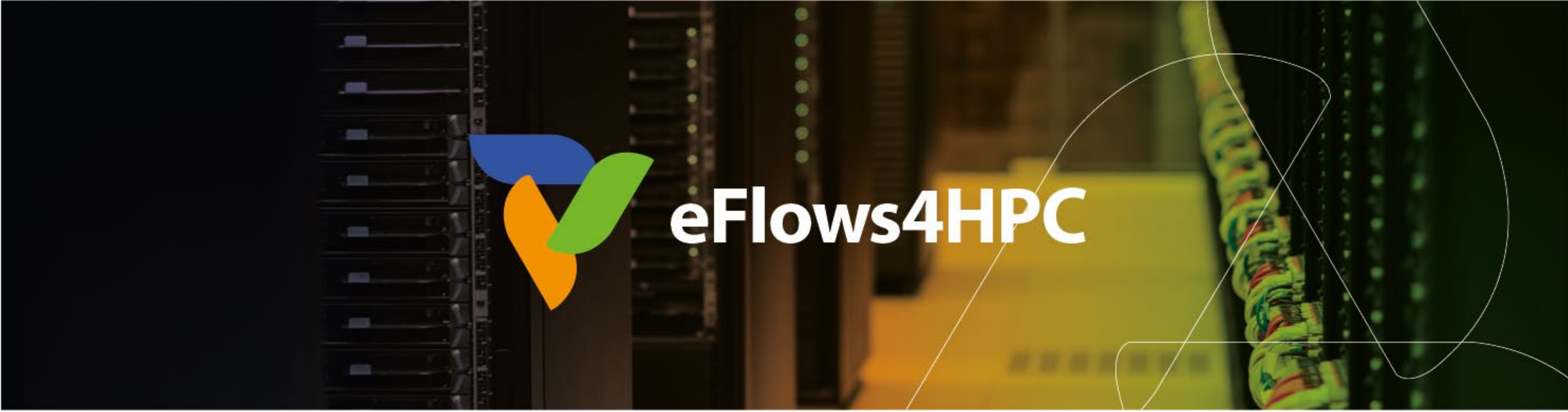


Demo Session: Deployment and Execution of a Workflow with HPCWaaS

Jorge Ejarque (BSC)

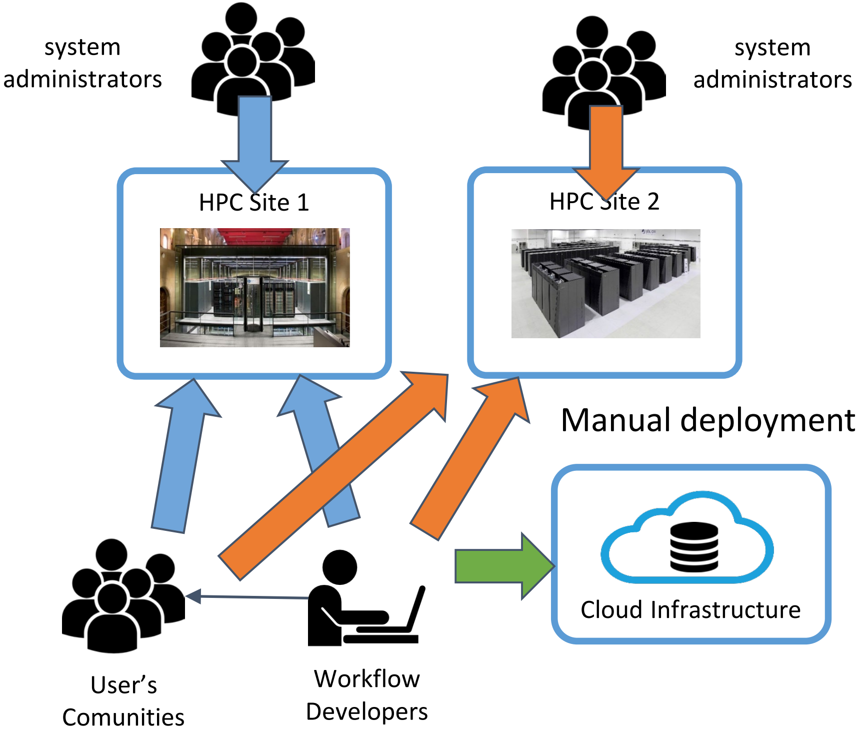
Innovative HPC workflows for industry

Munich, October 25, 2023

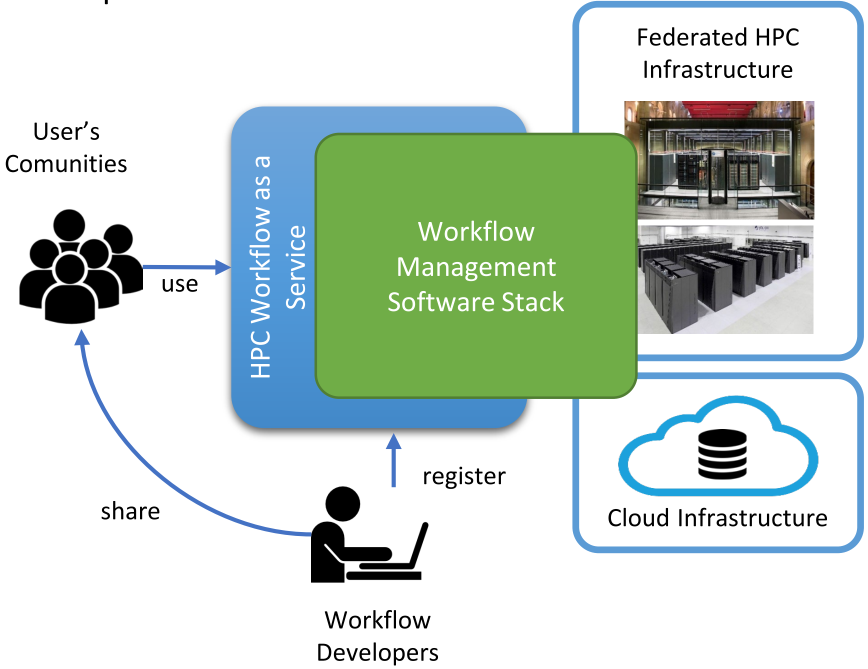
This project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 955558. The JU receives support from the European Union's Horizon 2020 research and innovation programme and Spain, Germany, France, Italy, Poland, Switzerland, Norway. MCIN/AEI/10.13039/501100011033 and the European Union NextGenerationEU/PRTR (PCI2021-121957)

Deployment in HPC Environments

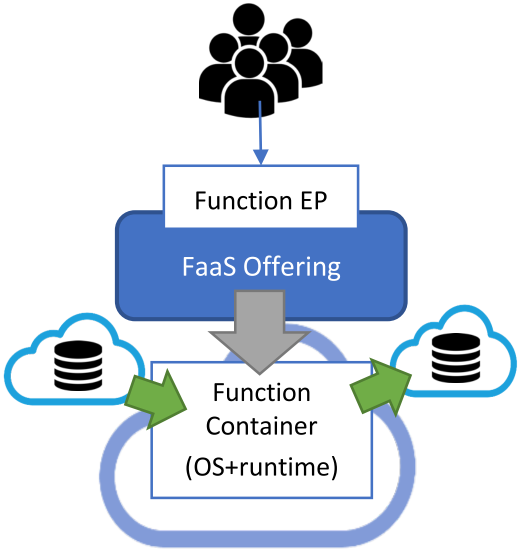
Current approach



Can we apply something like FaaS for Complex Workflows in HPC?


Federated HPC Infrastructure
User's Comunities
use
HPC Workflow as a Service
Workflow Management Software Stack
register
share
Cloud Infrastructure
Workflow Developers

FaaS vs. HPCWaaS

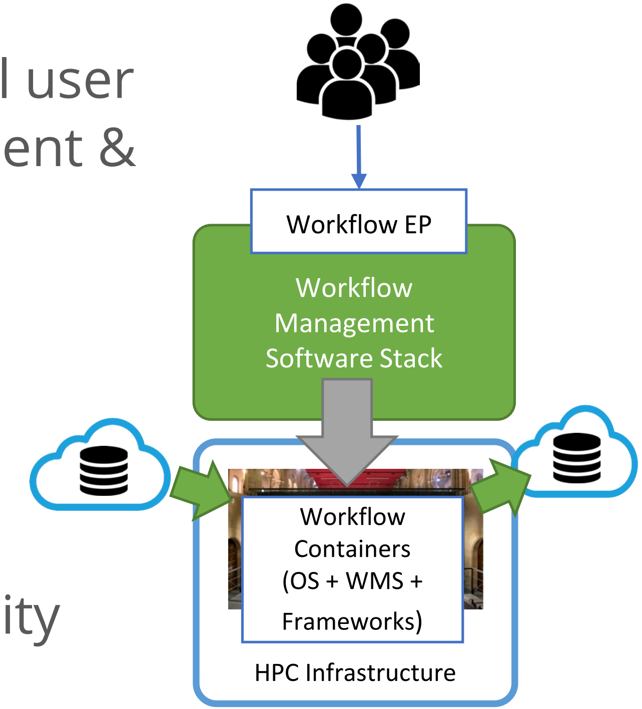


Similarities

- Easy to use for final user
- Automate deployment & execution
- Data integration
- Containers

Differences

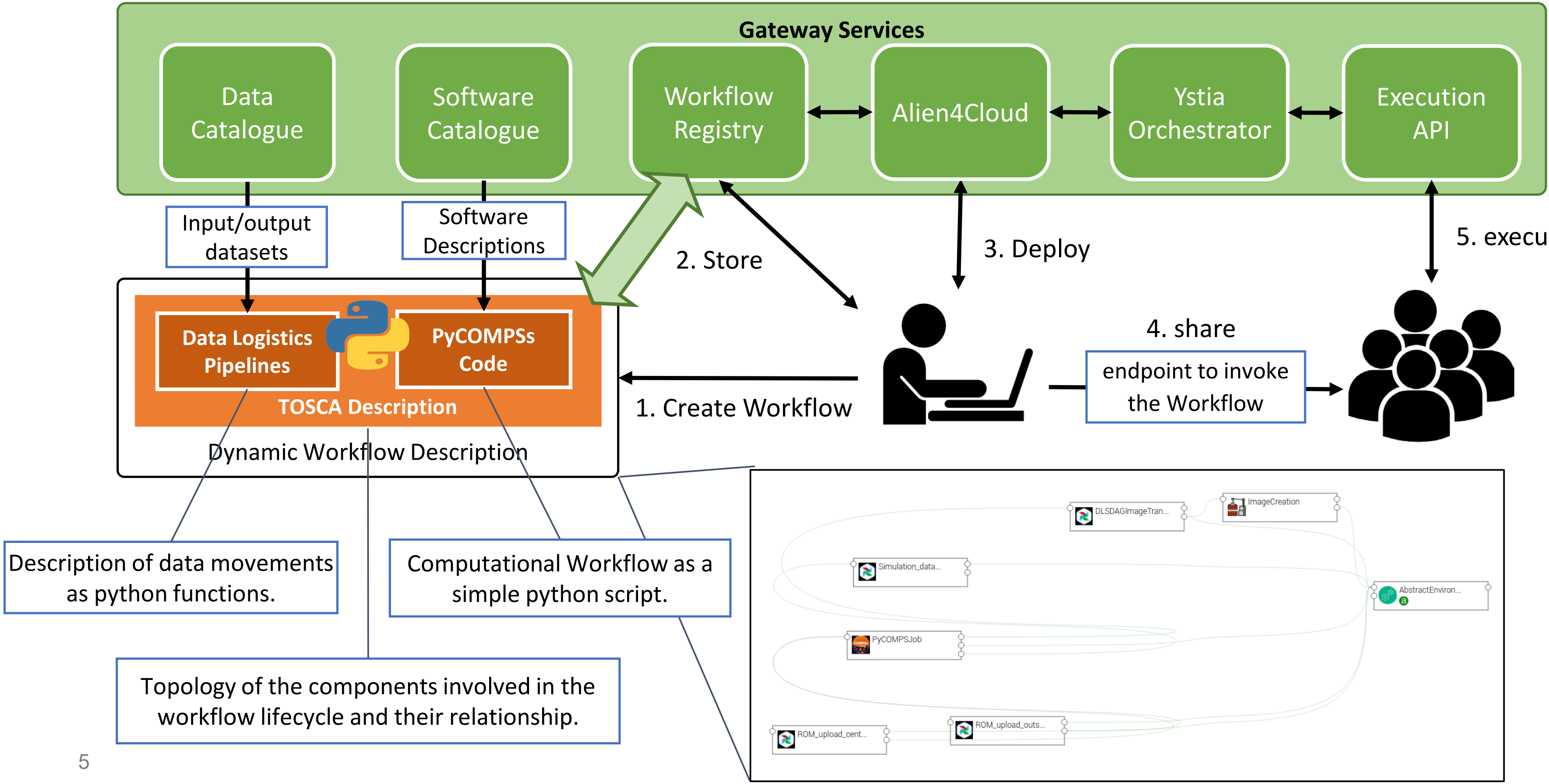
- Restrictions
- Deployment and Execution Complexity
- Performance


Workflow EP
Workflow Management Software Stack
Workflow Containers (OS + WMS + Frameworks)
HPC Infrastructure

ROM Creation Workflow Demo

- Computational Workflow
  - PyCOMPSs Implementation
- Data Management
  - Simulation configuration and meshes stored in the B2DROP and must be moved from/to HPC
  - Data Logistics Service and Data Catalogue
- Software Deployment
  - Workflows Code and required software in the HPC with Containers
  - Container Image Creation:
    - ✓ Build a container tailored for the target HPC machine
- Deployment and Execution Automation
  - TOSCA topology in the workflow registry
  - HPCWaaS:
    - ✓ Key management
    - ✓ Orchestration the Image creation, Data pipeline and PyCOMPS executions

Development Overview



Gateway Services

Data Catalogue

Software Catalogue

Workflow Registry

Alien4Cloud

Ystia Orchestrator

Execution API

Input/output datasets

Software Descriptions

Data Logistics Pipelines

PyCOMPSs Code

TOSCA Description

Dynamic Workflow Description

1. Create Workflow

2. Store

3. Deploy

4. share

endpoint to invoke the Workflow

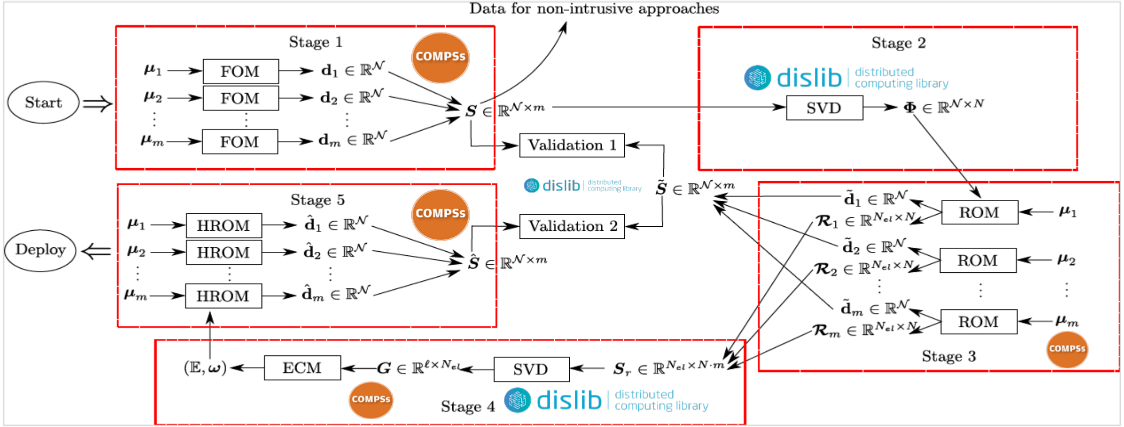
5. execute

Description of data movements as python functions.

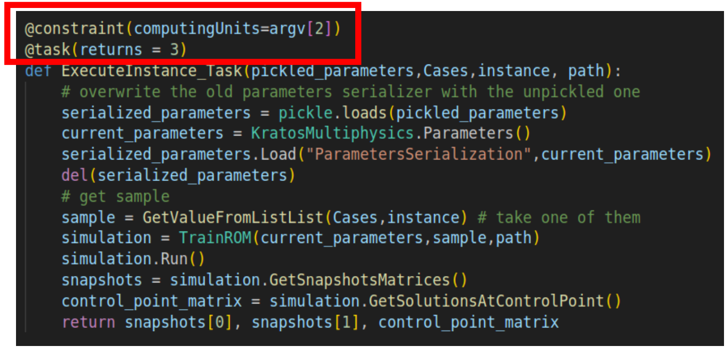
Computational Workflow as a simple python script.

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

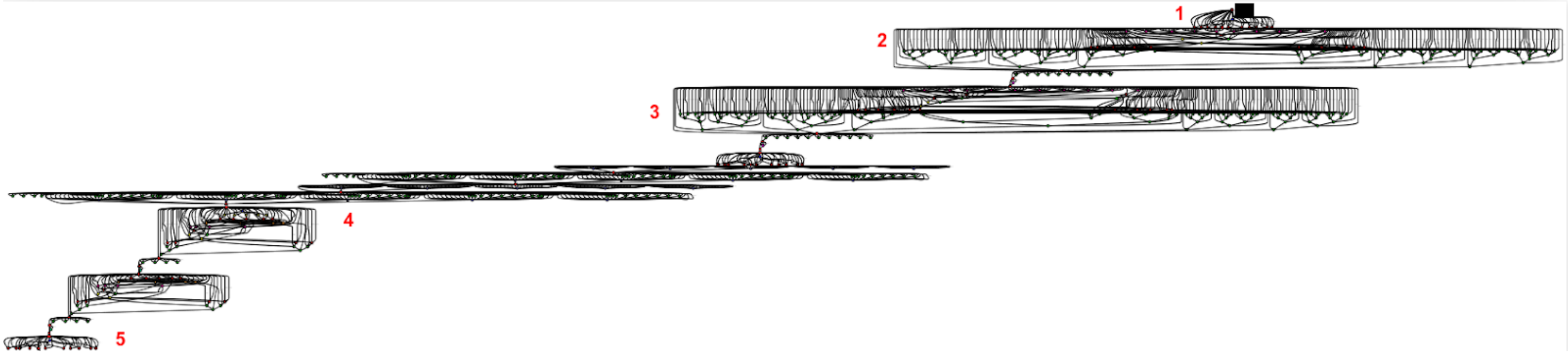
ROM Creation Workflow Implementation



Data for non-intrusive approaches
Start
Stage 1
COMPSs
μ_1 FOM $d_1 \in \mathbb{R}^{\mathcal{N}}$
μ_2 FOM $d_2 \in \mathbb{R}^{\mathcal{N}}$
μ_m FOM $d_m \in \mathbb{R}^{\mathcal{N}}$
$S \in \mathbb{R}^{\mathcal{N} \times m}$
Validation 1
Stage 2
dislib distributed computing library
SVD
$\Phi \in \mathbb{R}^{\mathcal{N} \times N}$
$\tilde{S} \in \mathbb{R}^{\mathcal{N} \times m}$
Stage 5
Deploy
μ_1 HROM $\hat{d}_1 \in \mathbb{R}^{\mathcal{N}}$
μ_2 HROM $\hat{d}_2 \in \mathbb{R}^{\mathcal{N}}$
μ_m HROM $\hat{d}_m \in \mathbb{R}^{\mathcal{N}}$
$\hat{S} \in \mathbb{R}^{\mathcal{N} \times m}$
Validation 2
$\tilde{d}_1 \in \mathbb{R}^{\mathcal{N}}$ $\mathcal{R}_1 \in \mathbb{R}^{N_{el} \times N}$ ROM μ_1
$\tilde{d}_2 \in \mathbb{R}^{\mathcal{N}}$ $\mathcal{R}_2 \in \mathbb{R}^{N_{el} \times N}$ ROM μ_2
$\tilde{d}_m \in \mathbb{R}^{\mathcal{N}}$ $\mathcal{R}_m \in \mathbb{R}^{N_{el} \times N}$ ROM μ_m
Stage 3
$(\mathbb{E}, \omega)$ ECM $G \in \mathbb{R}^{\ell \times N_{el}}$ SVD $S_r \in \mathbb{R}^{N_{el} \times N \cdot m}$
Stage 4

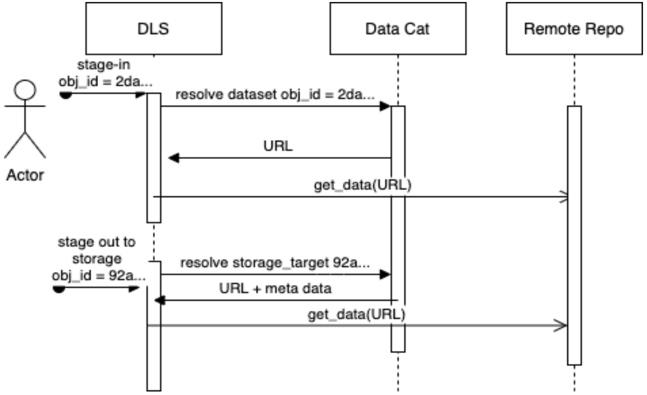


```
@constraint(computingUnits=argv[2])
@task(returns = 3)
def ExecuteInstance_Task(pickled_parameters,Cases,instance, path):
    # overwrite the old parameters serializer with the unpickled one
    serialized_parameters = pickle.loads(pickled_parameters)
    current_parameters = KratosMultiphysics.Parameters()
    serialized_parameters.Load("ParametersSerialization",current_parameters)
    del(serialized_parameters)
    # get sample
    sample = GetValueFromListList(Cases,instance) # take one of them
    simulation = TrainROM(current_parameters,sample,path)
    simulation.Run()
    snapshots = simulation.GetSnapshotsMatrices()
    control_point_matrix = simulation.GetSolutionsAtControlPoint()
    return snapshots[0], snapshots[1], control_point_matrix
```



Data pipelines

- Implemented in Data Logistics Service
- Reusable for multiple data/workflows
- Configured from Data Catalogue



DLS

Data Cat

Remote Repo

Actor

stage-in
obj_id = 2da...

resolve dataset obj_id = 2da...

URL

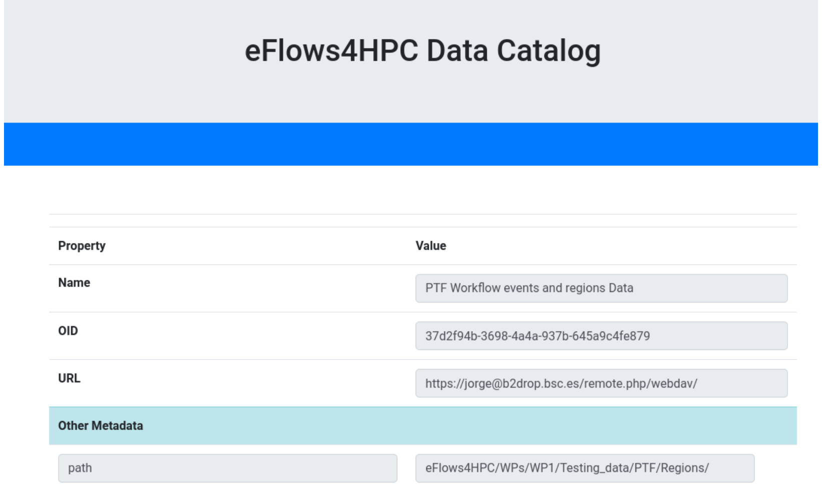
get_data(URL)

stage out to
storage
obj_id = 92a...

resolve storage_target 92a...

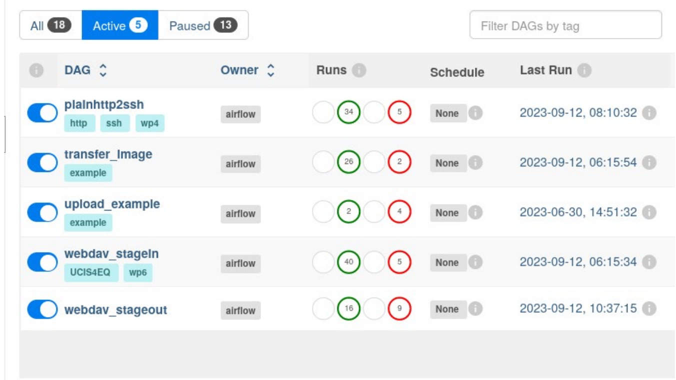
URL + meta data

get_data(URL)



eFlows4HPC Data Catalog

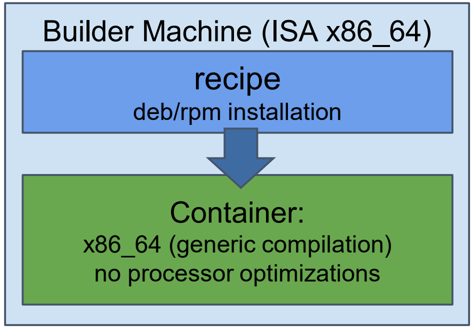
Property	Value
Name	PTF Workflow events and regions Data
OID	37d2f94b-3698-4a4a-937b-645a9c4fe879
URL	https://jorge@b2drop.bsc.es/remote.php/webdav/
Other Metadata	
path	eFlows4HPC/WPs/WP1/Testing_data/PTF/Regions/



DAG	Owner	Runs	Schedule	Last Run
plainhttp2ssh http ssh wp4	airflow	○ 34 ○ 5	None	2023-09-12, 08:10:32
transfer_Image example	airflow	○ 26 ○ 2	None	2023-09-12, 06:15:54
upload_example example	airflow	○ 2 ○ 4	None	2023-06-30, 14:51:32
webdav_stageIn UCIS4EQ wp6	airflow	○ 40 ○ 5	None	2023-09-12, 06:15:34
webdav_stageout	airflow	○ 16 ○ 9	None	2023-09-12, 10:37:15

Containers and HPC

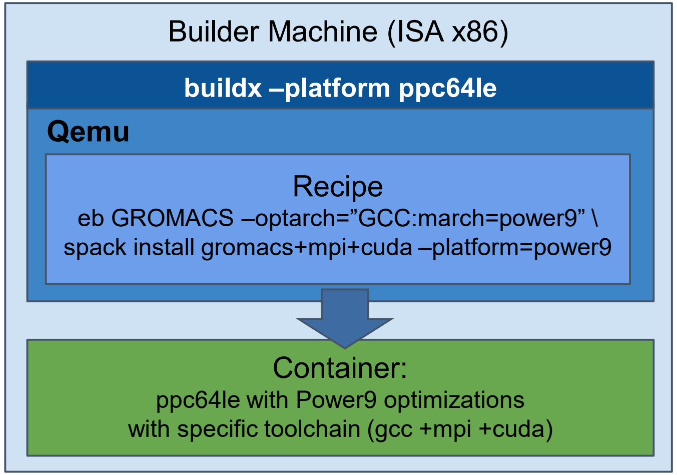
Standard container image creation


Builder Machine (ISA x86_64)
recipe
deb/rpm installation
Container:
x86_64 (generic compilation)
no processor optimizations

- **Simplicity for deployment**
  - Just pull or download the image
- **Trade-Off performance/portability**
  - Architecture Optimizations
- **Accessing Hardware from Containers**
  - MPI Fabric /GPUs
- **Host-Container Version Compatibility**

HPC Ready Containers

eFlows4HPC approach



Builder Machine (ISA x86)

buildx –platform ppc64le

Qemu

Recipe

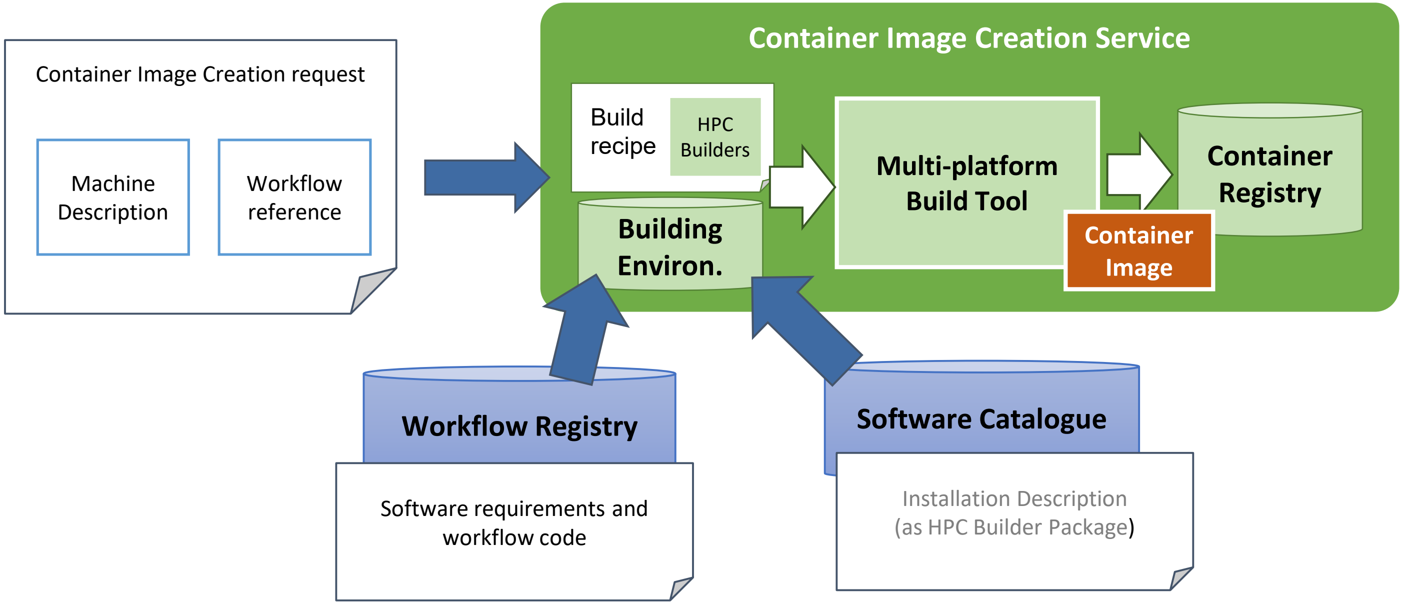
eb GROMACS –optarch="GCC:march=power9" \
spack install gromacs+mpi+cuda –platform=power9

Container:

ppc64le with Power9 optimizations
with specific toolchain (gcc +mpi +cuda)

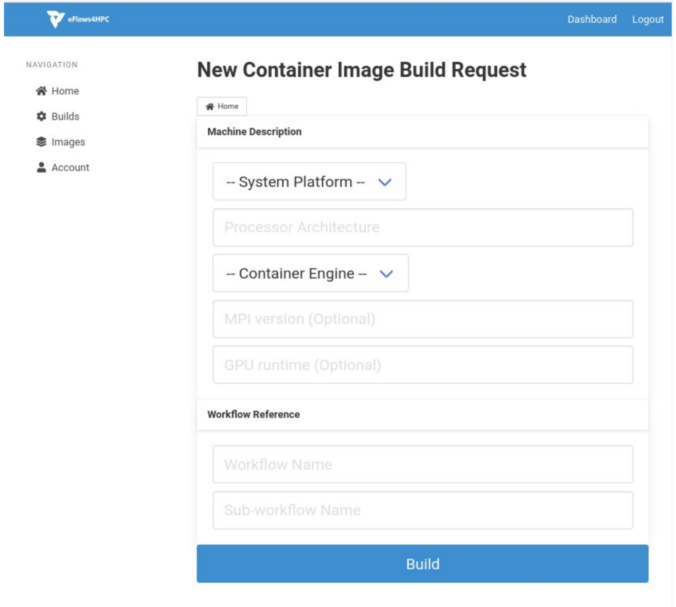
- **Methodology to allow the creation containers for specific HPC system**
  - Leverage HPC and Multi-platform container builders
- **It is tight to do by hand but let's automate!**

Container Image Creation Service


Container Image Creation request
Machine Description
Workflow reference
Container Image Creation Service
Build recipe
HPC Builders
Building Environ.
Multi-platform Build Tool
Container Image
Container Registry
Workflow Registry
Software requirements and workflow code
Software Catalogue
Installation Description (as HPC Builder Package)

Container Image Creation Service

- Web Interface



New Container Image Build Request

Machine Description

-- System Platform --

Processor Architecture

-- Container Engine --

MPI version (Optional)

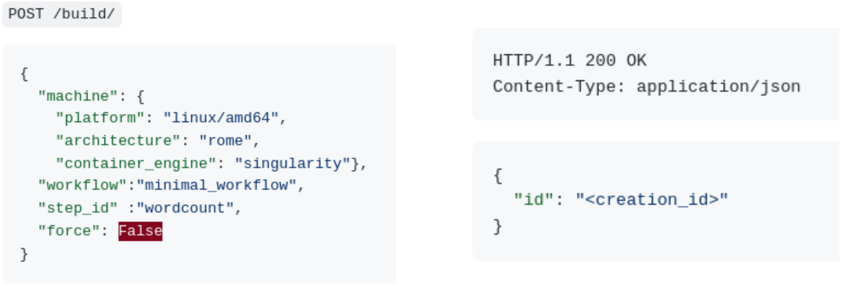
GPU runtime (Optional)

Workflow Reference

Workflow Name

Sub-workflow Name

- REST Interface and CLI

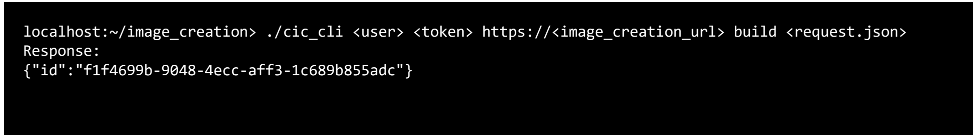


```
POST /build/
```

```
{
  "machine": {
    "platform": "linux/amd64",
    "architecture": "rome",
    "container_engine": "singularity"},
  "workflow":"minimal_workflow",
  "step_id" :"wordcount",
  "force": False
}
```

```
HTTP/1.1 200 OK
Content-Type: application/json
```

```
{
  "id": "<creation_id>"
}
```

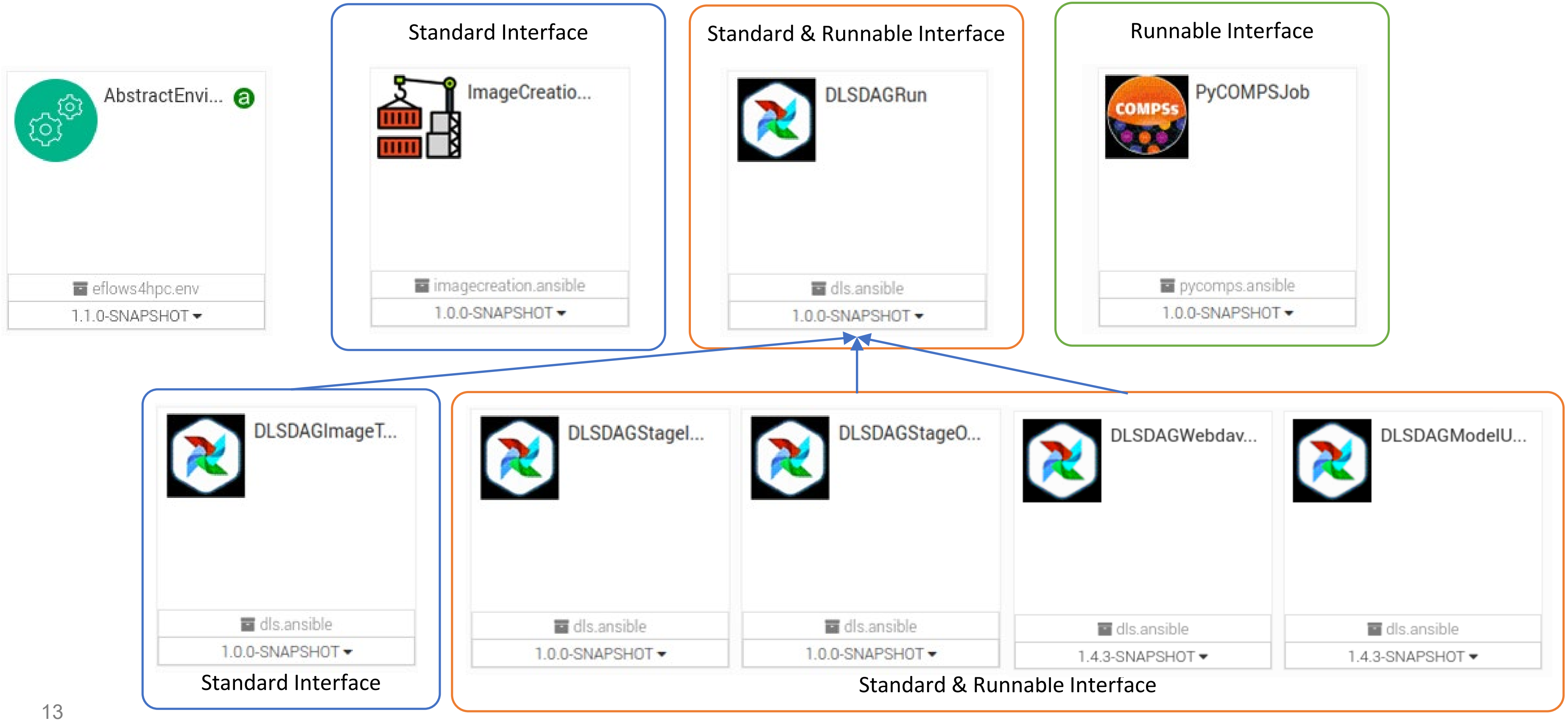


```
localhost:~/image_creation> ./cic_cli <user> <token> https://<image_creation_url> build <request.json>
Response:
{"id":"f1f4699b-9048-4ecc-aff3-1c689b855adc"}
```

TOSCA Model

- **Describe the orchestration of the application lifecycle management**
- **Topology of components with dependencies**
  - Application Component:
    - Describe what to do in every lifecycle step
      - ✓ Standard tosca steps (start, stop, delete,…)
      - ✓ Extended runnable (submit, run, cancel,…) Integrate jobs in Tosca.
    - The required input data and properties
  - Dependencies:
    - Describe the data exchanged between components.
- **Workflows**
  - Topology generate the standard TOSCA workflows to deploy/undeploy the application
  - Custom workflows

eFlows4HPC TOSCA Components



AbstractEnvi... a
eflows4hpc.env
1.1.0-SNAPSHOT ▾

Standard Interface

ImageCreatio...
imagecreation.ansible
1.0.0-SNAPSHOT ▾

Standard & Runnable Interface

DLSDAGRun
dls.ansible
1.0.0-SNAPSHOT ▾

Runnable Interface

PyCOMPSJob
pycomps.ansible
1.0.0-SNAPSHOT ▾

DLSDAGImageT...
dls.ansible
1.0.0-SNAPSHOT ▾

Standard Interface

DLSDAGStageI...
dls.ansible
1.0.0-SNAPSHOT ▾

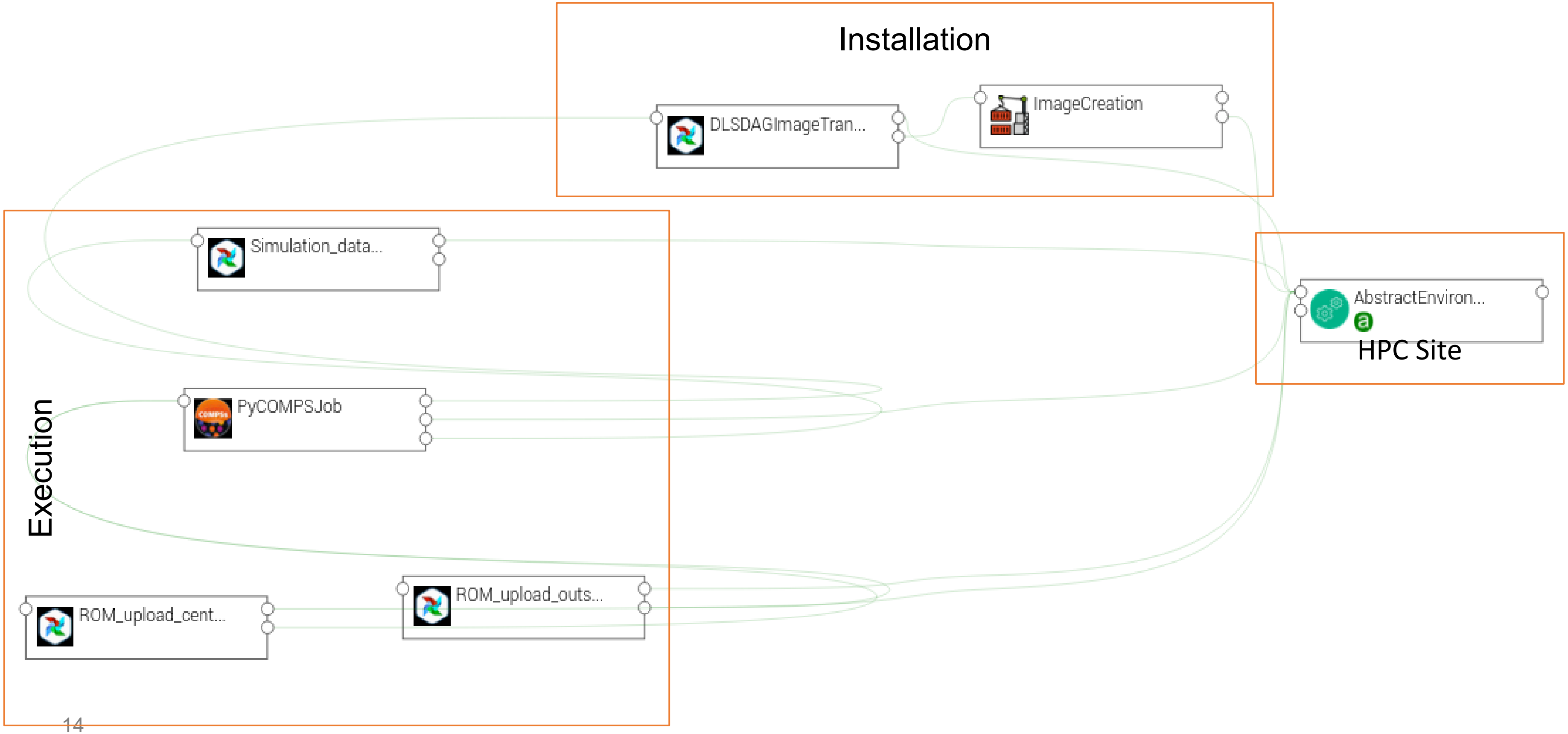
DLSDAGStageO...
dls.ansible
1.0.0-SNAPSHOT ▾

DLSDAGWebdav...
dls.ansible
1.4.3-SNAPSHOT ▾

DLSDAGModelU...
dls.ansible
1.4.3-SNAPSHOT ▾

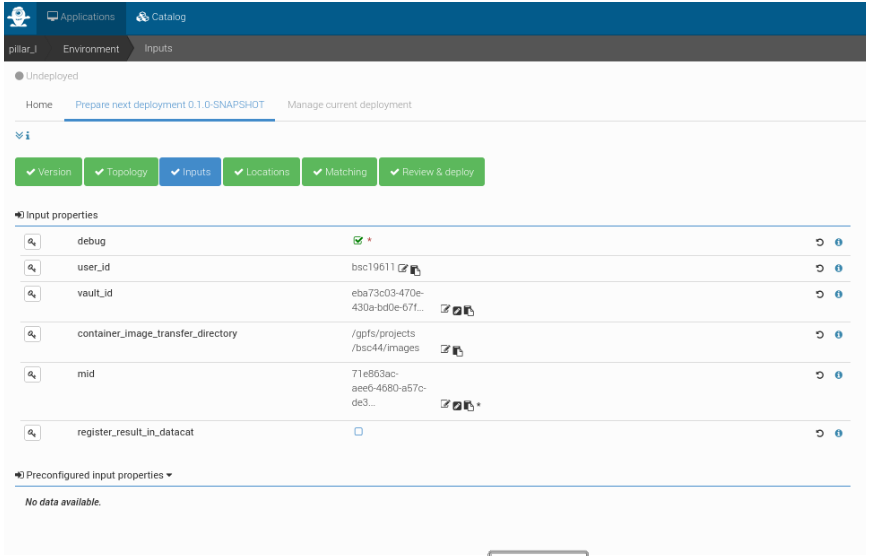
Standard & Runnable Interface

TOSCA Modelization



Workflow Deployment (done once per HPC site)

- Set deployment input parameters (user, credential, select HPC location)



pillar_I › Environment › Inputs

● Undeployed

Home | Prepare next deployment 0.1.0-SNAPSHOT | Manage current deployment

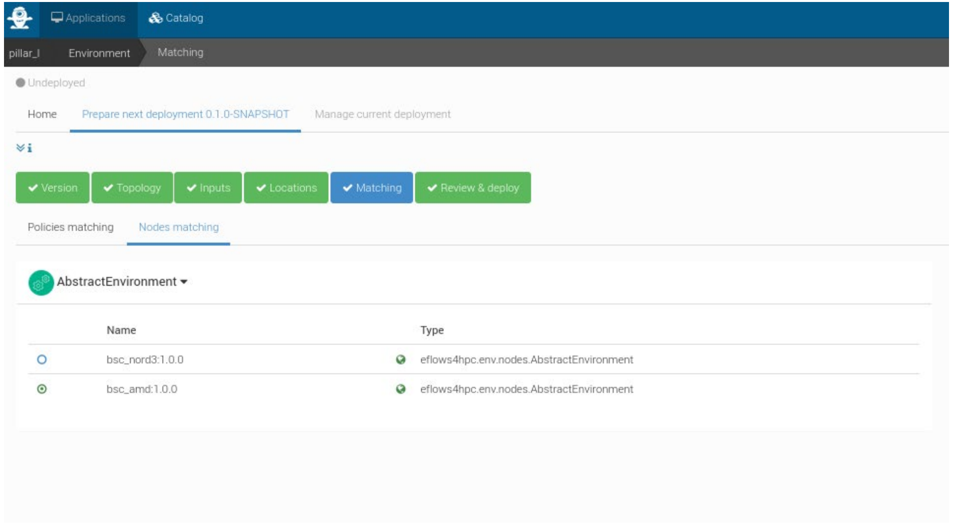
✓ Version | ✓ Topology | ✓ Inputs | ✓ Locations | ✓ Matching | ✓ Review & deploy

Input properties

debug	☑ *	
user_id	bsc19611	
vault_id	eba73c03-470e-430a-bd0e-67f...	
container_image_transfer_directory	/gpfs/projects/bsc44/images	
mid	71e863ac-aee6-4680-a57c-de3...	*
register_result_in_datacat	□	

Preconfigured input properties ▾

No data available.



pillar_I › Environment › Matching

● Undeployed

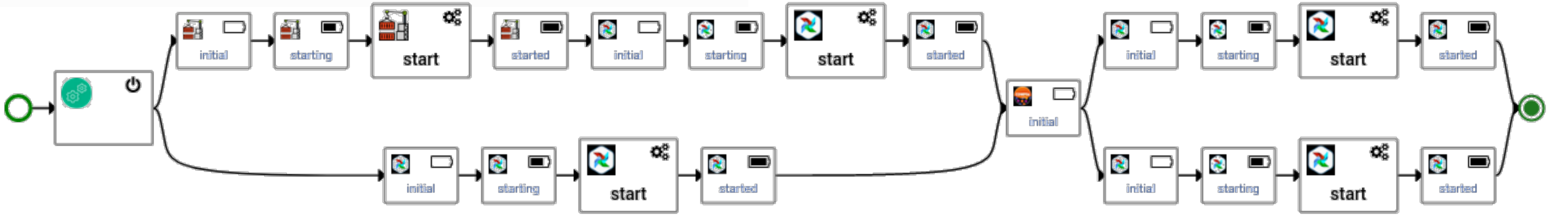
Home | Prepare next deployment 0.1.0-SNAPSHOT | Manage current deployment

✓ Version | ✓ Topology | ✓ Inputs | ✓ Locations | ✓ Matching | ✓ Review & deploy

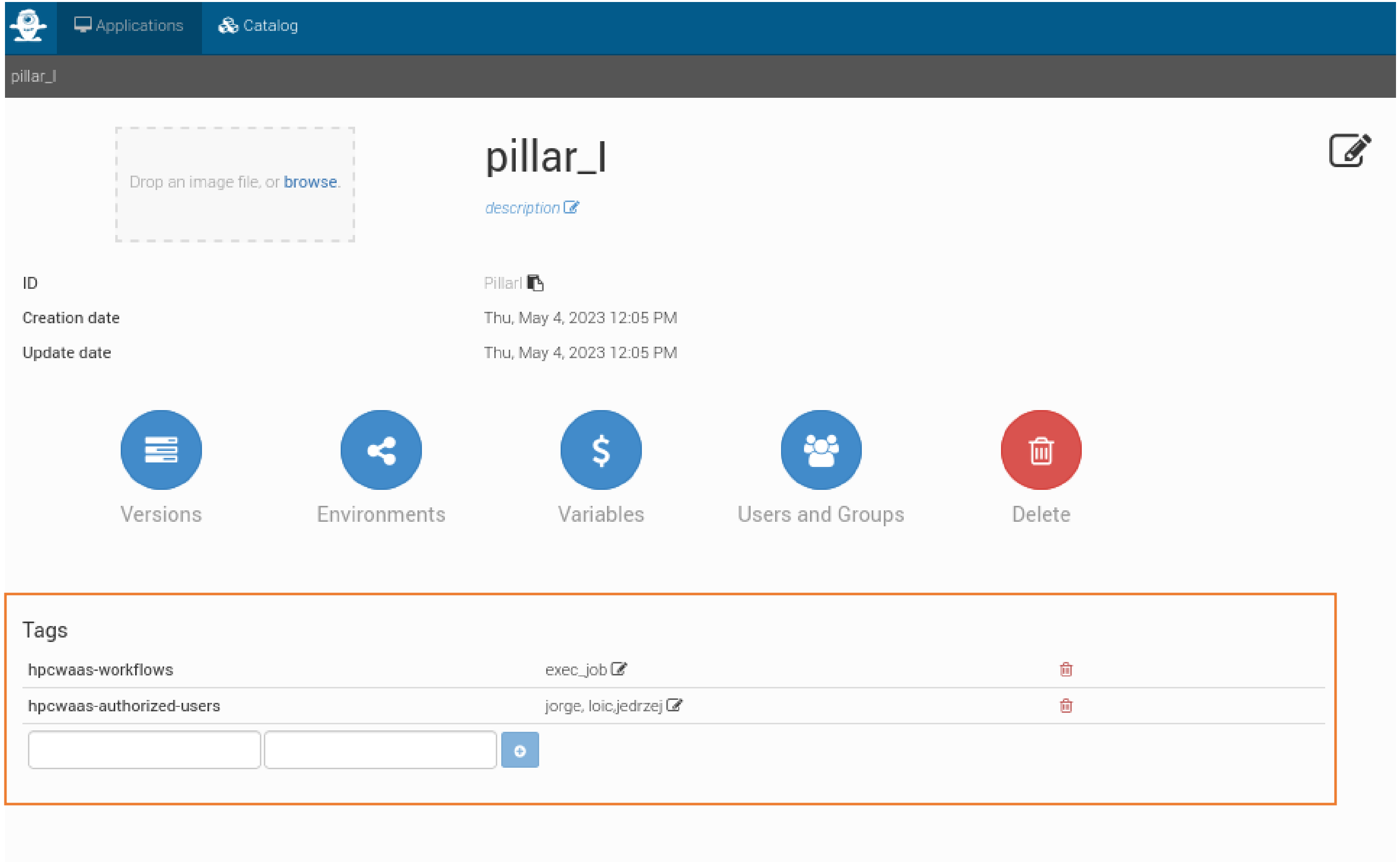
Policies matching | Nodes matching

AbstractEnvironment ▾

	Name	Type
○	bsc_nord3:1.0.0	eflows4hpc.env.nodes.AbstractEnvironment
◉	bsc_amd:1.0.0	eflows4hpc.env.nodes.AbstractEnvironment



Publish workflow and authorize users



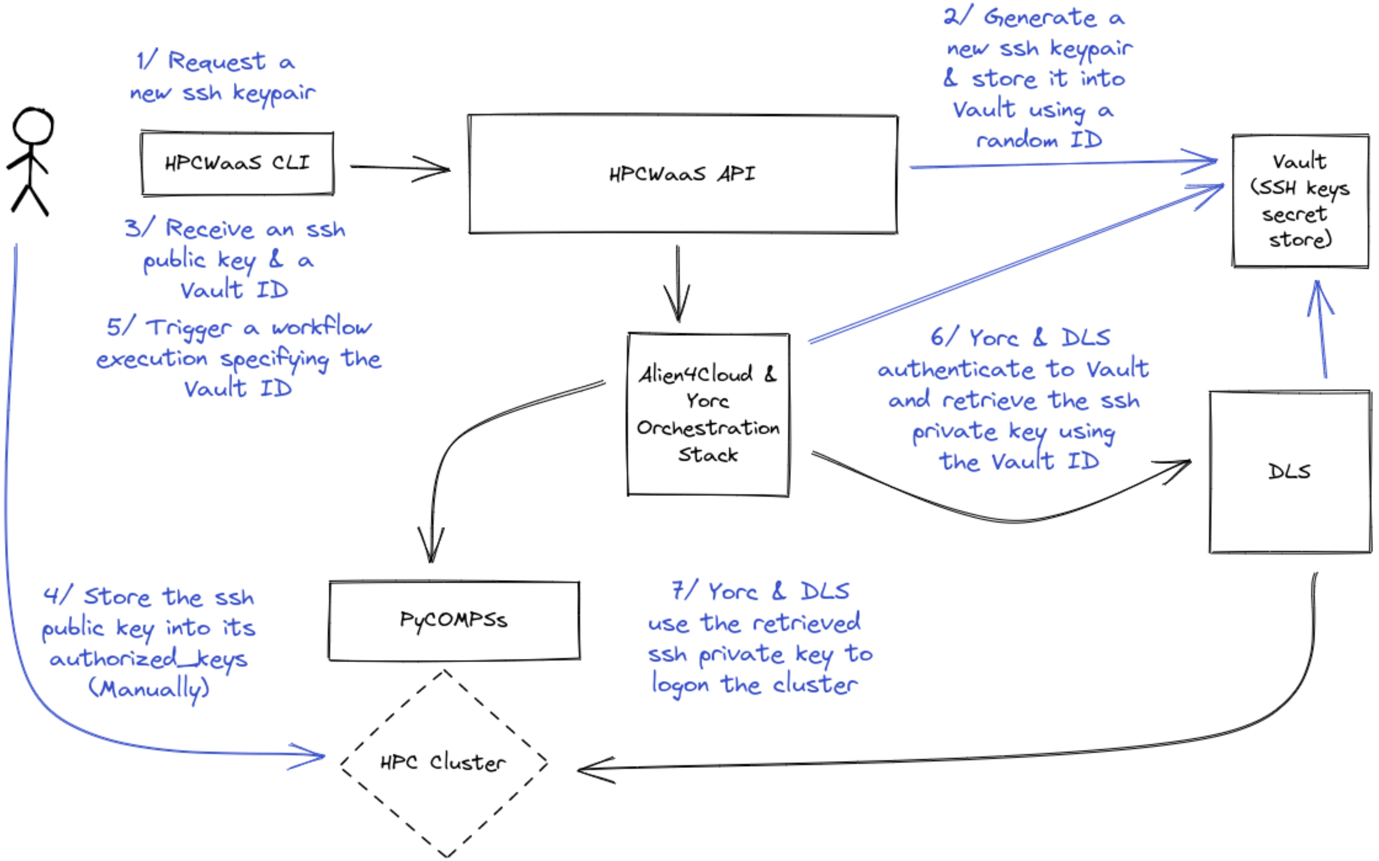
pillar_I

ID	PillarI
Creation date	Thu, May 4, 2023 12:05 PM
Update date	Thu, May 4, 2023 12:05 PM

Tags

hpcwaas-workflows	exec_job
hpcwaas-authorized-users	jorge, loic,jedrzej

Workflow Execution End user



1/ Request a new ssh keypair

2/ Generate a new ssh keypair & store it into Vault using a random ID

3/ Receive an ssh public key & a Vault ID

4/ Store the ssh public key into its authorized_keys (Manually)

5/ Trigger a workflow execution specifying the Vault ID

6/ Yorc & DLS authenticate to Vault and retrieve the ssh private key using the Vault ID

7/ Yorc & DLS use the retrieved ssh private key to logon the cluster

HPCWaaS CLI
HPCWaaS API
Vault (SSH keys secret store)
Alien4Cloud & Yorc Orchestration Stack
DLS
PyCOMPSs
HPC Cluster

Thank you

eFlows4HPC

Enabling dynamic and Intelligent workflows
in the future EuroHPC ecosystem

www.eFlows4HPC.eu

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This project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 955558. The JU receives support from the European Union’s Horizon 2020 research and innovation programme and Spain, Germany, France, Italy, Poland, Switzerland, Norway.