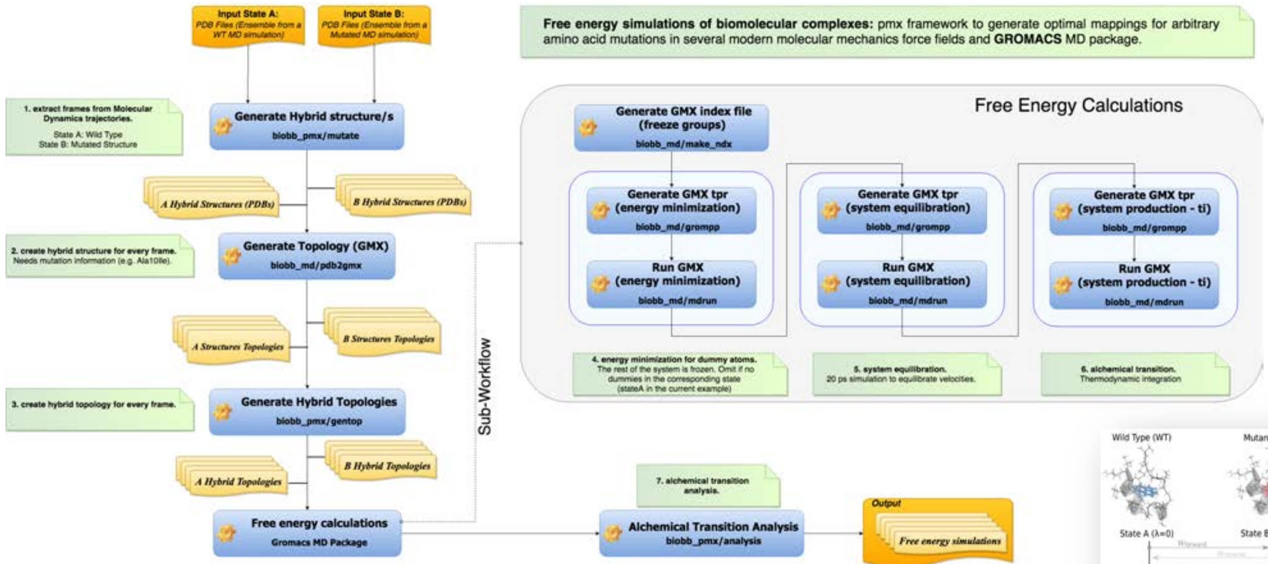
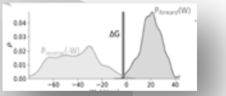
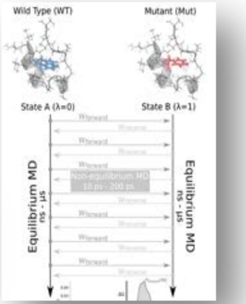
Pre-exascale workflows to explore COVID-19 Infectious Mechanisms and Host Selection Process





Impact of mutations in binding affinity





- **Fast-growth Thermodynamic Integration**
- **1000** independent **short MD simulations** (500 forward + 500 reverse)
- **GROMACS + pmx**
- **Extremely parallelizable**

GROMACS
FAST. FLEXIBLE. FREE.

pmx: generate hybrid protein structure and topology
Computational Biomolecular Dynamics Group

Molecular Dynamics simulation data

- For each mutation:
  - MD Simulations (RBD + ACE2 + Complex)
  - Free energy calculations

PRACE

Big Data Study:
PRACE computational power
Massive amount of data

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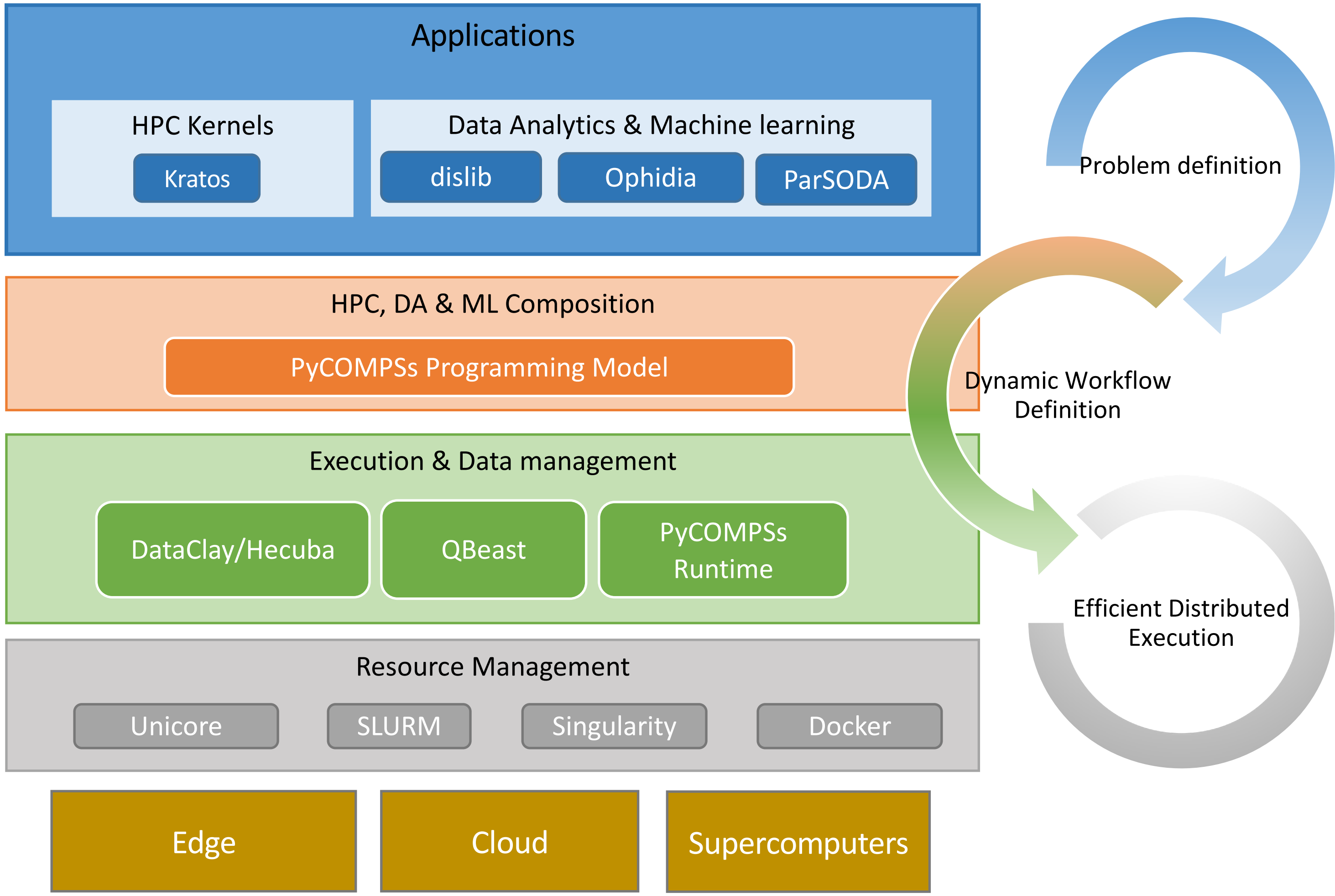
Conclusions

- PyCOMPSs 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 involved

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Center of Excellence for Computational Biomolecular Research

LAND SUPPORT

CLASS

ExaQUte
Exascale Quantification of Uncertainties for Technology and Science Simulation

ELASTIC

EXPERTISE

FUJITSU

Joint Laboratory for Extreme-Scale Computing
Inria NCSA Argonne BSC JÜLICH RIKEN

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- 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-ubuntu16/
- Applications

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

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

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Thank you

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