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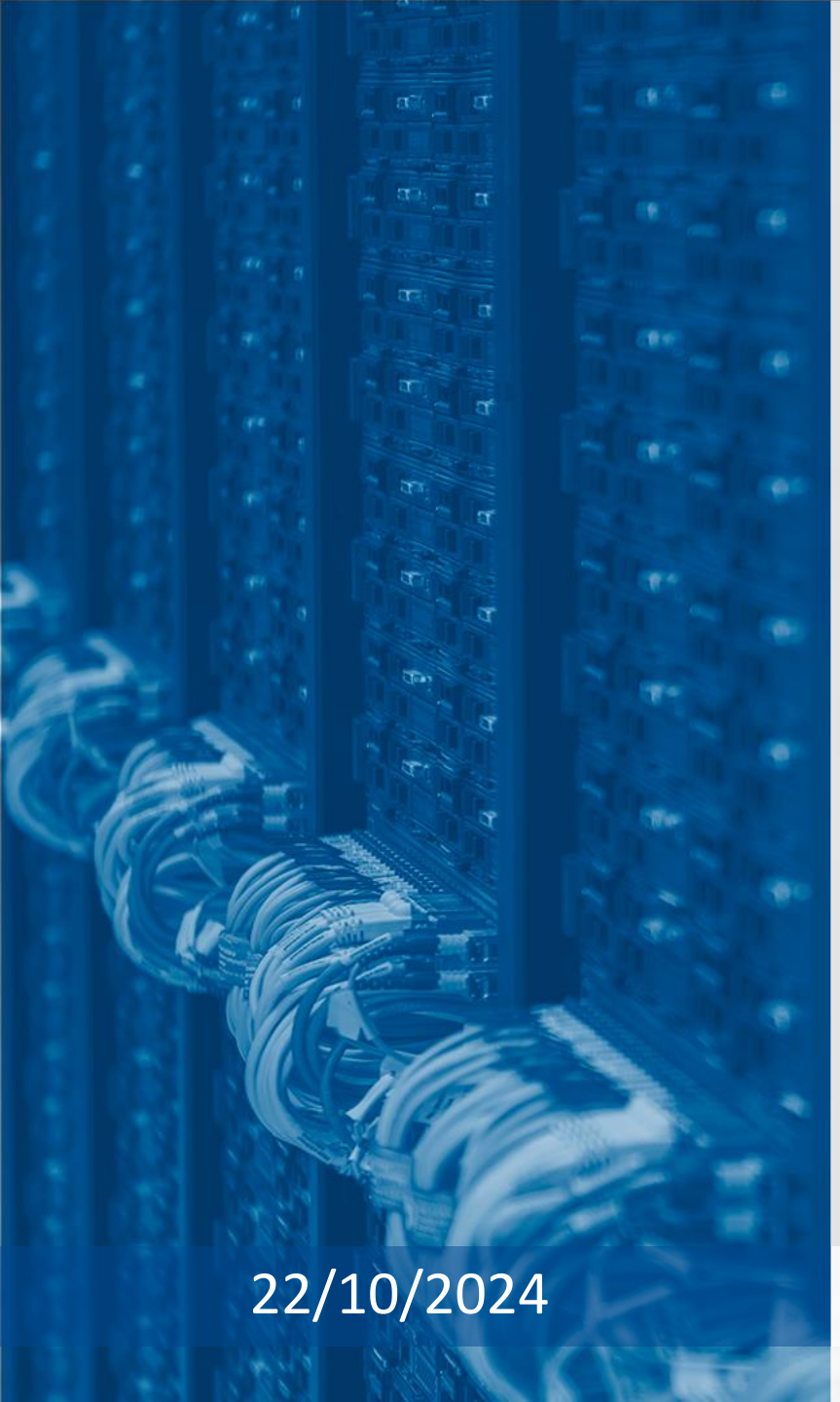

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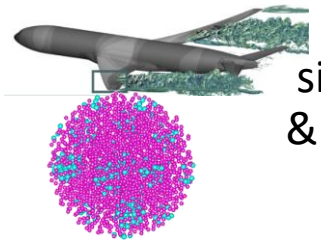
HPC+AI workflows at BSC

Rosa M Badia

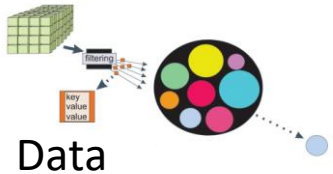
22/10/2024

86th HPC User Forum, Barcelona

Complex problems for complex computing infrastructures



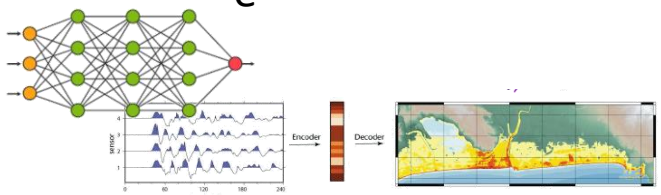
HPC simulation & modeling

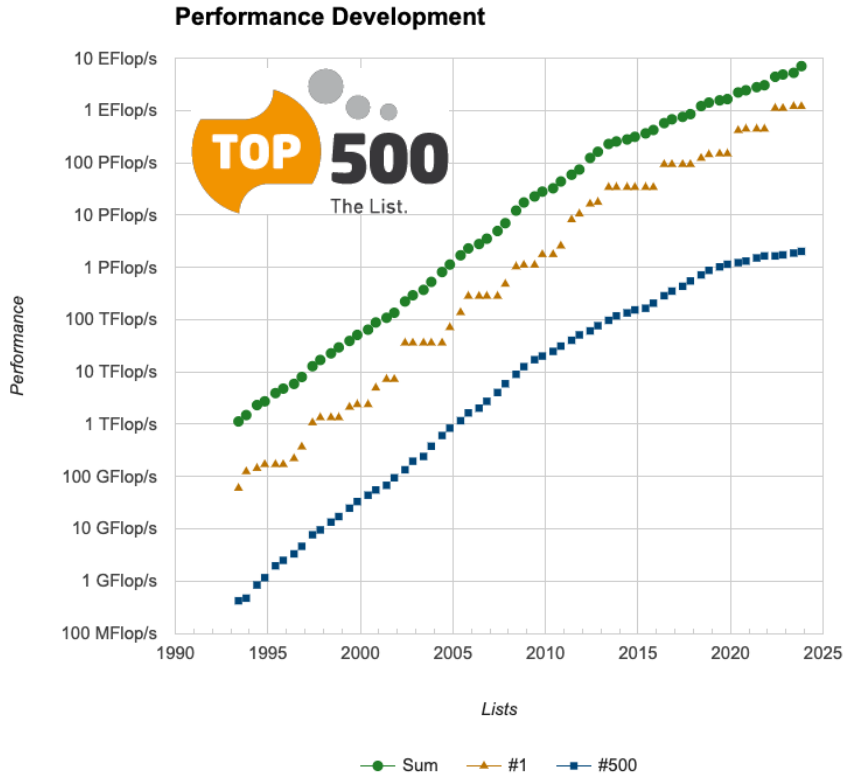


Data analytics

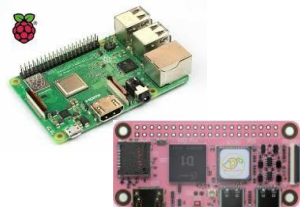
COMPLEX PROBLEMS

Artificial intelligence





Digital continuum



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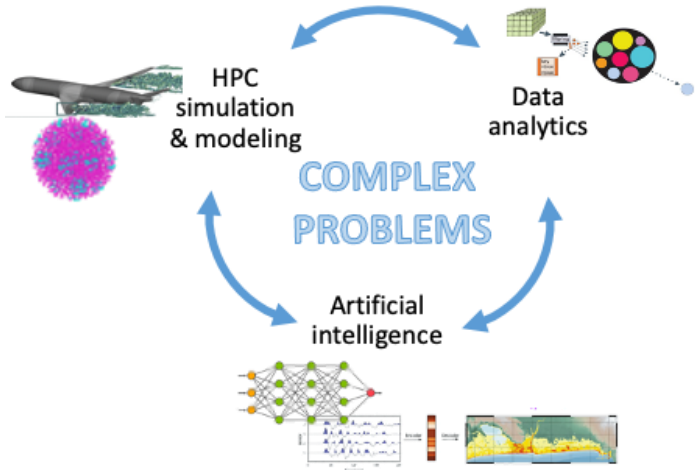
Workflow lifecyle challenges



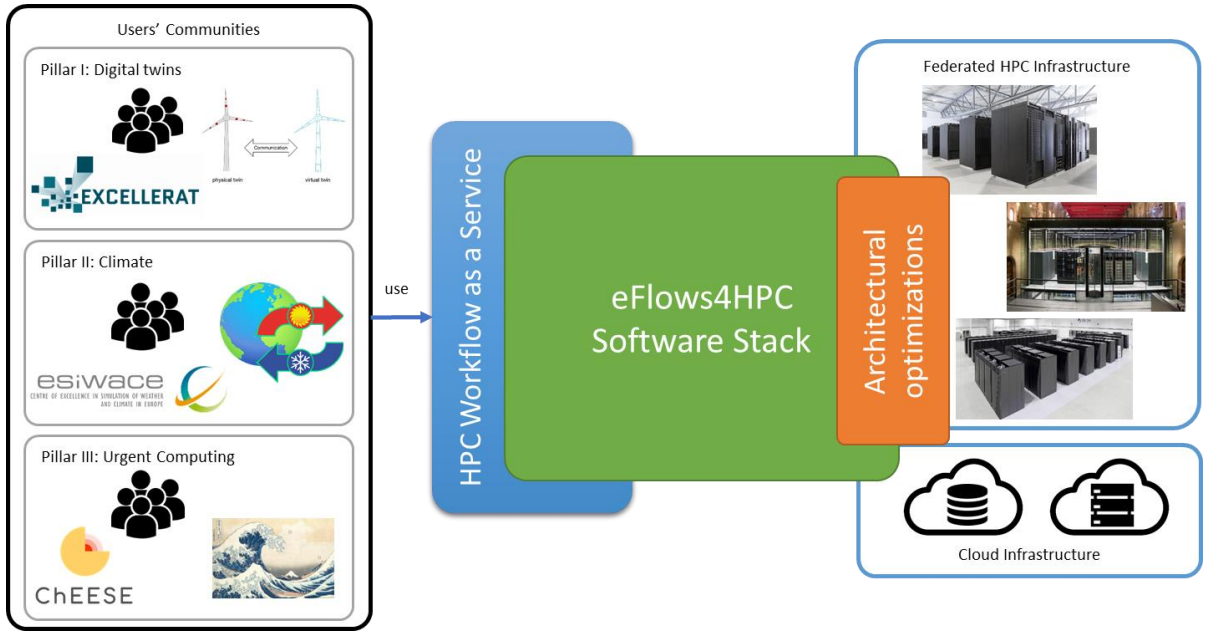
- Workflow development
  - Different programming models and environments
- Workflow deployment
  - Can we make it easier to new HPC users?
- Workflow operation
  - Go beyond static workflows
  - Not only computational aspects, data management as well

eFlows4HPC

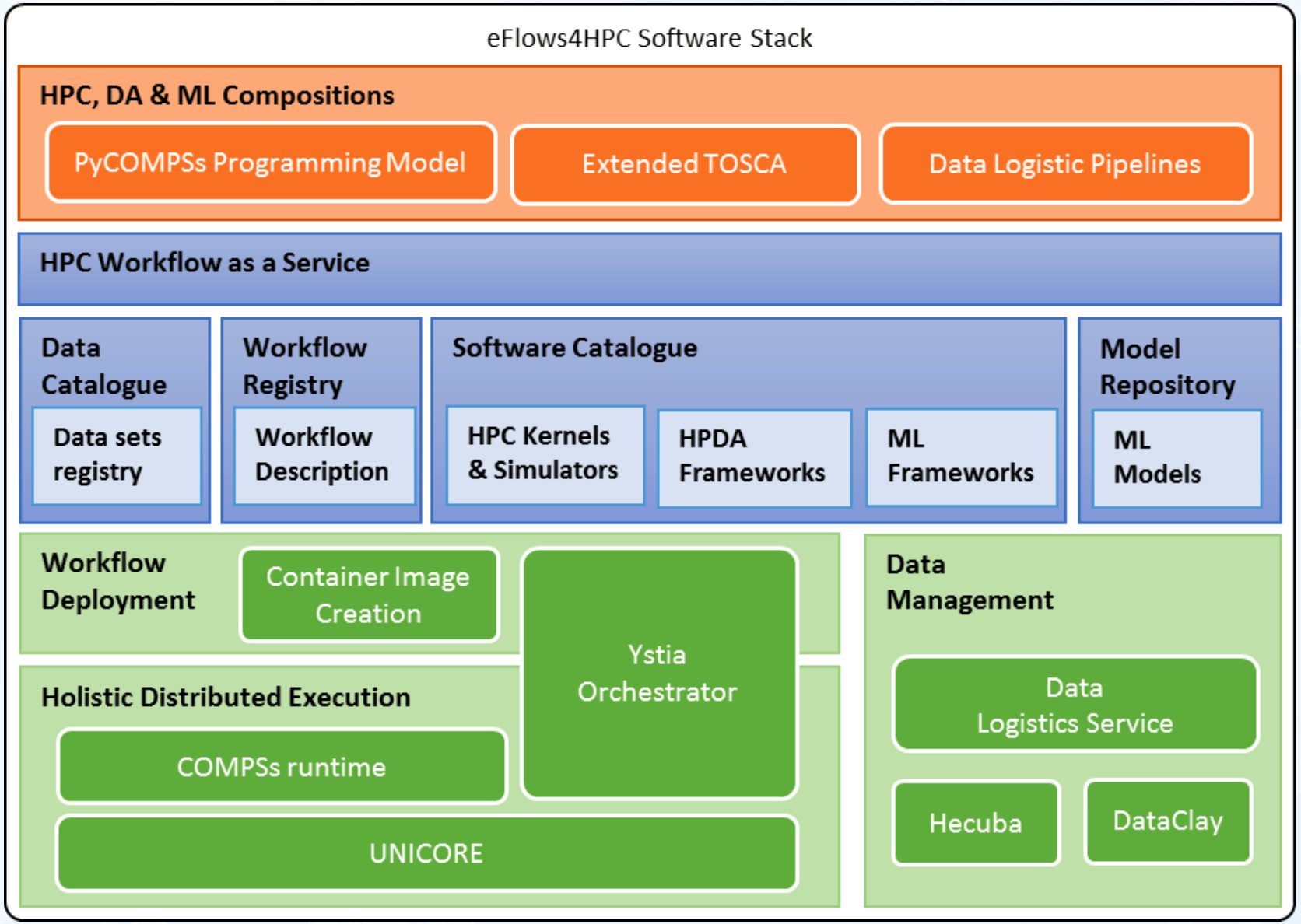
caelestis

eFlows4HPC in a nutshell

- Software tools stack that makes easier the development and management of complex workflows:
  - Combine different aspects
    - HPC, AI, data analytics
  - Reactive and dynamic workflows
    - Autonomous workflow steering
  - Full lifecycle management
    - Not just execution
    - Data logistics and Deployment
- HPC Workflows as a Service:
  - Mechanisms to make easier the use and reuse of HPC by wider communities
- Architectural Optimizations:
  - Selected HPC – AI Kernels Optimized for GPUs, FPGA, EPI
- Validation Pillar's
  - End-user workflows linked to CoEs

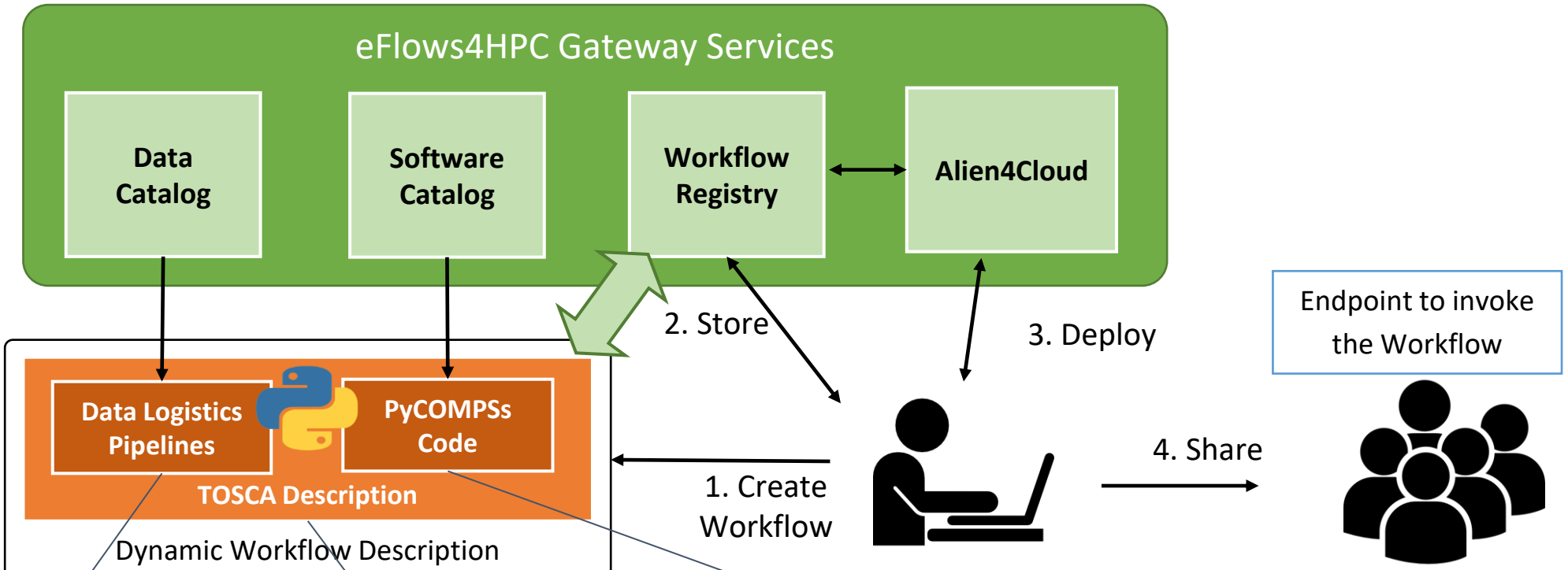


eFlows4HPC


eFlows4HPC Software Stack
HPC, DA & ML Compositions
PyCOMPSs Programming Model
Extended TOSCA
Data Logistic Pipelines
HPC Workflow as a Service
Data Catalogue
Data sets registry
Workflow Registry
Workflow Description
Software Catalogue
HPC Kernels & Simulators
HPDA Frameworks
ML Frameworks
Model Repository
ML Models
Workflow Deployment
Container Image Creation
Ystia Orchestrator
Holistic Distributed Execution
COMPSs runtime
UNICORE
Data Management
Data Logistics Service
Hecuba
DataClay


Dynamic Workflow Definition
Workflow Accessibility/ Re-usability
Efficient Distributed Execution

HPCWaaS: Workflow lifecycle overview



Description of data movements as Python functions. Input/output datasets described at Data Catalog

Computational Workflow as a simple Python script. Invocation of software described in the Software Catalog

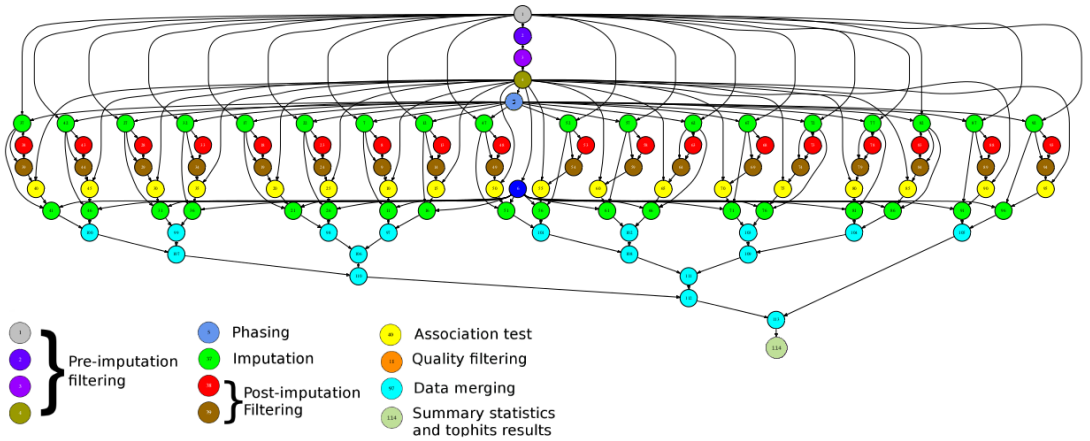
Topology of the components involved in the workflow lifecycle and their relationship.

3 levels of workflow: Computational, Data, Top-level

Computational Workflows in PyCOMPSs

- Sequential programming, parallel execution
  - General purpose programming language + annotations/hints
- Task-based parallelization
  - Automatic generation of task graph
  - Coarse grain tasks: methods and web services
  - Sequential and parallel tasks
- Offers a shared memory vision in a distributed system
  - Can address larger dataset than storage space
- Agnostic of computing platform
  - Clusters, clouds and containers cluster
- Based in Python

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



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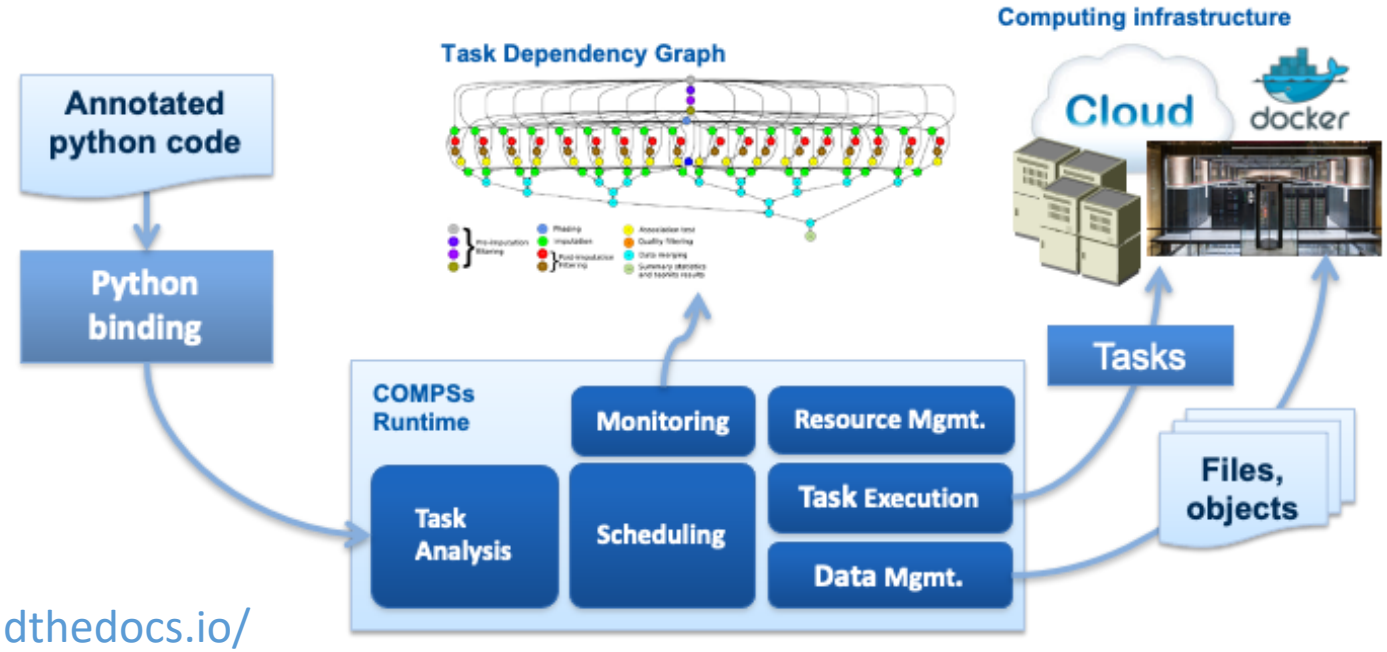
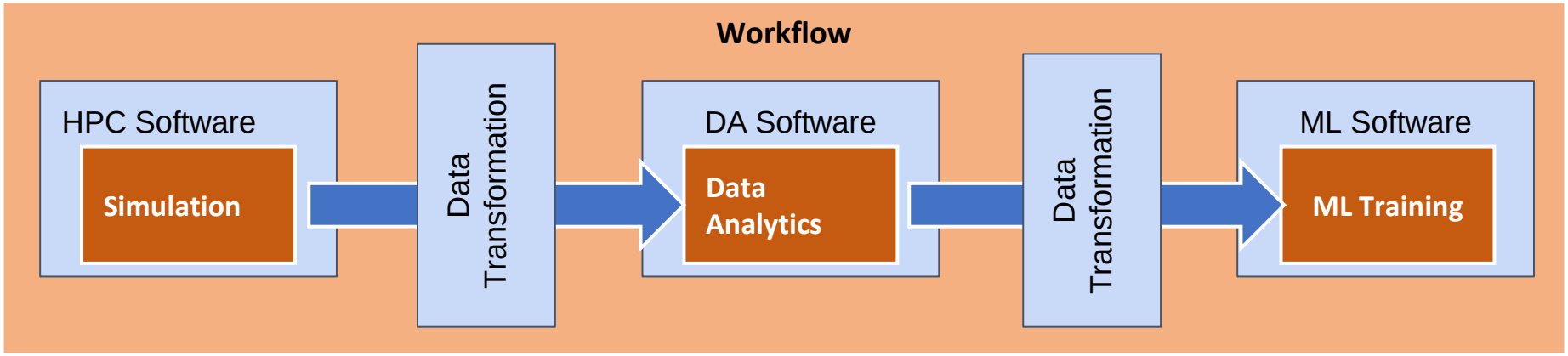
PyCOMPSs features and runtime

- Support for tasks' constraints – support for heterogeneous infrastructure
- Support for tasks' faults and tasks' exceptions
  - Enlarges the dynamicity of the type of workflows that we support
- Streamed data
  - ... and many others*
- PyCOMPSs applications deployed as a distributed master-worker
  - Executed in an allocation of an HPC system
- All data scheduling decisions and data transfers by the runtime
- Support for horizontal elasticity



*https://compss-doc.readthedocs.io/

Interfaces to integrate HPC/DA/ML



- Goal:
  - Reduce the required glue code to invoke multiple complex software steps
  - Developer can focus in the functionality, not in the integration
  - Enables reusability
- Two paradigms:
  - Software invocation
  - Data transformations

workflow steps defined as tasks

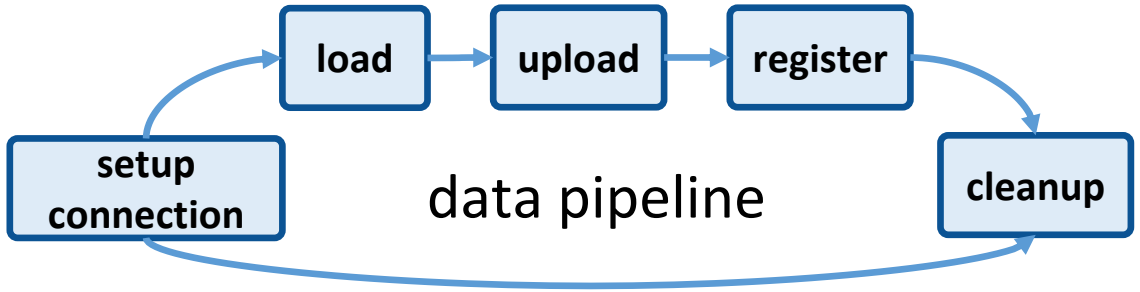
workflow body

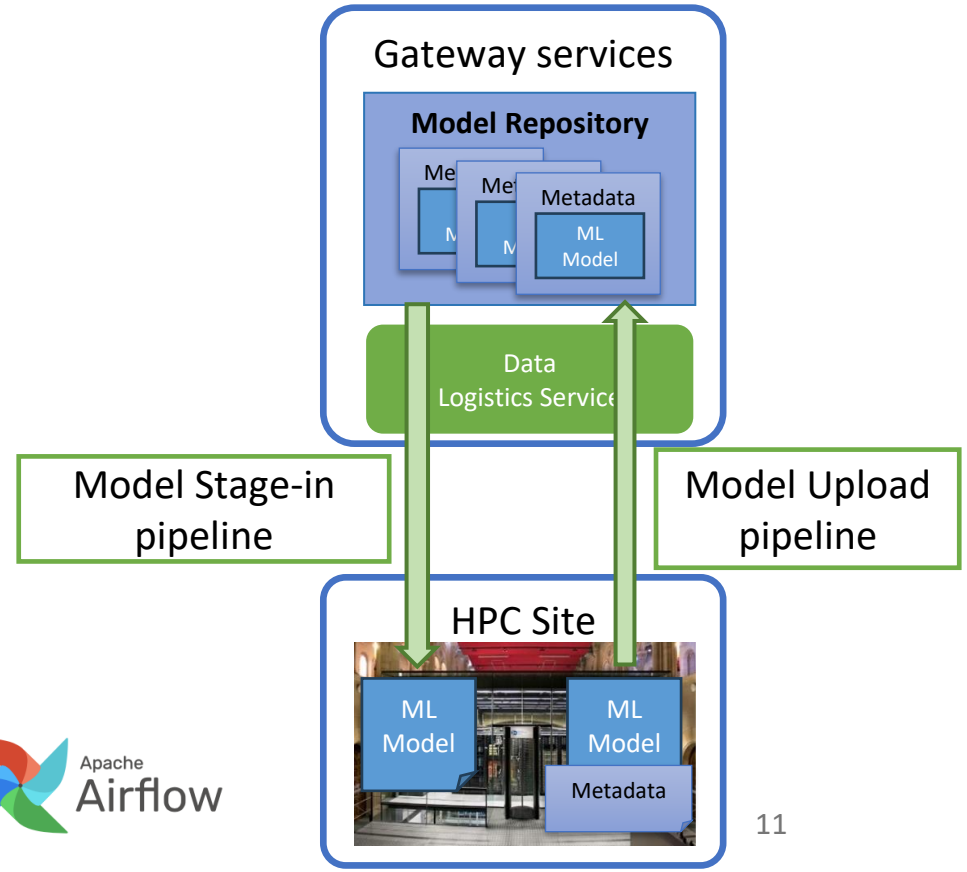
```
@data_transformation (input_data, transformation description)
@software (invocation description)
def data_analytics (input_data, result):
    pass

simulation (input_cfg, sim_out)
data_analytics (sim_out, analysis_result)
ml_training (analysis_result, ml_model)
```

Data workflows

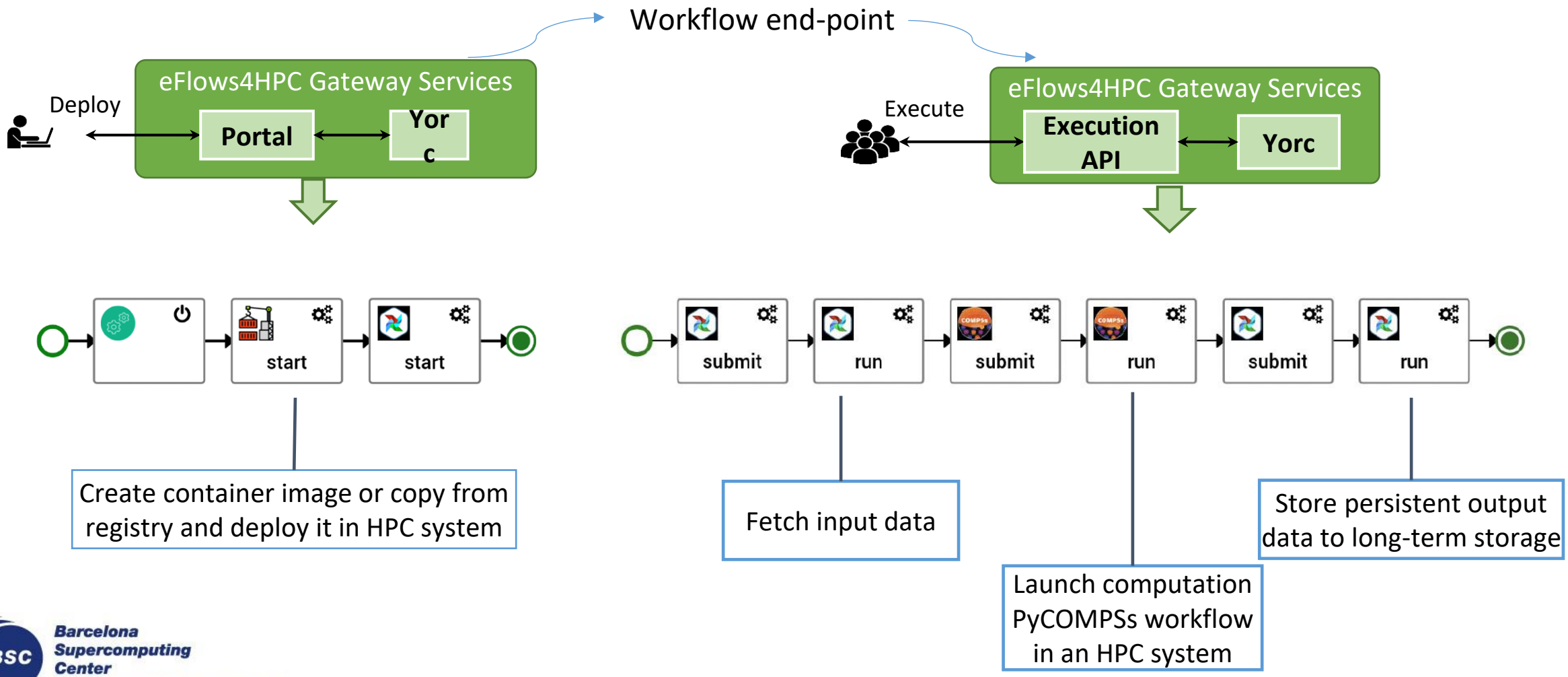
- Support to data movements from/to HPC system
- Use of data pipelines to specify and formalize them
  - Transparency and reusability
- Data catalogue
  - Lists datasets and provides metadata
  - Suppot to FAIR
- Data Logisitcs Service
  - Stage-in/out
  - **Container image transfer**
  - **AI trained models**





Top-level workflows

- Overall orchestration: Deployment and execution top-level workflows



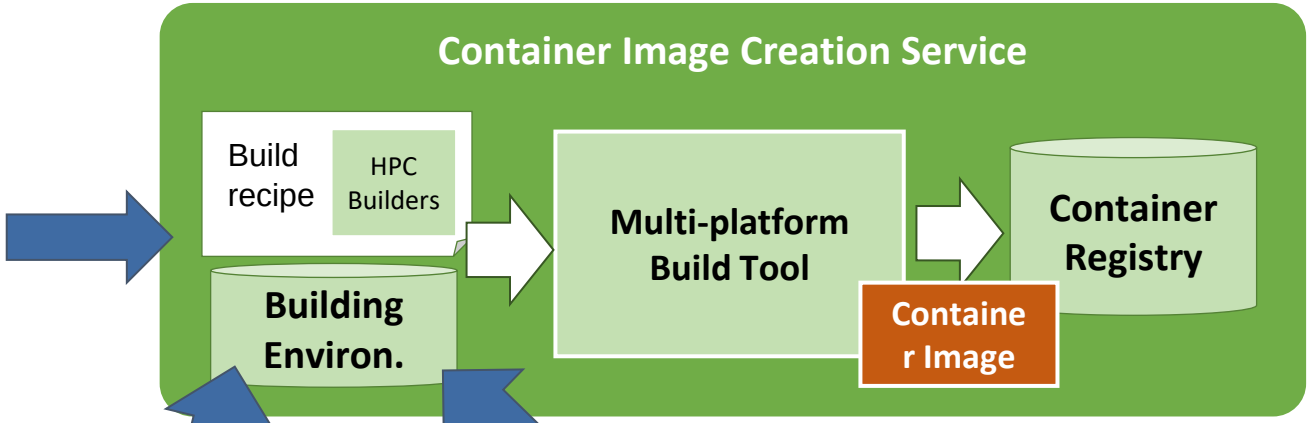
HPC Ready Containers

eFlows4HPC

Workflow step + target system

```
{
    "machine": {
        "platform": "linux/ppc64le",
        "architecture": "power9le",
        "container_engine":
    ↪ "singularity",
        "mpi": "openmpi@4",
        "gpu": "cuda@10.2"
        },
    "workflow": "pillar_III",
    "step_id": "ftrt"
}
```

Service request




```
spack:
    packages:
        all:
            compiler: [ gcc@8 ]
    specs:
        - t-hysea
        - t-hysea-lb
        - compss@eflows4hpc
```

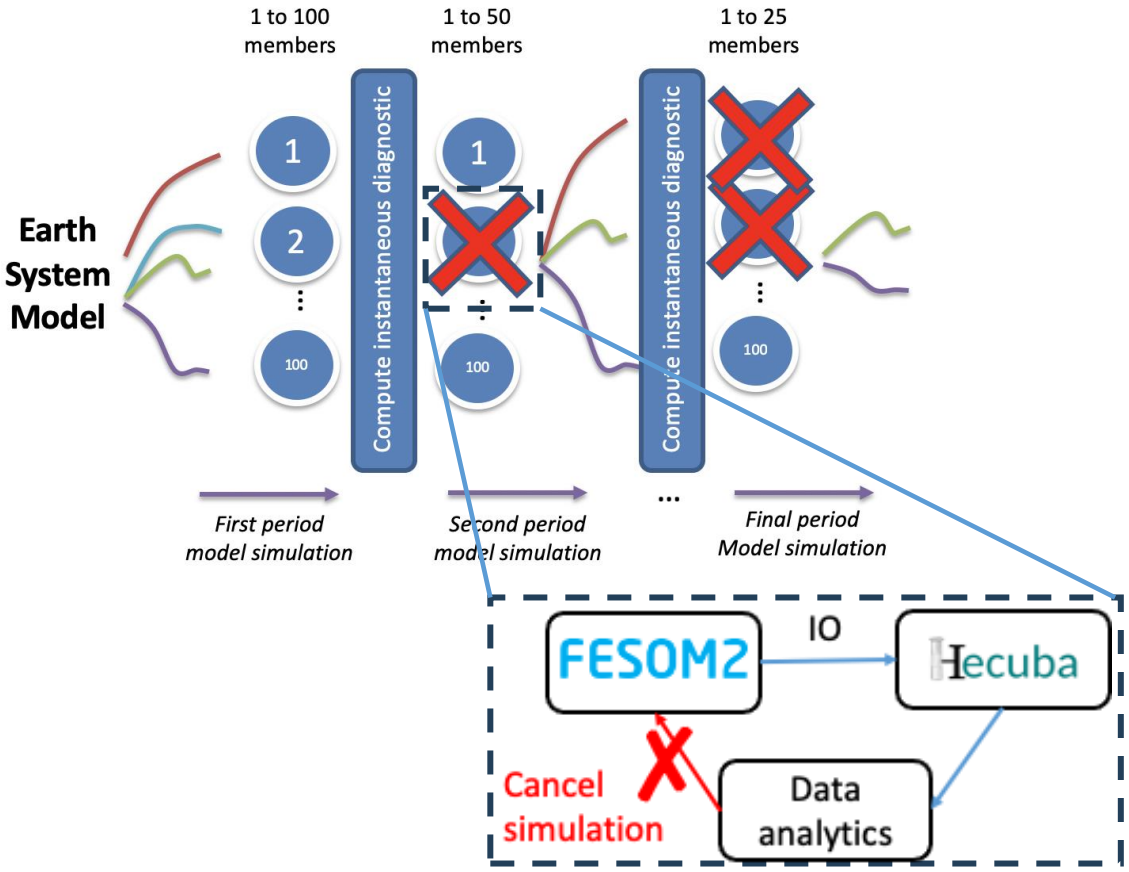
spack.yml

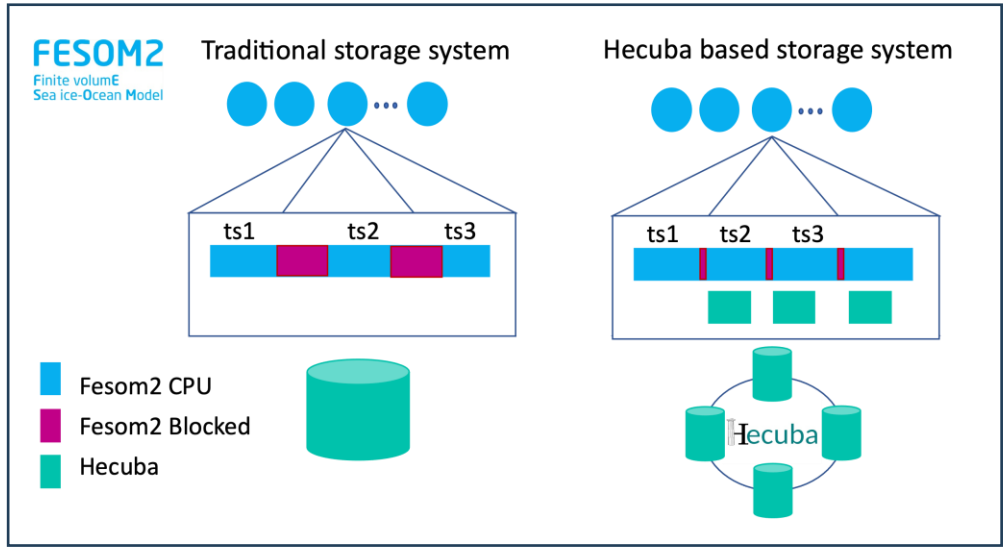
package.py

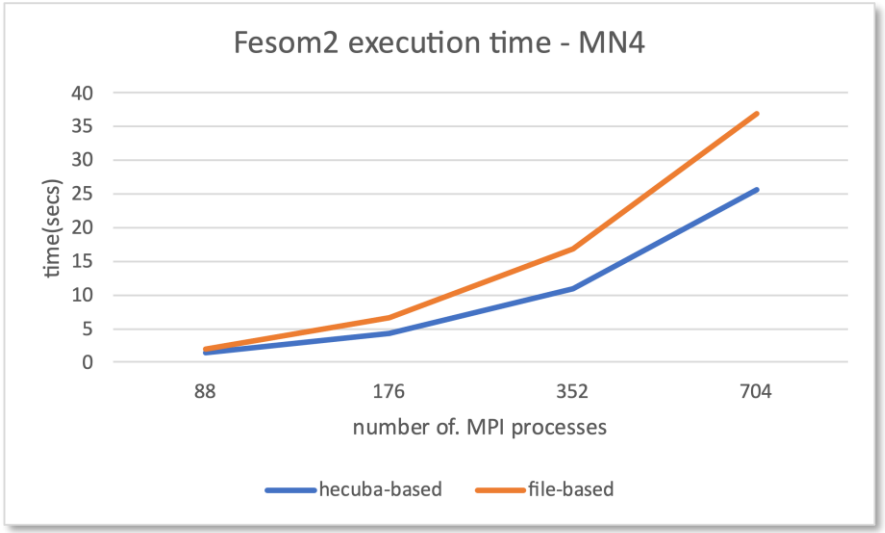
Up to 2X performace with respect standard container images!

DA-driven ensemble member pruning

Earth-System Model (ESM) workflow





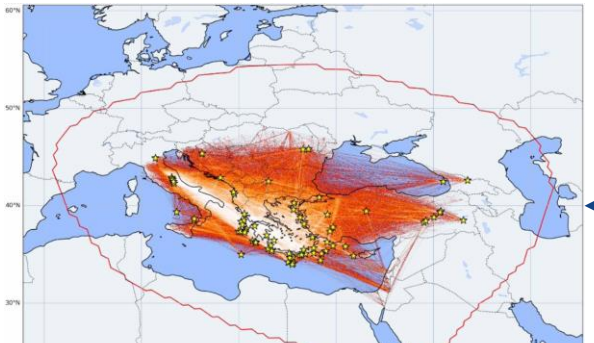


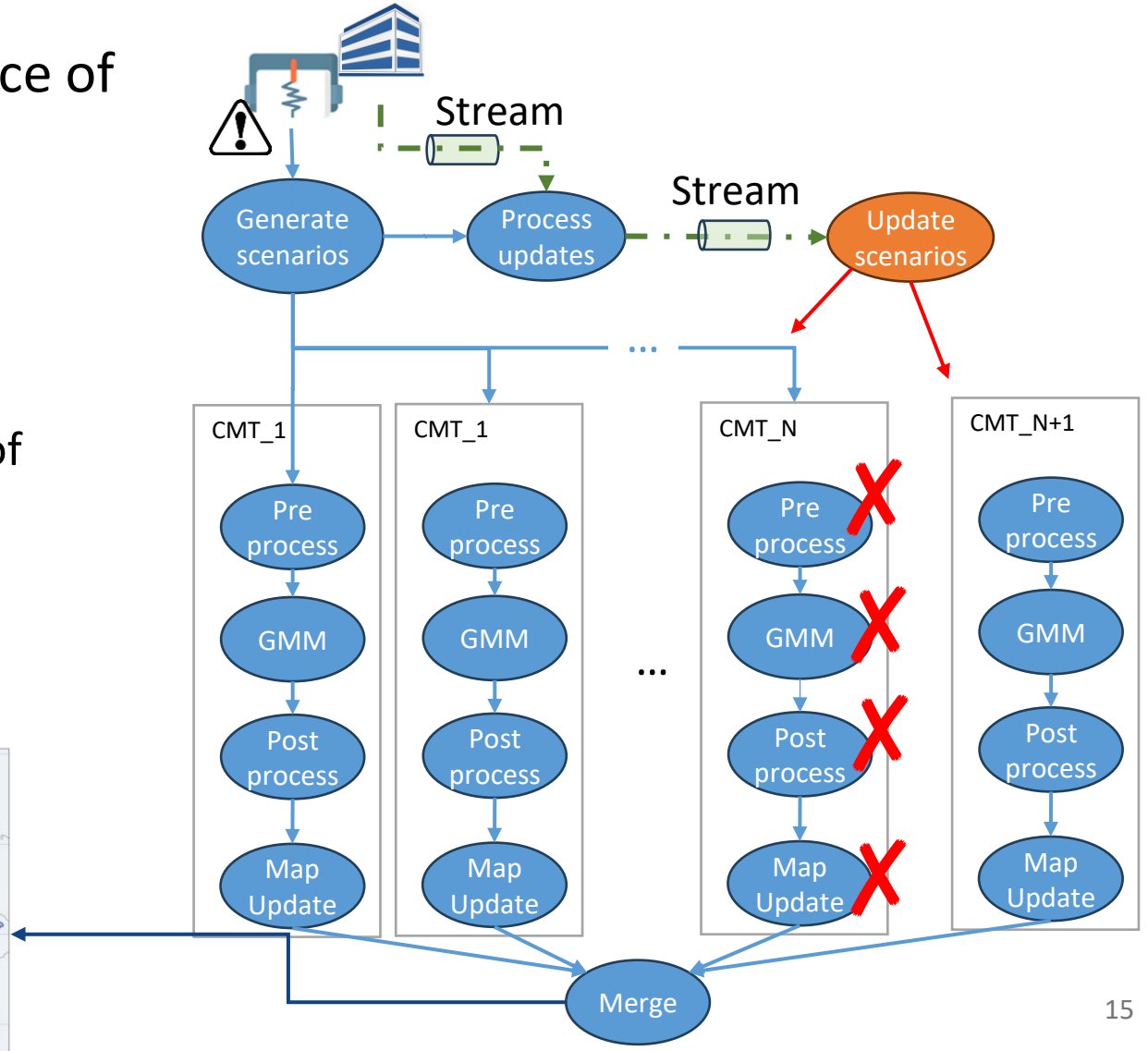
Hecuba support for a lambda architecture, allowing both batch processing and stream processing

Event-driven cancellation/creation

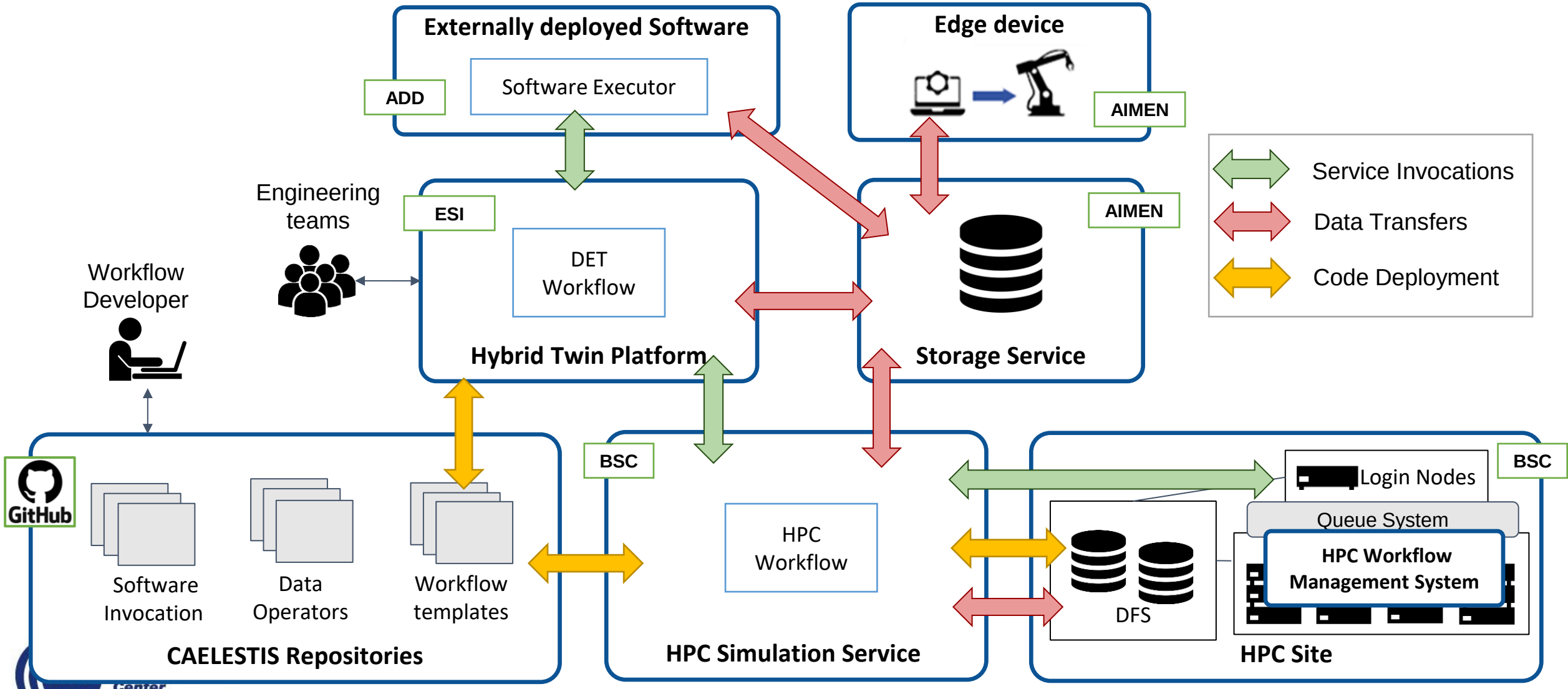
UCIS4EQ: HPC-based urgent seismic simulation workflow

- Evaluation of scenarios after the occurrence of a seismic event
- Combines multiple web services and HPC simulation (Salvus)
- Workflow Dynamicity:
  - Usage of **data streaming** for communication of events
  - On event occurrence API supports:
    - **Dynamic cancellation** of task groups
    - **Dynamic creation** of new set of tasks

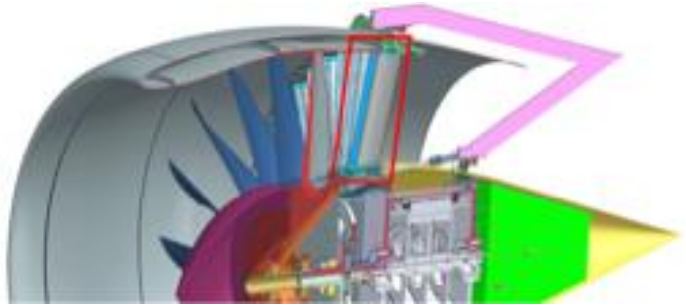




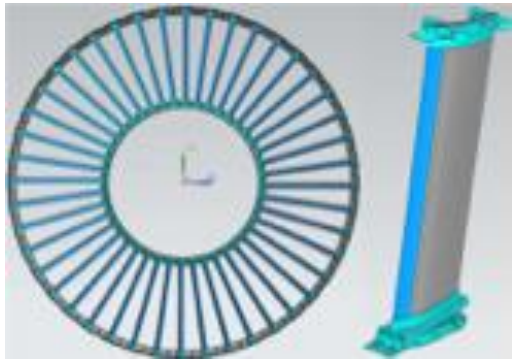
CAELESTIS Simulation Ecosystem Architecture



Use case: Outlet Guide Vane (OGV)



- Selected use case for real-world scenario (GKN)
- Manufacturing processes in composites:
  - Automated Fiber Placement (AFP)
  - Resin Transfer Moulding (RTM)
- Focus on manufacturing and mechanical test procedures
  - Manufacturing tests will assess process-induced defects: can impact the final mechanical properties of the components
    - Fibre misalignment
    - Tape overlaps and gaps
    - Void formation during RTM,
  - Mechanical tests will evaluate critical performance metrics
    - Tensile strength, stiffness, and fatigue resistance
    - To ensure that the simulated outcomes accurately reflect real-world performance
- Each of them implemented with workflows



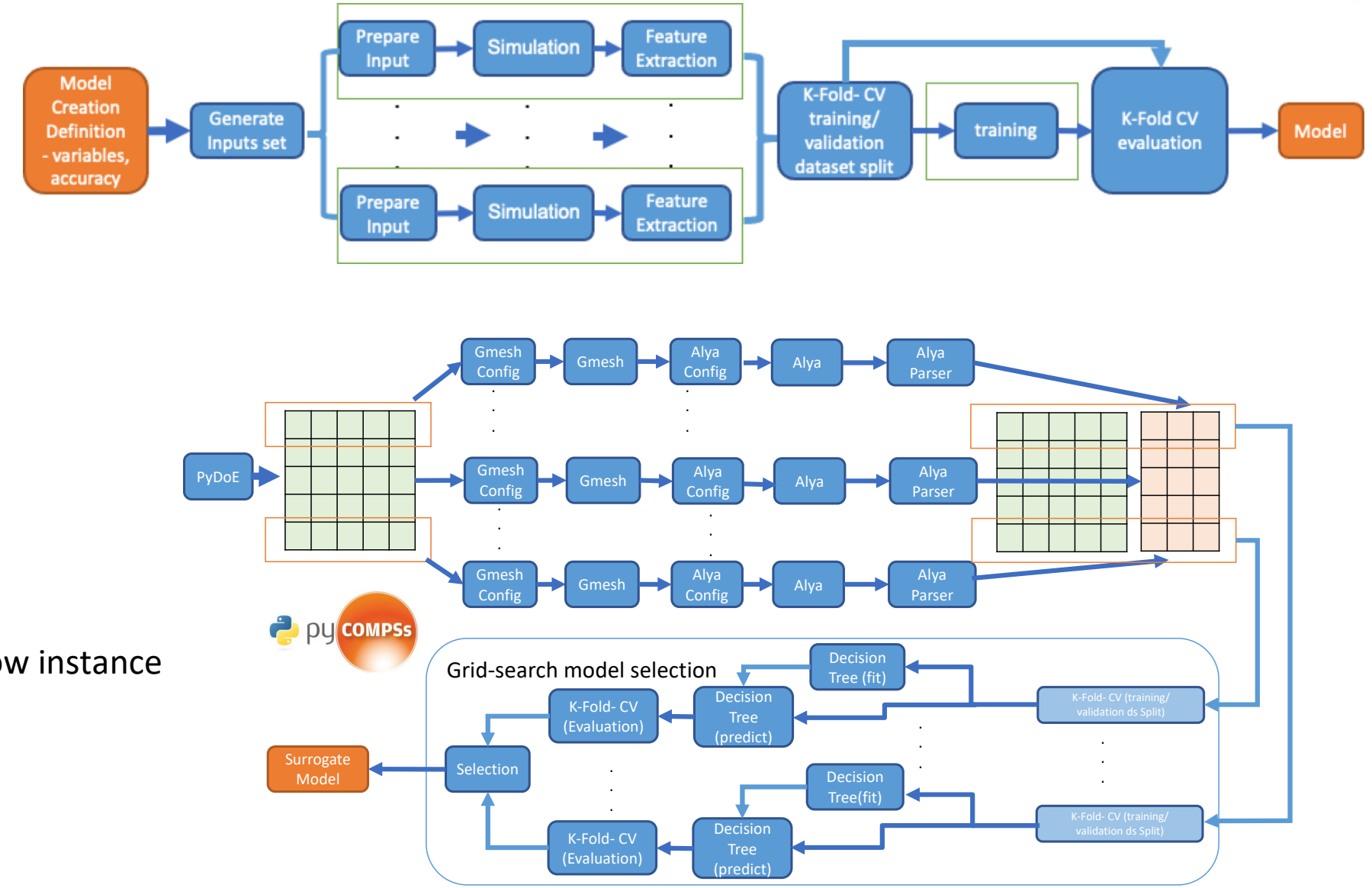
From workflow templates to instances

caelestis

Workflow template

Configuration

Workflow instance



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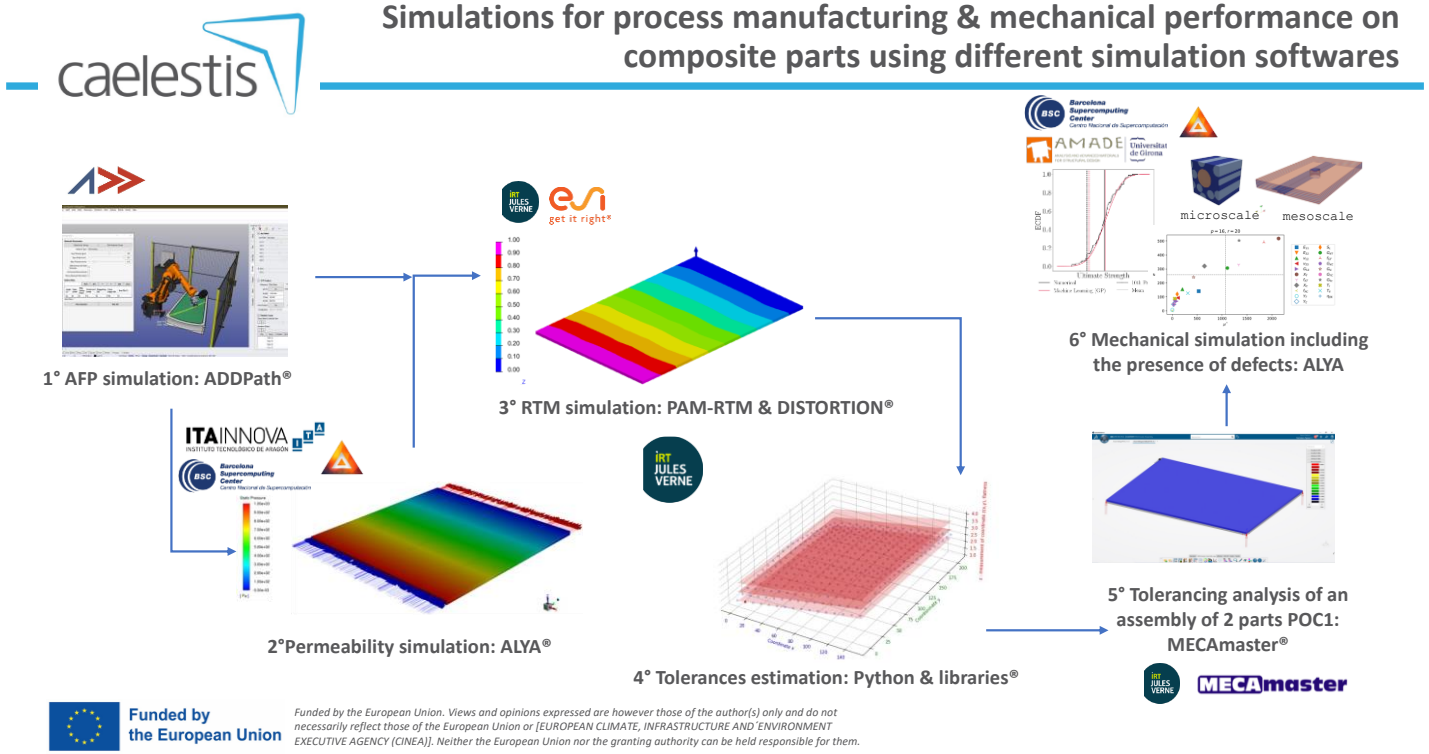
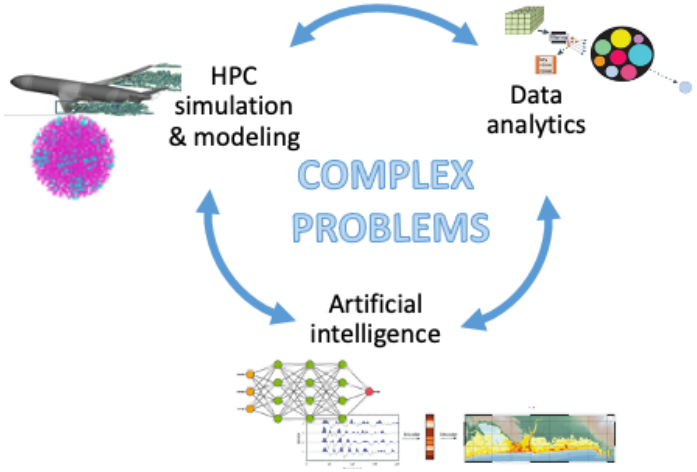
Workflow executions

- HPC simulation campaign for product and process optimization
- Multiple workflows execution
  - RTM simulation
  - Permeability simulation
  - Mechanical simulation
  - …
- Spanish RES allocation
  BSC MareNostrum 4 and MareNostrum 5
- Orchestrated with **PyCOMPSs** and involving **BSC Alya** simulations
- More than 50000 simulacions, 4.6 million CPU hours



Final thoughts and future work



- Workflows that compose HPC, AI and Data analytics steps are very useful to solve science and technology challenges
- Methodologies proposed in projects such as eFlows4HPC and CAELESTIS help on the goal of implementing, deploying and executing such workflows
- Evolution towards Digital twins!
  - Are appearing everywhere!
  - New category of applications that evolve from HPC+AI+DA workflows
  - Beyond the model, interaction between the digital twin and the physical object
  - There is a need for methodologies to avoid adhoc solutions and reinventing the wheel in each application

Further Information

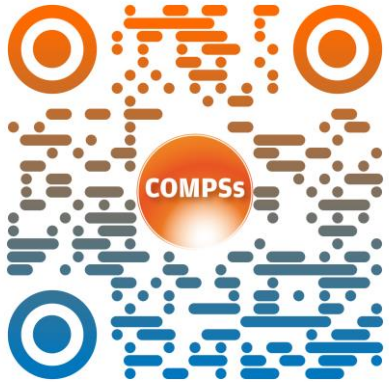
- Project page: http://www.bsc.es/compss
  - Documentation
  - Virtual Appliance for testing & sample applications
  - Tutorials
- Source Code

  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
- Dislib
  - https://dislib.readthedocs.io/en/latest/



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ACKs

HP2C-DT

CAELESTIS

MareNostrum 5

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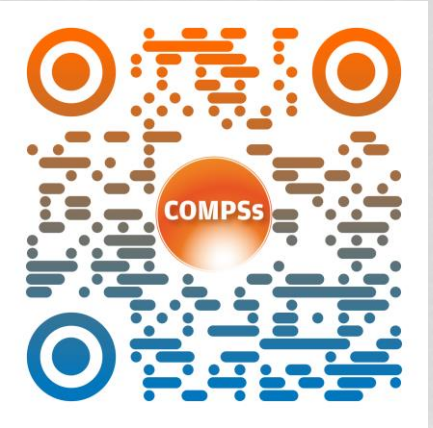
Thanks!



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