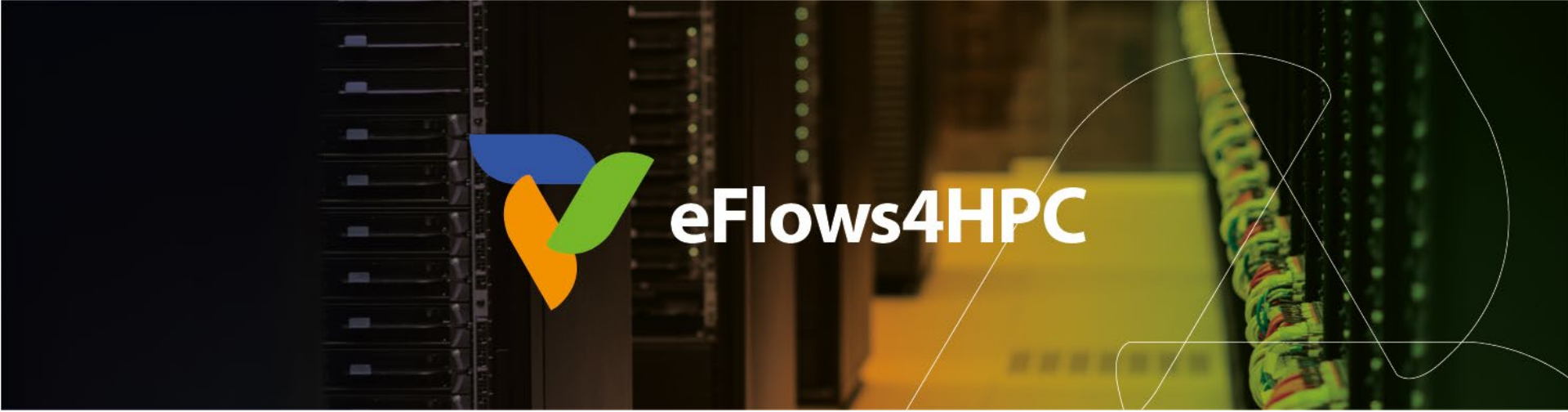

Demo Session: Deployment and Execution the PTF Workflow with HPCWaaS

Jorge Ejarque (BSC)

Next-generation HPC workflows for natural hazards

Barcelona, September 13, 2023

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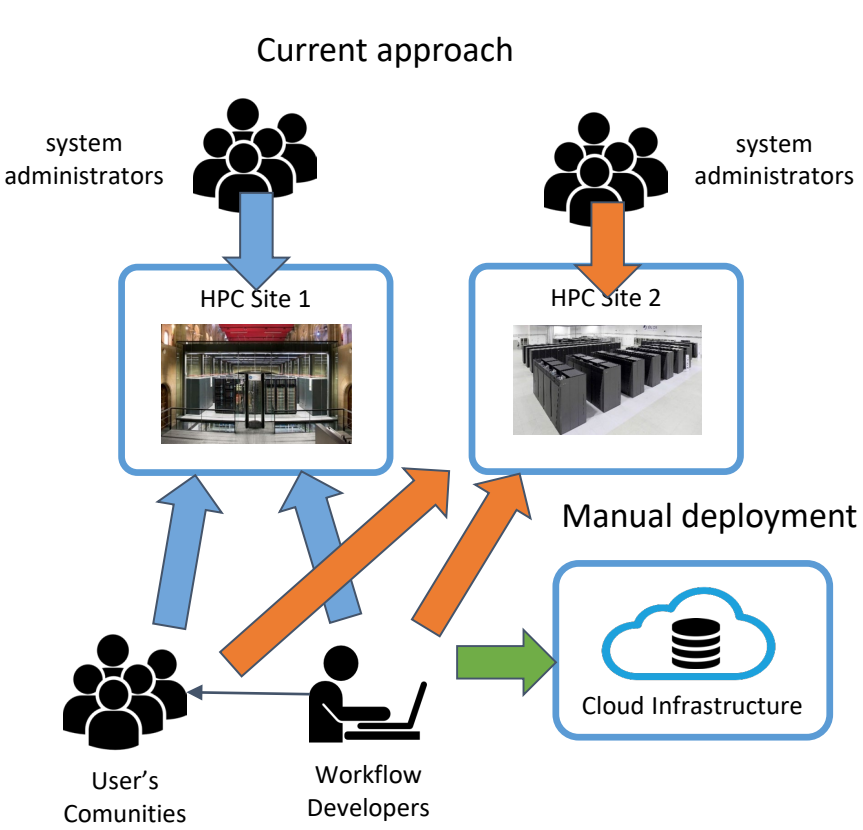
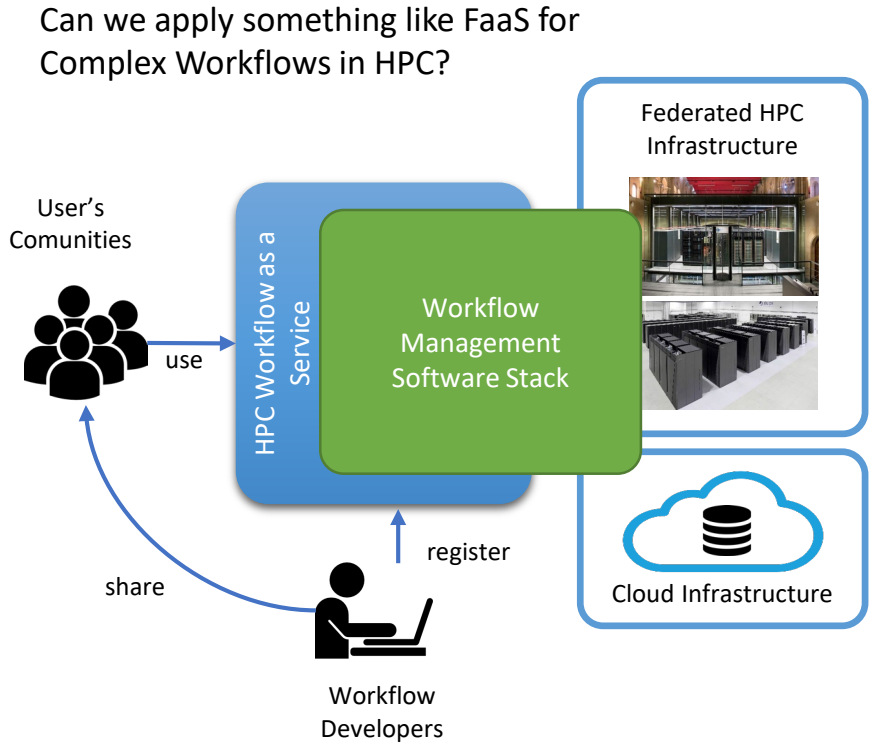
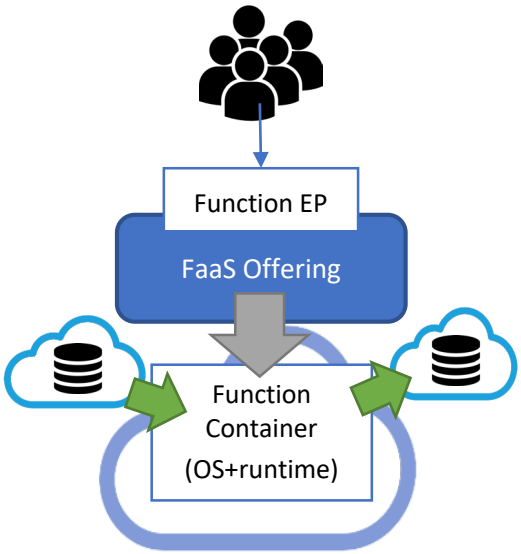
Deployment in HPC Environments





FaaS vs. HPCWaaS

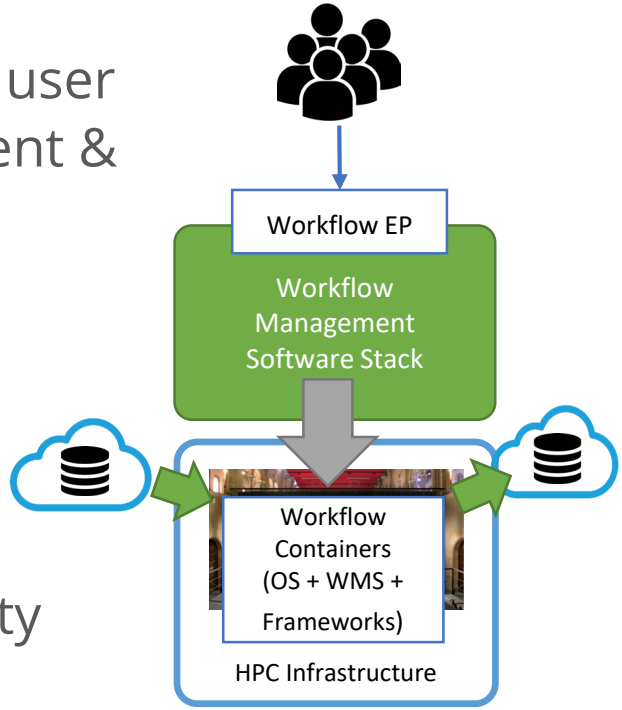


Similarities

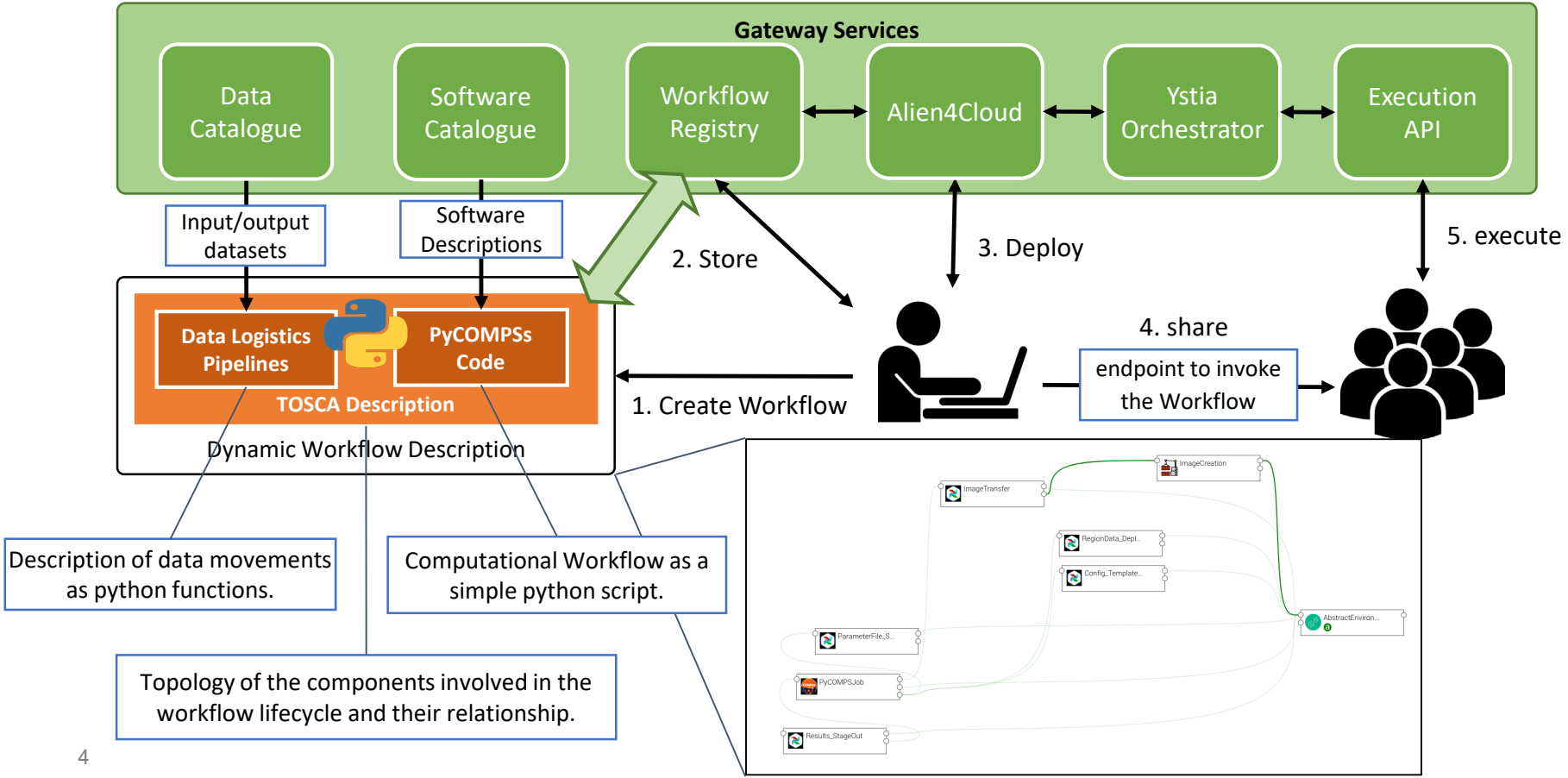
- Easy to use for final user
- Automate deployment & execution
- Data integration
- Containers

Differences

- Restrictions
- Deployment and Execution Complexity
- Performance



Development Overview



PTF Workflow

- Data Management
  - Required data and Results 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

PyCOMPSs

```
@binary(binary=config_bin)
@task(config_file=FILE_OUT)
def build_config(config_template, config_file, data_dir, files_step2, par_file, kag, tsu, event_id):
    pass
```

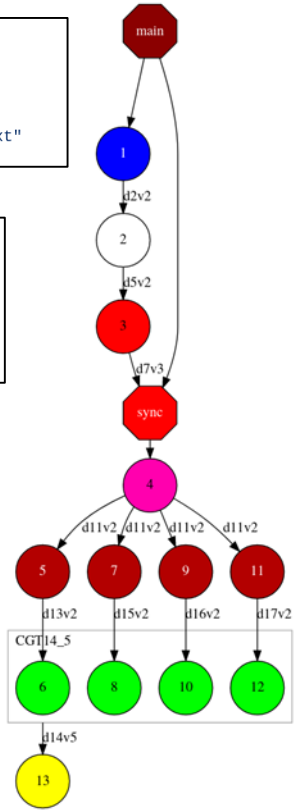
```
@task(config_file=FILE_IN, returns=1)
def step1_func(args, config_file, seistype, sim_files_step1):
    args.cfg=config_file
    run_step1_init(args,sim_files_step1)
    return sim_files_step1 + "/Step1_scenario_list_"+seistype+".txt"
```

```
@binary(binary=simulBS_bin, working_dir="{{wdir}}")
@task(sim_files_step2=FILE_OUT)
def build_structure(seistype, grid, hours, group, sim_files_step2, load_balancing, pois_ts_file,
    pass
```

```
@constraint(processors=[{'processorType':'CPU', 'computingUnits':'1'},
                        {'processorType':'GPU', 'computingUnits':'1'}])
@mpi(binary=tsunamiHySEA_bin, args="{{file_in}}", runner="mpirun", processes=gpus_per_exec, processes_per_node=gpus_per_node,working_dir="{{wdir}}")
@task(file_in=FILE_IN,returns=1)
def mpi_func(file_in, wdir):
     pass
```

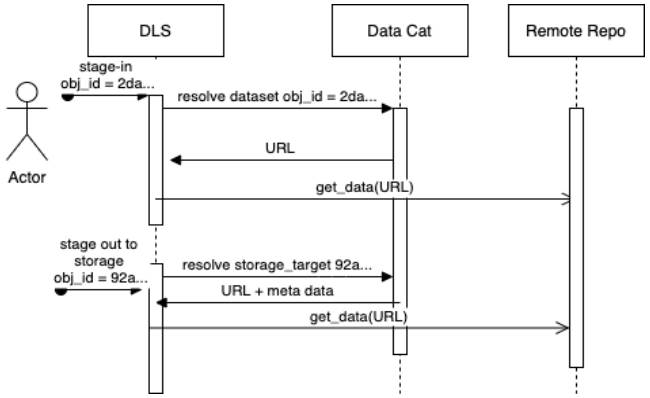
```
@task(ptf_files=COMMUTATIVE, config_file=FILE_IN)
def append_and_evaluate(ptf_files, ptf_file, args, config_file, sim_files_step1, out_step2_path, out_update_path, out_final, depth_file, log_file, sim_pois_ts, num_sims, kag, tsu,
    args.cfg = config_file
    ptf_files.append(ptf_file)
    if (num_sims != 0) and (len(ptf_files) % num_sims == 0):
        step2_create_ptf_input(ptf_files, out_step2_path, depth_file, log_file)
        if kag>0:
            run_step_kagan(args,sim_files_step1,out_update_path)
            sim_files_input=out_update_path
        elif tsu>0:
            run_step_mare(args, sim_files_step1, out_update_path, sim_pois_ts, ptf_files)
            sim_files_input=out_update_path
        else:
            sim_files_input=sim_files_step1
        run_step3_init(args, sim_files_input, out_final, sim_pois_ts, ptf_files)
```

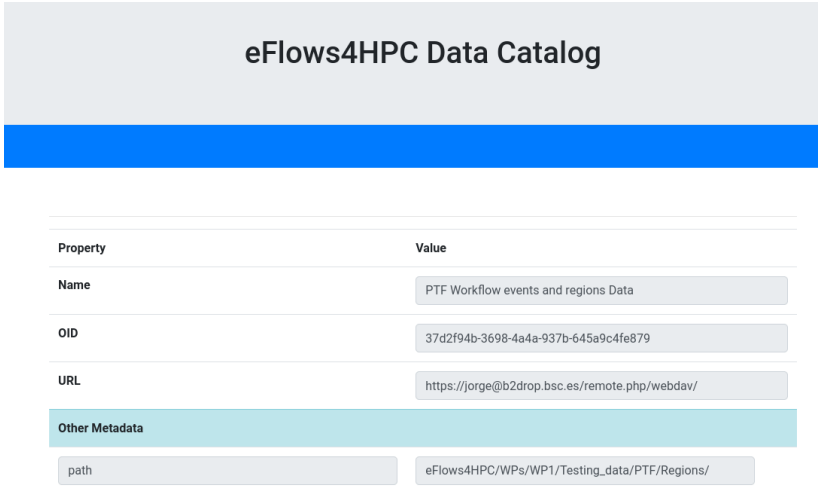
```
@binary(binary="tar", args="zcvf {{outfile}} {{folder}}")
@task(outfile=FILE_OUT)
def compress(folder, outfile, ptf_files):
    pass
```

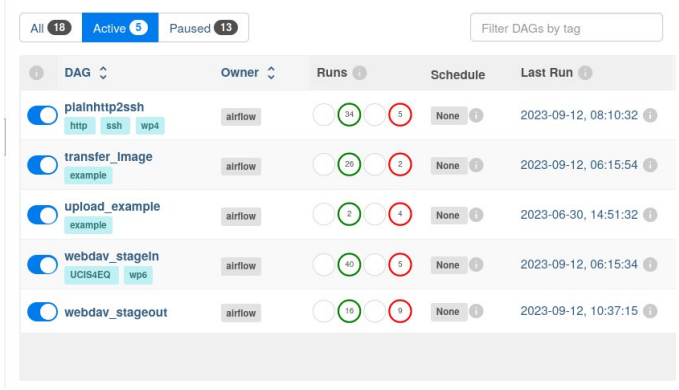


Data pipelines

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

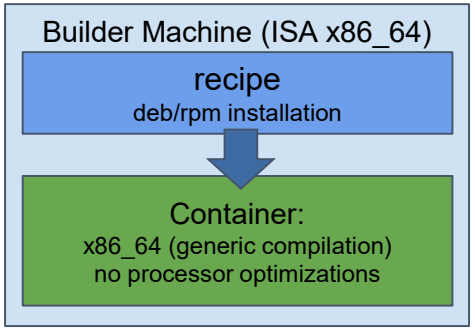






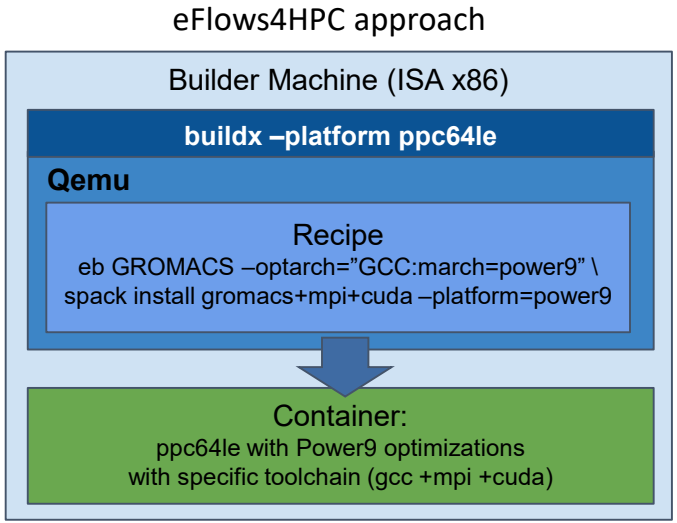
Containers and HPC

Standard container image creation



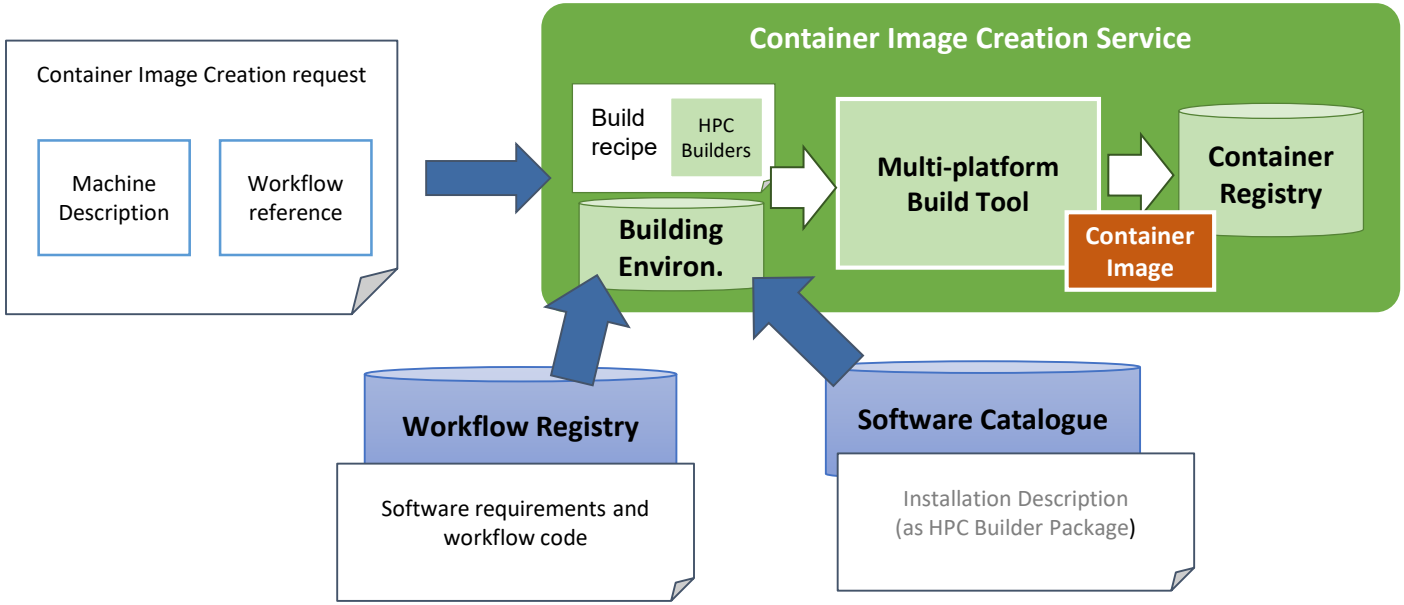
- **Simplicity for deployment**
  - Just pull or download the image
- **Trade-Off performance/portability**
  - Architecture Optimizations
- **Accessing Hardware from Containers**
  - MPI Fabric /GPUs
- **Host-Container Version Compatibility**

HPC Ready Containers



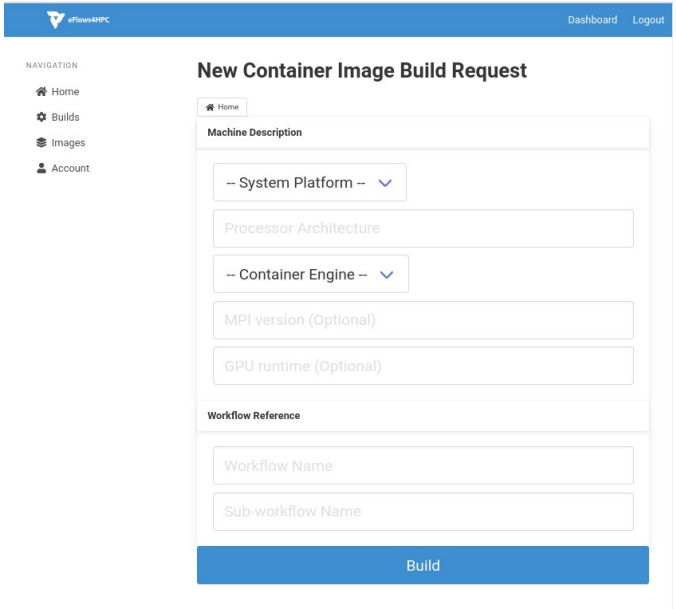
- **Methodology to allow the creation containers for specific HPC system**
  - Leverage HPC and Multi-platform container builders
- **It is tight to do by hand but let’s automate!**

Container Image Creation Service



Container Image Creation Service

- Web Interface



- 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
```

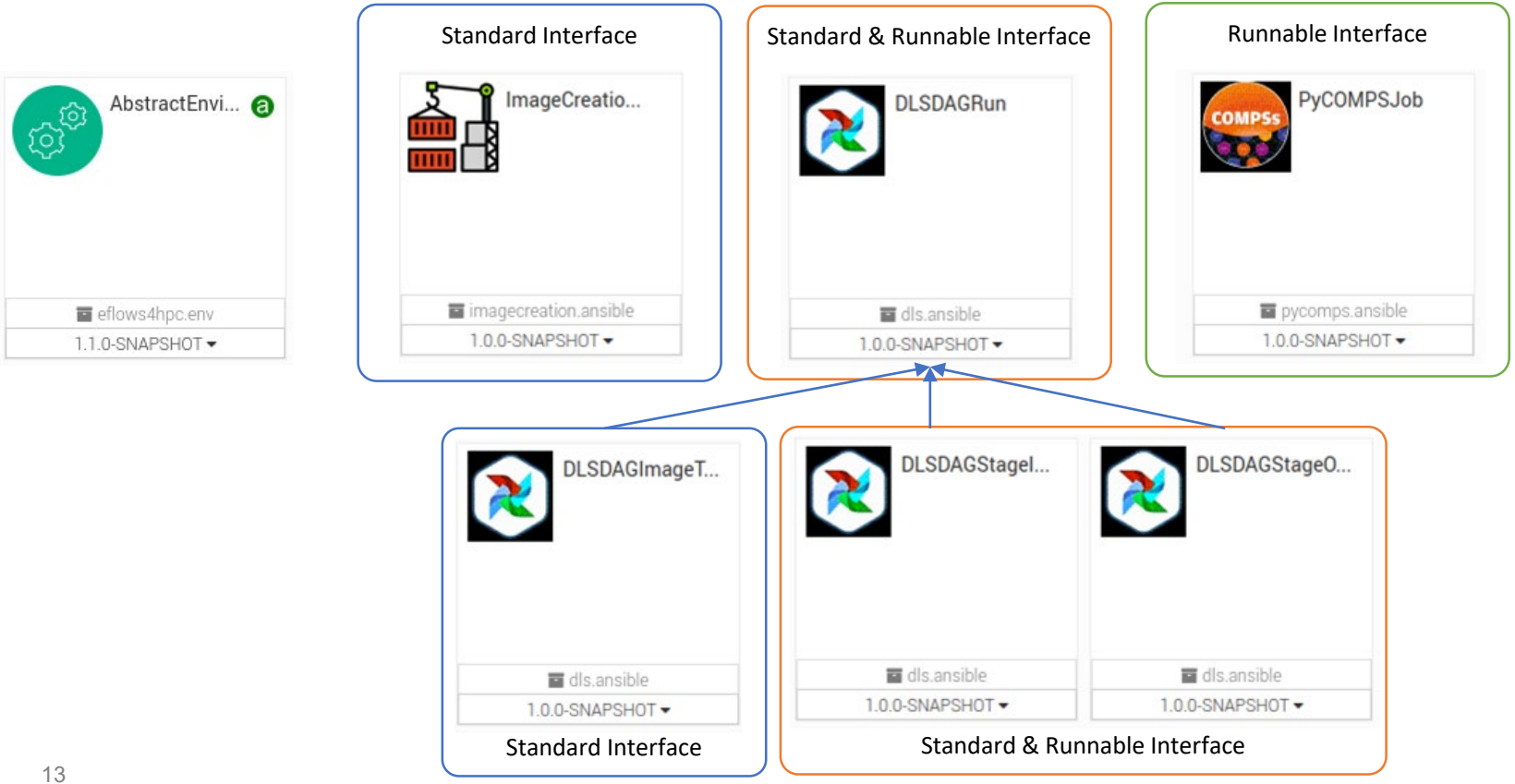
```
{
  "id": "<creation_id>"
}
```

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

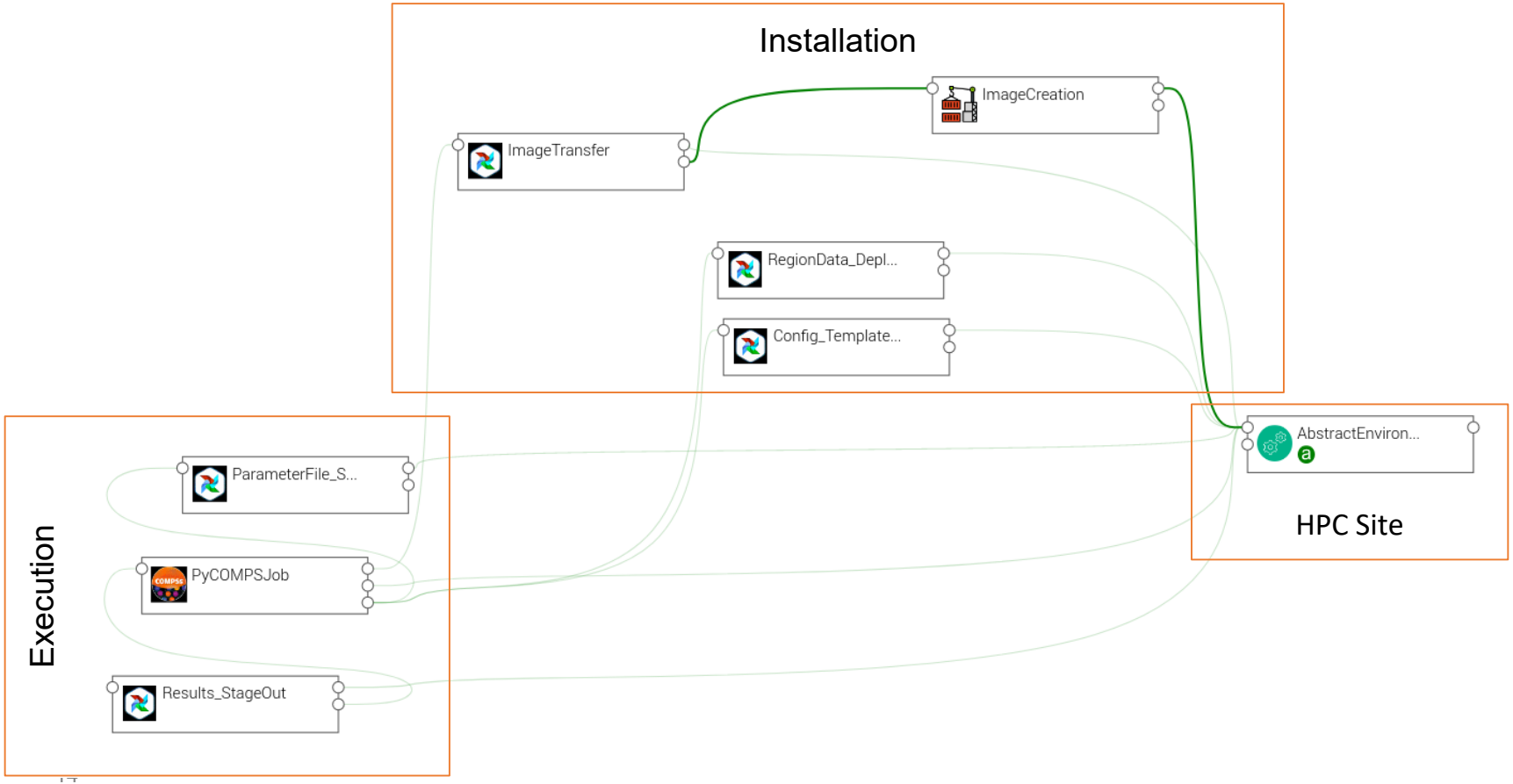
TOSCA Model

- **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

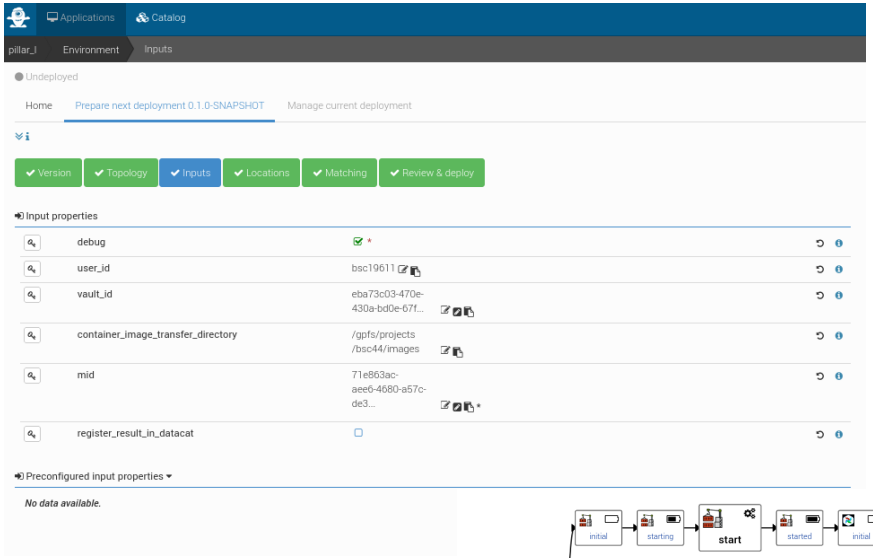


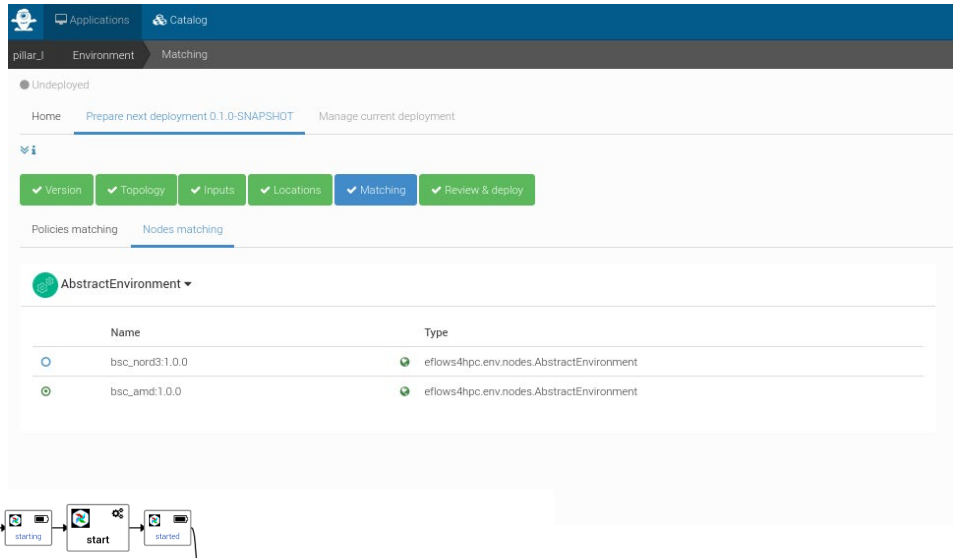
TOSCA Modelization

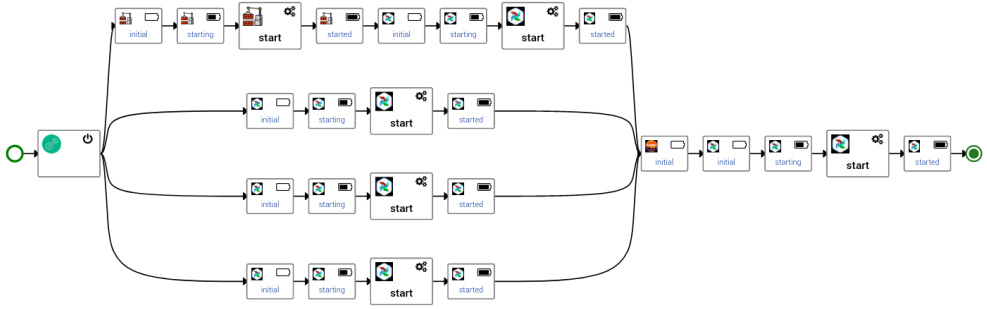


Workflow Deployment (done once per HPC site)

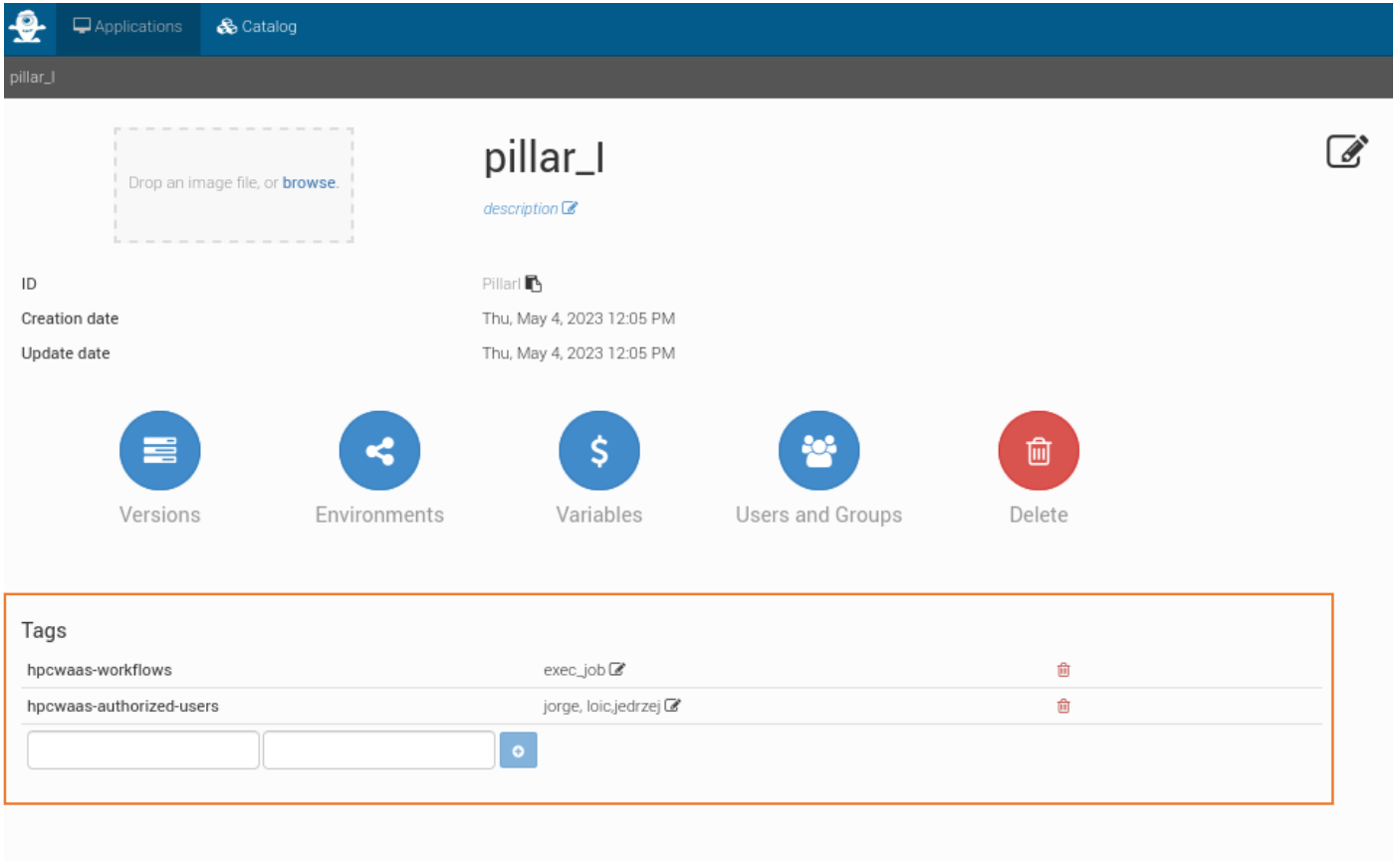
- Set deployment input parameters (user, credential, select HPC location)



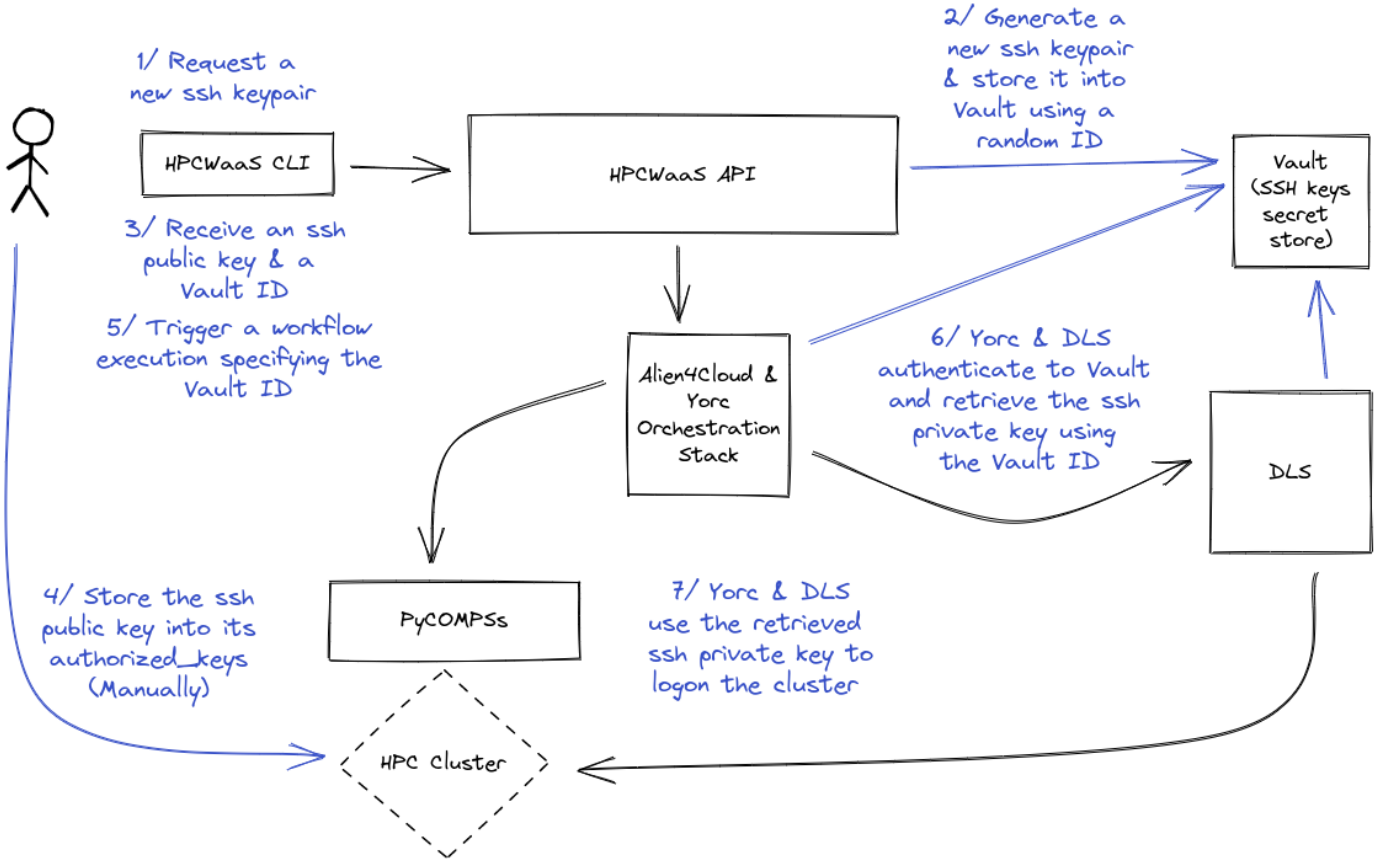




Publish workflow and authorize users



Workflow Execution End user



Thank you

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in the future EuroHPC ecosystem

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