Easy Development and Execution of Workflows with eFlows4HPC

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21ST INTERNATIONAL SYMPOSIUM ON PARALLEL & DISTRIBUTED COMPUTING,
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Complex workflows and complex infrastructures

- EuroHPC aims at developing a World Class Supercomputing Ecosystem in Europe
  - Procuring and deploying pre-exascale and petascale systems in Europe
- These systems will be capable of running large and complex applications
- Applications demand the composition of HPC, artificial intelligence and data analytics

EuroHPC systems

eFlows4HPC

Pre-Exascale

	Status	Country	Peak performance	Architecture
LUMI	Operational	Finland	552 petaflops	64-core AMD EPYC™ CPUs + AMD Instinct™ GPU
Leonardo	Under construction	Italy	322.6 petaflops	Intel Ice-Lake, Intel Sapphire Rapids + NVIDIA Ampere
MareNostrum 5	Contract signed	Spain	314 petaflops	Bull Sequana XH3000 and Lenovo ThinkSystem
Meluxina	Operational	Luxembourg	15 petaflops	AMD EP NVIDIA Ampere A100
Vega	Operational	Sl		12 + Nvidia A100
Karolina				Nvidia A100
Discoverer	C	Bulgaria	6 petaflops	AMD EPYC
Deucalion	Under construction	Portugal	10 petaflops	A64FX, AMD EPYC +Nvidia Ampere

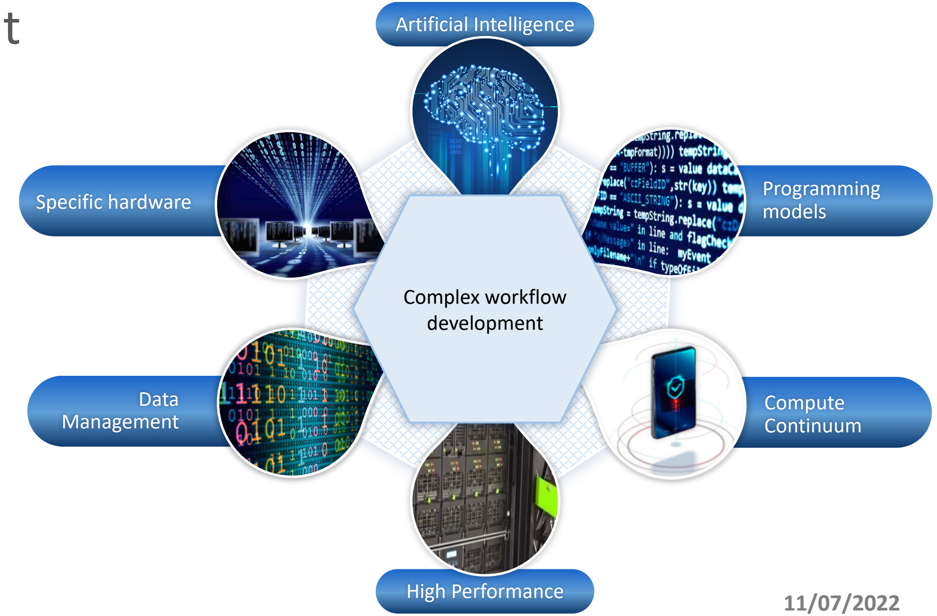
Petascale

First European Exascale Supercomputer announced to be installed in Jülich

https://eurohpc-ju.europa.eu/about/our-supercomputers_en

Main objectives

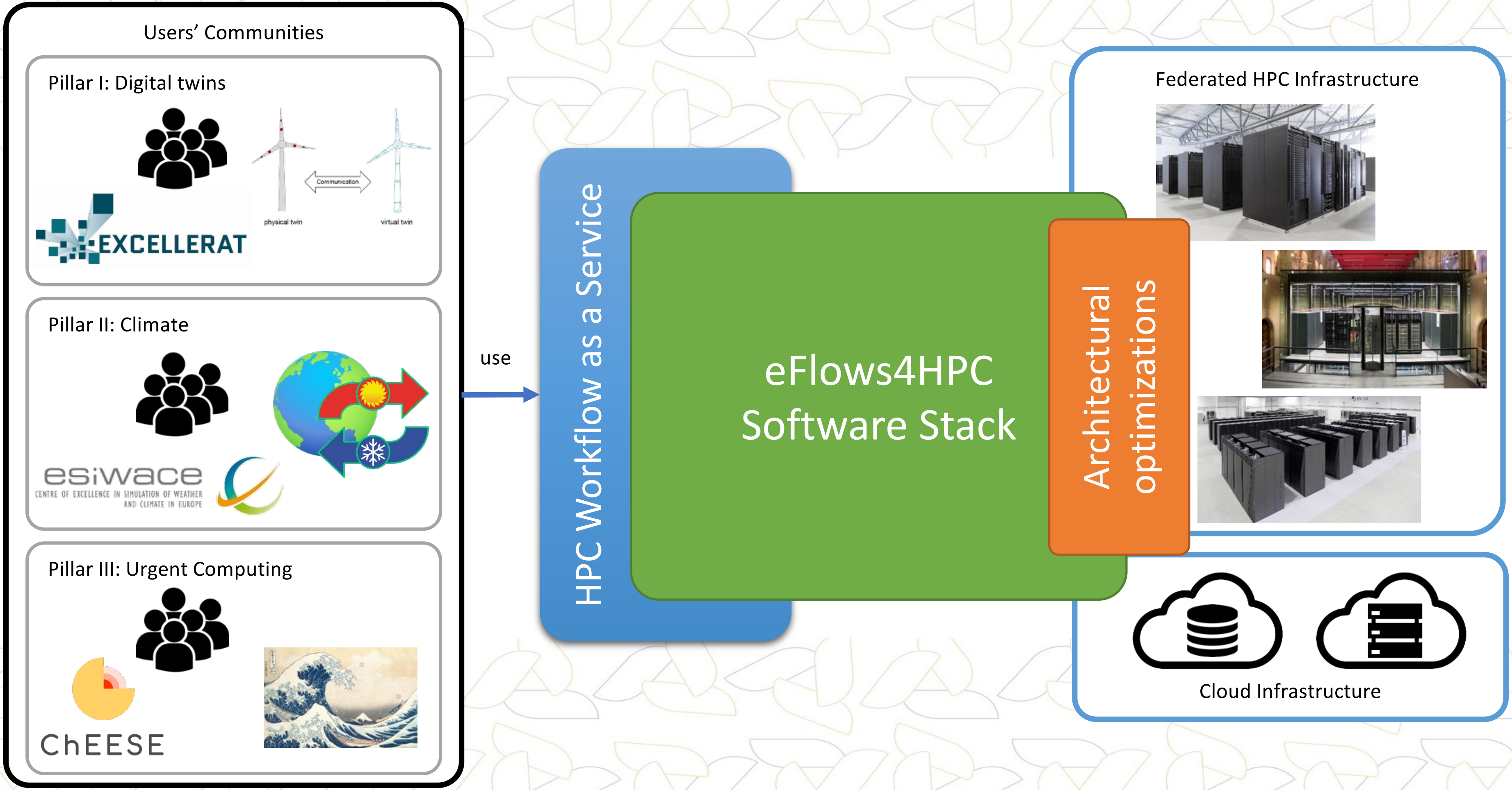
- Software tools stack that make it easier the development of workflows
  - HPC, AI + data analytics
  - Reactive and dynamic workflows
  - Efficient resource management
- HPC Workflows as a Service:
  - Mechanisms to make it easier the use and reuse of HPC by wider communities



Outline

- Project architecture
  - Software stack
  - HPC Workflows as a Service
- Pillar applications

PROJECT ARCHITECTURE



Users' Communities

Pillar I: Digital twins

Communication
physical twin
virtual twin
EXCELLERAT

Pillar II: Climate

esiwace
CENTRE OF EXCELLENCE IN SIMULATION OF WEATHER AND CLIMATE IN EUROPE

Pillar III: Urgent Computing

use

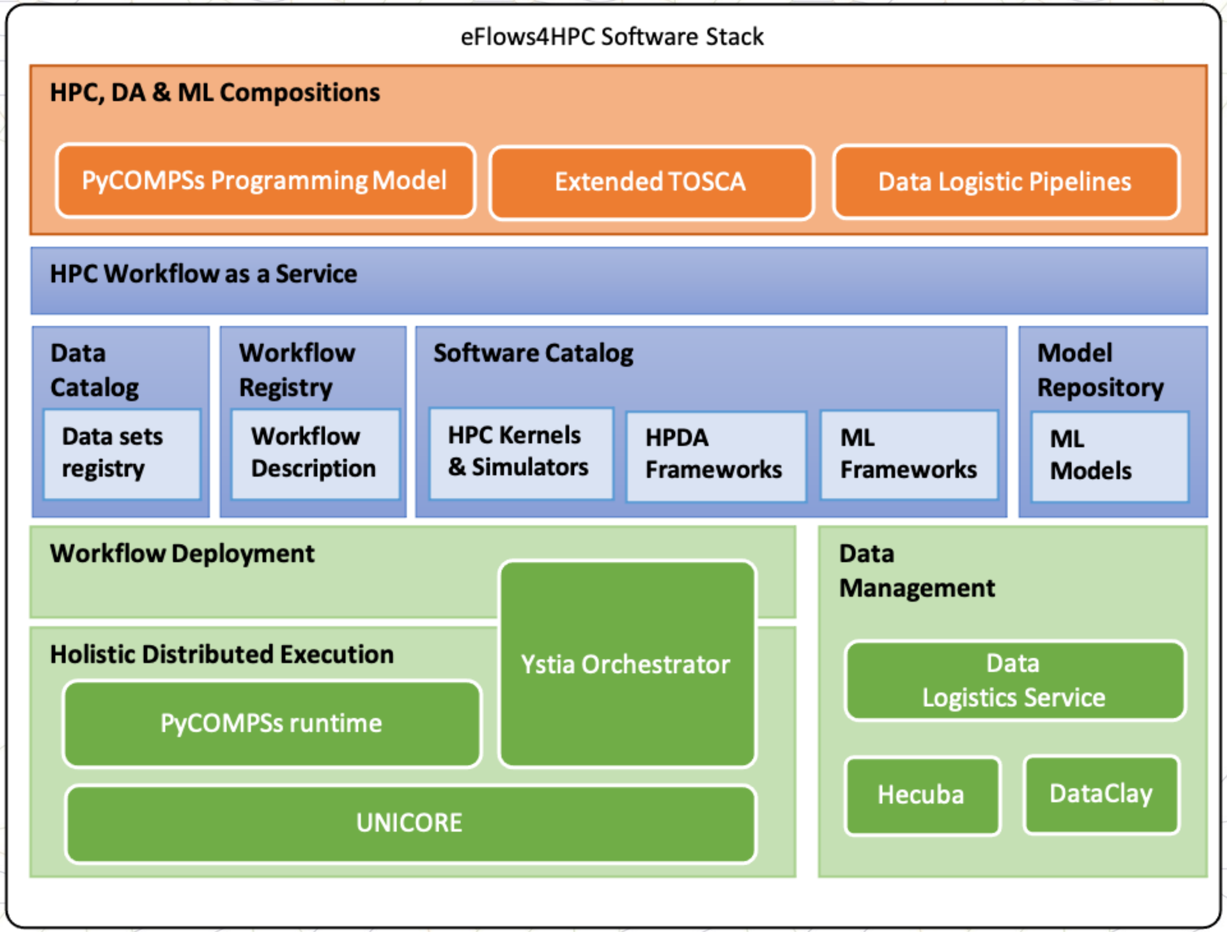
HPC Workflow as a Service

eFlows4HPC Software Stack

Architectural optimizations

Federated HPC Infrastructure

Cloud Infrastructure



eFlows4HPC Software Stack

HPC, DA & ML Compositions

PyCOMPSs Programming Model

Extended TOSCA

Data Logistic Pipelines

HPC Workflow as a Service

Data Catalog

Data sets registry

Workflow Registry

Workflow Description

Software Catalog

HPC Kernels & Simulators

HPDA Frameworks

ML Frameworks

Model Repository

ML Models

Workflow Deployment

Holistic Distributed Execution

PyCOMPSs runtime

Ystia Orchestrator

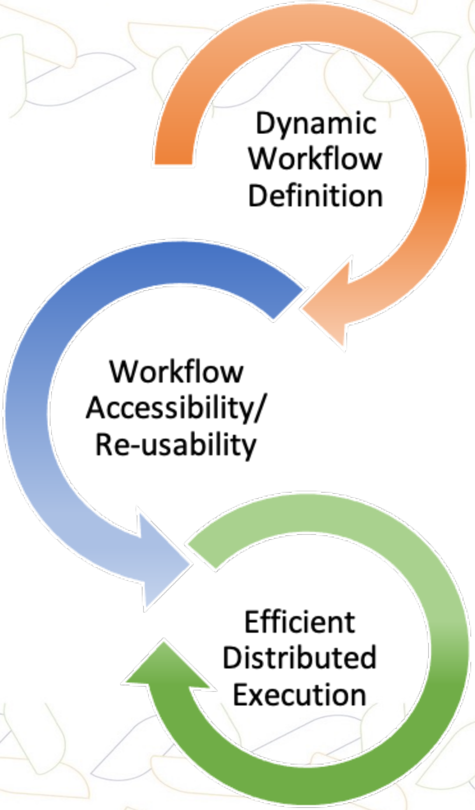
UNICORE

Data Management

Data Logistics Service

Hecuba

DataClay



Dynamic Workflow Definition

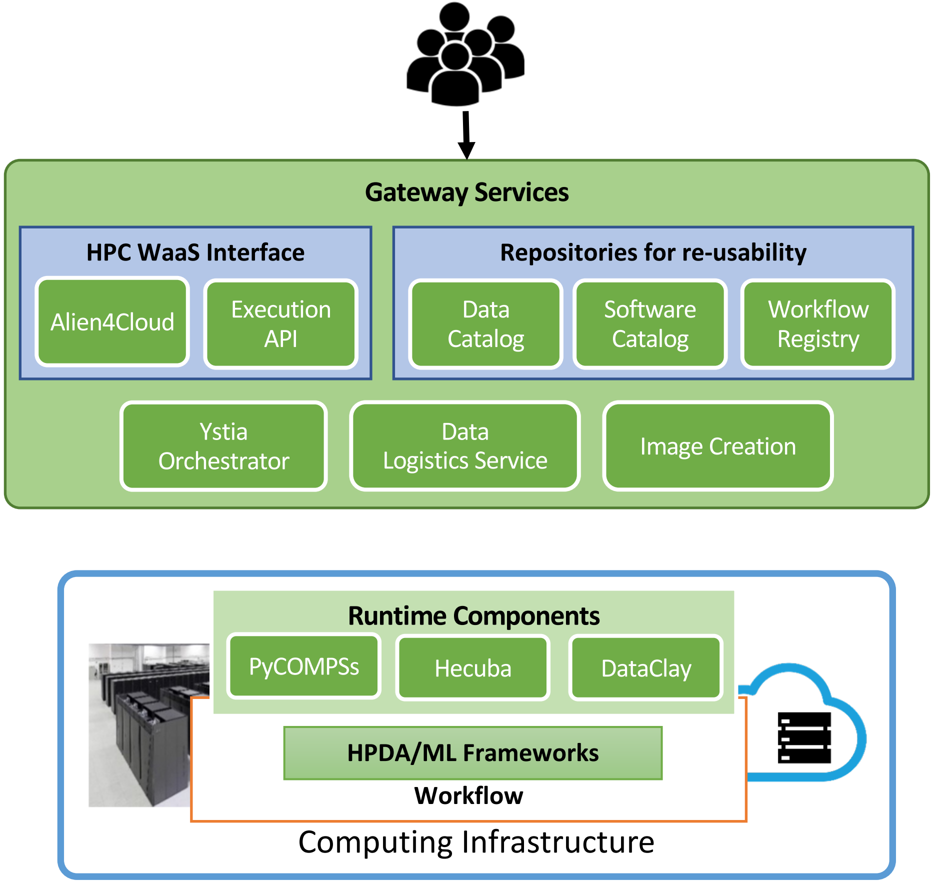
Workflow Accessibility/ Re-usability

Efficient Distributed Execution

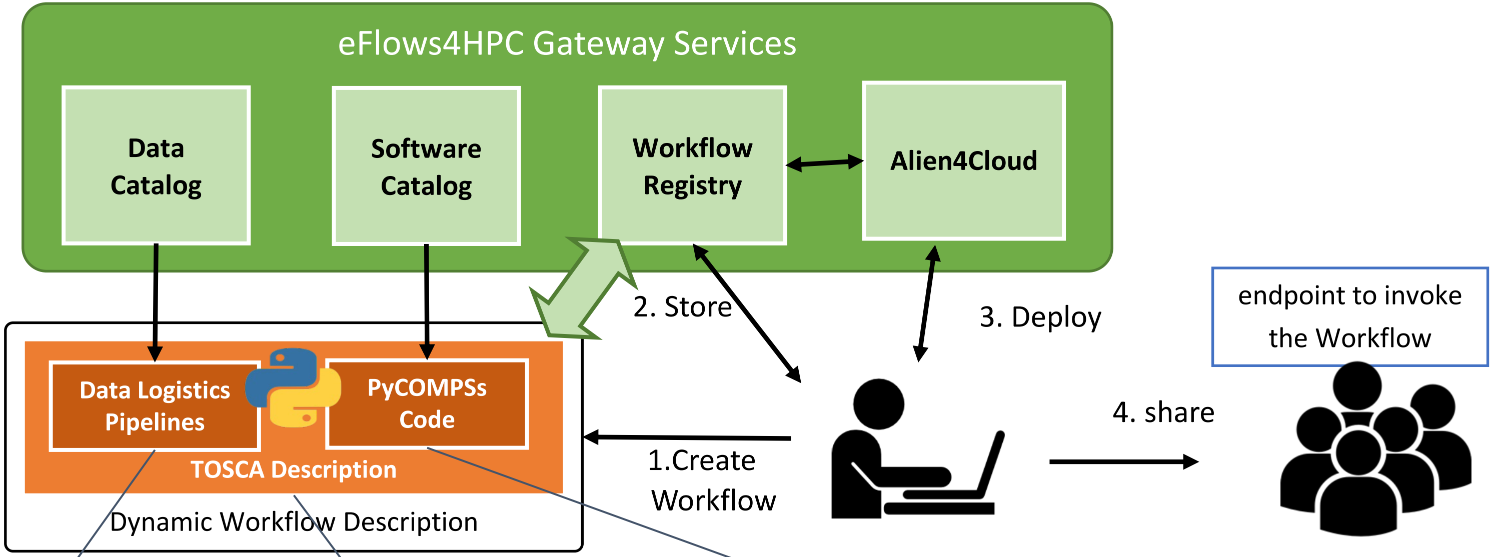
eFlows4HPC software stack and HPCWaaS

- Gateway services
  - Components deployed outside the computing infrastructure.
  - Managing external interactions and workflow lifecycle

- Runtime Components
  - Deployed inside the computing infrastructure to manage the workflow execution



Workflow development overview



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

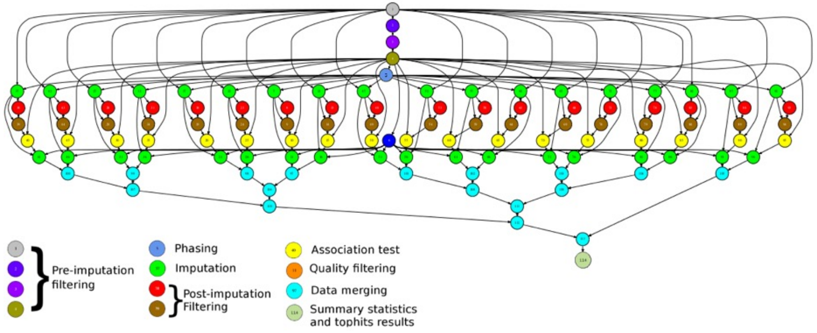
Computational Workflow as a simple python script.
Invocation of software described in the Software Catalog

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

Main element: Workflows in PyCOMPSs

- Sequential programming, parallel execution
- General purpose programming language + annotations/hints
  - To identify tasks and directionality of data
- Builds a task graph at runtime that express potential concurrency
- Tasks can be sequential, parallel (threaded or MPI)
- Offers to applications a shared memory illusion in a distributed system
  - The application can address larger data than storage space: support for Big Data apps
  - Support for persistent storage
- Agnostic of computing platform
  - Enabled by the runtime for clusters, clouds and container managed clusters

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



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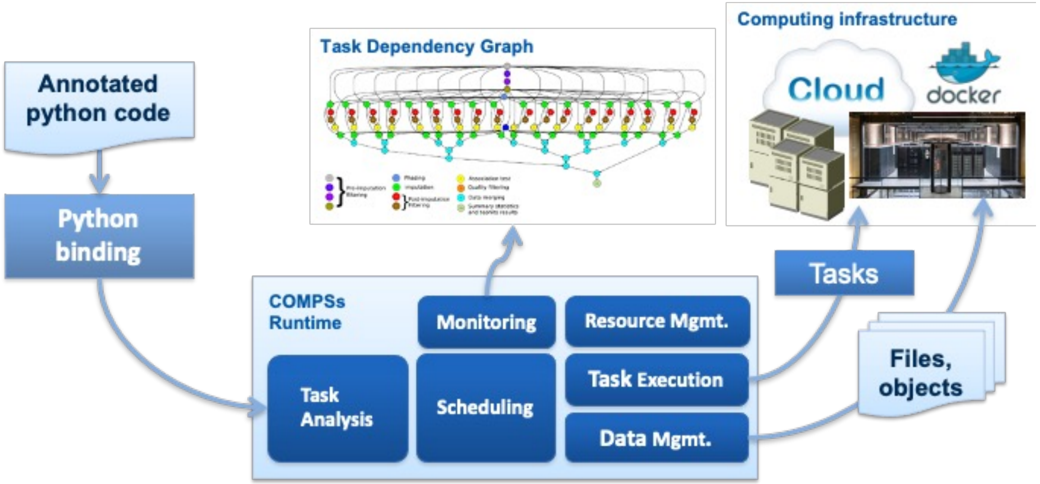
PyCOMPSs features and runtime

- 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
- Runtime deployed as a distributed master-worker
- All data scheduling decisions and data transfers are performed by the runtime
- Support for elasticity



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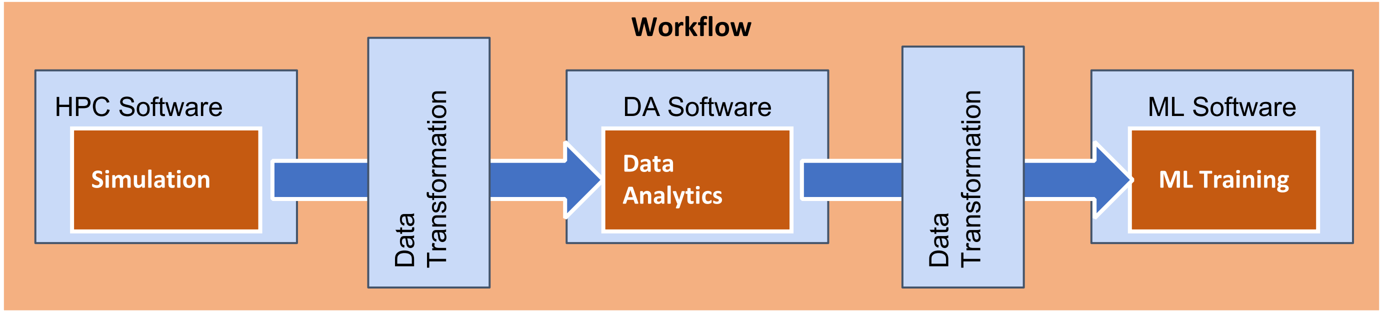
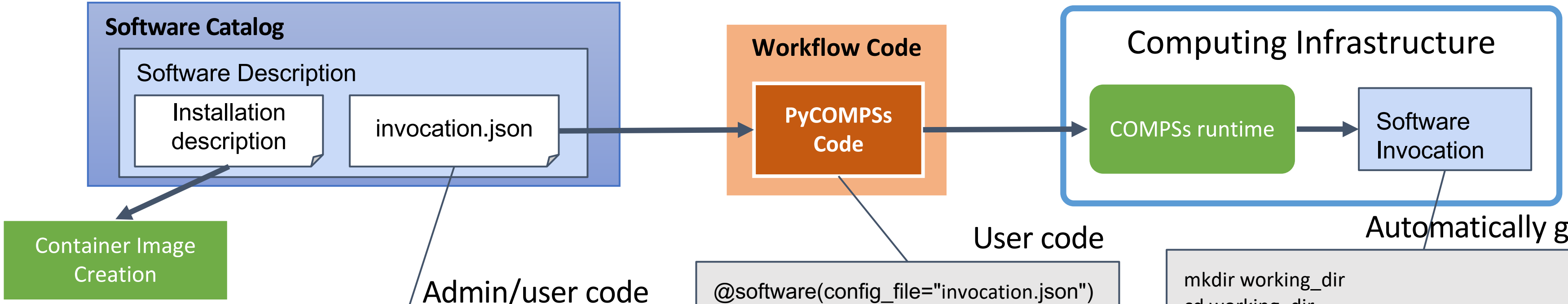
Interfaces to integrate HPC/DA/ML



- Goal:
  - Reduce glue code
  - Developer focuses in the functionality, not in the integration
  - Reusability
- Two paradigms:
  - Software integration
  - Data transformations

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

#Worflow

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

Software Invocation description



Software Catalog

Software Description

Installation description

invocation.json

Container Image Creation

Workflow Code

PyCOMPSs Code

Computing Infrastructure

COMPSs runtime

Software Invocation

Admin/user code

```
{
 "type":"mpi",
  "properties":{
     "runner": "mpirun",
    “processes”: “$SW_PROCS”
     "binary": "mpi_sofware.x",
     "params": "-d {{param}}",
    “working_dir”: “{{working_dir}}”},
  "prolog":{
       "binary":"mkdir",
       "params":"{{working_dir}}"},
    "epilog":{
       "binary":"tar",
       "params":"zcvf {{out_tgz}}" {{working_dir}}},
  "constraints":{
     "computing_units": $SW_THREADS}
}
```

User code

```
@software(config_file="invocation.json")
def mpi_exec(work_dir, param, out_tgz):
    pass

#Call to the task function:

mpi_exec('my_folder', 'hello_world')
```

Automatically generated

```
mkdir working_dir
cd working_dir
export OMP_NUM_THREADS=$SW_THREADS
mpirun -n $SW_PROCS mpi_software.x -d param
tar zcvf out_tgz working_dir
```

- Converts a python function of a software invocation to a PyCOMPSs task
- Reused in different workflows

Data Catalogue and Data Logistics Service

Data Catalogue:

- Lists datasets used and created by the workflow according to FAIR principles
- Provides metadata to make data movement pipelines more generic

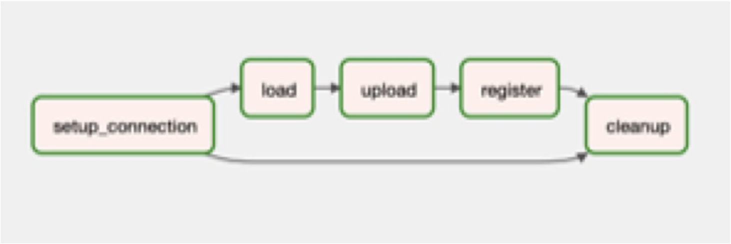
Data Pipelines:

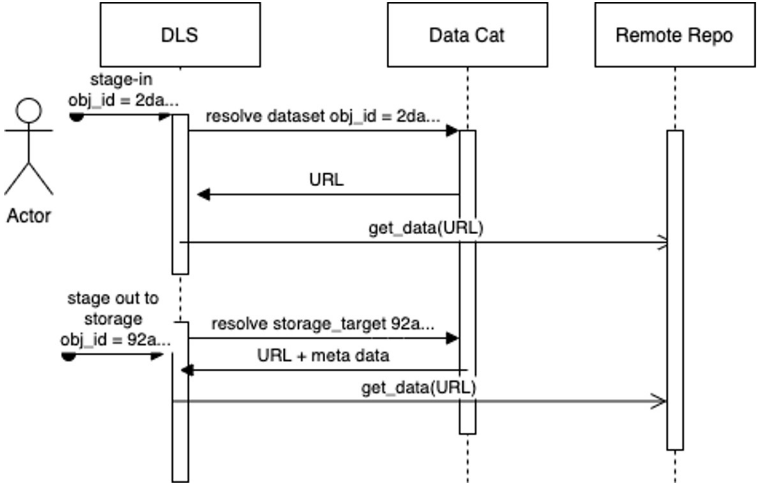
- Formalization of data movements for transparency and reusability
- Stage-in/out, image transfer

Data Logistics Services (DLS):

- Performs the execution of data pipelines to fuel Pillars’ computations

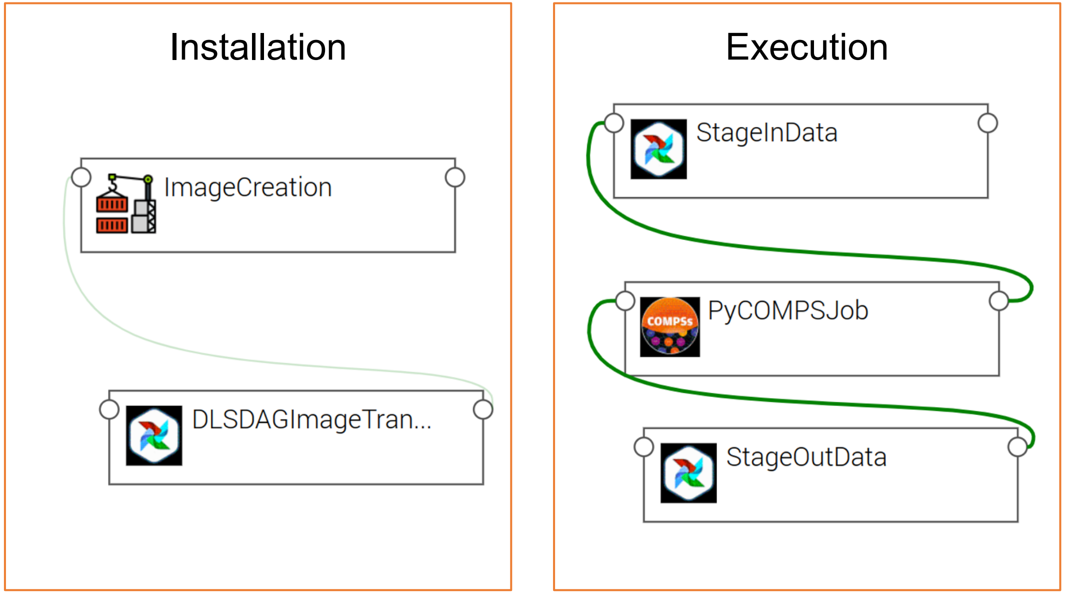
Data pipeline





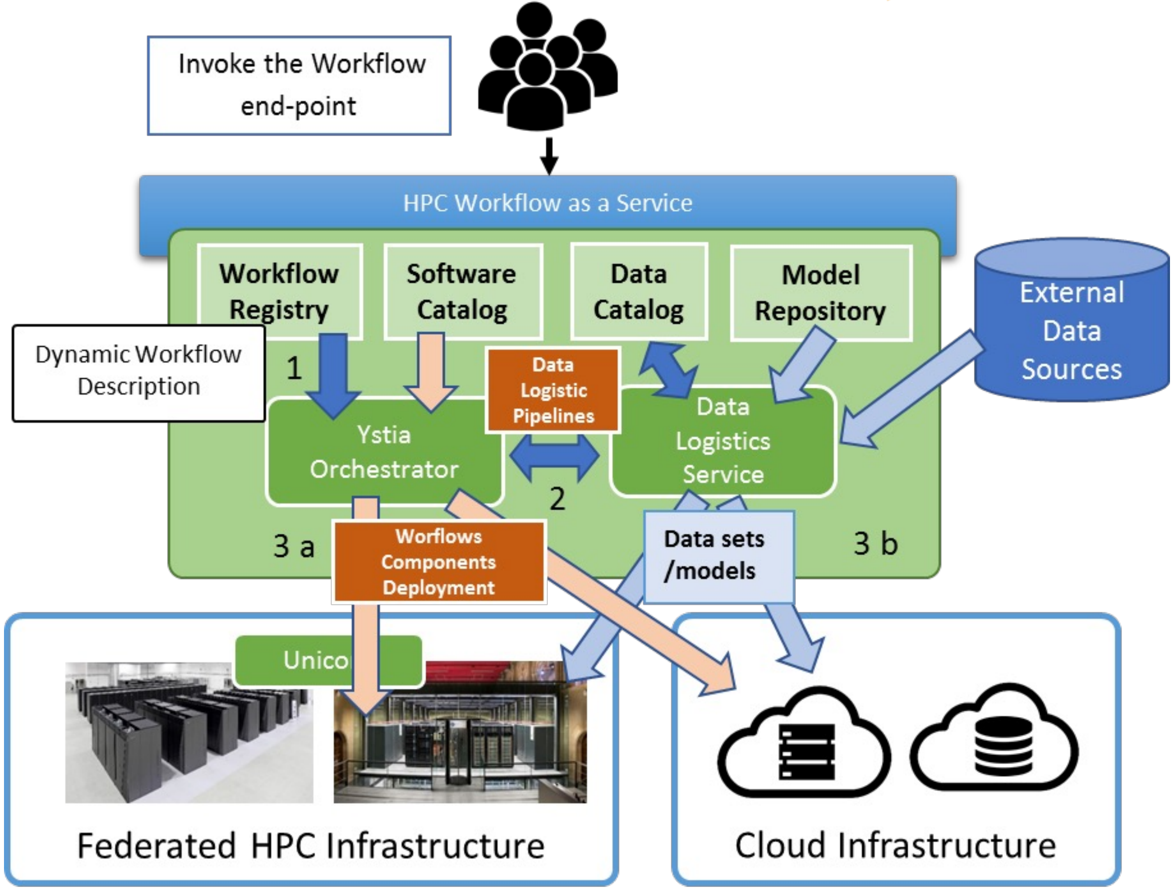
TOSCA Modelization

Topology of the different components involved in the Workflow lifecycle



Deployment

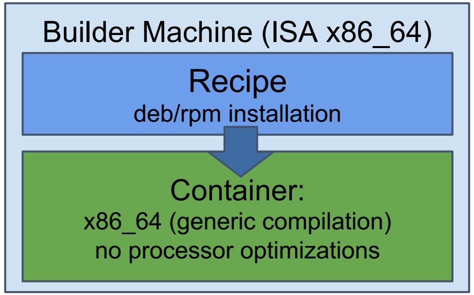
- Invocation of a workflow
- Deployment orchestrated by Ystia Orchestrator (Yorc)
- Workflow retrieved from registry
- Data Logistic Service – data stage-in and stage-out
  - Periodical transfers of data outside HPC systems
- Deployment of workflow components in the computing infrastructures
  - HPC containers built with easybuild/Spack



HPC Ready Containers

eFlows4HPC

Standard container image creation

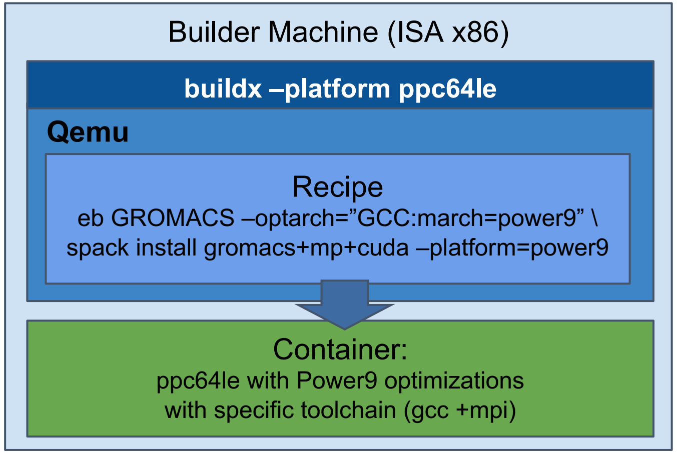


Builder Machine (ISA x86_64)

Recipe
deb/rpm installation

Container:
x86_64 (generic compilation)
no processor optimizations

eFlows4HPC approach



Builder Machine (ISA x86)

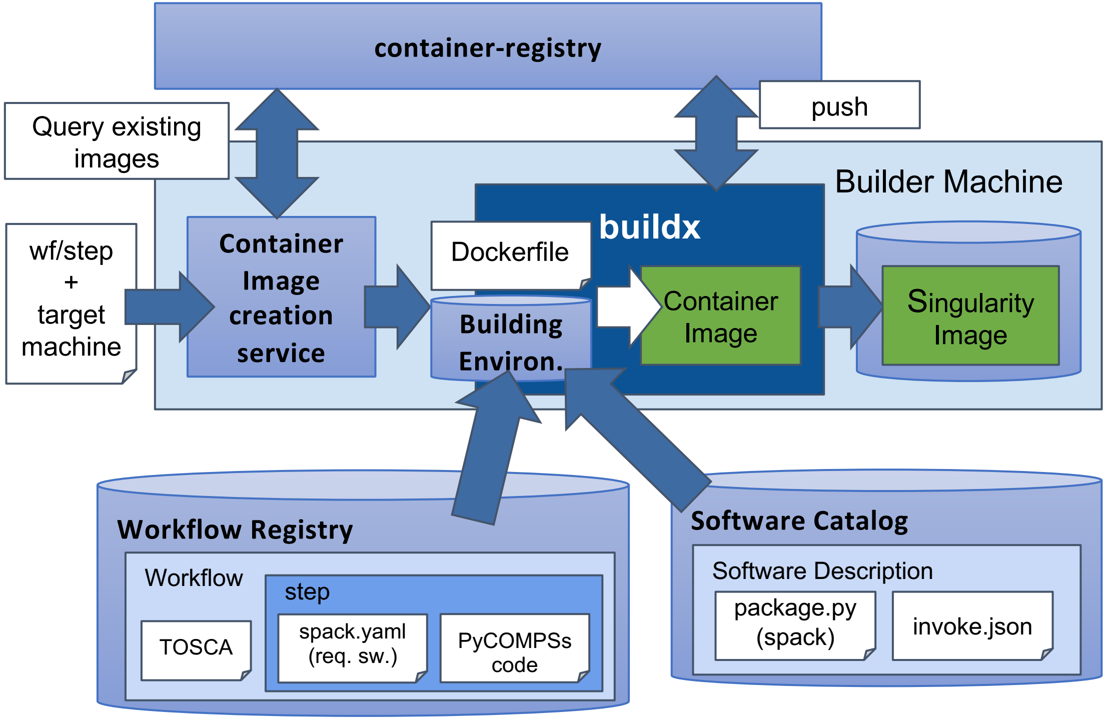
buildx –platform ppc64le

Qemu

Recipe
eb GROMACS –optarch=”GCC:march=power9” \
spack install gromacs+mp+cuda –platform=power9

Container:
ppc64le with Power9 optimizations
with specific toolchain (gcc +mpi)

Service to automate the Container Image Creation



container-registry

Query existing images

push

Builder Machine

wf/step + target machine

Container Image creation service

Dockerfile

Building Environ.

buildx

Container Image

Singularity Image

Workflow Registry

Workflow

TOSCA

step

spack.yaml (req. sw.)

PyCOMPSs code

Software Catalog

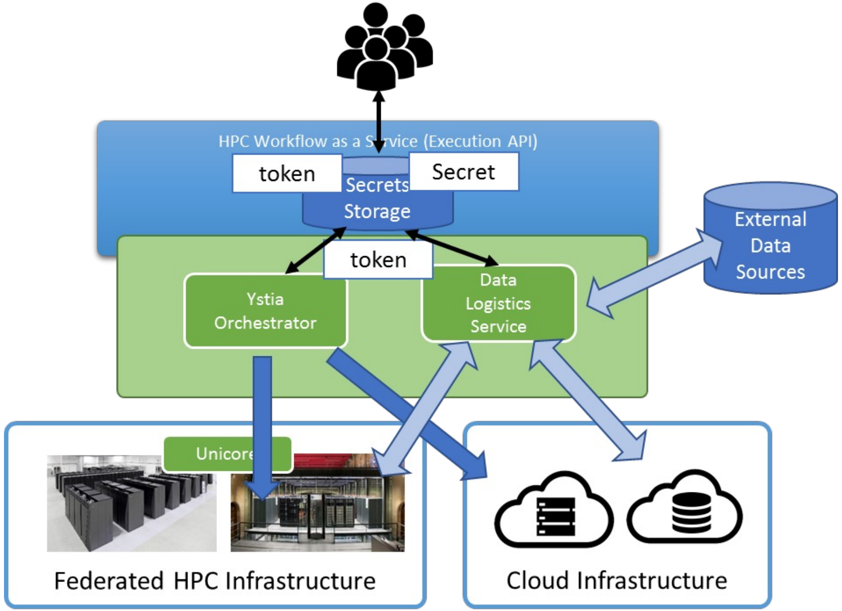
Software Description

package.py (spack)

invoke.json

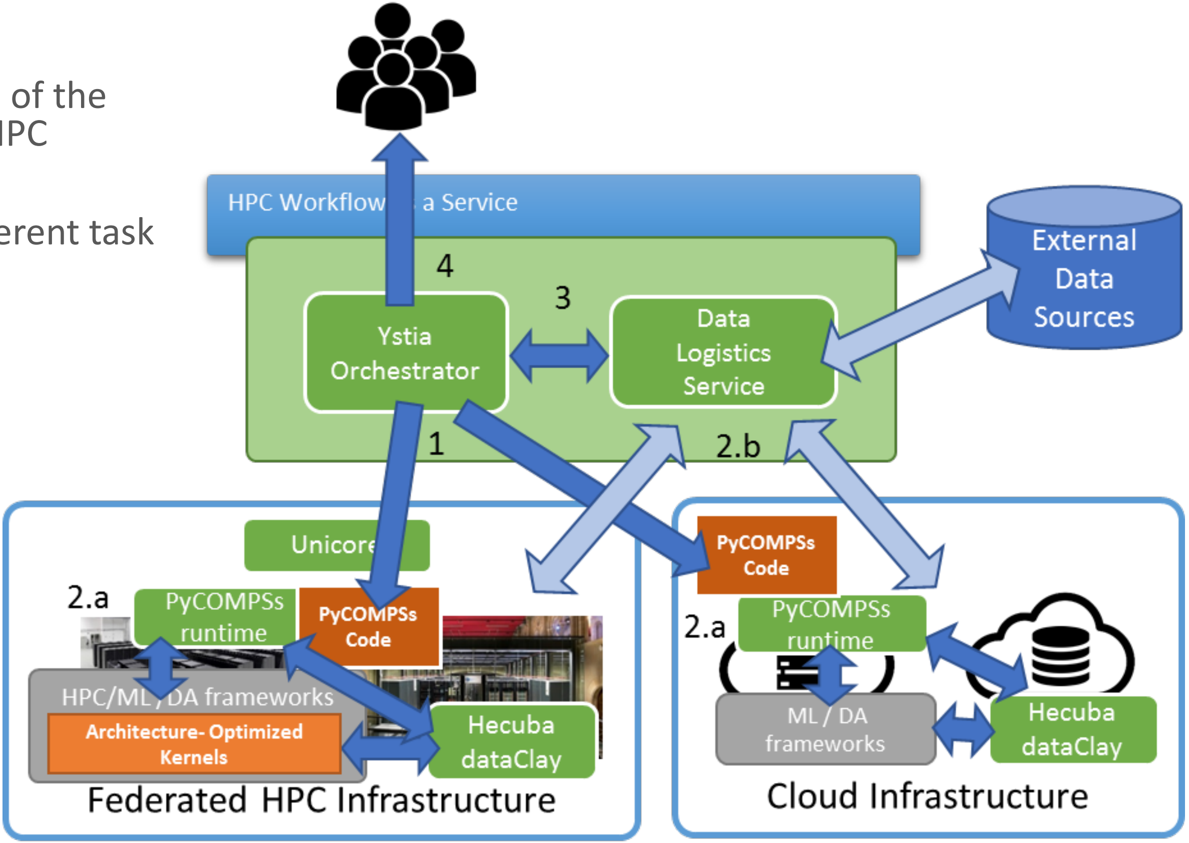
Credential management

- Prior to executing the registered workflows, the users have to configure the infrastructure access credentials
- Usernames, public-key certificates, passwords
- Users' certificates managed by an Execution API
    - Provides a few methods to register and access credentials or generate a new secret
    - HashiCorp Vault for secret (SSH keys) management
- User authorizes adding credentials in the HPC cluster
- Credentials identified by a token attached to the user's workflow invocation.



Operation- Workflow Execution

- Submission of the execution of the workflow processes to the HPC infrastructure
- PyCOMPSs orchestrates different task types
  - HPC (MPI), ML, DA
- Dynamic execution
  - Runtime task-graph
  - Task-level FT
  - Exceptions
- Data management
  - Persistent storage
- Optimized kernels
  - EPI, GPU, FPGA



PILLAR APPLICATIONS

Pillar I: Manufacturing

CIMNE

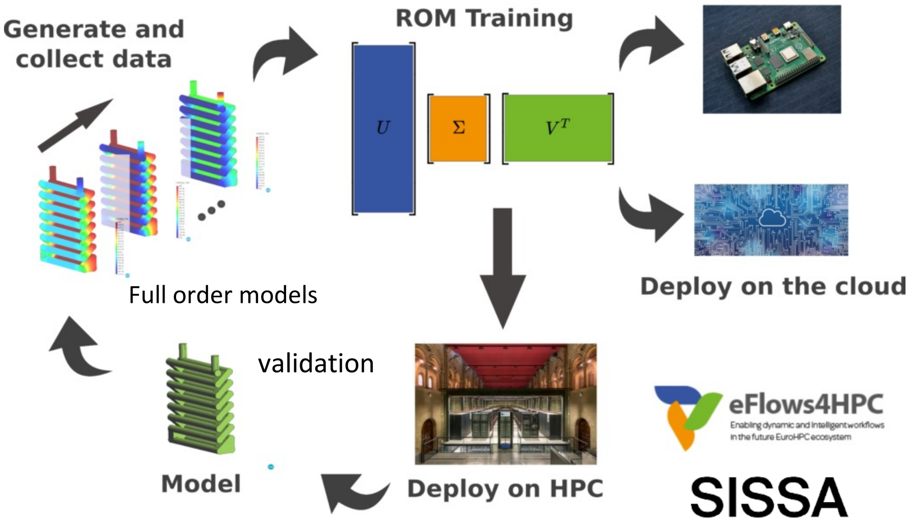
KRATOS MULTI-PHYSICS

Inria

Upgrade your meshes

ParMMg

SIEMENS

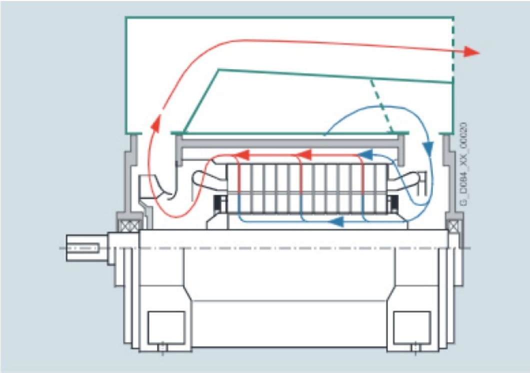


eFlows4HPC
Enabling dynamic and intelligent workflows in the future EuroHPC ecosystem

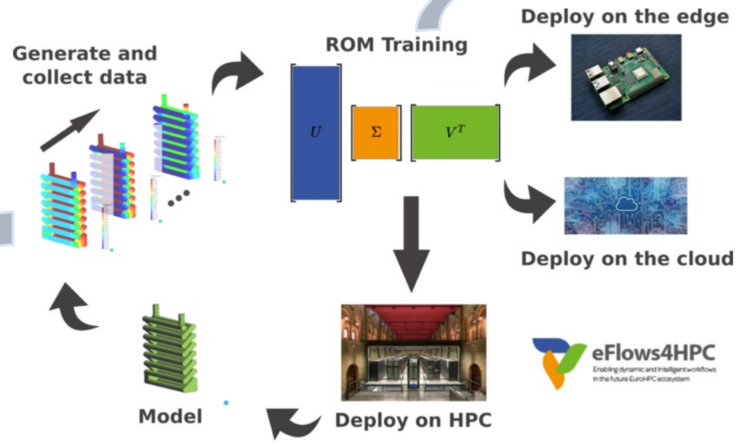
SISSA
Scuola Internazionale Superiore di Studi Avanzati

Pillar I focuses on the construction of DigitalTwins for the prototyping of complex manufactured objects:

- Integrating state-of-the-art adaptive solvers with machine learning and data-mining
- Contributing to the Industry 4.0 vision



Integration of HPC and data analytics in a single workflow

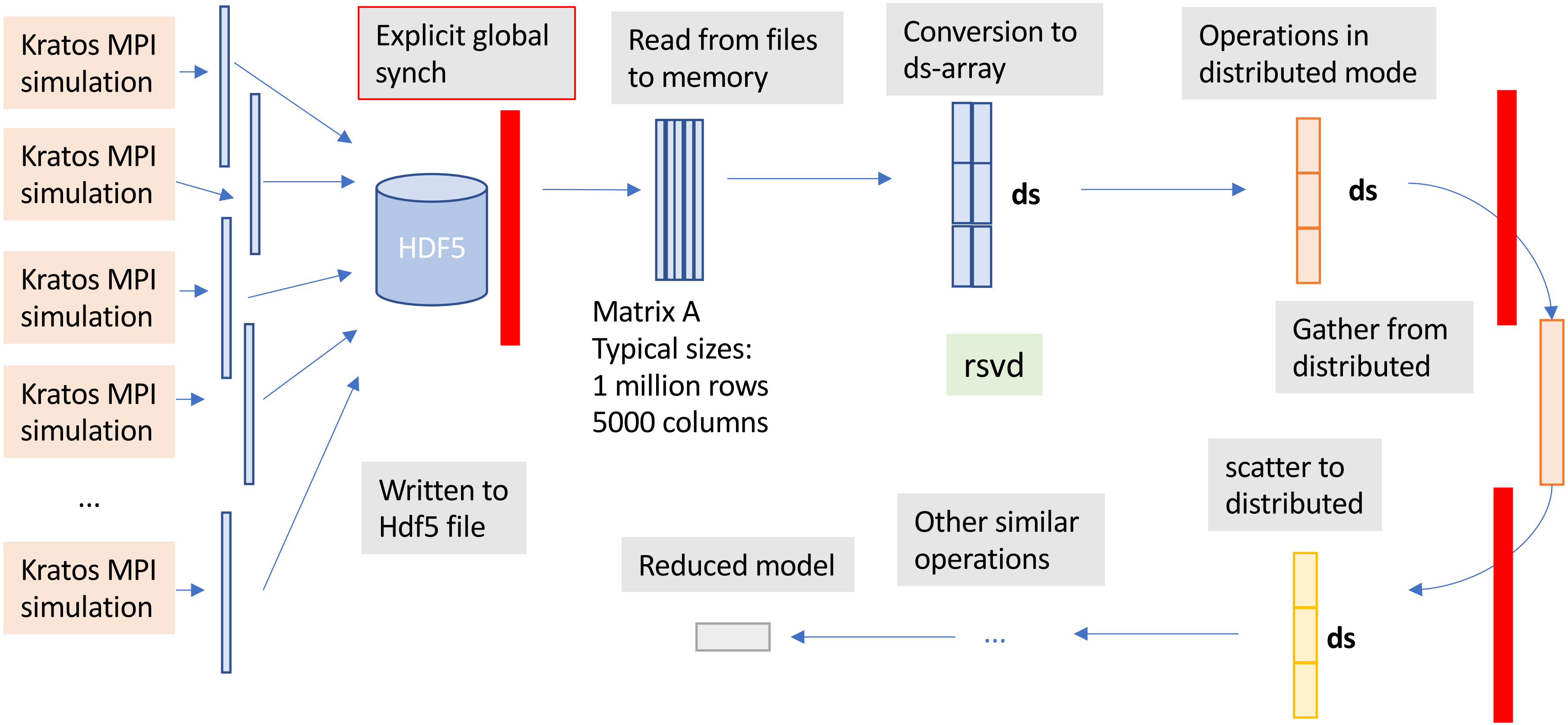

Generate and collect data
ROM Training
U
Σ
V^T
Deploy on the edge
Deploy on the cloud
Model
Deploy on HPC
eFlows4HPC
Enabling dynamic and intelligent workflows in the future EuroHPC ecosystem

```
import dislib as ds

@constraint(computingUnits=8)
@task(Y_blocks={Type: COLLECTION_IN, Depth: 2},
def my_qr(Y_blocks):
    Y = np.block(Y_blocks)
    Q,R = np.linalg.qr(Y, mode='reduced')
    return Q,R

def rsvd(A, desired_rank):
    k = desired_rank
    ...
    Y = A @ Omega
    Q,R = my_qr(Y._blocks)
    Q=load_blocks_rechunk([Q], ...)
    ...
    R = Q.T @ A
```

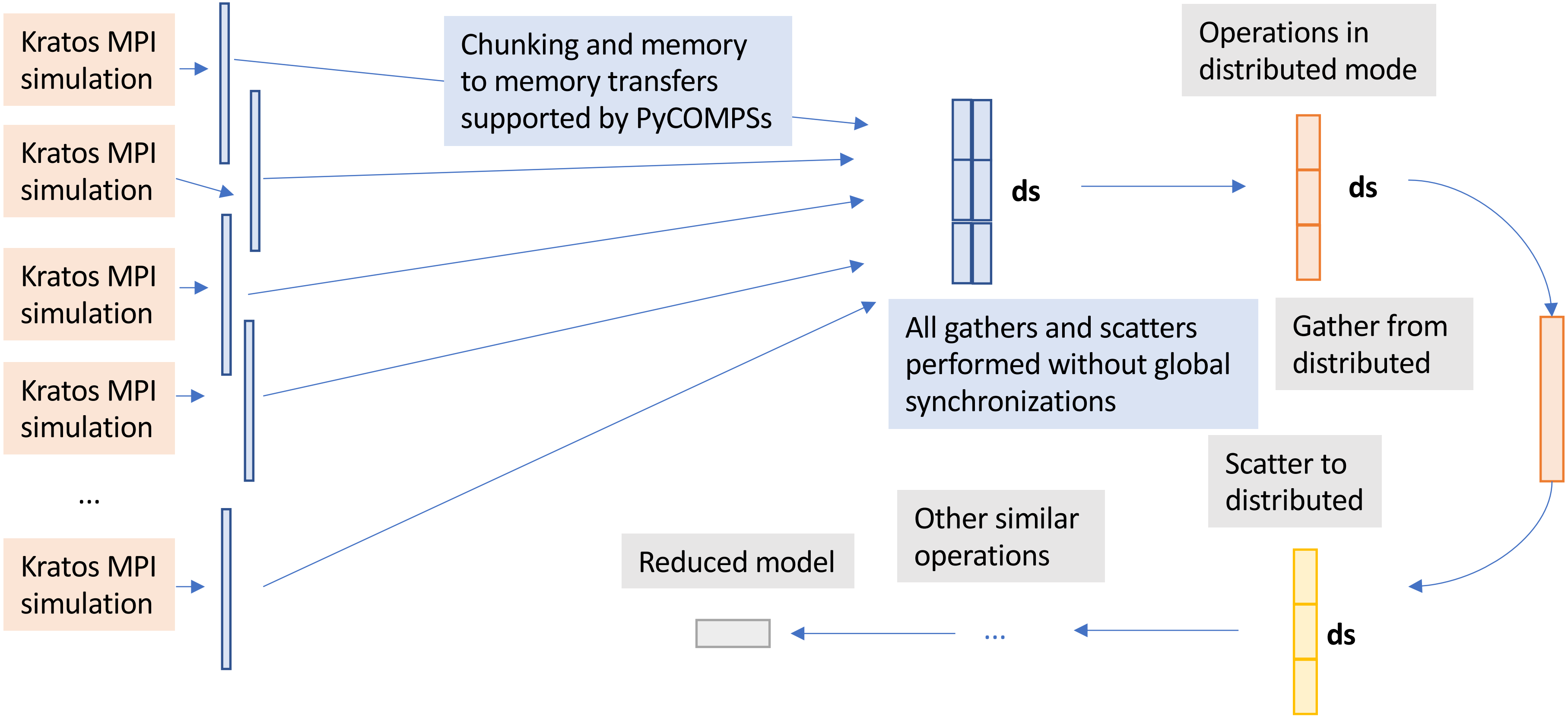
```
@constraint(computing_units="8")
@mpi(runner="mpirun", processes="16")
@task(returns = np.array)
def ExecuteInstance_Task(
    ...
    current_parameters =
    ...
    simulation = GetTrai
    simulation.Run()
    return simulation.GetSnapshotsMatrix()
```

```
....
for instance in range (0,TotalNumberOFCases):
    blocks.append(ExecuteInstance_Task(model, parameters, pars, inst
...
U, s = rsvd(A, desired_rank)
...
```

Pillar I sample workflow – initial version



Pillar I sample workflow – optimized version



Chunking and memory to memory transfers supported by PyCOMPSs

Operations in distributed mode

All gathers and scatters performed without global synchronizations

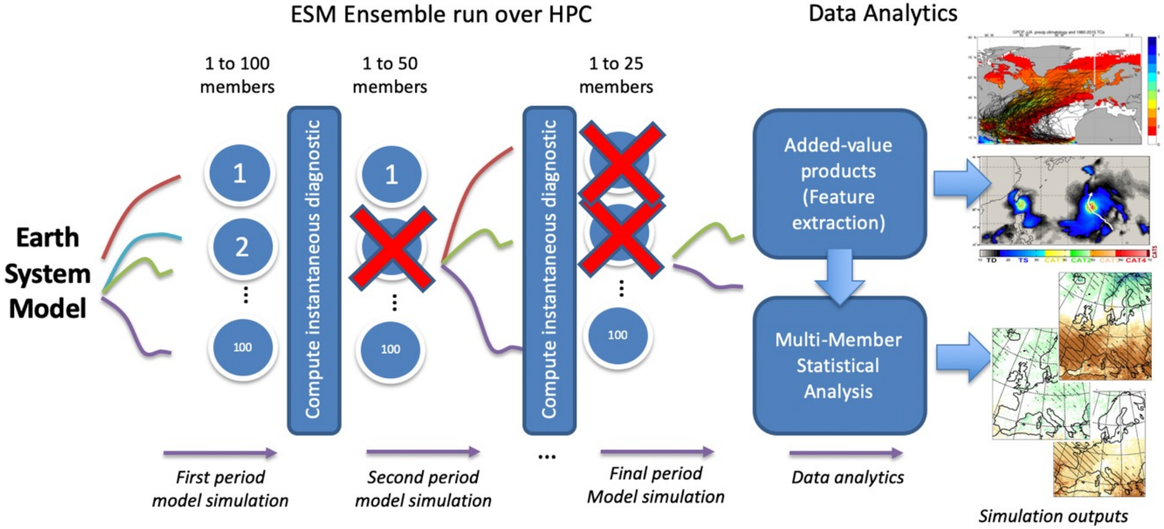
Gather from distributed

Scatter to distributed

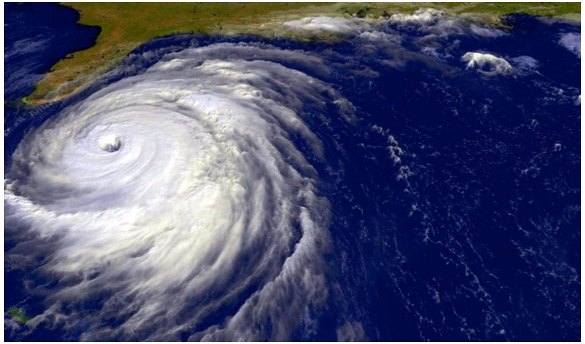
Other similar operations

Reduced model

Pillar II: Climate



ESM Ensemble run over HPC
Data Analytics
1 to 100 members
1 to 50 members
1 to 25 members
Earth System Model
1
2
100
Compute instantaneous diagnostic
1
100
Compute instantaneous diagnostic
100
Added-value products (Feature extraction)
Multi-Member Statistical Analysis
First period model simulation
Second period model simulation
...
Final period Model simulation
Data analytics
Simulation outputs



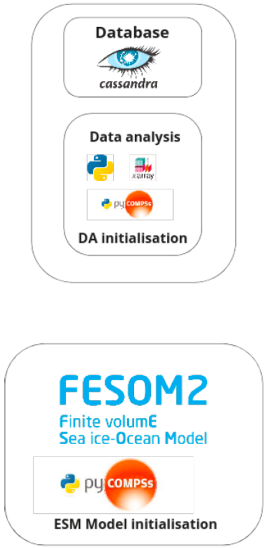
Dynamic (AI-assisted) workflow

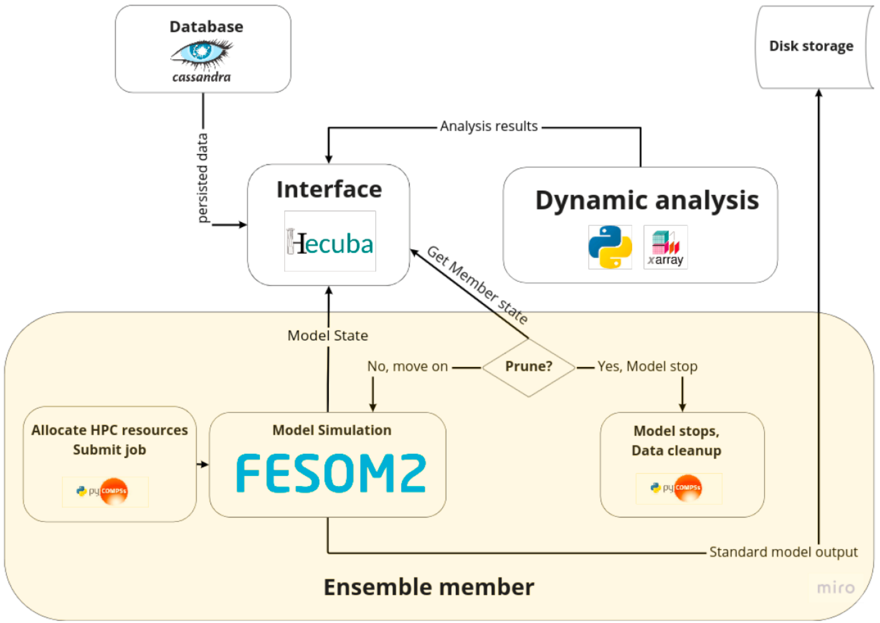
HPDA & ML/DL

- Perform climate predictions: temperature, precipitation or wind speed
- AI-assisted pruning of the ESM workflow
- Study of Tropical Cyclones (TC) in the North Pacific, with in-situ analytics

ESM Dynamic Workflow

- Ensemble of FESOM simulations
- Intermediate simulation results stored persistently to Hecuba
- Pruning mechanism cancels given simulations based on dynamic anaysis of data stored in Hecuba

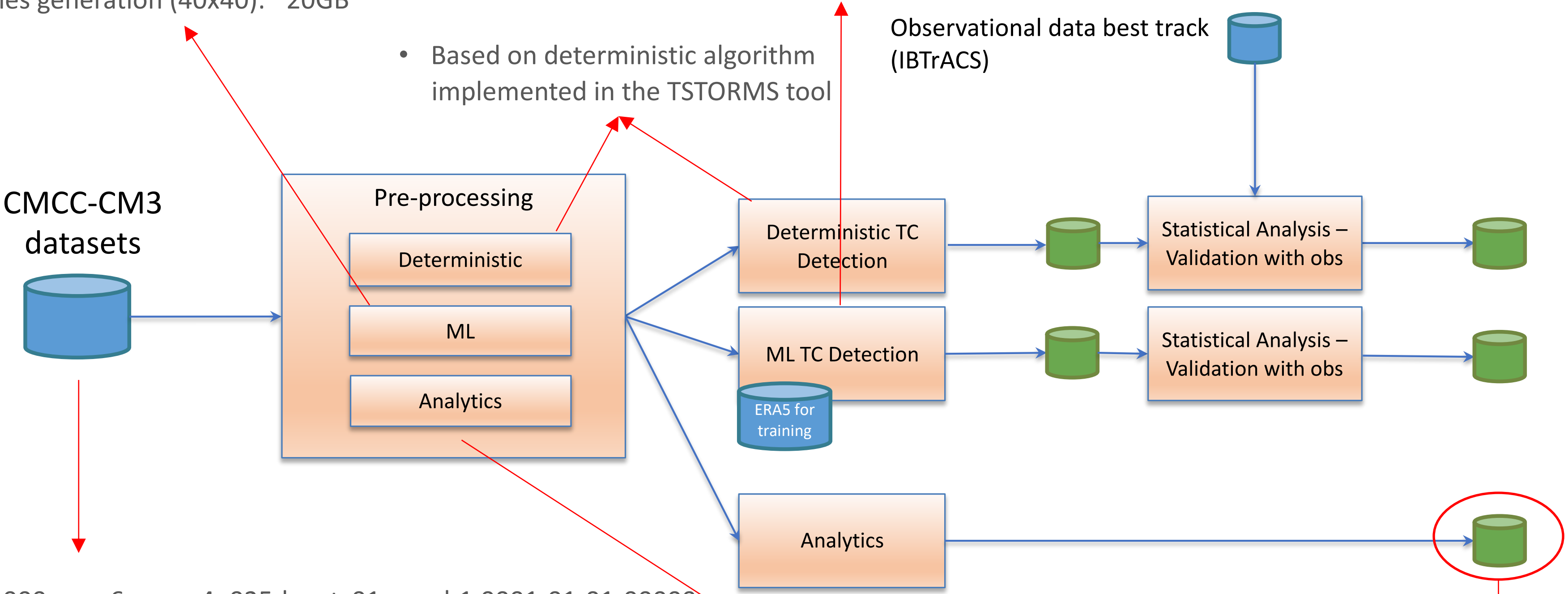




Use case 1 – CMCC-CM3 based

- Selection of input data for NN training ERA5 NetCDF (North Pacific region): ~240GB
- Patches generation (40x40): ~20GB

- NN defined and trained
- Inference on CMCC-CM3 datasets under testing



- Based on deterministic algorithm implemented in the TSTORMS tool

Observational data best track (IBTrACS)

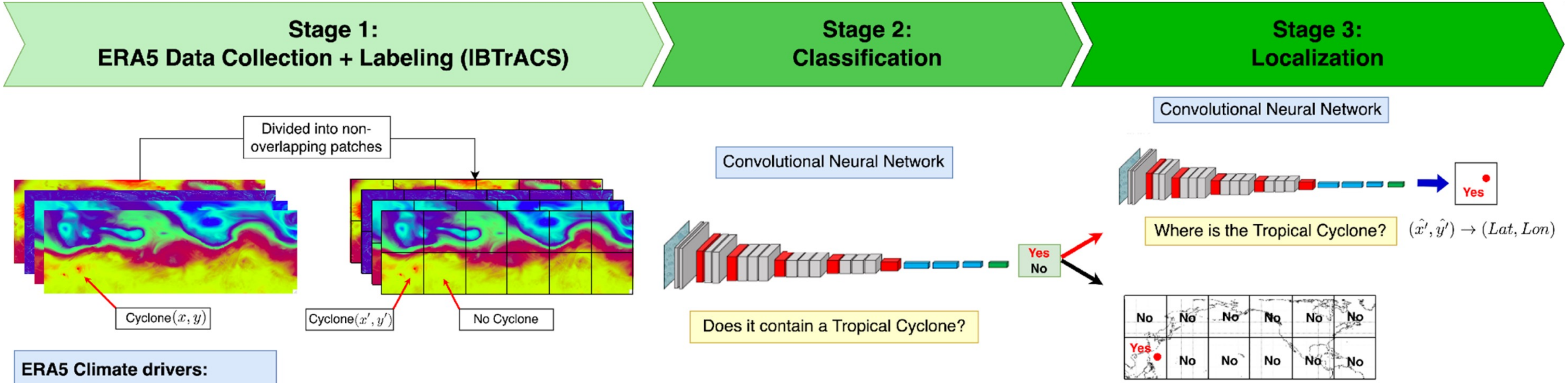
CMCC-CM3 datasets
Pre-processing
Deterministic
ML
Analytics
Deterministic TC Detection
ML TC Detection
ERA5 for training
Analytics
Statistical Analysis – Validation with obs
Statistical Analysis – Validation with obs

NetCDF: 2000_cam6-nemo4_025deg_tc01.cam.h1.0001-01-01-00000.nc ~200MB, 4 timesteps (6 hourly), Global domain

Climate indicators defined and implemented

Outputs: Maps (png, jpeg) and NetCDF

Tropical Cyclones Detection ML Workflow: Training Phase

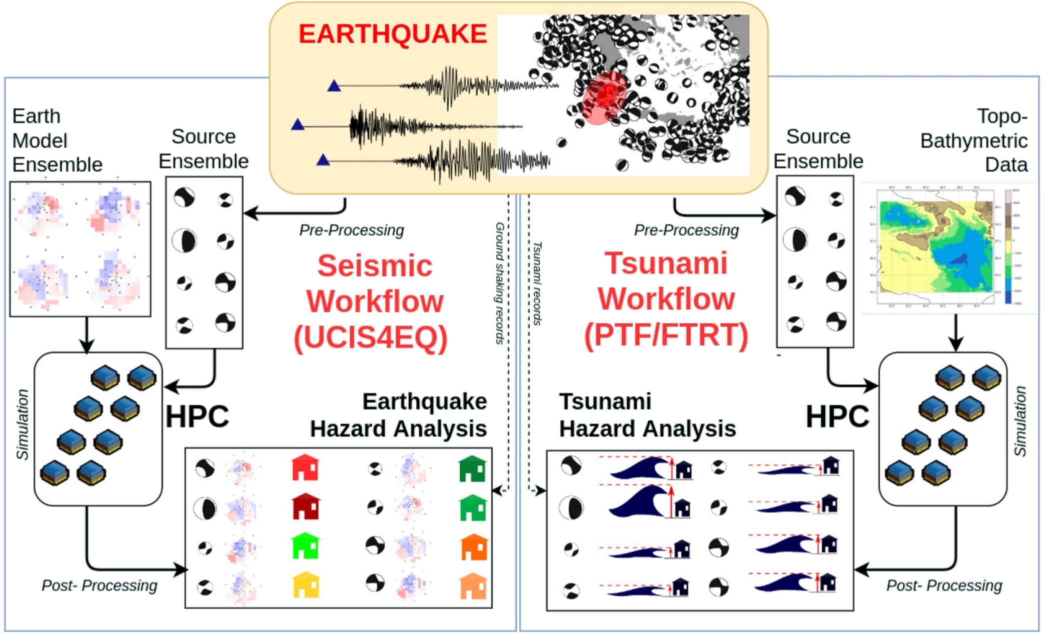

Stage 1:
ERA5 Data Collection + Labeling (IBTrACS)
Stage 2:
Classification
Stage 3:
Localization
Divided into non-overlapping patches
Cyclone(x, y)
Cyclone(x', y')
No Cyclone
Convolutional Neural Network
Does it contain a Tropical Cyclone?
Yes
No
Convolutional Neural Network
Yes
Where is the Tropical Cyclone?
$(\hat{x}', \hat{y}') \rightarrow (Lat, Lon)$
No
No
No
No
No
No
Yes
No
No
No
No
No

ERA5 Climate drivers:

- 10 m wind gust
- Temperature at 500 hPa
- Temperature at 300 hPa
- Mean sea level pressure

- Three main stages:
  - STAGE 1: Gathering of ERA5 climatic maps and generation of patches containing at most 1 tropical Cyclone (TC) each
  - STAGE 2: Classification of TC presence/absence inside the patch
  - STAGE 3: Localization of TC center coordinates in the patches in which the TC was previously classified as present

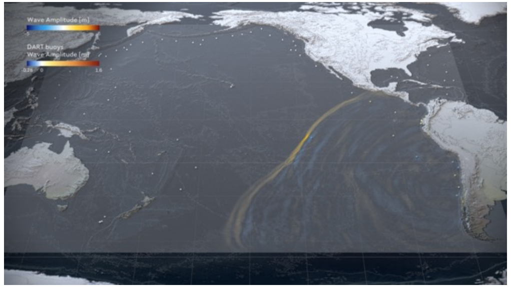
Pillar III: Urgent computing for natural hazards



Pillar III explores the modelling of natural catastrophes:

- Earthquakes and their associated tsunamis shortly after such an event is recorded
- Use of AI to estimate intensity maps
- Use of DA and AI tools to enhance event diagnostics
- Areas: Mediterranean basin, Mexico, Iceland and Chile

Tsunami-HySEA GPU-based code



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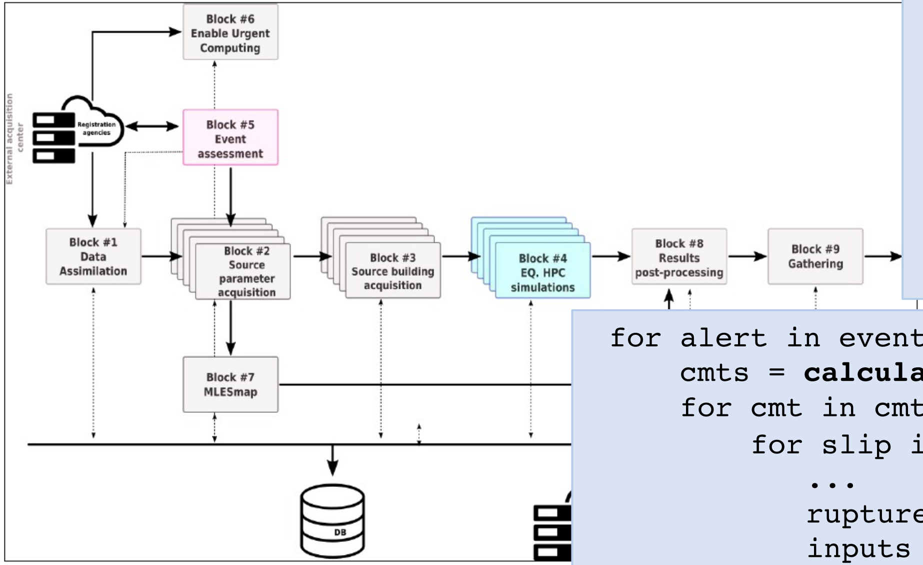
NGI

UCIS4EQ workflow: http services as tasks

Urgent Computing Integrated Services for Earthquakes: UCIS4EQ



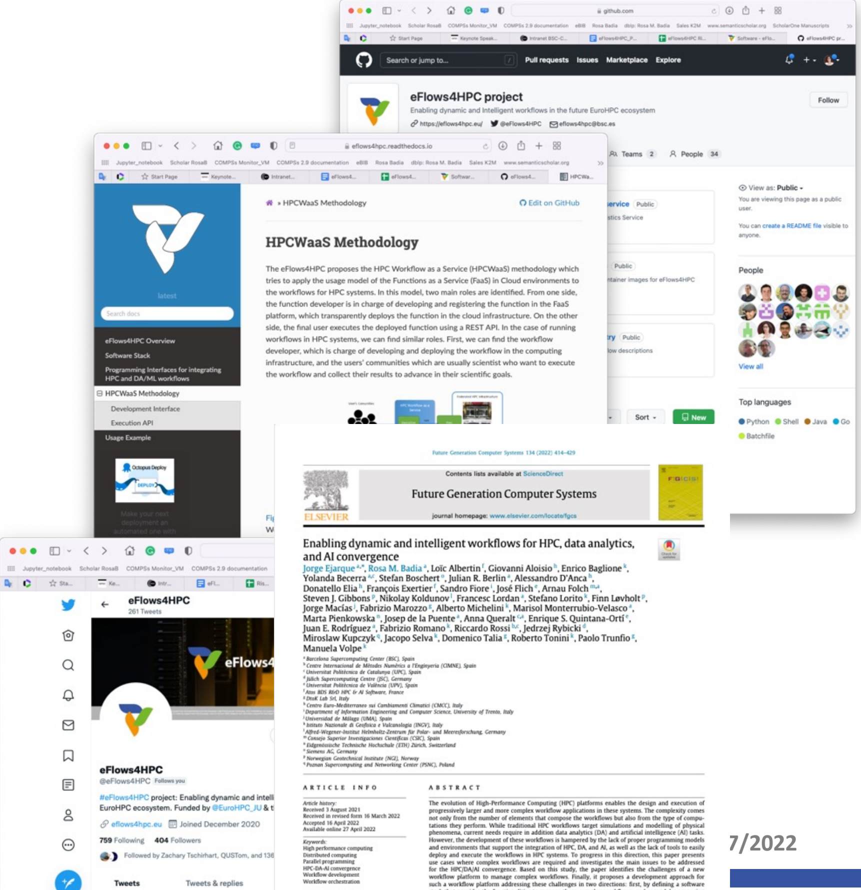
```
@http(request="POST", resource="SalvusRun", ...')
@task(returns=1)
def run_salvus(event_id, trial, input, resources):
    """
    """
    pass
@http(request="POST", resource="cmt",...)
@task(returns=1)
def calculate_cmt(alert, event_id, domain, precmt):
    """
    """
    pass
...
```

```
for alert in event['alerts’]:
    cmts = calculate_cmt(alert, eid, domain, precmt)
    for cmt in cmts.keys():
        for slip in range(1, region['GPSetup']['trials']+1)
            ...
            rupture = compute_graves_pitarka(eid, alert, ...)
            inputs = build_input_parameters( eid, alert, ...)
            salvus_inputs = build_salvus_parameters( eid, path, ...)
            result = run_salvus( eid, path, ...)
            all_results.append(run_salvus_post(eid, result, ...))
result = run_salvus_plots(eid, basename, domain, resources)
```

Project main achievements

https://eflows4hpc.eu/software/

- Requirements and software architecture
- Definition and implementation of abstractions to support the integration of different stack components
- Design and development of a minimal workflow
- Design and first version of the HPCWaaS methodology
- Design and implementation of the Data Catalogue
- Definition of first version of Pillars’ workflows. Implementation in progress
- First release of project software and documentation available
- Set of internal trainings about software stack components and HPCWaaS
- Good visibility: articles, keynote presentations, media



eFlows4HPC project

Enabling dynamic and Intelligent workflows in the future EuroHPC ecosystem

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» HPCWaaS Methodology

HPCWaaS Methodology

The eFlows4HPC proposes the HPC Workflow as a Service (HPCWaaS) methodology which tries to apply the usage model of the Functions as a Service (FaaS) in Cloud environments to the workflows for HPC systems. In this model, two main roles are identified. From one side, the function developer is in charge of developing and registering the function in the FaaS platform, which transparently deploys the function in the cloud infrastructure. On the other side, the final user executes the deployed function using a REST API. In the case of running workflows in HPC systems, we can find similar roles. First, we can find the workflow developer, which is charge of developing and deploying the workflow in the computing infrastructure, and the users’ communities which are usually scientist who want to execute the workflow and collect their results to advance in their scientific goals.

eFlows4HPC

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Enabling dynamic and intelligent workflows for HPC, data analytics, and AI convergence

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ABSTRACT

The evolution of High-Performance Computing (HPC) platforms enables the design and execution of progressively larger and more complex workflow applications in these systems. The complexity comes not only from the number of elements that compose the workflows but also from the type of computations they perform. While traditional HPC workflows target simulations and modelling of physical phenomena, current needs require in addition data analytics (DA) and artificial intelligence (AI) tasks. However, the development of these workflows is hampered by the lack of proper programming models and environments that support the integration of HPC, DA, and AI, as well as the lack of tools to easily deploy and execute the workflows in HPC systems. To progress in this direction, this paper presents use cases where complex workflows are required and investigates the main issues to be addressed for the HPC/DA/AI convergence. Based on this study, the paper identifies the challenges of a new workflow platform to manage complex workflows. Finally, it proposes a development approach for such a workflow platform addressing these challenges in two directions: first, by defining a software

Conclusions

- There is a need for providing tools for the development of complex workflows that include HPC modeling and simulation, artificial intelligence components and big data
- eFlows4HPC aims at providing a software stack that supports the development, deployment and execution of complex and dynamic workflows
- The HPCWaaS aims to provide a functionality similar for FaaS in cloud for complex workflows in HPC to make it easier the adoption of HPC technologies

Project partners

BSC Barcelona Supercomputing Center
Centro Nacional de Supercomputación

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eFlows4HPC Project

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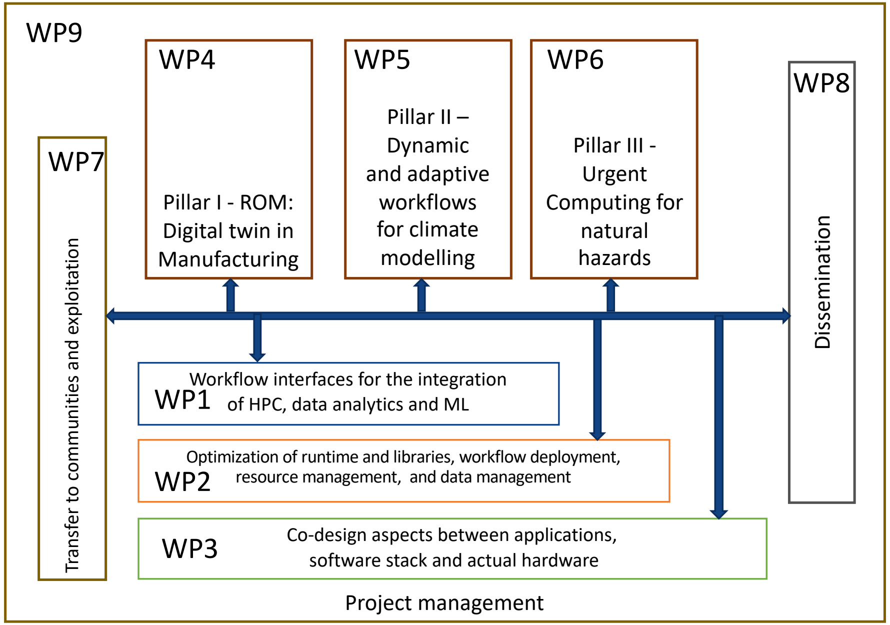
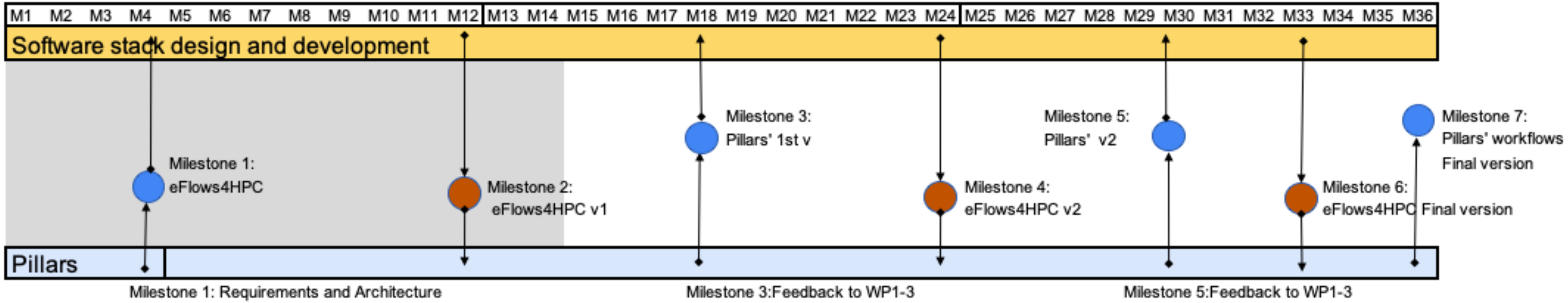
Project WP Structure


WP9
WP4
Pillar I - ROM: Digital twin in Manufacturing
WP5
Pillar II – Dynamic and adaptive workflows for climate modelling
WP6
Pillar III - Urgent Computing for natural hazards
WP7
Transfer to communities and exploitation
WP8
Dissemination
WP1
Workflow interfaces for the integration of HPC, data analytics and ML
WP2
Optimization of runtime and libraries, workflow deployment, resource management, and data management
WP3
Co-design aspects between applications, software stack and actual hardware
Project management

Project RoadMap



M1 M2 M3 M4 M5 M6 M7 M8 M9 M10 M11 M12 M13 M14 M15 M16 M17 M18 M19 M20 M21 M22 M23 M24 M25 M26 M27 M28 M29 M30 M31 M32 M33 M34 M35 M36

Software stack design and development

Milestone 1: eFlows4HPC

Milestone 2: eFlows4HPC v1

Milestone 3: Pillars' 1st v

Milestone 4: eFlows4HPC v2

Milestone 5: Pillars' v2

Milestone 6: eFlows4HPC Final version

Milestone 7: Pillars' workflows Final version

Pillars

Milestone 1: Requirements and Architecture

Milestone 3:Feedback to WP1-3

Milestone 5:Feedback to WP1-3