Can Python do for HPC what it did for machine learning?
PyCOMPSs support to HPC + AI workflows

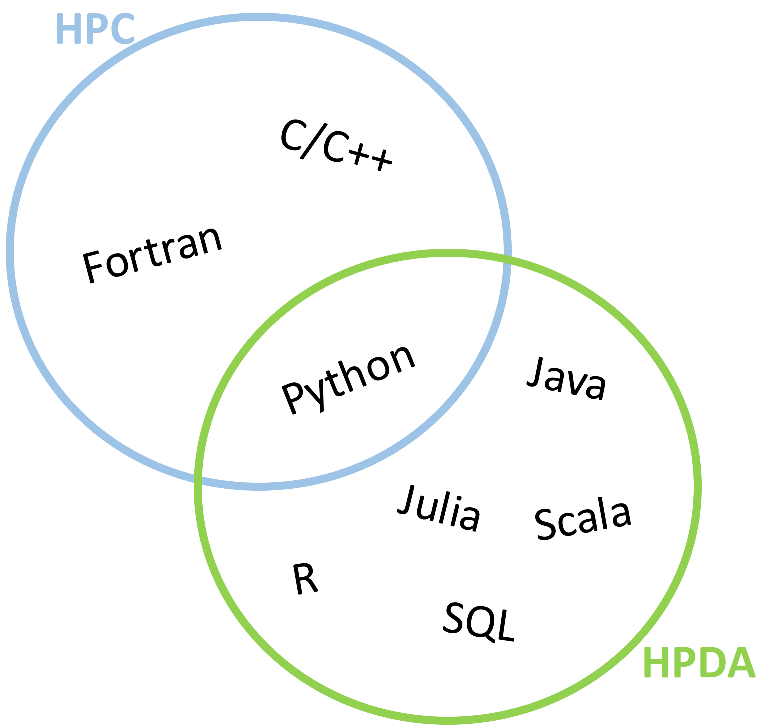
Rosa M Badia, Barcelona Supercomputing Center

SC24
Atlanta, GA | hpc creates.

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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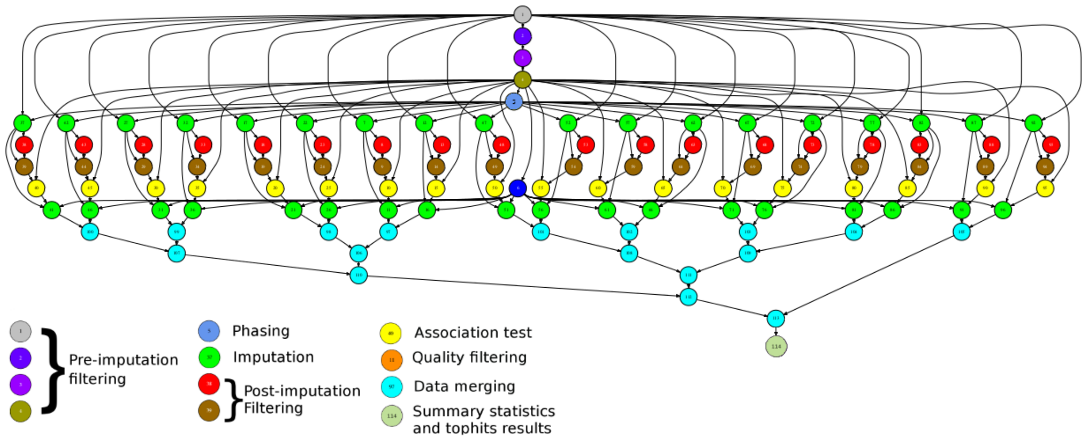
* From python.org

Computational Workflows in PyCOMPSs

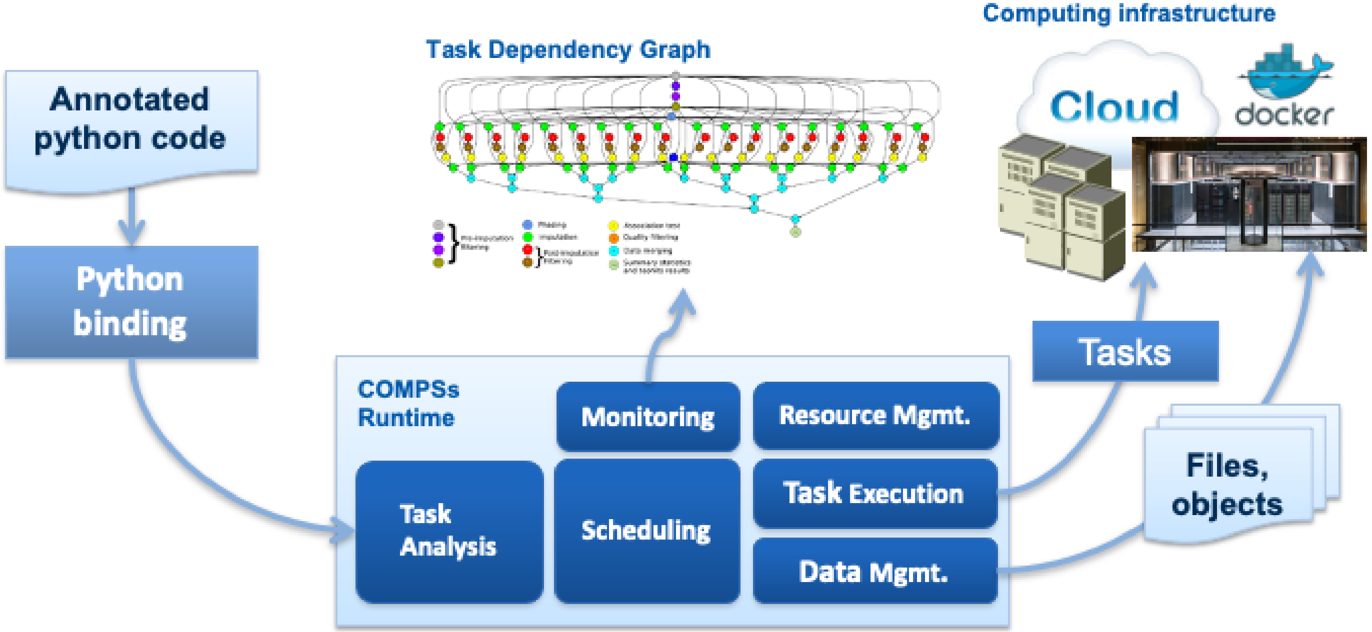
- Sequential programming, parallel execution
  - General purpose programming language + annotations/hints
- Task-based parallelization
  - Automatic generation of task graph
  - Coarse grain tasks: methods and web services
  - Sequential and parallel tasks
- Offers a shared memory vision in a distributed 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
```



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/

Support for MPI and MPMD tasks

- Resource manager aware of multi-node tasks

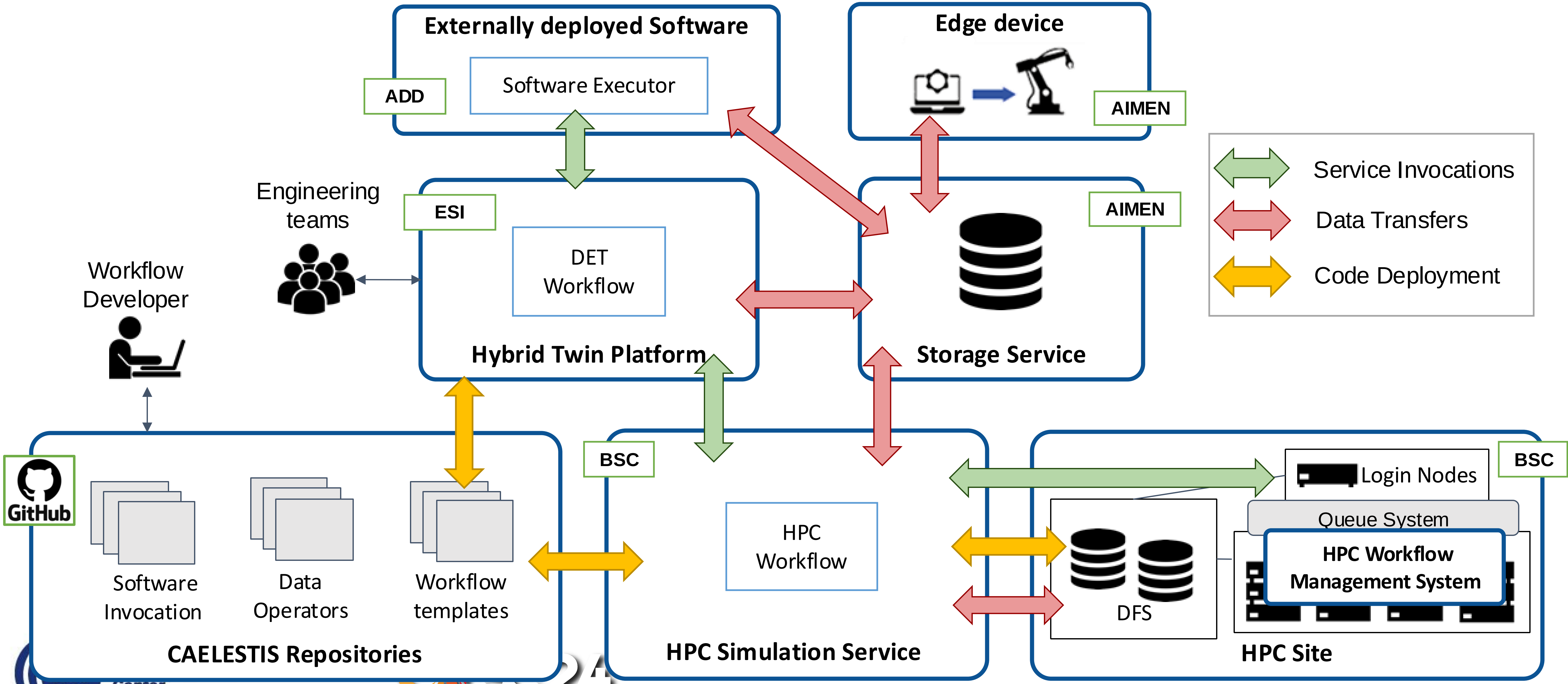
```
@mpi (binary="mySimulator", runner="mpirun", processes= "32", processes_per_node=8)
@task (returns=int, stdOutFile=FILE_OUT_STDOUT, stdErrFile=FILE_OUT_STDERR)
def nems(stdOutFile, stdErrFile):
    pass
```

Launches MPI execution with
32 processes
8 processes per node

```
@mpmd_mpi(runner="mpirun", working_dir = {{working_dir_exe}},
          programs=[{binary="fesom.x", processes = "$FESOM_PROCS" },
                    {binary="oifs", args="-v ecmwf -e awi3", processes = "$OIFS_PROCS" },
                    {binary="rnfma", processes = "$RNFMA_PROCS"}])
@task(log_file={Type:FILE_OUT, StdIOStream:STDOUT}, working_dir_exe=DIRECTORY_INOUT)
def esm_simulation(log_file, working_dir_exe):
   pass
```

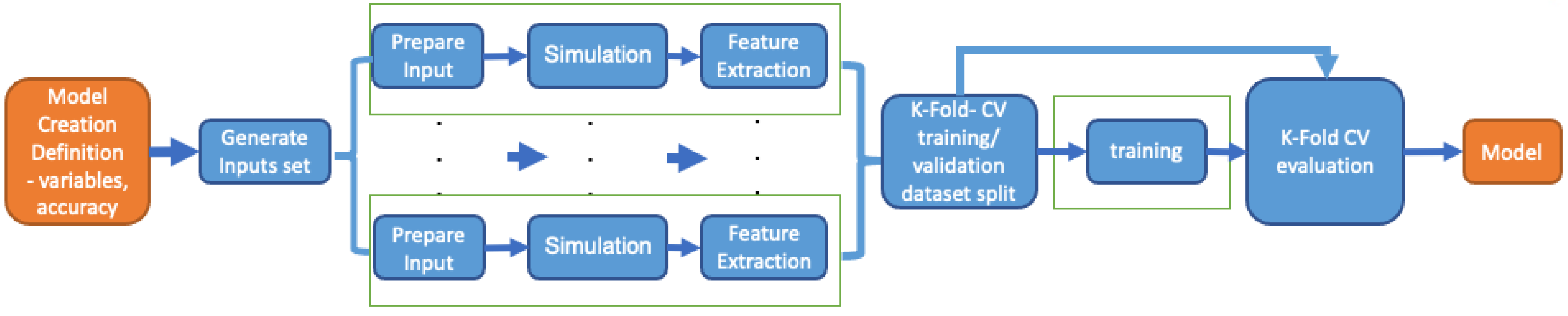
Launches coupled MPI
execution of FESOM, OpenIFS
and RNFMAP

CAELESTIS Simulation Ecosystem Architecture



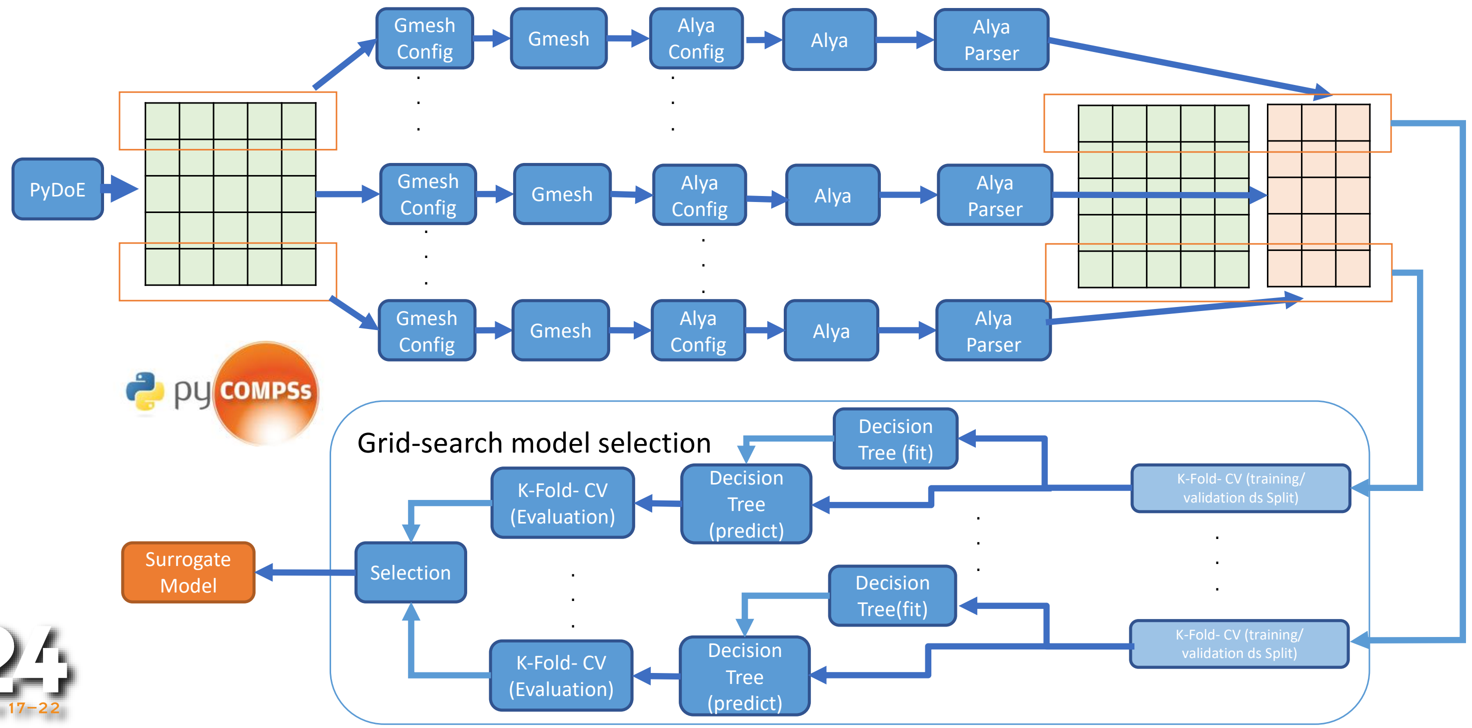
From workflow templates to instances

Workflow template

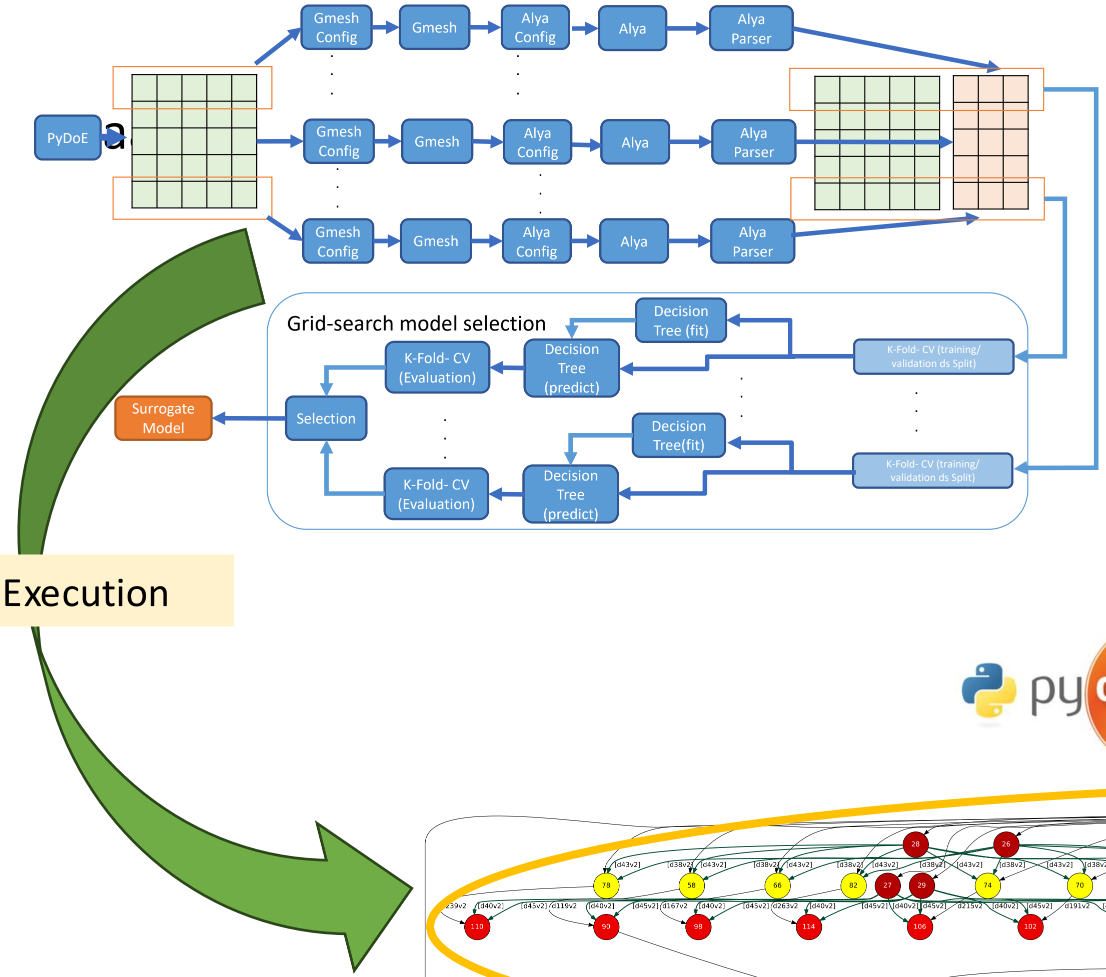


Configuration

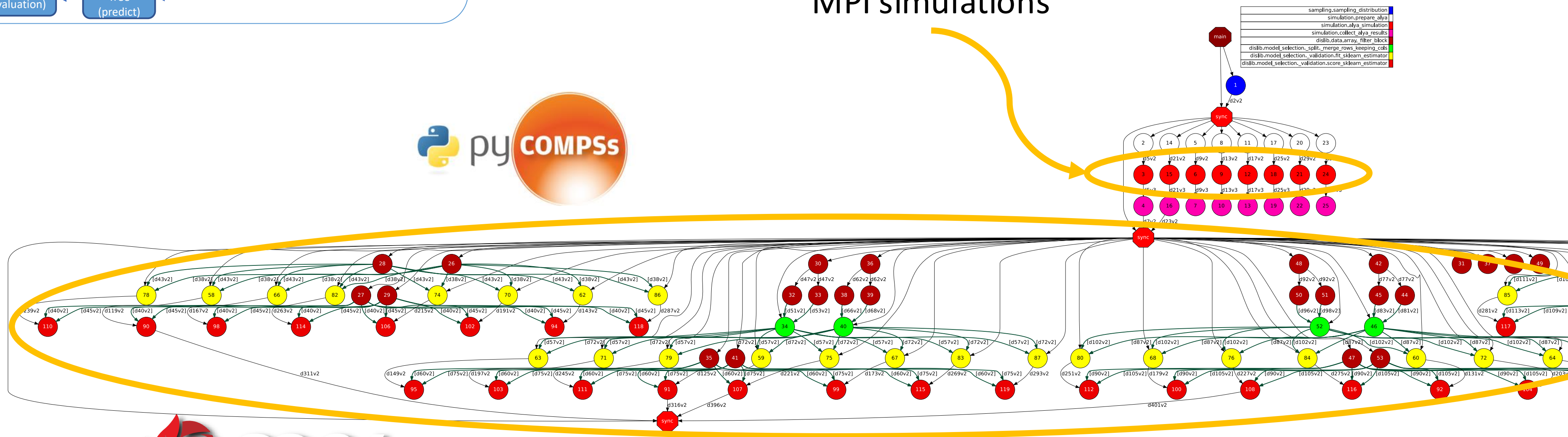
Workflow instance



From workflow templates to instances

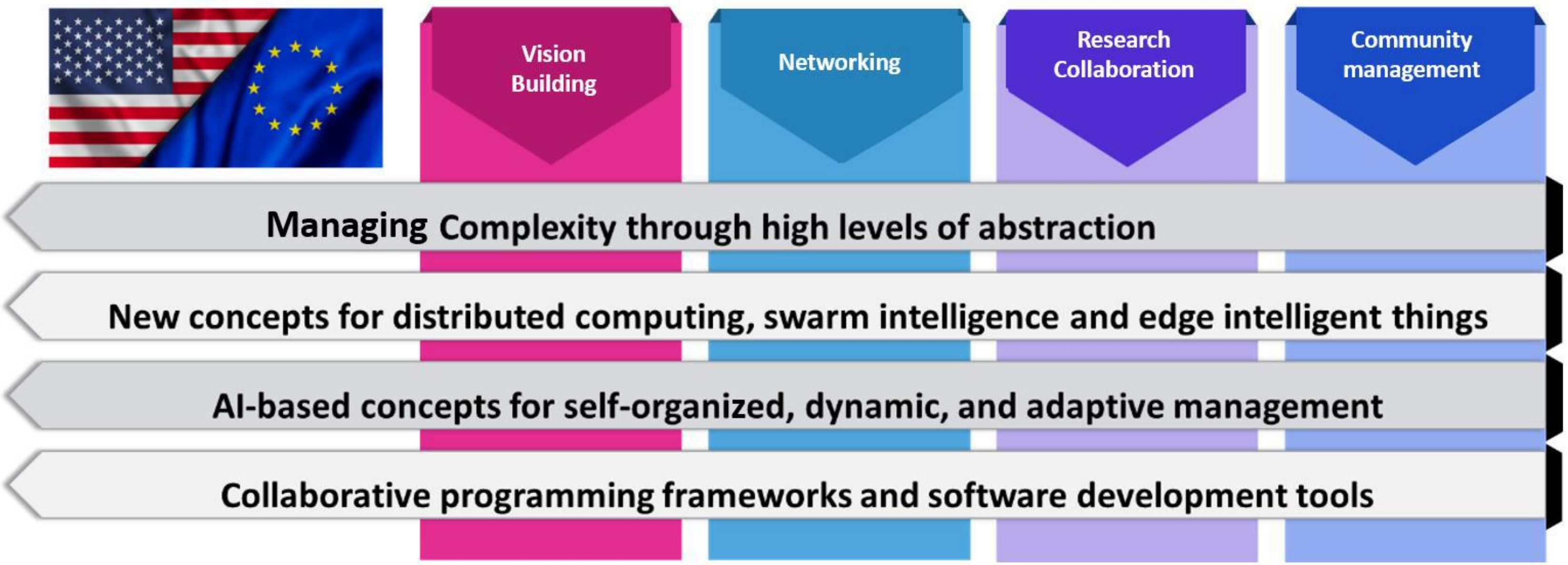


Execution



DISCOVER US

- Strengthen long-term collaboration between the EU and the US on new concepts and visions for the computing continuum, distributed computing and swarm intelligence.
  - By creating networking and collaboration opportunities to promote cooperation
- Organization of networking events, exchange and fellowship programs, training
- 66 members from 18 countries
- First call for exchanges already closed
  - 23 submissions
- Next calls in April 2025 and October 2025



Key research topics

Project duration: 30 months
Involve 100 senior researchers funding 20 pre-competitive transatlantic research collaborations.

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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/

ACKs

eFlows4HPC

DT-GEO

CEEC

Colmena

HP2C-DT

CyclOps

DISCOVER US

CAELESTIS

ICOS

Joint Laboratory for Extreme-Scale Computing

Inria NCSA Argonne BSC JÜLICH RIKEN

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Generalitat de Catalunya
Departament de Recerca i Universitats

MINISTERIO DE CIENCIA E INNOVACIÓN

Financiado por la Unión Europea NextGenerationEU

Plan de Recuperación, Transformación y Resiliencia

AGENCIA ESTATAL DE INVESTIGACIÓN

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Thanks!

rosa.m.badia@bsc.es

- The Edge nodes interface with real-world elements in the power grid (Devices)
- A Device can be a Sensor, an Actuator, or both.
- Sensors make measurements available to the Digital Twin and can trigger functions.
- Actuators allow actions from de Digital Twin into the real world.
- Such actuations can be determined automatically by Edge functions or manually from the User Interface.