



eFlows4HPC

eFlow4HPC project results

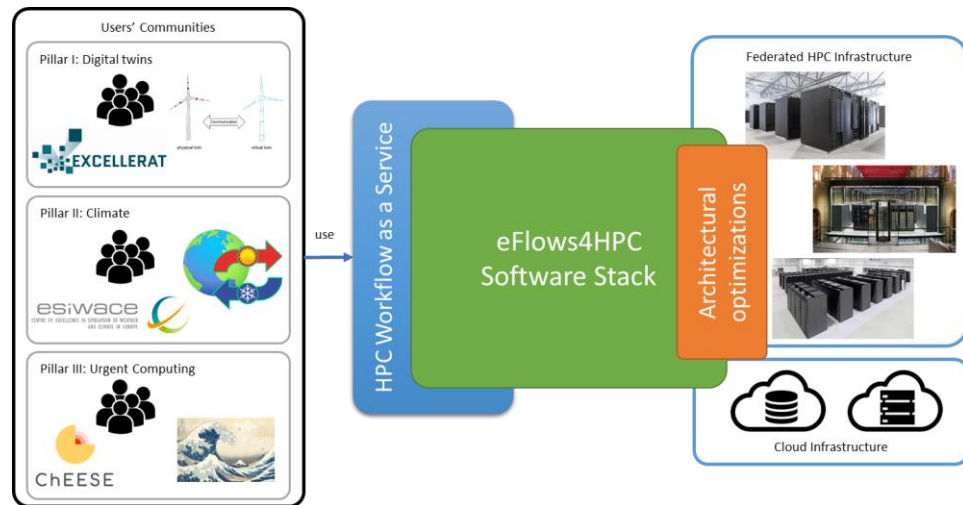
HiPEAC Conference 2023

Jorge Ejarque (BSC)



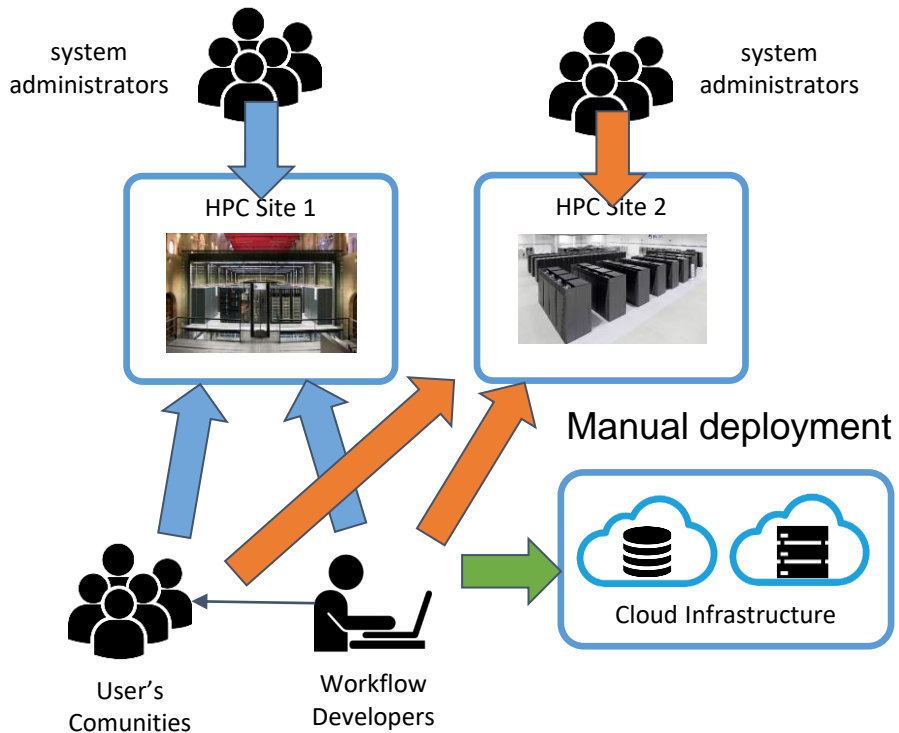
This project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 955558. The JU receives support from the European Union's Horizon 2020 research and innovation programme and Spain, Germany, France, Italy, Poland, Switzerland, Norway.

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

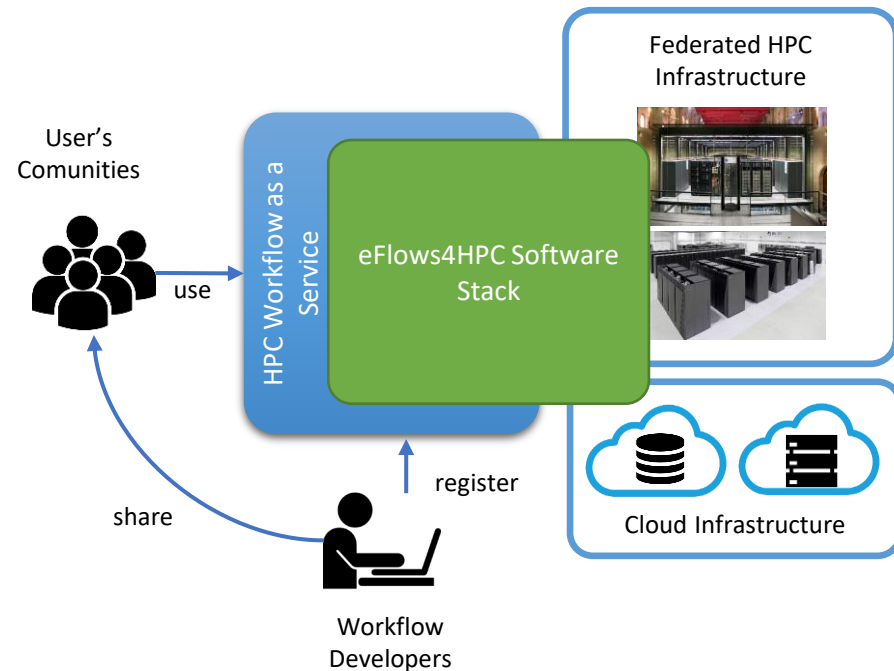


Motivation

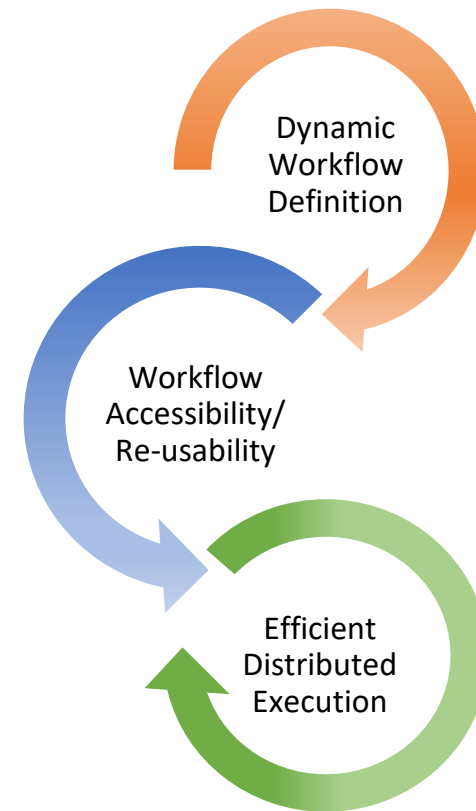
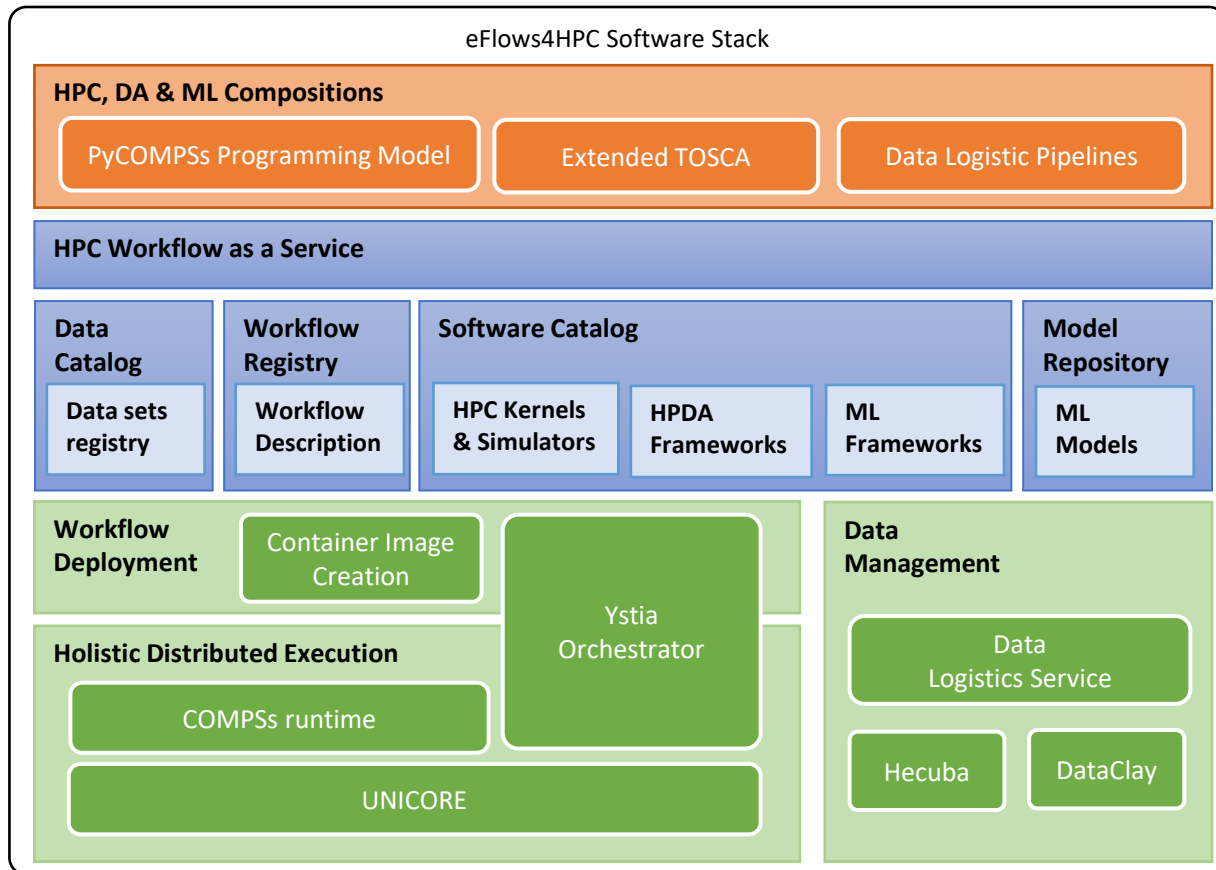
Current approach



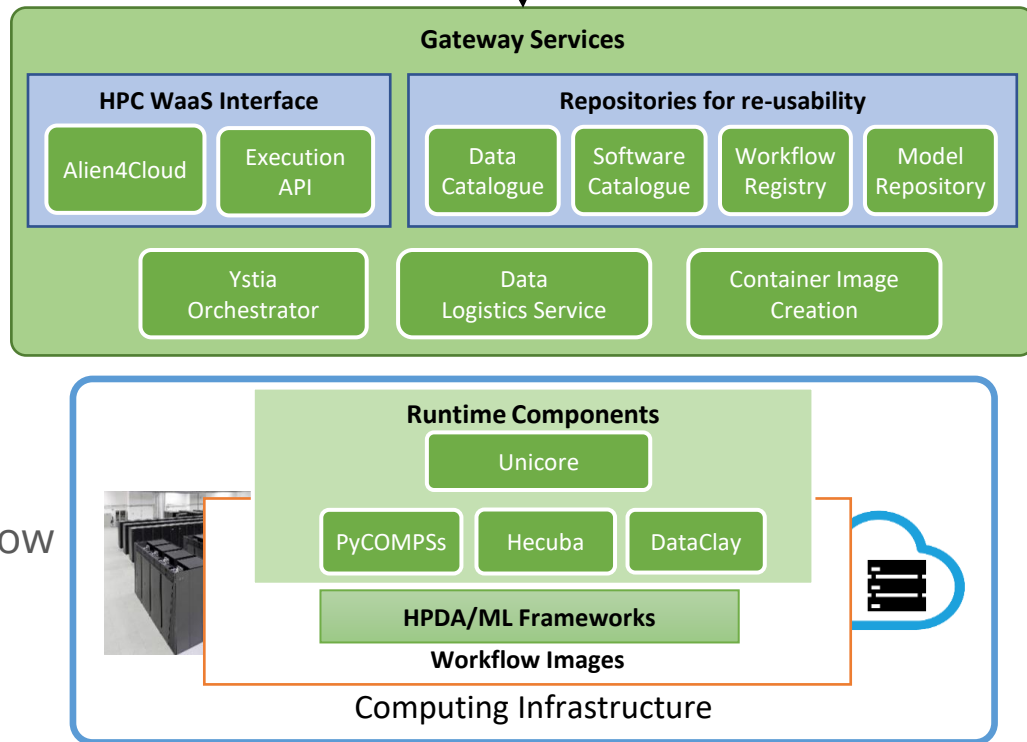
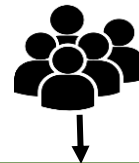
eFlows4HPC approach



Software Stack overview



eFlows4HPC software stack and HPCWaaS



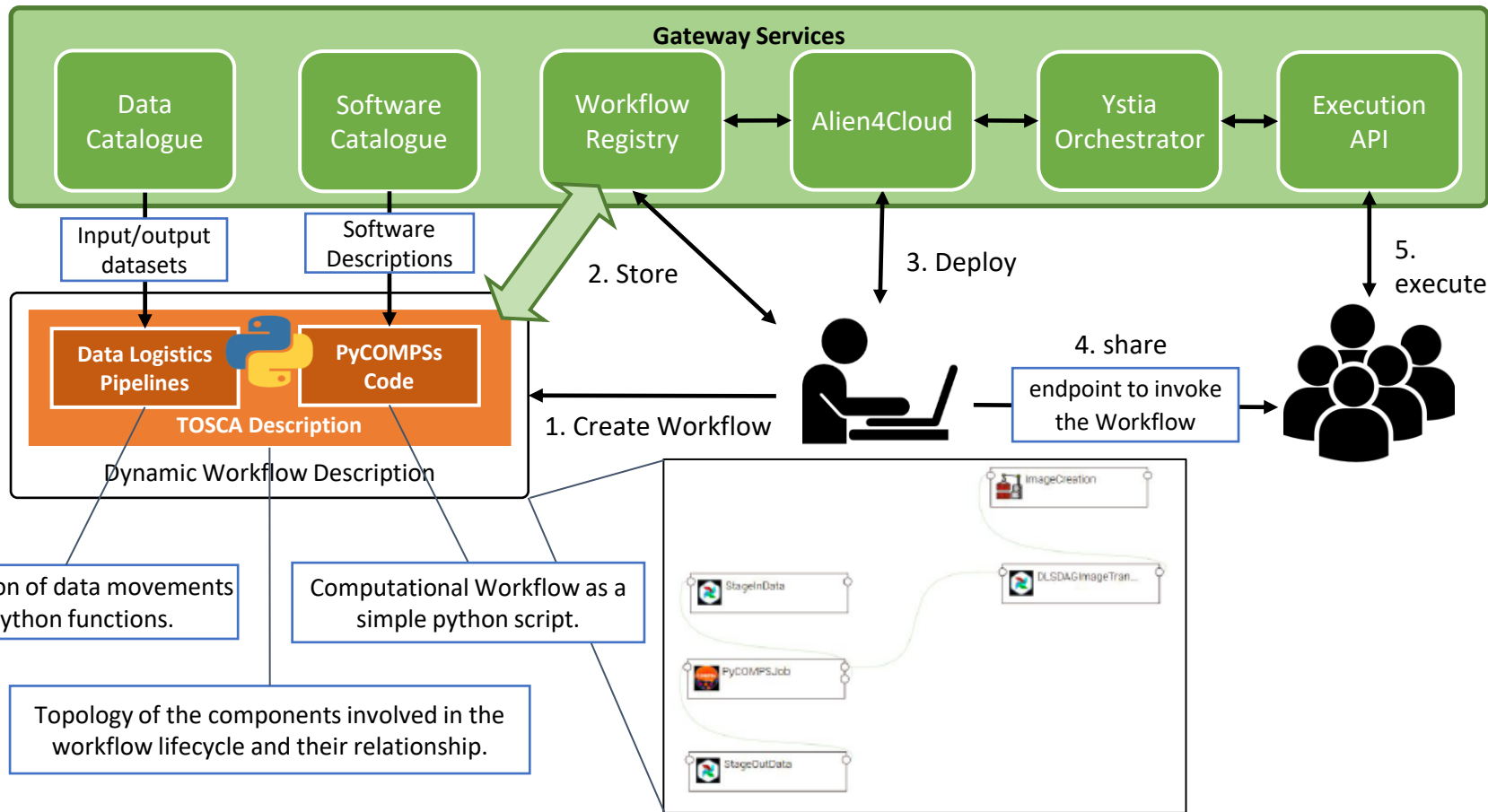
Gateway services

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

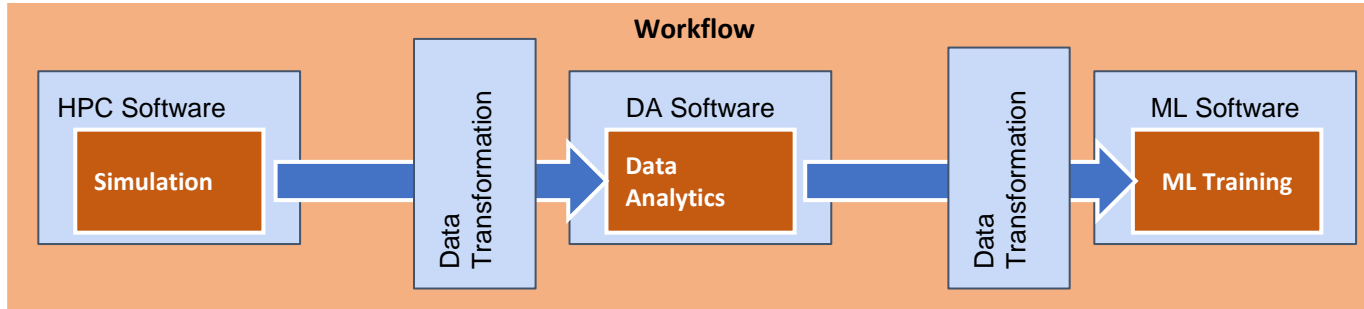
Runtime Components

- Deployed inside the computing infrastructure to manage the workflow execution

HPCWaaS Overview



Interfaces to integrate HPC/DA/ML



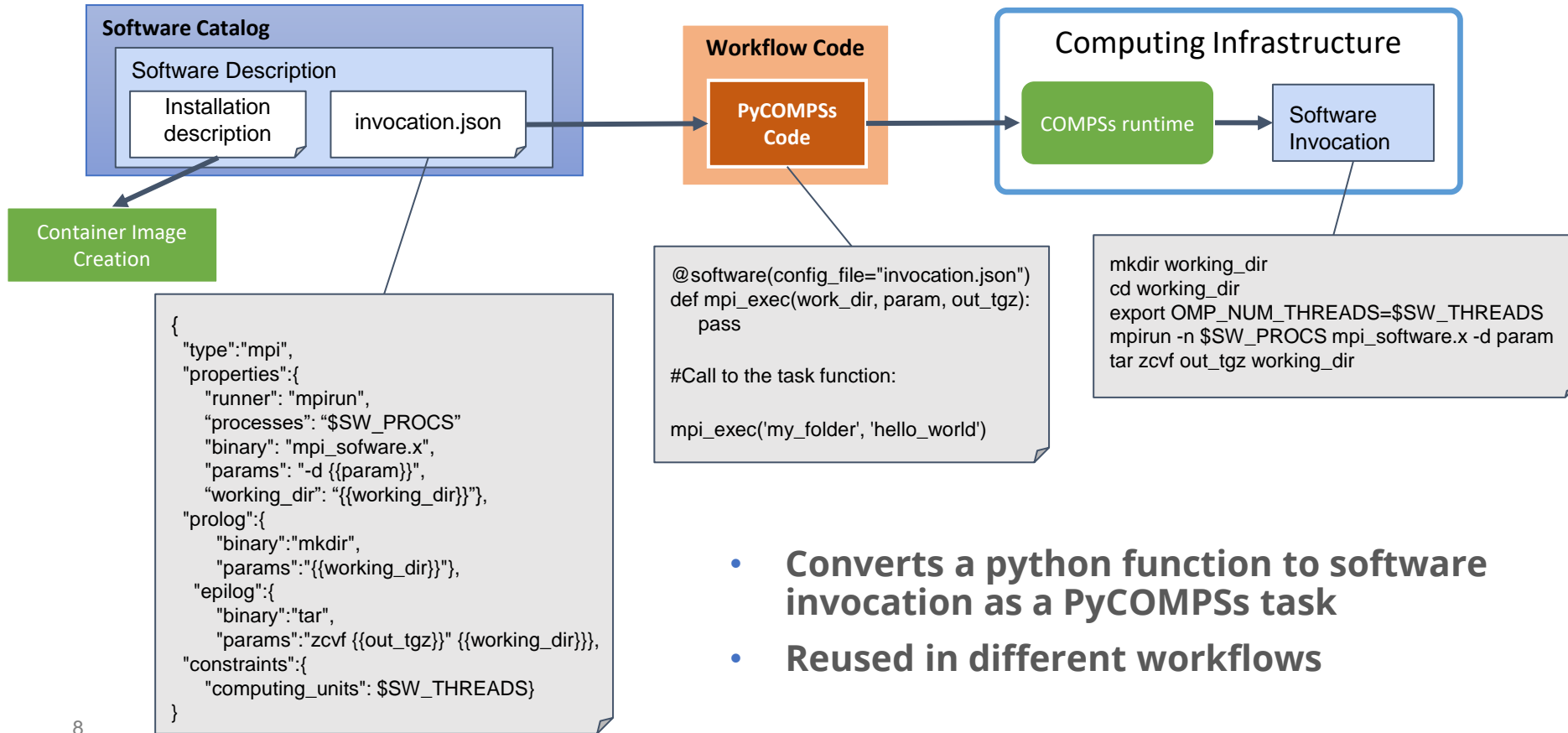
- **Goal:**
 - Reduce glue code
 - Focus on the functionality, not in the integration
 - Reusability
- **First phase:** software integration
- **Second phase:** data transformations

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

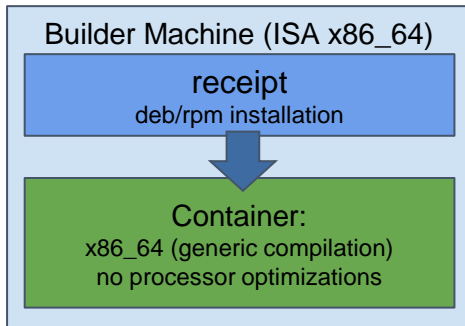
#Workflow

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

Software Invocation description



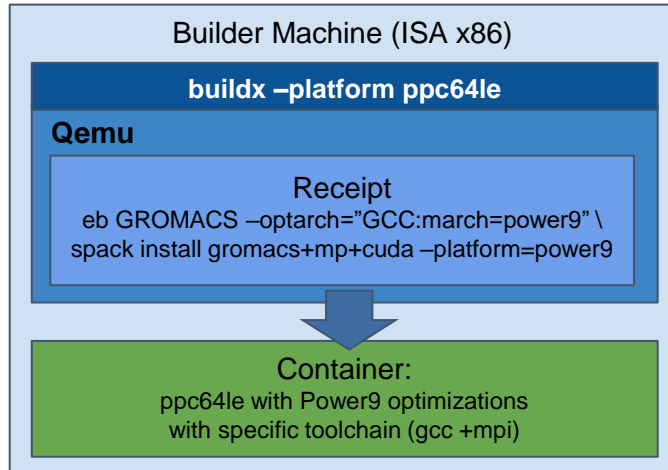
Standard container image creation



- **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

eFlows4HPC approach

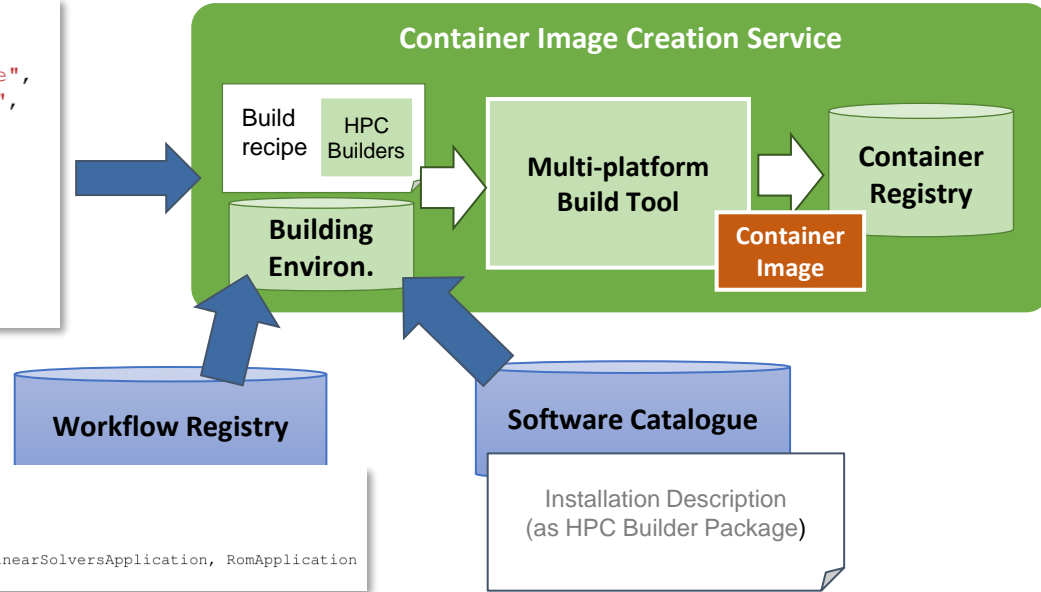


- **Methodology to allow the creation containers for specific HPC system**
 - Leverage HPC and Multi-platform container builders
- **It is tight to do by hand but let's automate!**

HPC Ready Containers

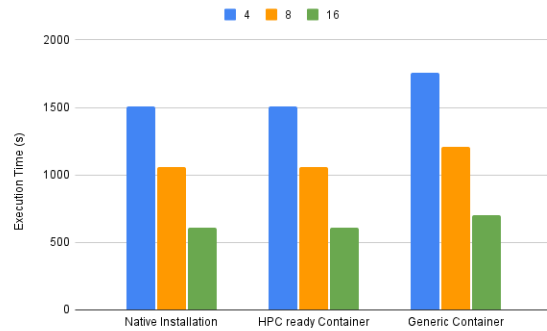
```
1 {  
2   "machine": {  
3     "platform": "linux/ppc64le",  
4     "architecture": "power9le",  
5     "container_engine":  
6     ↪ "singularity",  
7     "mpi": "openmpi@4",  
8     "gpu": "cuda@10.2"  
9   },  
10  "workflow": "pillar_III",  
11  "step_id": "ftrt"  
}
```

```
1 spack:  
2   specs:  
3     - compss  
4     - py-dislib  
5     - kratos apps=LinearSolversApplication, RomApplication
```

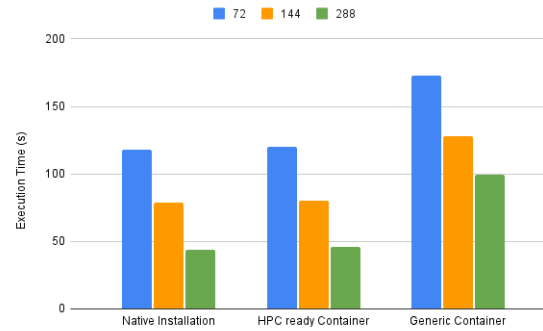


HPC-Ready Containers

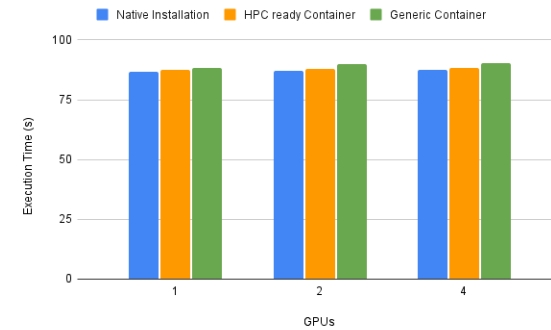
Kratos Multiphysics (shared memory)



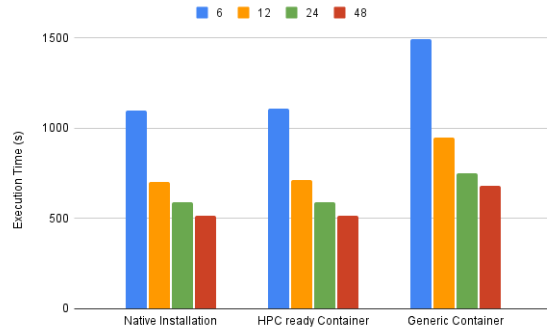
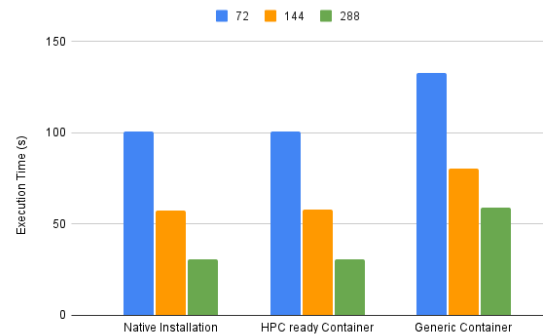
FESOM2 (MPI)



Tsunami-HySEA

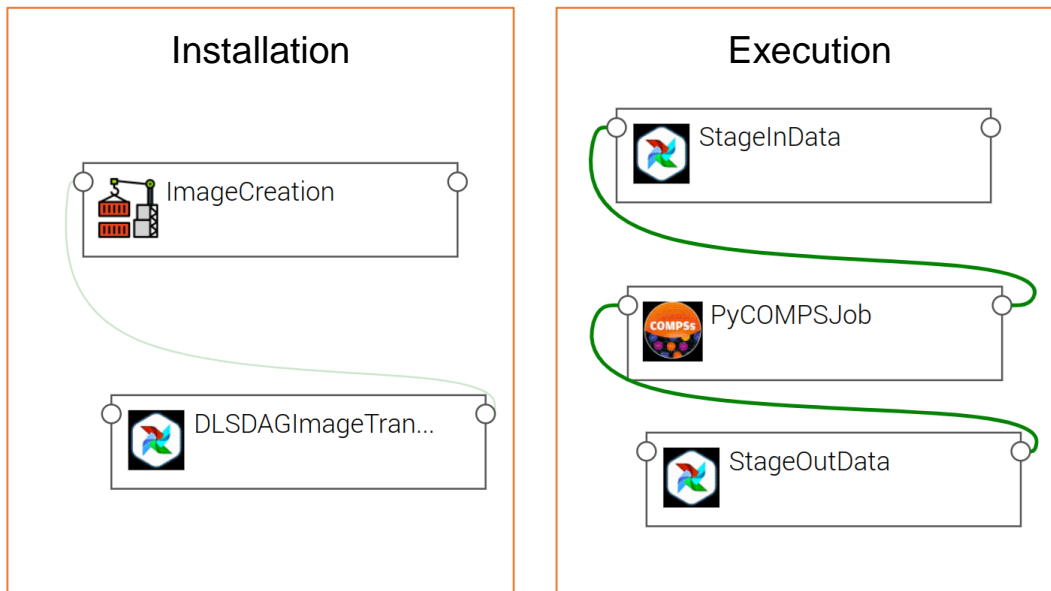


CTE-Power



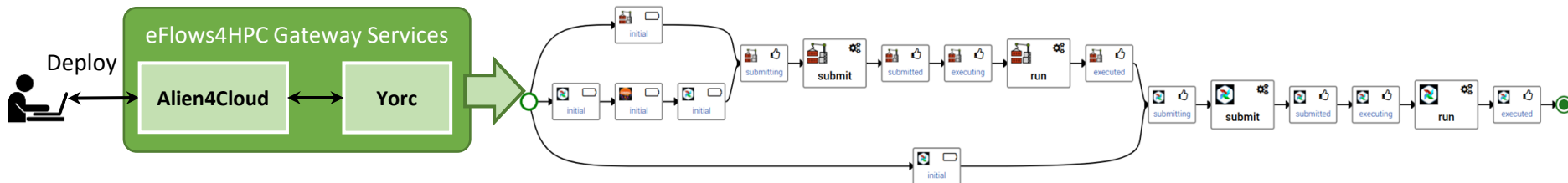
TOSCA Modelization

Topology of the different components involved in the Workflow lifecycle

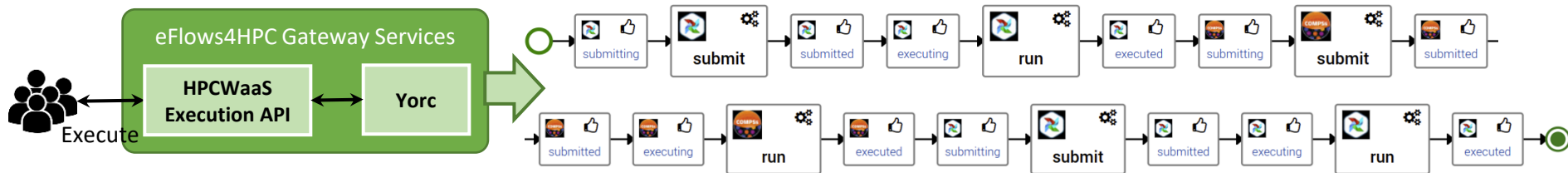


TOSCA Modelization

Application deployment workflow (done once)



End-User workflow (multiple executions)



Conclusion



- **eFlows4HPC**
 - Software stack and HPCWaaS
 - manage complex workflows in the whole lifecycle
 - Enable reusability of workflows and their components
 - Facilitate the deployment through HPC-Ready containers
 - Facilitates the accessibility of HPC systems
 - Reduce workflow management efforts
- **Other eFlows4HPC Sessions at HiPEAC**
 - WAPCO: Moday 11:55 - 12:20: *Toward Matrix Multiplication for Deep Learning Inference on the Xilinx Versal* (Jie Lei, José Flich and Enrique S. Quintana-Ortí, UPV)
 - AccML: Wednesday 11:30 – 12:10 *Convolutional Neural Networks: One Matrix Product to Rule them All!* (Enrique S. Quintana-Ortí, UPV)

Thank you



www.eFlows4HPC.eu



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