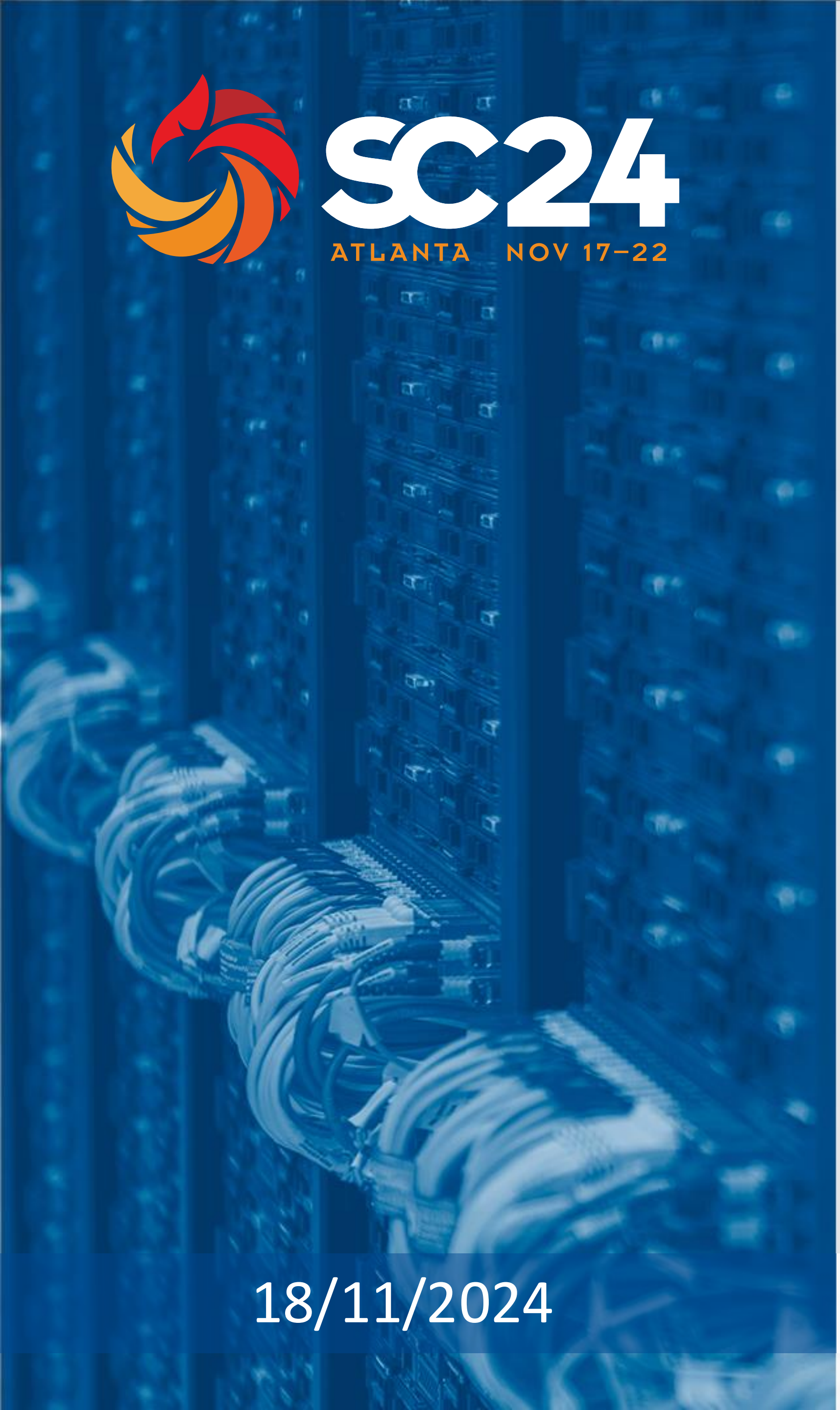

SC24

ATLANTA NOV 17–22

Barcelona
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Optimising workflow lifecycle management: development, HPC-ready containers deployment and reproducibility

Raül Sirvent, Rosa M Badia

18/11/2024

SC24 tutorial, Atlanta, 18 Novembre 2024

Tutorial website

https://github.com/bsc-wdc/Tutorial_SC24

Agenda

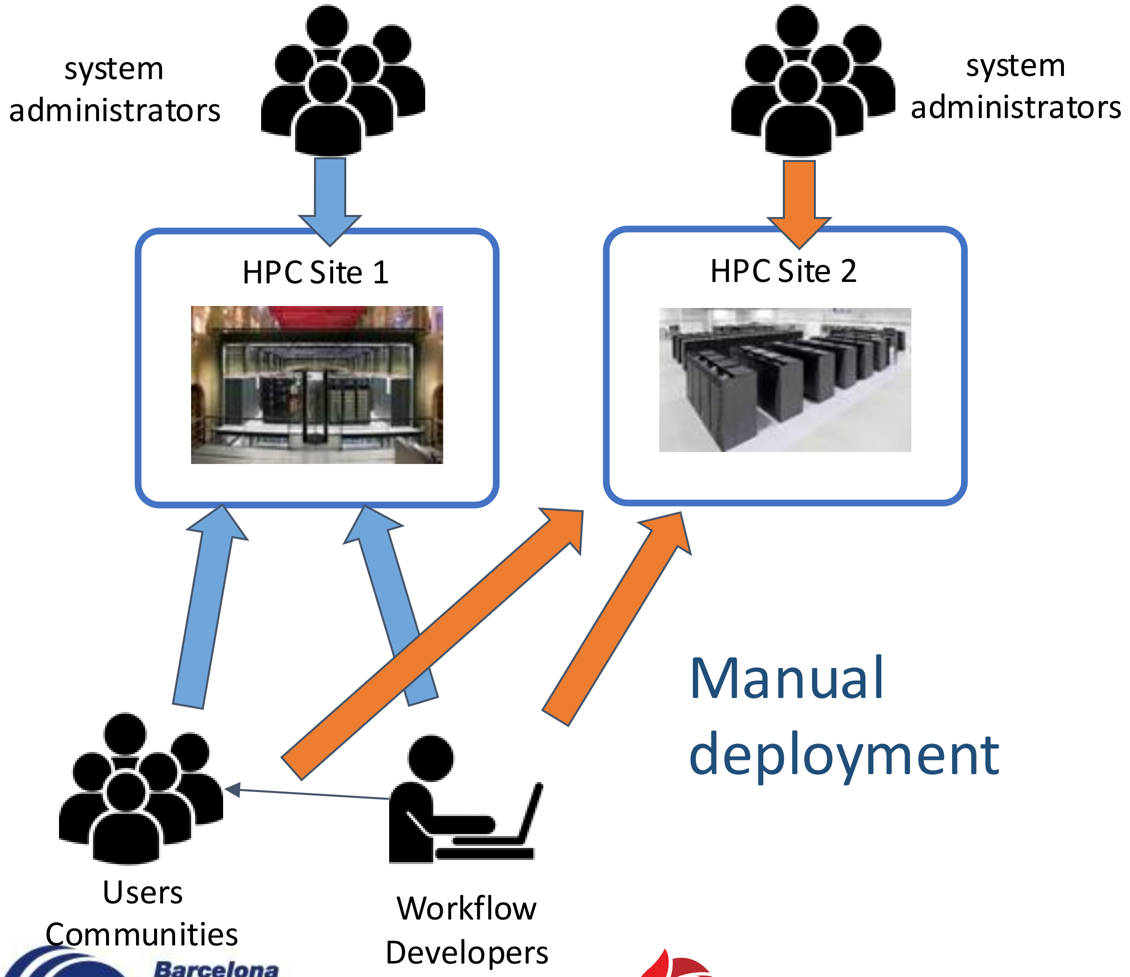
8:30 – 8:45	Overview of tutorial agenda	Rosa M Badia
8:45 – 9:15	Part 1.1: Hybrid HPC+AI+DA workflow development with PyCOMPSs - Context of the workflows at BSC - Overview of workflow development with PyCOMPSs - Extensions for the integration of HPC with AI and DA - Sample workflows	Rosa M Badia
9:15 – 9:45	Part 1.2: Workflows' reproducibility through provenance - Motivation for workflow provenance - Design of the recording mechanism - Sharing experiments for reproducibility	Raül Sirvent
9:45 - 10:00	Part 1.3: HPC ready container images - Motivation for architecture specific containers - Overview of the Container Image Creation service - Example of HPC ready container generation	Rosa M Badia
10:00 - 10:30	Coffee break	

Agenda

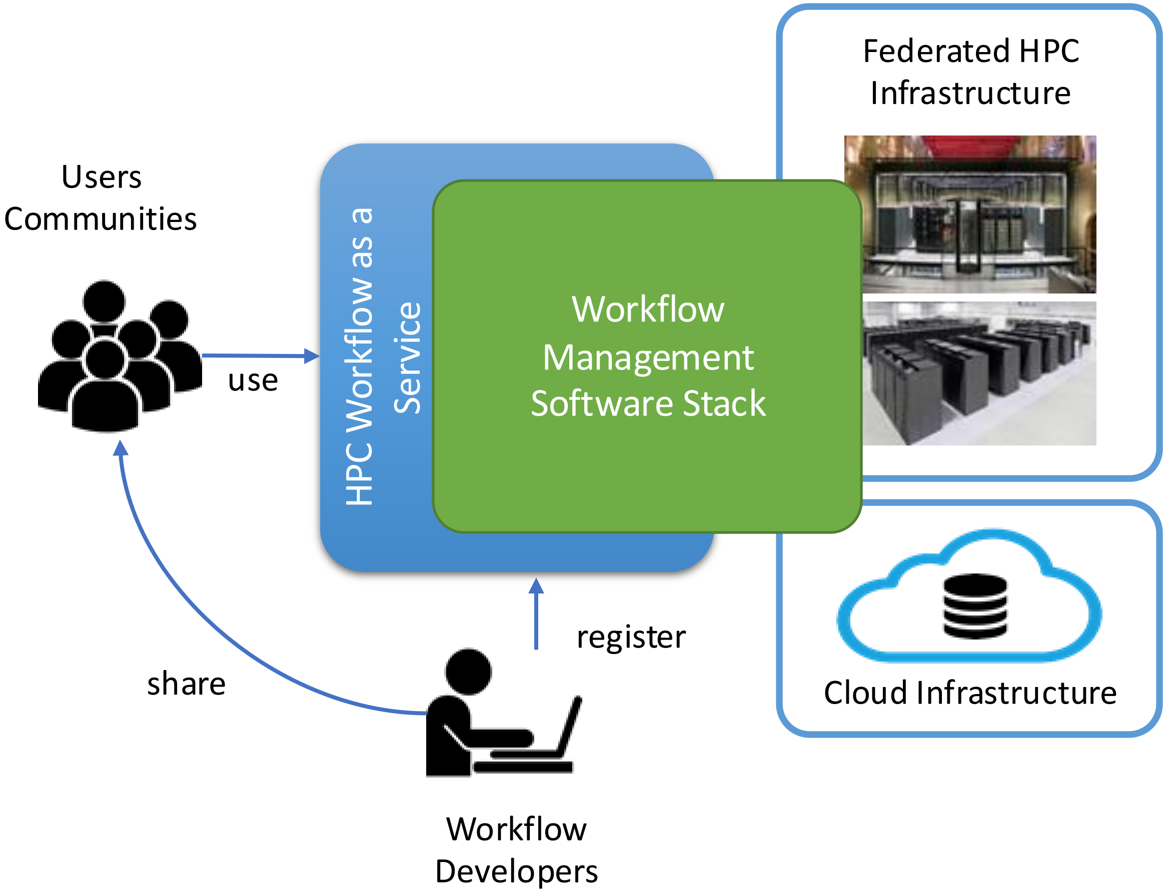
10:30 – 10:45	Hands-on preparation (credentials distribution, how to access, etc)	All presenters
10:45 – 11:15	Part 2.1: Hands-on session: Sample workflows with PyCOMPSs, execution with containers, task-graph generation, tracefile generation (optional)	Rosa M Badia
11:15 – 11:55	Part 2.2: Hands-on session: How to automatically record workflow provenance and use it to share experiments in WorkflowHub	Raül Sirvent
11:55 - 12:00	Tutorial conclusions	All presenters

Deployment in HPC Environments

Current approach

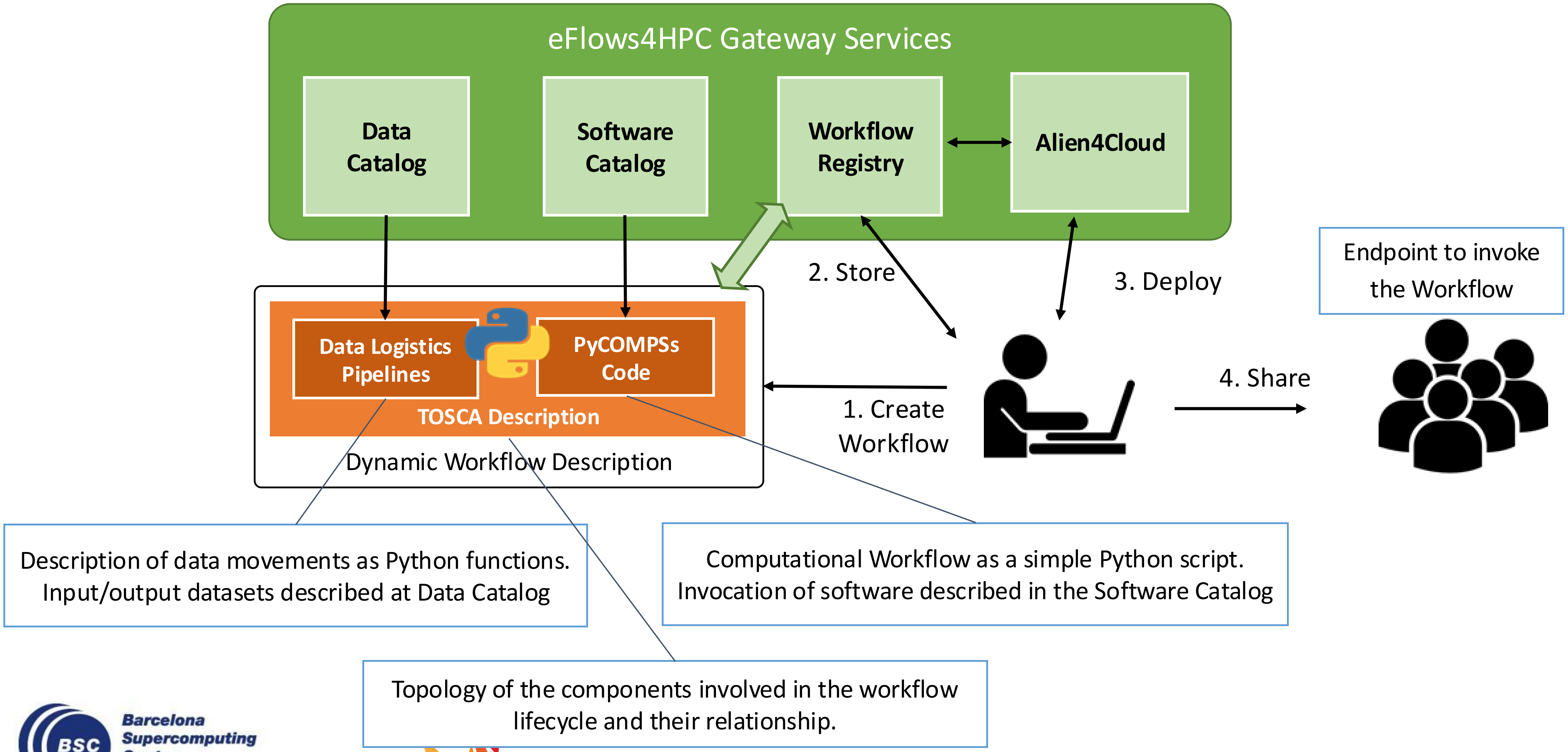


Manual deployment


Users Communities
use
HPC Workflow as a Service
Workflow Management Software Stack
Federated HPC Infrastructure
Cloud Infrastructure
register
share
Workflow Developers

Can we design something like FaaS for Complex Workflows for HPC?

HPCWaaS: Workflow lifecycle overview



eFlows4HPC Gateway Services

Data Catalog

Software Catalog

Workflow Registry

Alien4Cloud

Data Logistics Pipelines

PyCOMPSs Code

TOSCA Description

Dynamic Workflow Description

1. Create Workflow

2. Store

3. Deploy

4. Share

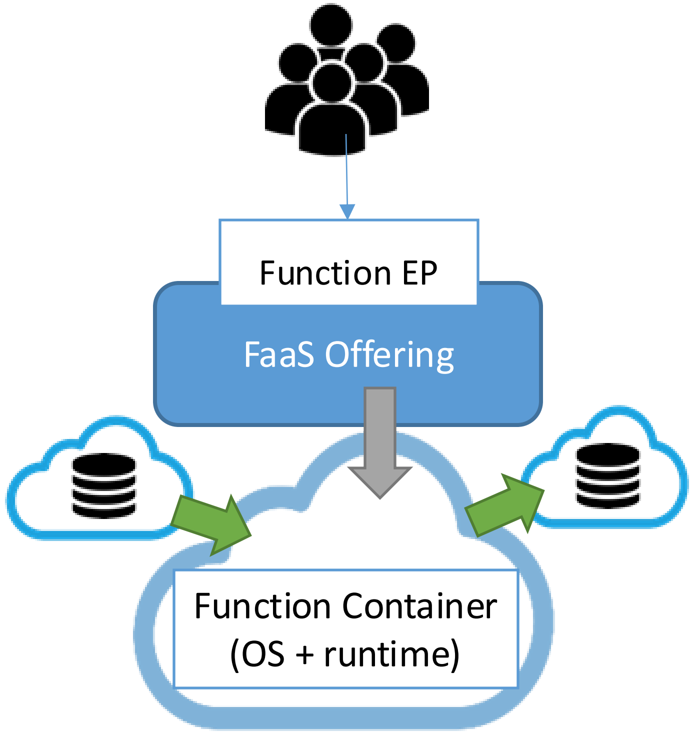
Endpoint to invoke the Workflow

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.

FaaS vs HPCWaaS

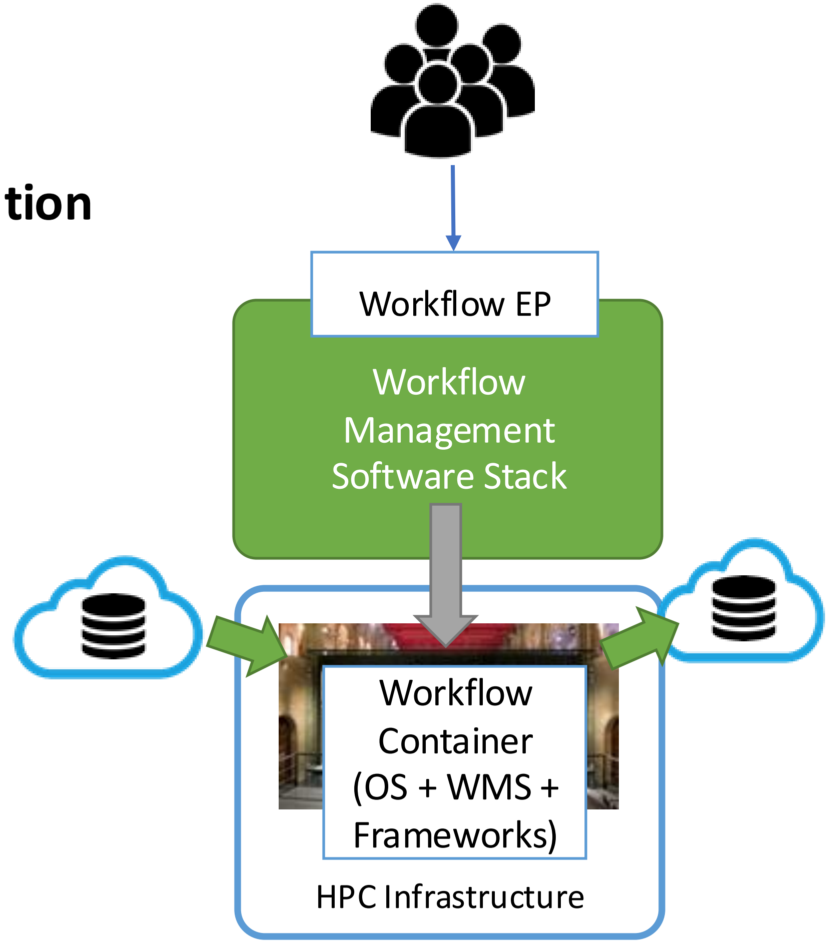


Similarities

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

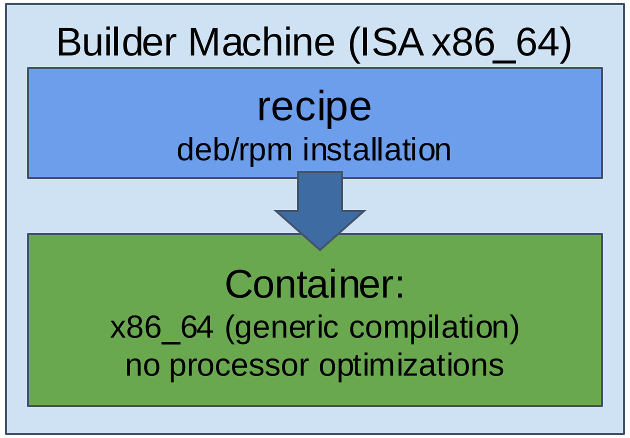
Differences

- HPC policies & requirements
- Deployment and Execution Complexity
- **Performance needs**



Containers and HPC

Standard container image creation



Builder Machine (ISA x86_64)

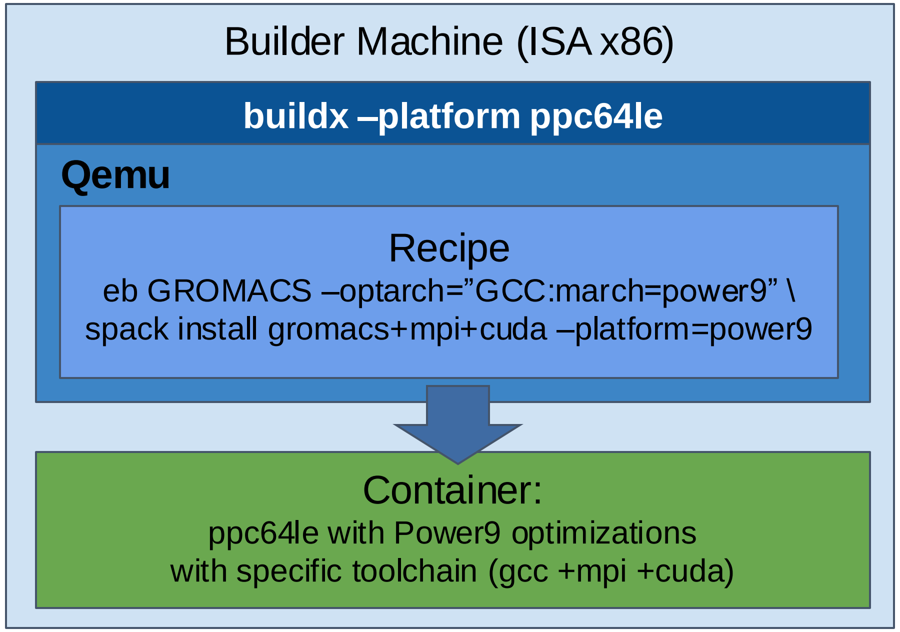
recipe
deb/rpm installation

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)

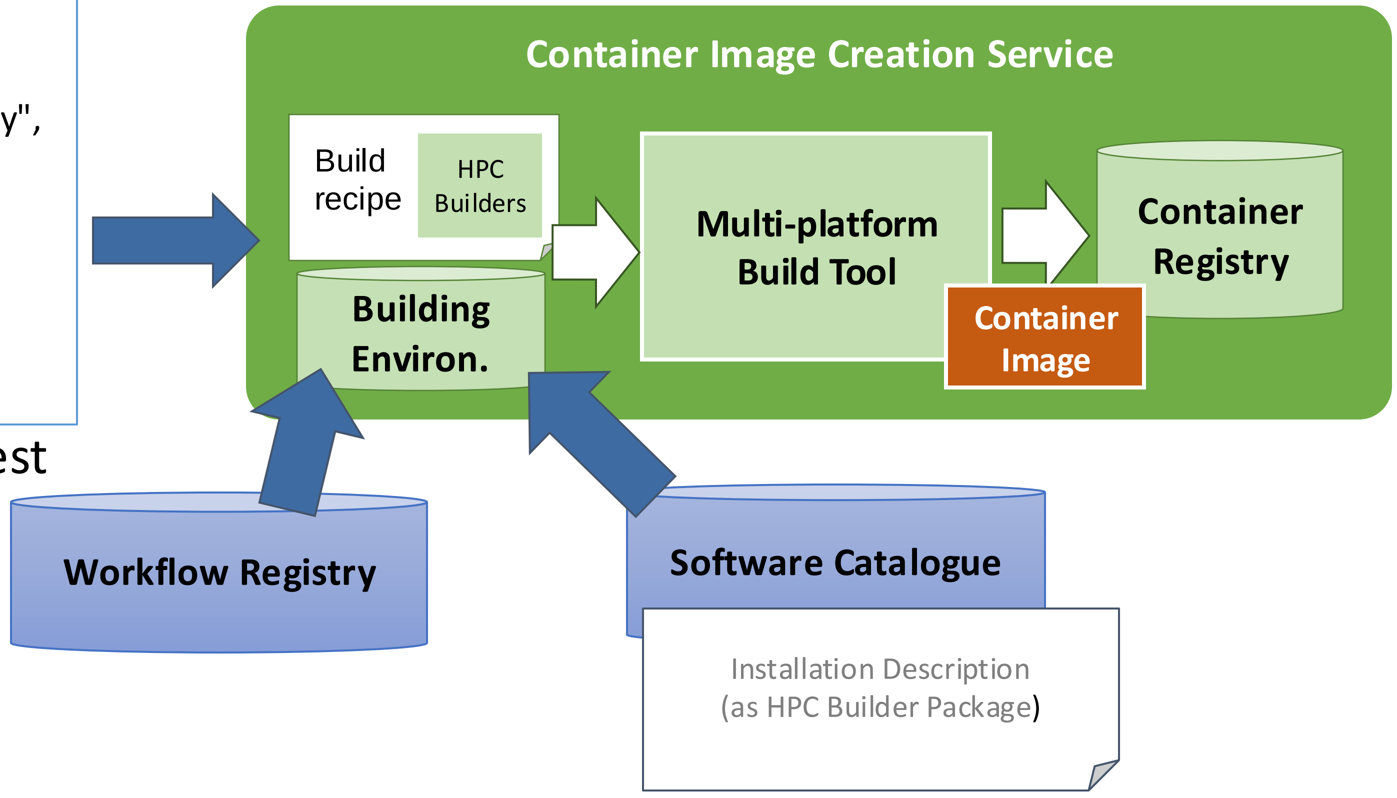
- Methodology to allow the creation containers for specific HPC system
  - Leverage HPC and Multi-platform container builders
- It is tight to do by hand but let's automate!

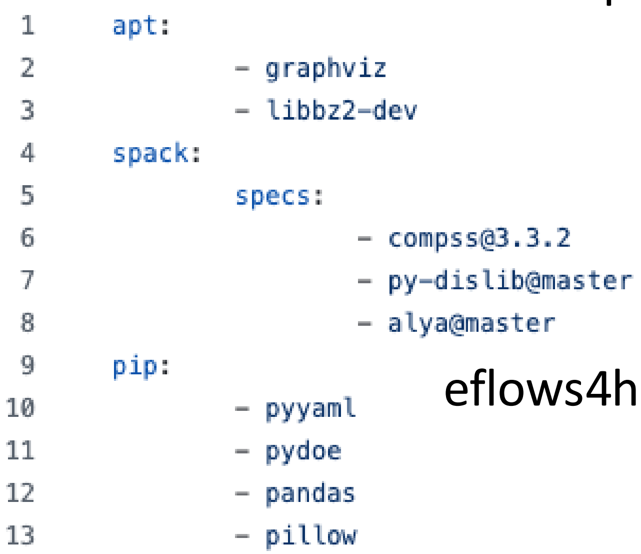
HPC Ready Containers

Workflow step + target system

```
{
"machine": {
                "platform": "linux/amd64",
                "architecture": "skylake",
                "container_engine": "singularity",
                "mpi":"openmpi@4.1.1"
},
"workflow":”tutorial",
"step_id" : " HPC_AI_training",
"workflow_yaml" : "eflows4hpc.yaml",
}
```

Service request





```
apt:
          - graphviz
          - libbz2-dev
spack:
          specs:
                    - compss@3.3.2
                    - py-dislib@master
                    - alya@master
pip:
          - pyyaml
          - pydoe
          - pandas
          - pillow
```

eflows4hpc.yaml

package.py

CAELESTIS workflow

https://github.com/eflows4hpc

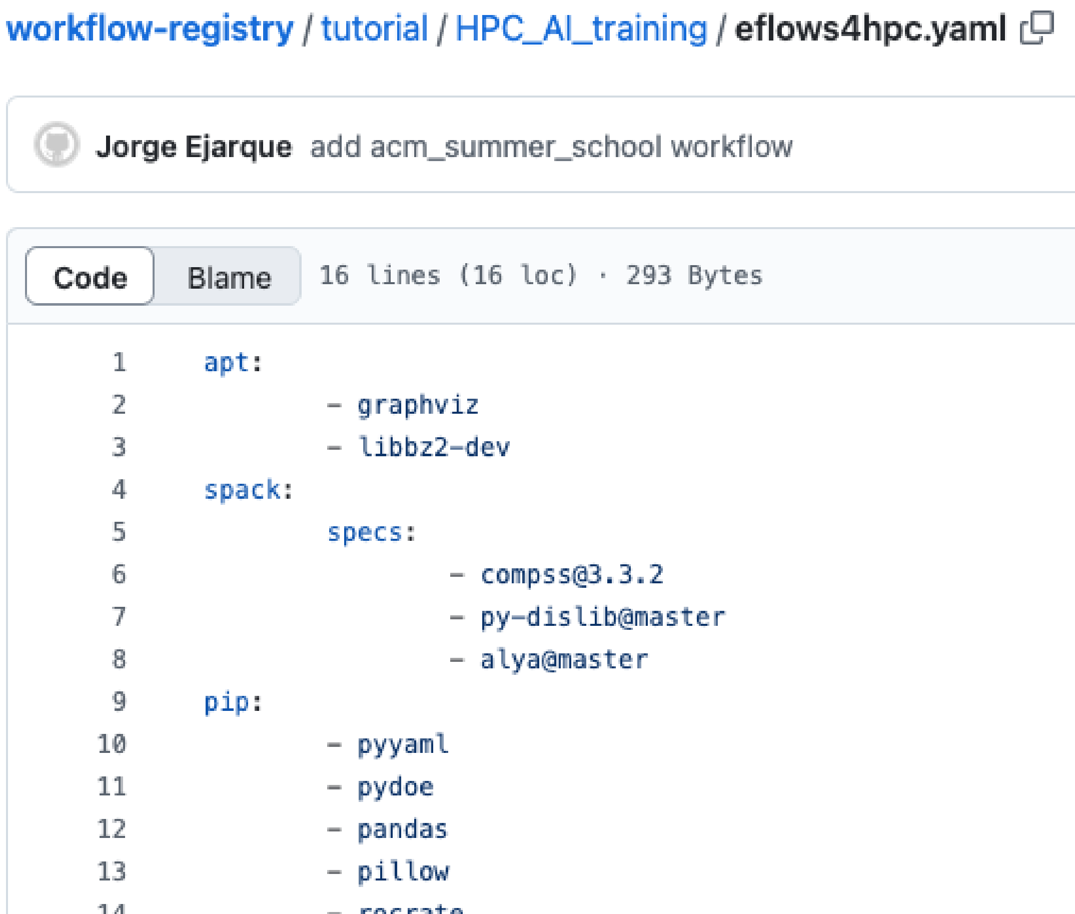
- Example of HPC ready container generation
- Sample request (json):

Target: MareNostrum4 architecture

```
{
"machine": {
            "platform": "linux/amd64",
            "architecture": "skylake",
            "container_engine": "singularity",
            "mpi":"openmpi@4.1.1"
},
"workflow":”tutorial",
"step_id" : "HPC_AI_training",
"workflow_yaml" : "eflows4hpc.yaml",
"force" : "True",
"push" : "False"
}
```

Location in workflow-registry

Yaml file describing modules involved in the workflow



workflow-registry / tutorial / HPC_AI_training / eflows4hpc.yaml

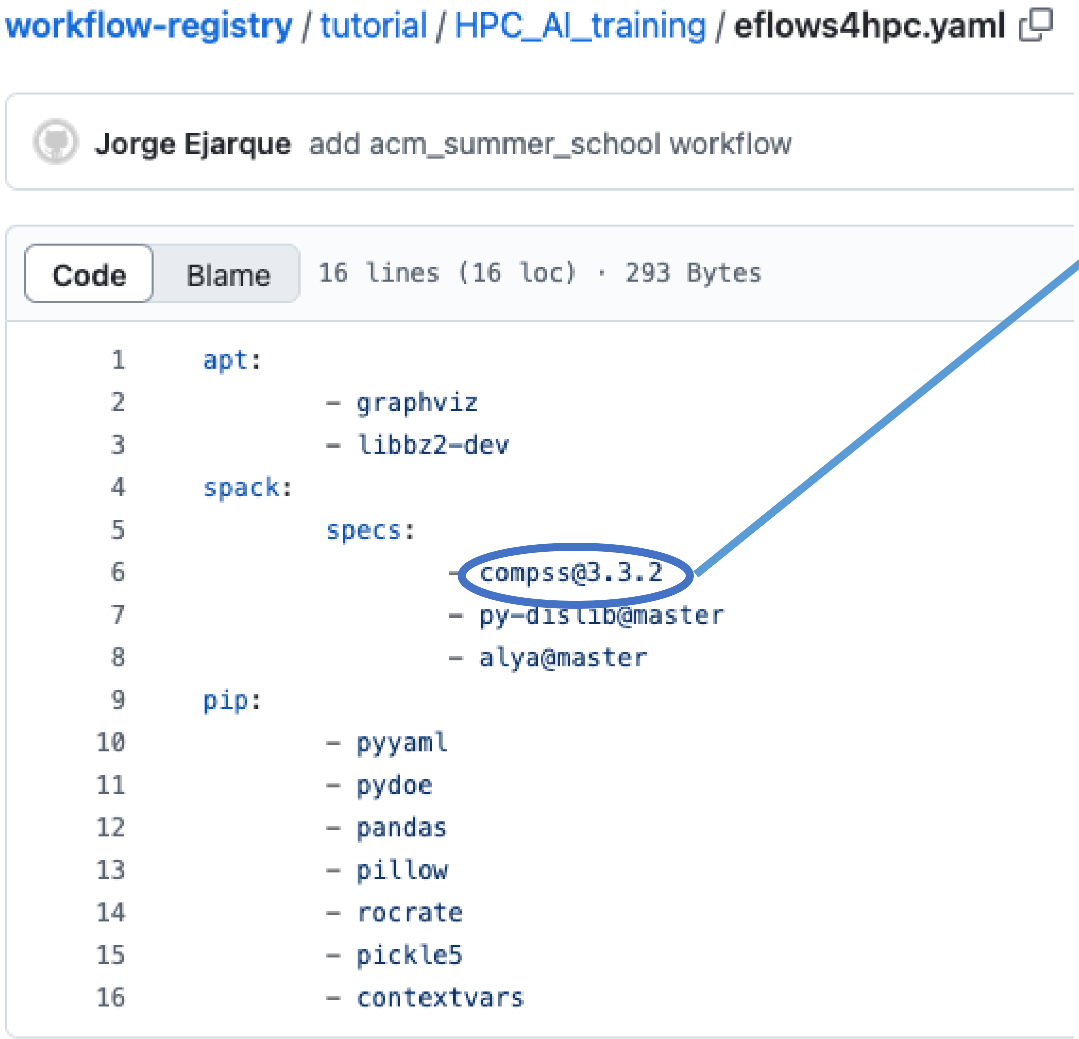
Jorge Ejarque add acm_summer_school workflow

16 lines (16 loc) · 293 Bytes

```
apt:
        - graphviz
        - libbz2-dev
spack:
        specs:
                - compss@3.3.2
                - py-dislib@master
                - alya@master
pip:
        - pyyaml
        - pydoe
        - pandas
        - pillow
        - rocrate
```

CAELESTIS workflow

https://github.com/eflows4hpc



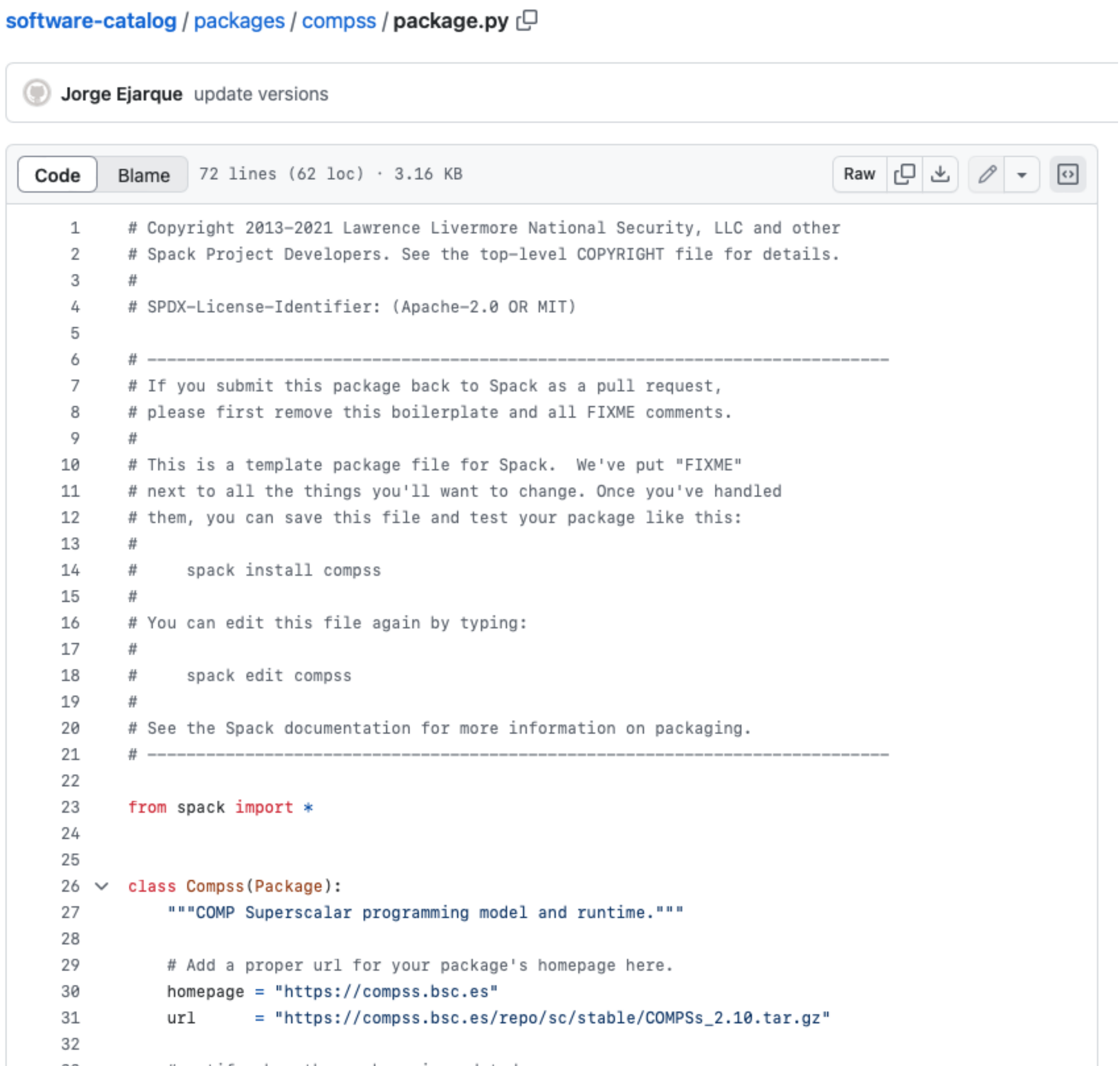
workflow-registry / tutorial / HPC_AI_training / eflows4hpc.yaml

Jorge Ejarque add acm_summer_school workflow

16 lines (16 loc) · 293 Bytes

```yaml
apt:
        - graphviz
        - libbz2-dev
spack:
        specs:
                - compss@3.3.2
                - py-dislib@master
                - alya@master
pip:
        - pyyaml
        - pydoe
        - pandas
        - pillow
        - rocrate
        - pickle5
        - contextvars
```

Specific spack packages



software-catalog / packages / compss / package.py

Jorge Ejarque update versions

72 lines (62 loc) · 3.16 KB

```python
# Copyright 2013-2021 Lawrence Livermore National Security, LLC and other
# Spack Project Developers. See the top-level COPYRIGHT file for details.
#
# SPDX-License-Identifier: (Apache-2.0 OR MIT)

# ----------------------------------------------------------------------------
# If you submit this package back to Spack as a pull request,
# please first remove this boilerplate and all FIXME comments.
#
# This is a template package file for Spack.  We've put "FIXME"
# next to all the things you'll want to change. Once you've handled
# them, you can save this file and test your package like this:
#
#     spack install compss
#
# You can edit this file again by typing:
#
#     spack edit compss
#
# See the Spack documentation for more information on packaging.
# ----------------------------------------------------------------------------

from spack import *


class Compss(Package):
    """COMP Superscalar programming model and runtime."""

    # Add a proper url for your package's homepage here.
    homepage = "https://compss.bsc.es"
    url      = "https://compss.bsc.es/repo/sc/stable/COMPSs_2.10.tar.gz"

```

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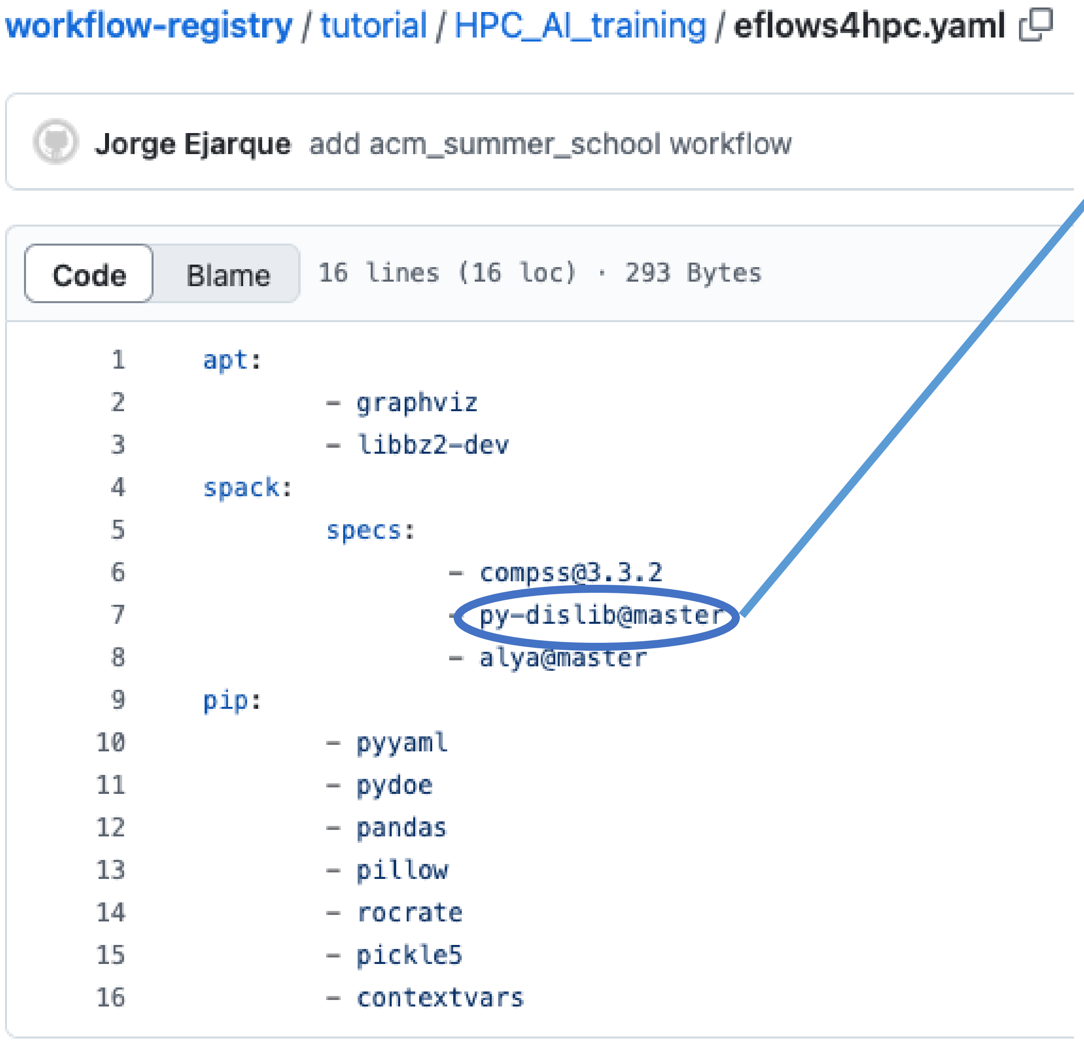
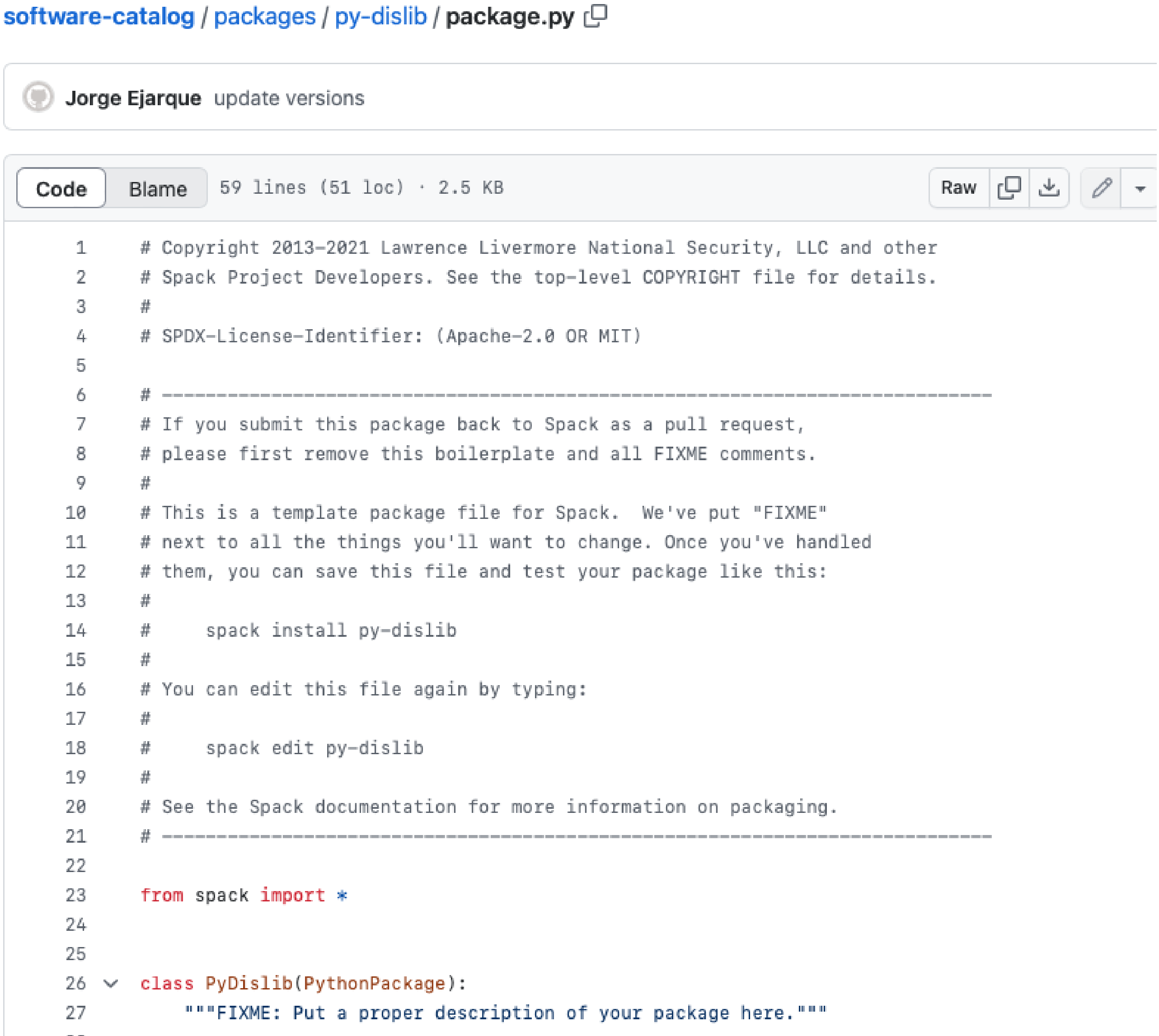
CAELESTIS workflow

https://github.com/eflows4hpc


workflow-registry / tutorial / HPC_AI_training / eflows4hpc.yaml
Jorge Ejarque add acm_summer_school workflow
Code
Blame
16 lines (16 loc) · 293 Bytes

```yaml
apt:
        - graphviz
        - libbz2-dev
spack:
        specs:
                - compss@3.3.2
                - py-dislib@master
                - alya@master
pip:
        - pyyaml
        - pydoe
        - pandas
        - pillow
        - rocrate
        - pickle5
        - contextvars
```

Specific spack packages


software-catalog / packages / py-dislib / package.py
Jorge Ejarque update versions
Code
Blame
59 lines (51 loc) · 2.5 KB
Raw

```python
# Copyright 2013-2021 Lawrence Livermore National Security, LLC and other
# Spack Project Developers. See the top-level COPYRIGHT file for details.
#
# SPDX-License-Identifier: (Apache-2.0 OR MIT)

# ----------------------------------------------------------------------------
# If you submit this package back to Spack as a pull request,
# please first remove this boilerplate and all FIXME comments.
#
# This is a template package file for Spack.  We've put "FIXME"
# next to all the things you'll want to change. Once you've handled
# them, you can save this file and test your package like this:
#
#     spack install py-dislib
#
# You can edit this file again by typing:
#
#     spack edit py-dislib
#
# See the Spack documentation for more information on packaging.
# ----------------------------------------------------------------------------

from spack import *


class PyDislib(PythonPackage):
    """FIXME: Put a proper description of your package here."""
```

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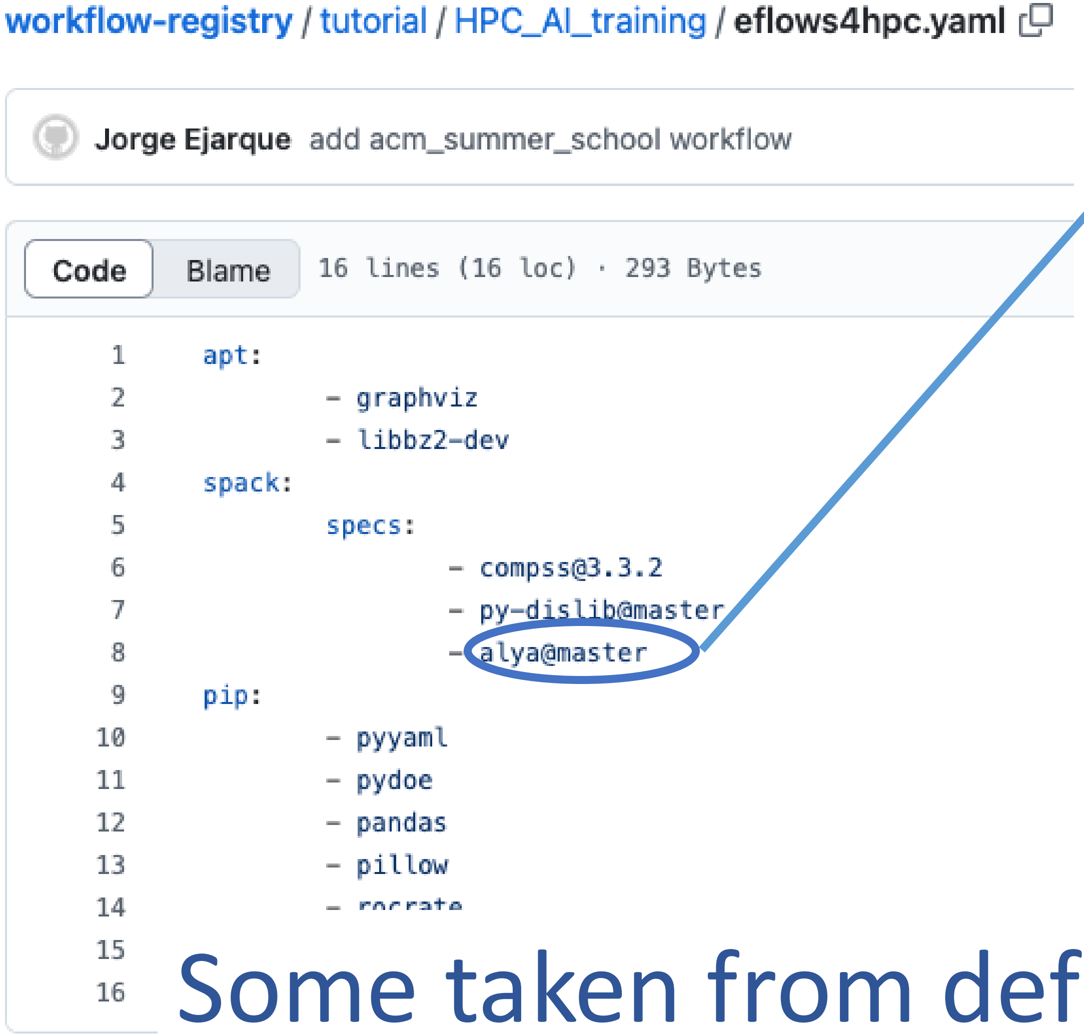
CAELESTIS workflow

https://github.com/eflows4hpc

Specific spack packages

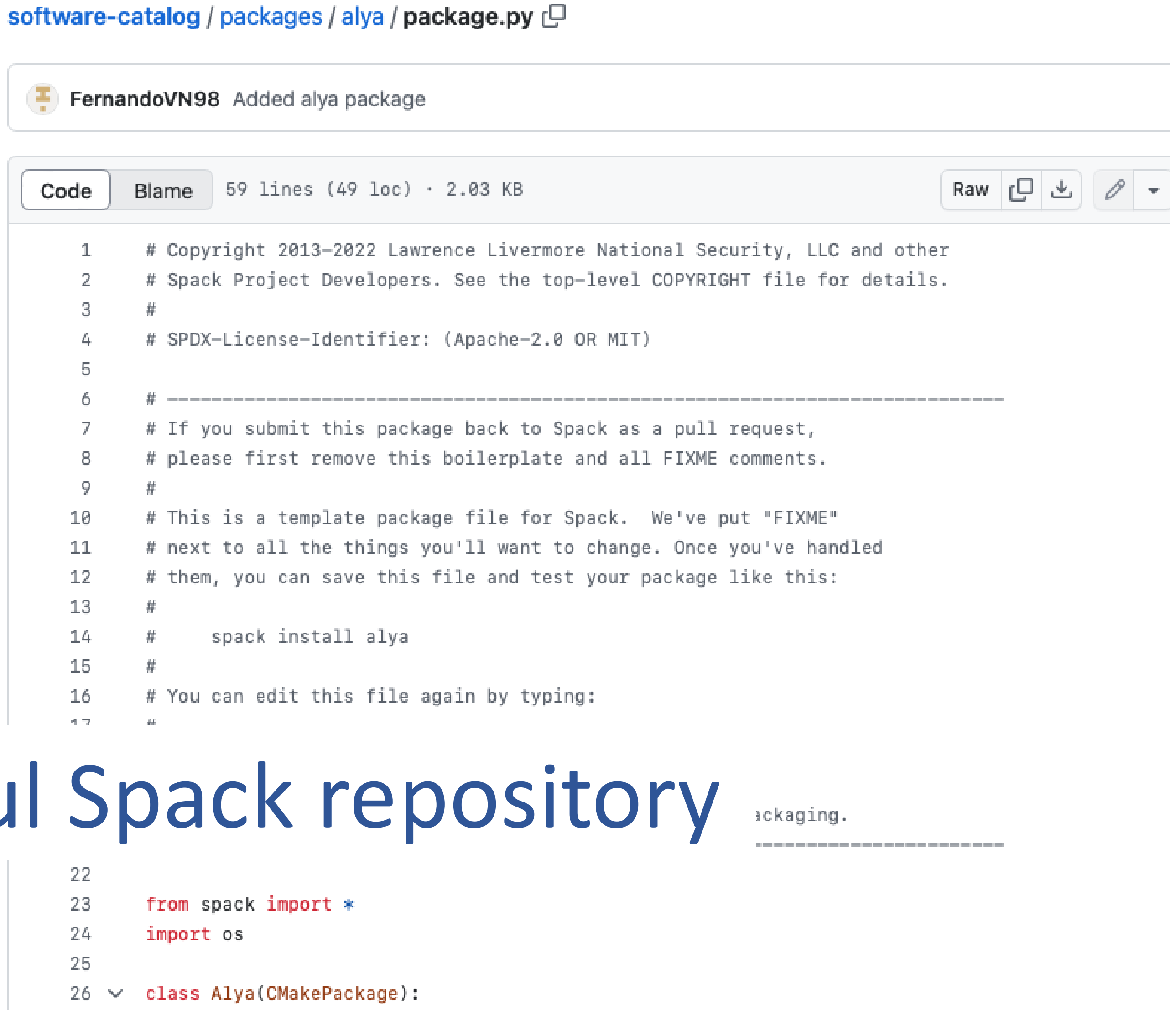


workflow-registry / tutorial / HPC_AI_training / eflows4hpc.yaml

Jorge Ejarque add acm_summer_school workflow

Code Blame 16 lines (16 loc) · 293 Bytes

```
apt:
        - graphviz
        - libbz2-dev
spack:
        specs:
                - compss@3.3.2
                - py-dislib@master
                - alya@master
pip:
        - pyyaml
        - pydoe
        - pandas
        - pillow
        - rocrate
```



software-catalog / packages / alya / package.py

FernandoVN98 Added alya package

Code Blame 59 lines (49 loc) · 2.03 KB

```
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#
# SPDX-License-Identifier: (Apache-2.0 OR MIT)

# ----------------------------------------------------------------------------
# If you submit this package back to Spack as a pull request,
# please first remove this boilerplate and all FIXME comments.
#
# This is a template package file for Spack.  We've put "FIXME"
# next to all the things you'll want to change. Once you've handled
# them, you can save this file and test your package like this:
#
#     spack install alya
#
# You can edit this file again by typing:
#
ackaging.
------------------------

from spack import *
import os

class Alya(CMakePackage):
```
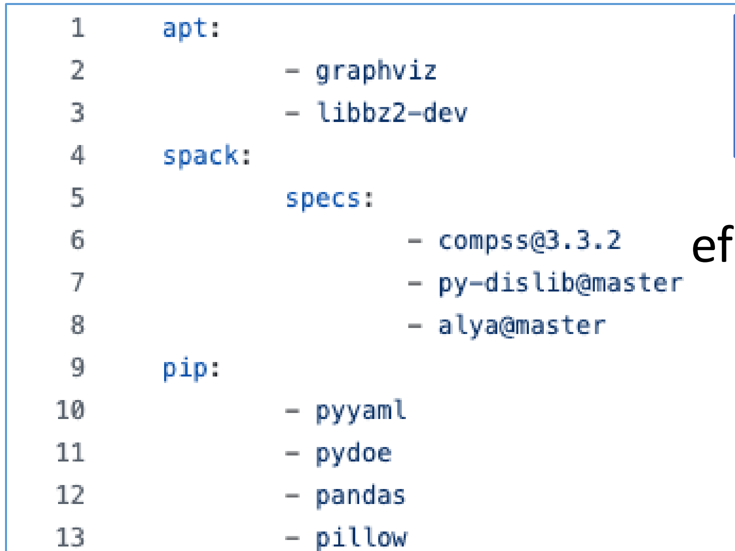

Some taken from defaul Spack repository

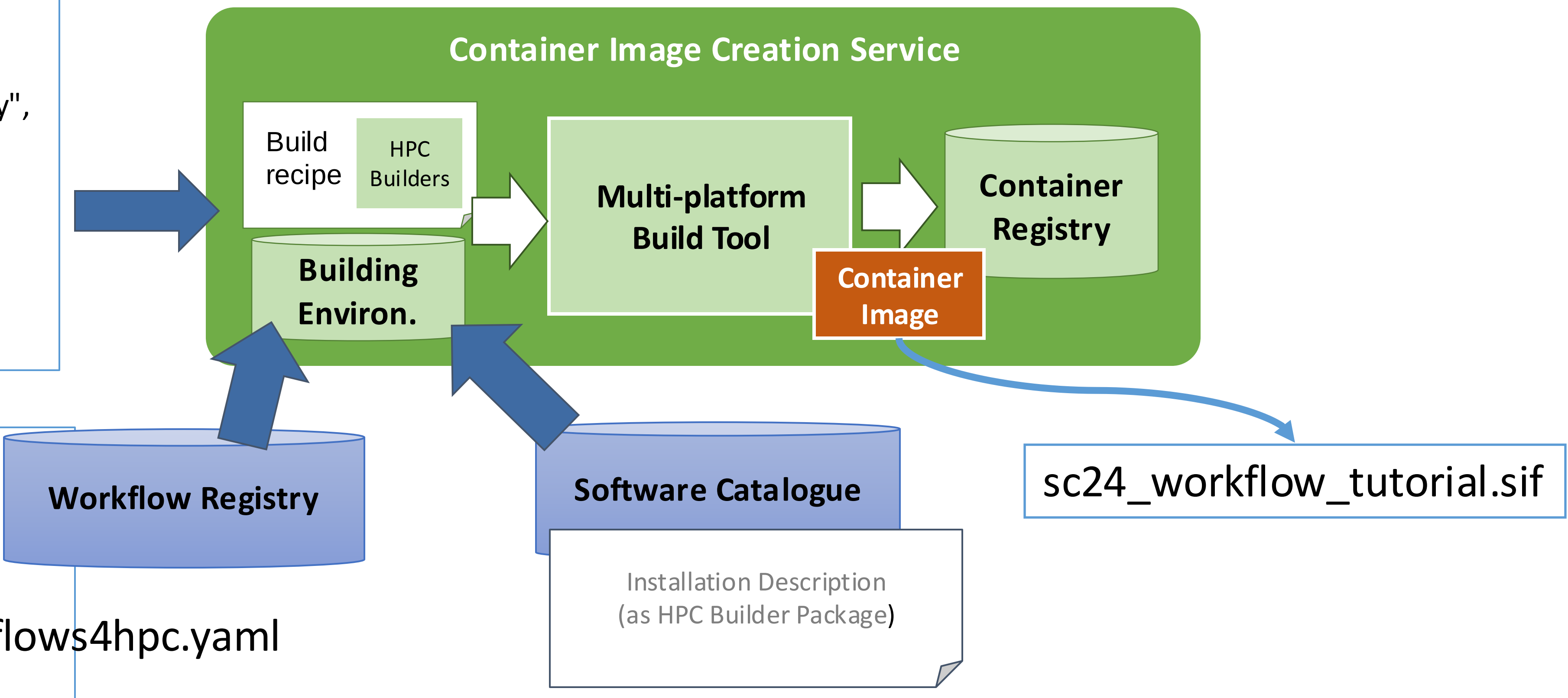
HPC Ready Containers

Service request

```
{
"machine": {
                "platform": "linux/amd64",
                "architecture": "skylake",
                "container_engine": "singularity",
                "mpi":"openmpi@4.1.1"
},
"workflow":”tutorial",
"step_id" : ”HPC_AI_training",
"workflow_yaml" : "eflows4hpc.yaml",
}
```



```
apt:
        - graphviz
        - libbz2-dev
spack:
        specs:
                - compss@3.3.2
                - py-dislib@master
                - alya@master
pip:
        - pyyaml
        - pydoe
        - pandas
        - pillow
```



eflows4hpc.yaml

package.py

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

DT-GEO

CEEC

Colmena

HP2C-DT

CyclOps

DISCOVER US

CAELESTIS

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for Extreme-Scale Computing
Inria NCSA Argonne BSC JÜLICH RIKEN

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Resiliencia

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Thanks!

COMPSs

rosa.m.badia@bsc.es