HPC WORKFLOWS AS A SERVICE AND SOFTWARE STACK HANDS-ON

Jedrzej Rybicki (j.rybicki@fz-juelich.de), Albertin, Loïc (loic.albertin@atos.net)
Jorge Ejarque (jorge.ejarque@bsc.es)

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Hands-on setup

For this hands-on you need:

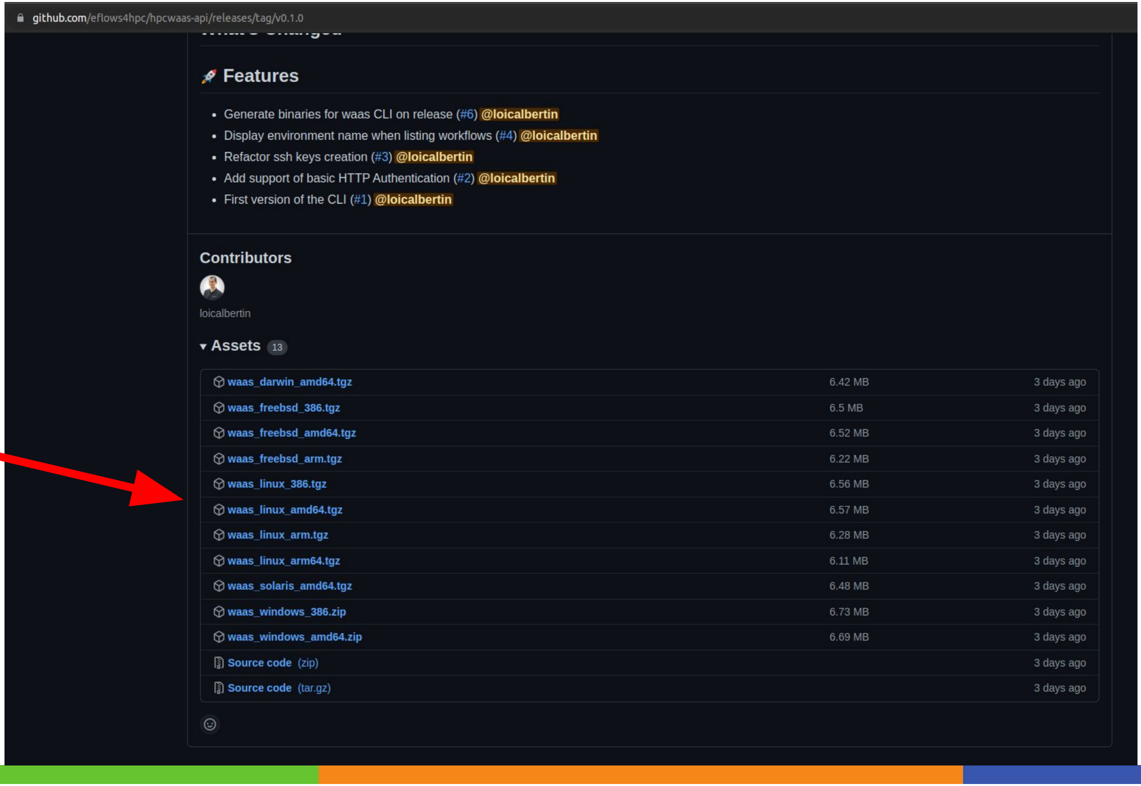
- A computer
- An internet connection
- A user in an HPC cluster and eFlow4HPC services

First things first ensure that you can reach BSC platforms

```
ssh -o PreferredAuthentications=password -o
PubkeyAuthentication=no <user_name>@nord3.bsc.es


# Create some directories that will be used
later

mkdir -p /gpfs/projects/nct01/<user_id>

mkdir -p /home/nct01/<user_id>/data/inputs

mkdir -p /home/nct01/<user_id>/data/results
```

Get the HPCWaaS CLI from github

Explore https://github.com/eflows4hpc/hpcwaas-api/releases/tag/v0.1.0 to get a binary that matches your computer.



github.com/eflows4hpc/hpcwaas-api/releases/tag/v0.1.0

🚀 Features

- Generate binaries for waas CLI on release (#6) @loicalbertin
- Display environment name when listing workflows (#4) @loicalbertin
- Refactor ssh keys creation (#3) @loicalbertin
- Add support of basic HTTP Authentication (#2) @loicalbertin
- First version of the CLI (#1) @loicalbertin

Contributors

loicalbertin

▾ Assets 13

waas_darwin_amd64.tgz	6.42 MB	3 days ago
waas_freebsd_386.tgz	6.5 MB	3 days ago
waas_freebsd_amd64.tgz	6.52 MB	3 days ago
waas_freebsd_arm.tgz	6.22 MB	3 days ago
waas_linux_386.tgz	6.56 MB	3 days ago
waas_linux_amd64.tgz	6.57 MB	3 days ago
waas_linux_arm.tgz	6.28 MB	3 days ago
waas_linux_arm64.tgz	6.11 MB	3 days ago
waas_solaris_amd64.tgz	6.48 MB	3 days ago
waas_windows_386.zip	6.73 MB	3 days ago
waas_windows_amd64.zip	6.69 MB	3 days ago
Source code (zip)		3 days ago
Source code (tar.gz)		3 days ago

Alternatively get the docker version

Simply run:

```
docker run -ti --rm ghcr.io/eflows4hpc/hpcwaas-api:main-cli help
```

this is equivalent to

```
./waas help
```

We will use the later form in this hands-on.

Generate an SSH keypair

```
./waas --api_url https://eflows4hpc.bsc.es/waas -u <user>:<password> ssh_keys
key-gen

INFO: Below is your newly generated SSH public key.

INFO: Take note of it as you will not see it again.

INFO: You are responsible for adding it to the authorized_keys file on the systems you want to run your
workflows.

INFO: SSH key ID:      31…3f

INFO: SSH Public key: ssh-rsa AAA…mH
```

Credentials are the same as for your bsc account.

The private key is stored in Vault and never provided to you.

Copy the public key on nord3 in ~/.ssh/authorized_keys file to allow access to your account by the stack.

Also copy the SSH Key ID that identifies your keypair and which is required to deploy and run workflows.

Now let’s create, configure and deploy a workflow

The goal in this hands-on is not to learn how to develop an application in TOSCA.

For today we will focus on how to use the stack.

We did a TOSCA tutorial during the first year of eFlows4HPC.

This tutorial is publically available on github: https://github.com/eflows4hpc/tosca-tutorial

Now let’s create, configure and deploy a workflow

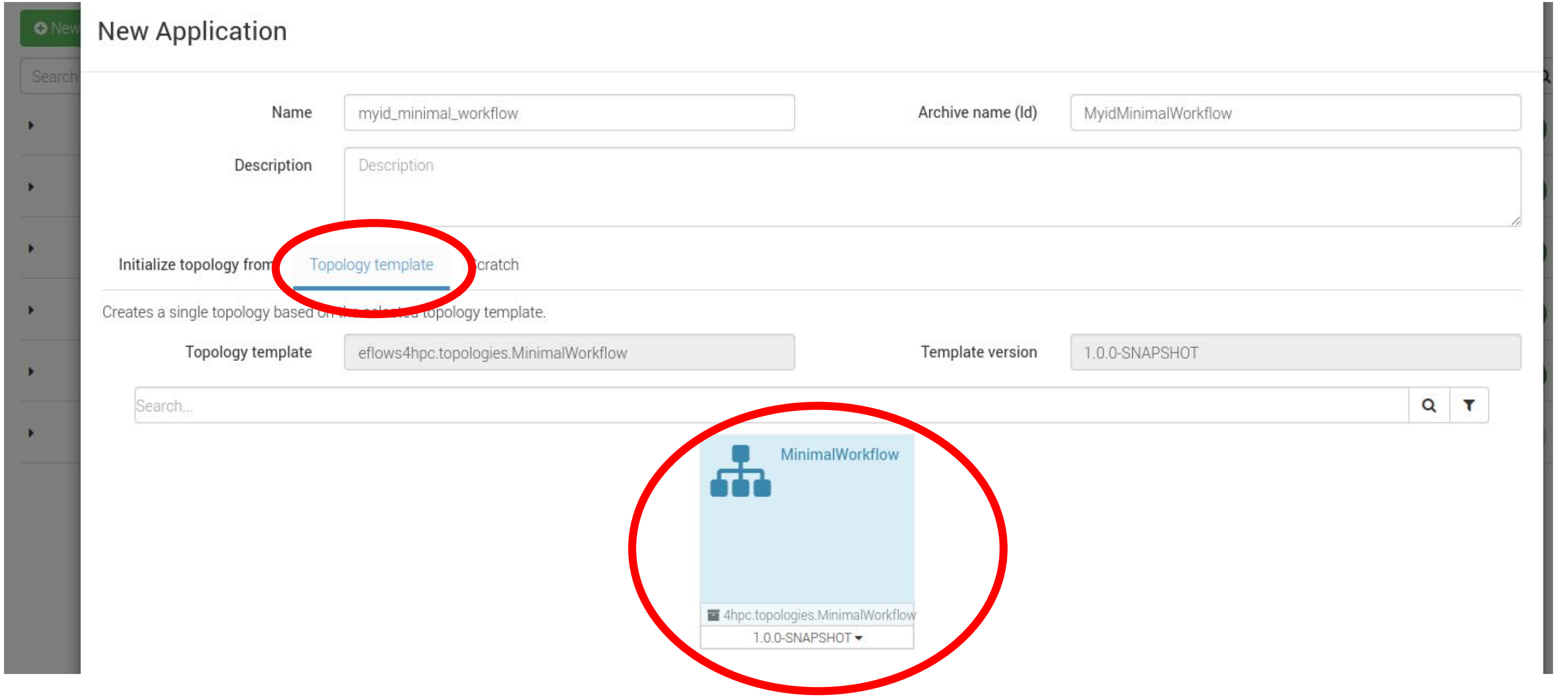
Navigate to https://eflows4hpc.bsc.es/alien/#/

And log into Alien4Cloud. Credentials are the same as your BSC account.

Click on “Applications” on top left tab, then click on “New Application”.

Now let's create, configure and deploy a workflow

Give a name (should be unique) to your application. And initialize it from the minimal workflow template



New Application

Name: myid_minimal_workflow

Archive name (Id): MyidMinimalWorkflow

Description: Description

Initialize topology from: Topology template | Scratch

Creates a single topology based on the selected topology template.

Topology template: eflows4hpc.topologies.MinimalWorkflow

Template version: 1.0.0-SNAPSHOT

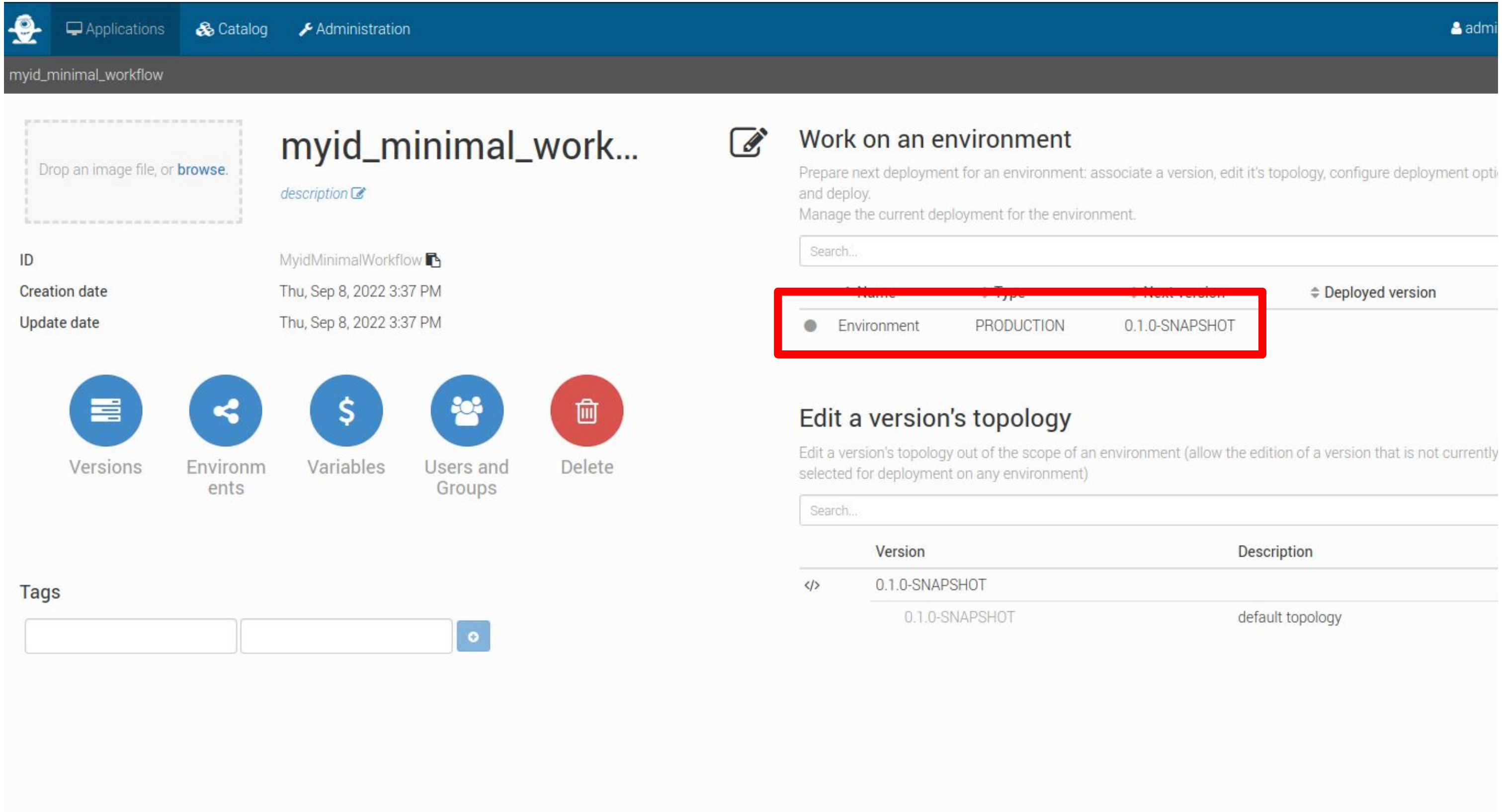
Search...

MinimalWorkflow

4hpc.topologies.MinimalWorkflow

1.0.0-SNAPSHOT

Now let’s create, configure and deploy a workflow



myid_minimal_work...

ID	MyidMinimalWorkflow
Creation date	Thu, Sep 8, 2022 3:37 PM
Update date	Thu, Sep 8, 2022 3:37 PM

Work on an environment

Prepare next deployment for an environment: associate a version, edit it's topology, configure deployment opti and deploy.

Manage the current deployment for the environment.

Search...

	Name	Type	Next version	Deployed version
●	Environment	PRODUCTION	0.1.0-SNAPSHOT	

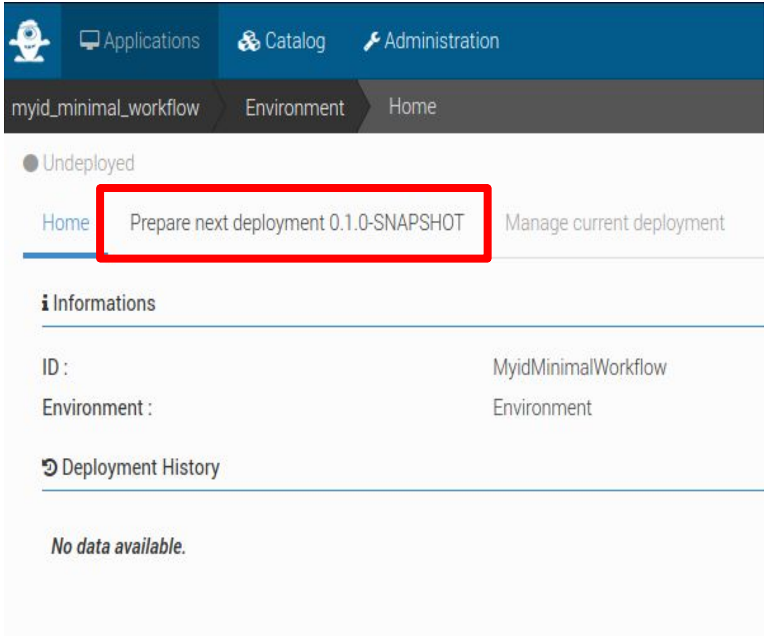
Edit a version's topology

Edit a version's topology out of the scope of an environment (allow the edition of a version that is not currently selected for deployment on any environment)

Search...

	Version	Description
</>	0.1.0-SNAPSHOT	
	0.1.0-SNAPSHOT	default topology

Now let’s create, configure and deploy a workflow

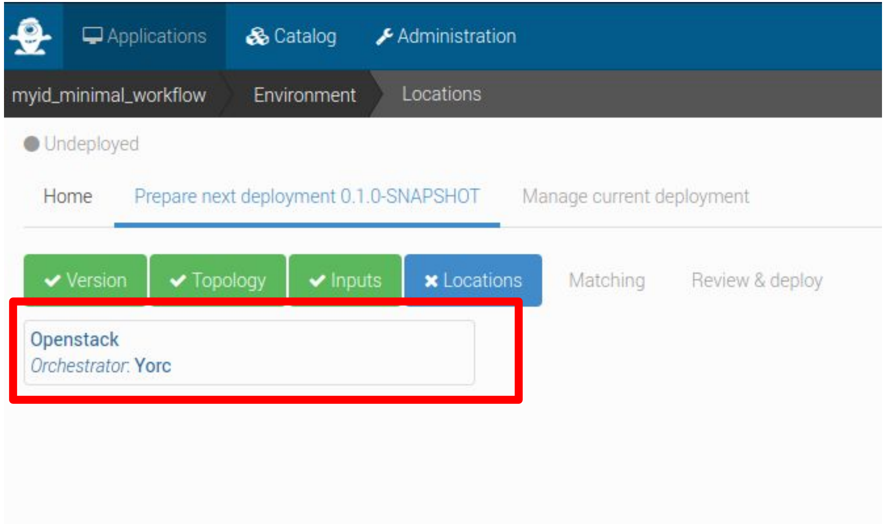


i Informations

ID :	MyidMinimalWorkflow
Environment :	Environment

Deployment History

No data available.

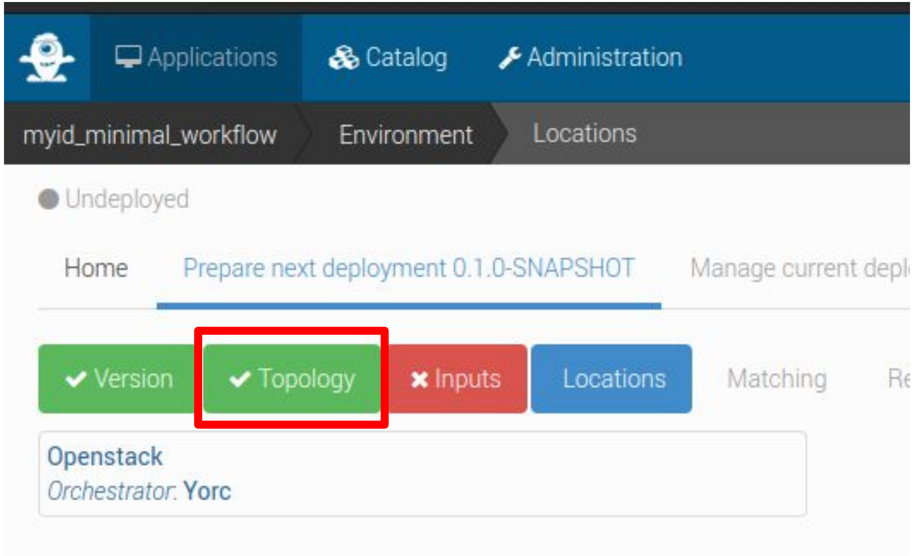


Openstack
Orchestrator: Yorc

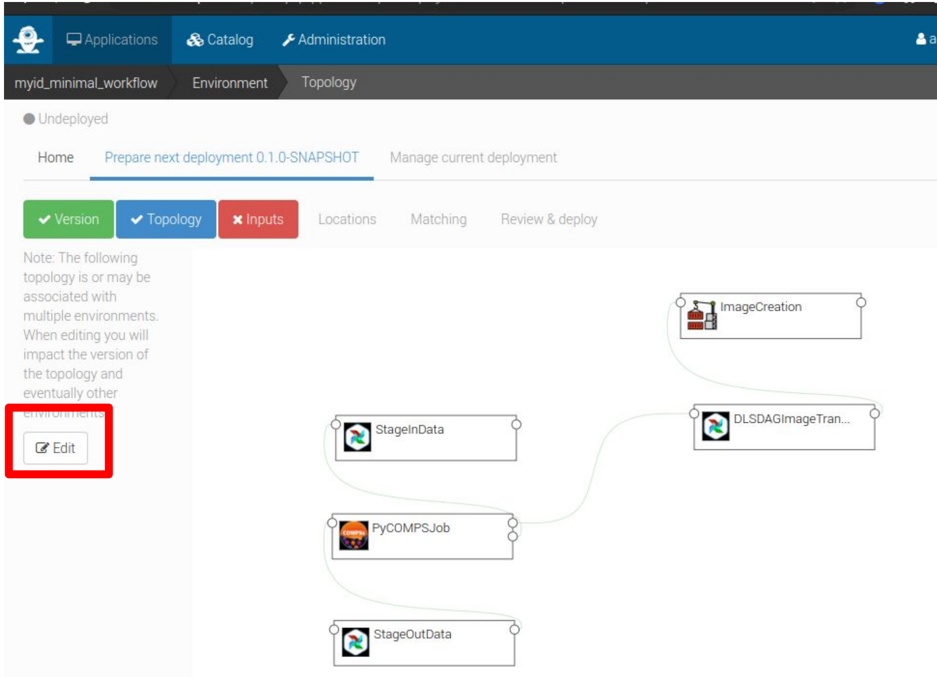
Now let’s create, configure and deploy a workflow

At this point you can have a break to explore the topology of your application.

But make sure to not change it ;)

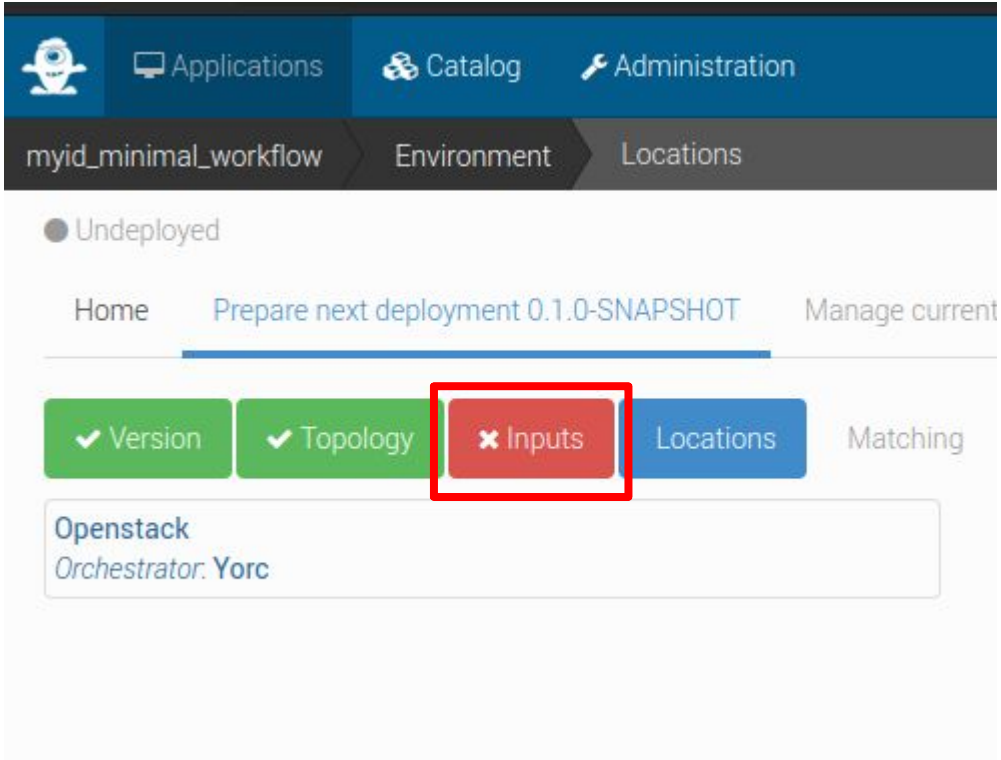


Openstack
Orchestrator: Yorc

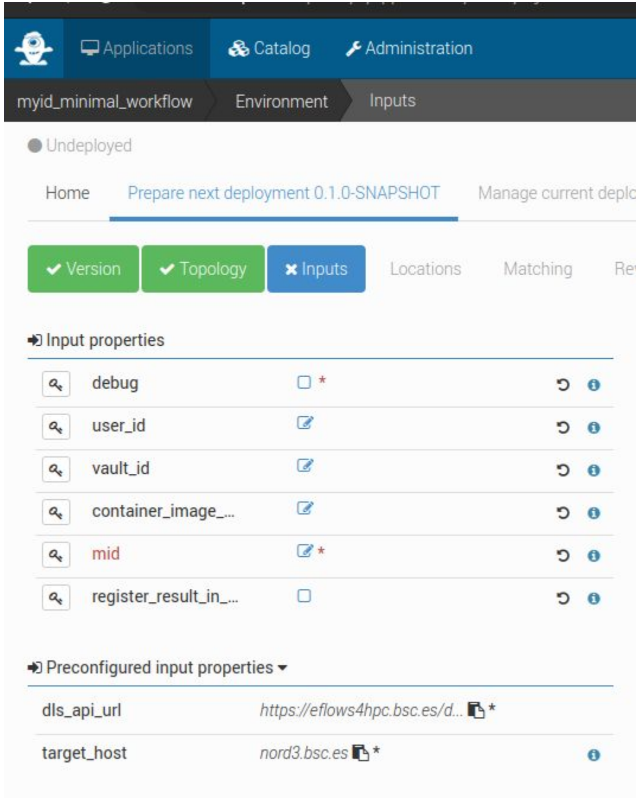


Note: The following topology is or may be associated with multiple environments. When editing you will impact the version of the topology and eventually other environments

Now let's create, configure and deploy a workflow



Openstack
Orchestrator: Yorc



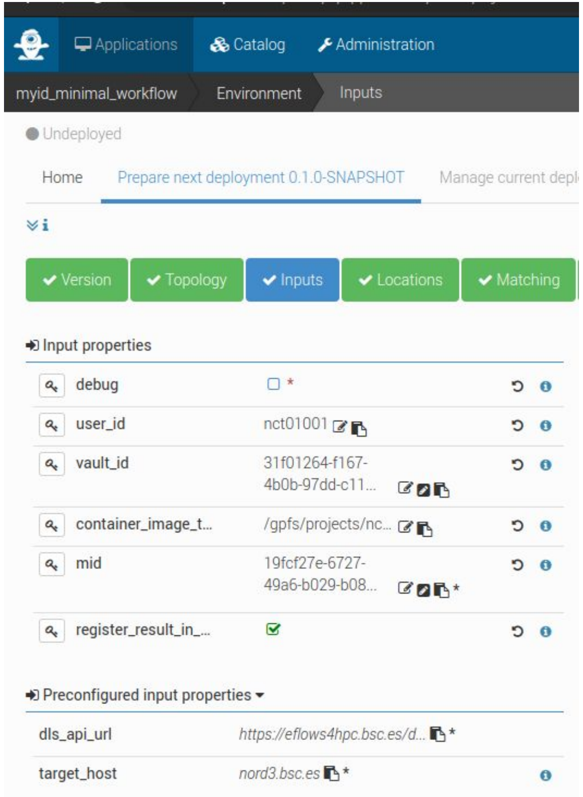
Input properties

debug	□ *	
user_id		
vault_id		
container_image_...		
mid	*	
register_result_in_...	□	

Preconfigured input properties

dls_api_url	*https://eflows4hpc.bsc.es/d...* *
target_host	*nord3.bsc.es* *

Now let's create, configure and deploy a workflow



Input properties

debug	□ *
user_id	nct01001
vault_id	31f01264-f167-4b0b-97dd-c11...
container_image_t...	/gpfs/projects/nc...
mid	19fcf27e-6727-49a6-b029-b08... *
register_result_in_...	☑

Preconfigured input properties

dls_api_url	https://eflows4hpc.bsc.es/d... *
target_host	nord3.bsc.es *

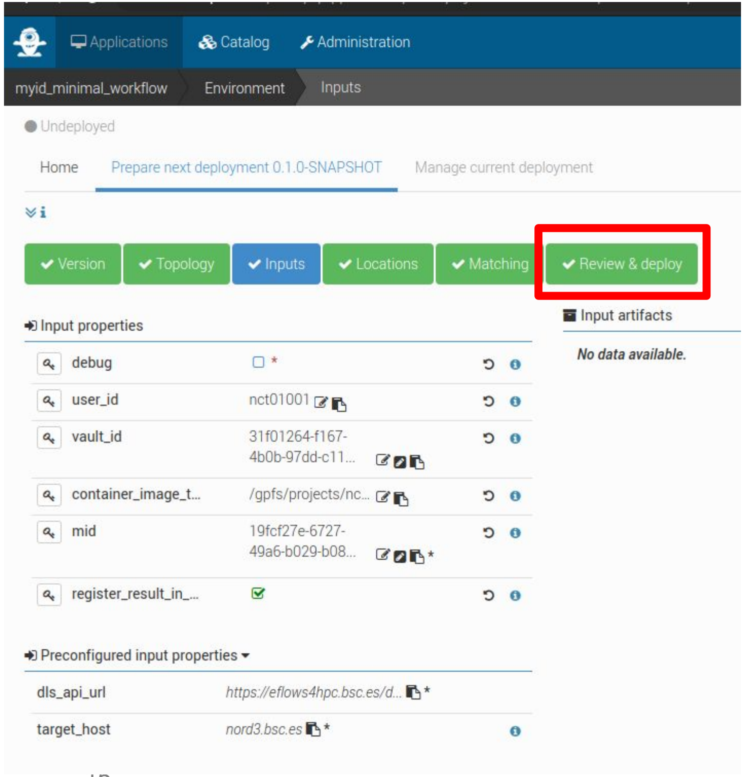
user_id is the user account that will be use to connect to nord3 to transfer the generated container image (it's your BSC account)

vault_id is the SSH keypair id you generated using waas CLI - remember we asked to keep it next to you ;)

container_image_transfer_directory is where the image will be transferred. Keep in mind that you are the developer for this workflow but not necessarily the unique end-user. So you should store it in a shared folder. On nord3 the path /gpfs/projects/nct01/<user_id> will do. The directory SHOULD EXIST before deploying.

mid is a metadata id that is used to store the results of the workflow execution to the data catalogue. For today it should be 19fcf27e-6727-49a6-b029-b08c59e8e38b

Now let’s create, configure and deploy a workflow



Input properties

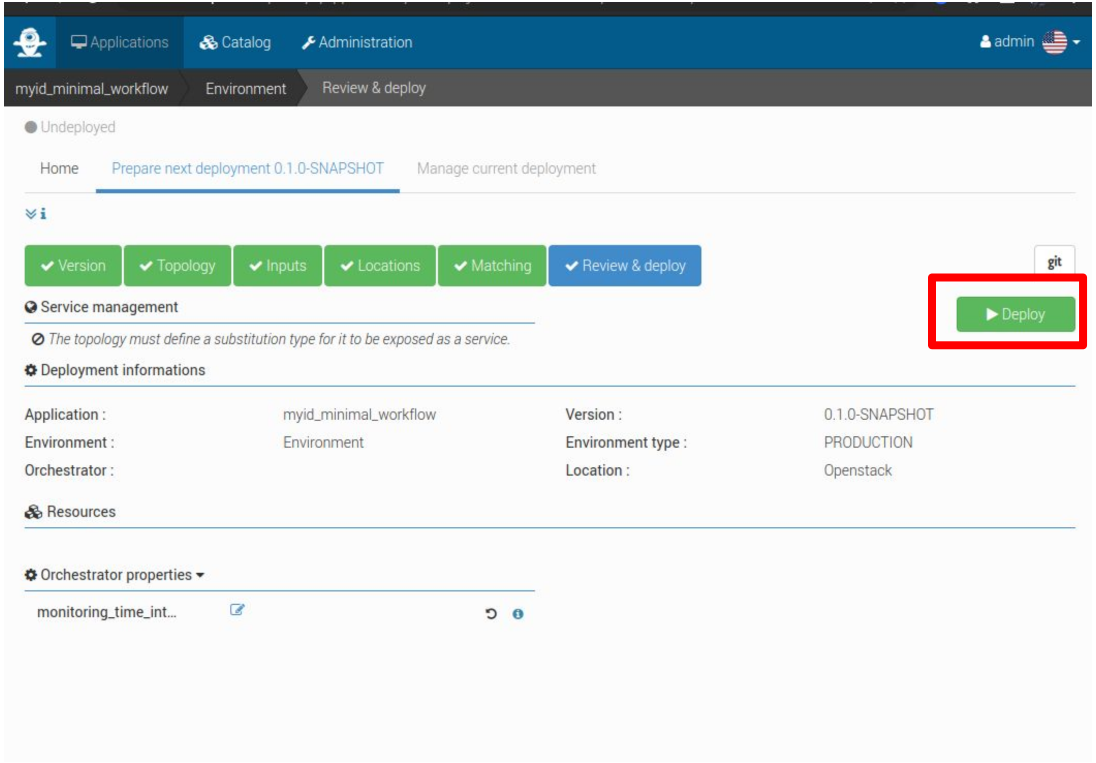
debug	□ *	
user_id	nct01001	
vault_id	31f01264-f167-4b0b-97dd-c11...	
container_image_t...	/gpfs/projects/nc...	
mid	19fcf27e-6727-49a6-b029-b08...	*
register_result_in_...	☑	

Input artifacts

No data available.

Preconfigured input properties ▾

dls_api_url	*https://eflows4hpc.bsc.es/d...* *
target_host	*nord3.bsc.es* *



Service management

The topology must define a substitution type for it to be exposed as a service.

Deployment informations

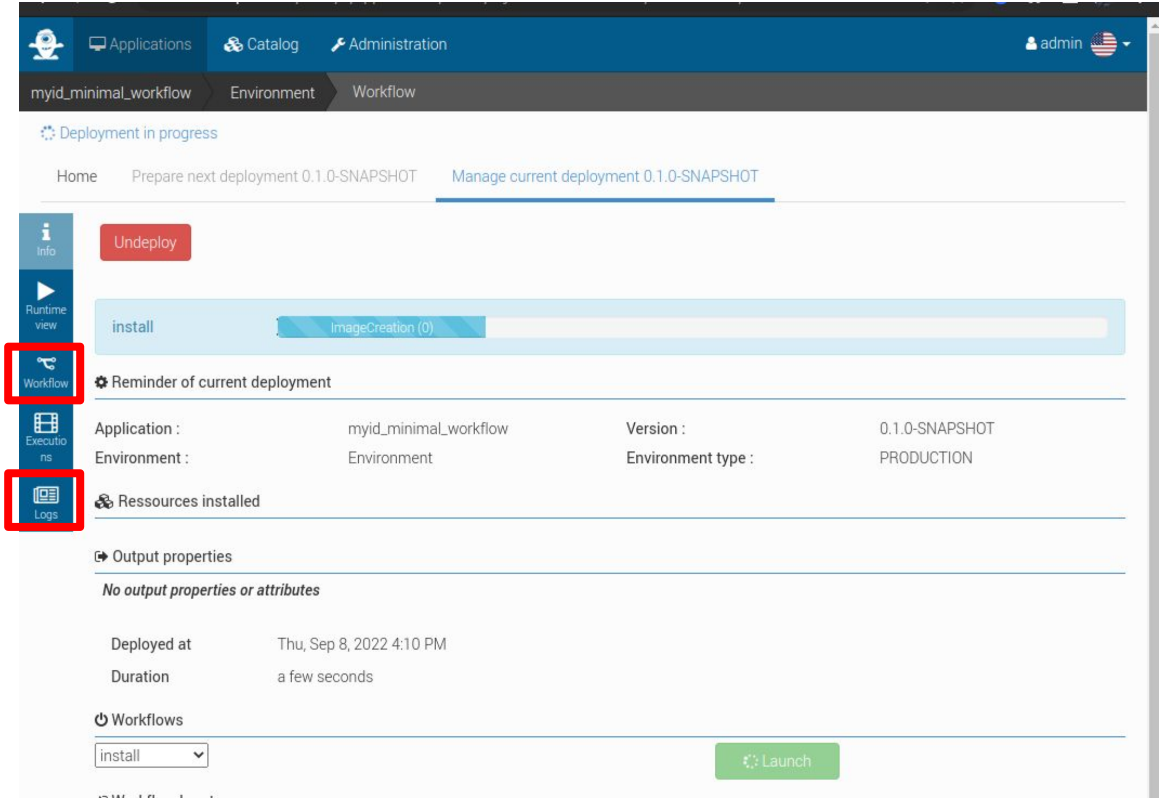
Application :	myid_minimal_workflow	Version :	0.1.0-SNAPSHOT
Environment :	Environment	Environment type :	PRODUCTION
Orchestrator :		Location :	Openstack

Resources

Orchestrator properties ▾

monitoring_time_int...

Now let's create, configure and deploy a workflow



Deployment in progress

install ImageCreation (0)

Reminder of current deployment

Application :	myid_minimal_workflow	Version :	0.1.0-SNAPSHOT
Environment :	Environment	Environment type :	PRODUCTION

Ressources installed

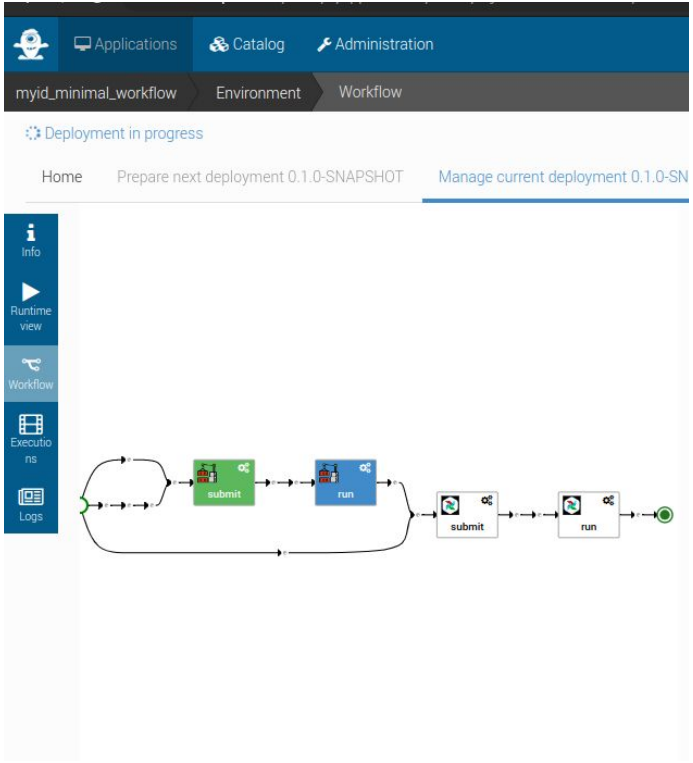
Output properties

No output properties or attributes

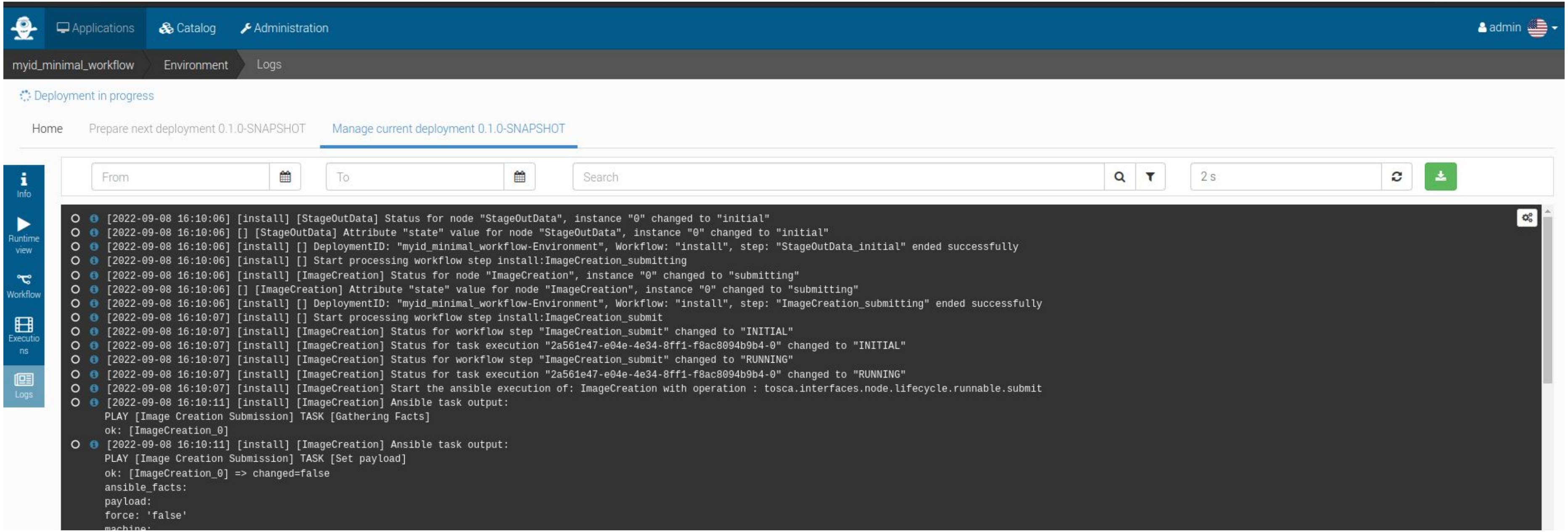
Deployed at	Thu, Sep 8, 2022 4:10 PM
Duration	a few seconds

Workflows

install

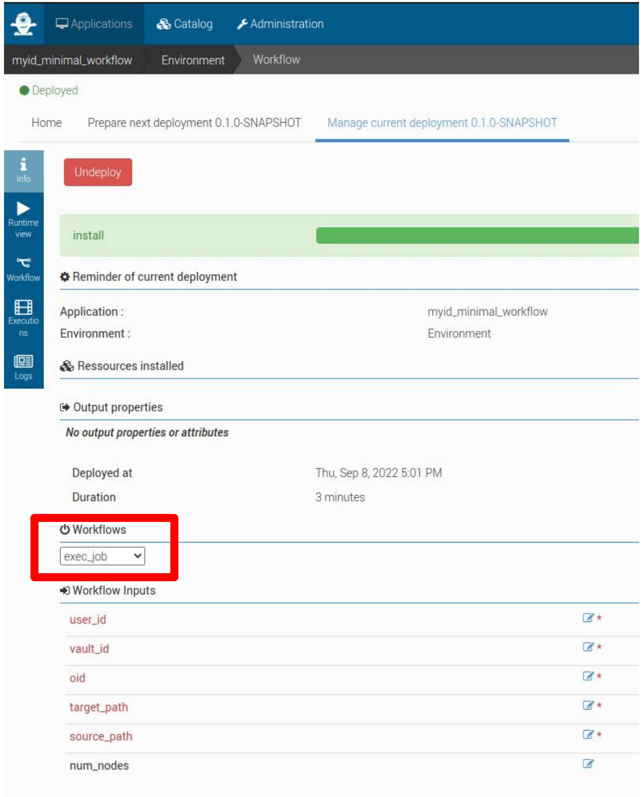


Now let’s create, configure and deploy a workflow



```
○ [2022-09-08 16:10:06] [install] [StageOutData] Status for node "StageOutData", instance "0" changed to "initial"
○ [2022-09-08 16:10:06] [] [StageOutData] Attribute "state" value for node "StageOutData", instance "0" changed to "initial"
○ [2022-09-08 16:10:06] [install] [] DeploymentID: "myid_minimal_workflow-Environment", Workflow: "install", step: "StageOutData_initial" ended successfully
○ [2022-09-08 16:10:06] [install] [] Start processing workflow step install:ImageCreation_submitting
○ [2022-09-08 16:10:06] [install] [ImageCreation] Status for node "ImageCreation", instance "0" changed to "submitting"
○ [2022-09-08 16:10:06] [] [ImageCreation] Attribute "state" value for node "ImageCreation", instance "0" changed to "submitting"
○ [2022-09-08 16:10:06] [install] [] DeploymentID: "myid_minimal_workflow-Environment", Workflow: "install", step: "ImageCreation_submitting" ended successfully
○ [2022-09-08 16:10:07] [install] [] Start processing workflow step install:ImageCreation_submit
○ [2022-09-08 16:10:07] [install] [ImageCreation] Status for workflow step "ImageCreation_submit" changed to "INITIAL"
○ [2022-09-08 16:10:07] [install] [ImageCreation] Status for task execution "2a561e47-e04e-4e34-8ff1-f8ac8094b9b4-0" changed to "INITIAL"
○ [2022-09-08 16:10:07] [install] [ImageCreation] Status for workflow step "ImageCreation_submit" changed to "RUNNING"
○ [2022-09-08 16:10:07] [install] [ImageCreation] Status for task execution "2a561e47-e04e-4e34-8ff1-f8ac8094b9b4-0" changed to "RUNNING"
○ [2022-09-08 16:10:07] [install] [ImageCreation] Start the ansible execution of: ImageCreation with operation : tosca.interfaces.node.lifecycle.runnable.submit
○ [2022-09-08 16:10:11] [install] [ImageCreation] Ansible task output:
    PLAY [Image Creation Submission] TASK [Gathering Facts]
    ok: [ImageCreation_0]
○ [2022-09-08 16:10:11] [install] [ImageCreation] Ansible task output:
    PLAY [Image Creation Submission] TASK [Set payload]
    ok: [ImageCreation_0] => changed=false
    ansible_facts:
    payload:
    force: 'false'
    machine:
```

Now as a Developer let’s test our workflow



Reminder of current deployment

Application : myid_minimal_workflow

Environment : Environment

Ressources installed

Output properties

No output properties or attributes

Deployed at Thu, Sep 8, 2022 5:01 PM

Duration 3 minutes

Workflows

exec_job

Workflow Inputs

- user_id *
- vault_id *
- oid *
- target_path *
- source_path *
- num_nodes

Select the “exec_job” workflow and fill inputs:

user_id **&** ***vault_id*** **are the account credential used to run the job just use the same values as just before deploying**

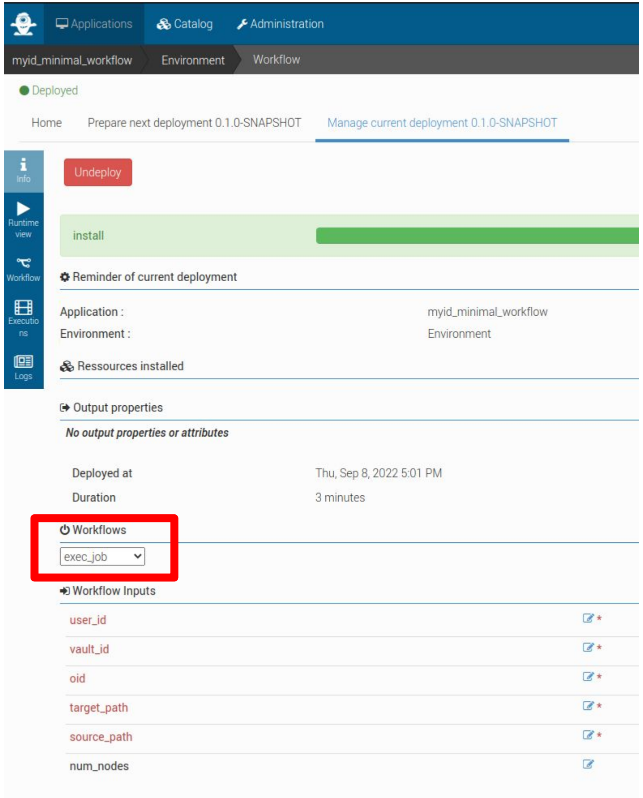
oid **is an object id in the data catalogue referencing the workflow input data. For today it should be 2c2463377aac4aa59381c6b06fe800f3**

target_path **is the path to a directory where the DLS will store input data and will be used as input for the PyCOMPSs job. Typically use some directory in your home, like /home/nct01/<user_id>/data/inputs . This directory SHOULD exist before running the workflow.**

source_path **is the path to a directory where the PyCOMPSs job produces results and which is uploaded to the data catalogue by the DLS. Typically use some directory in your home, like /home/nct01/<user_id>/data/results . This directory SHOULD exist before running the workflow.**

num_nodes **is the number of compute nodes used to run the PyCOMPSs job. Use “2” for this input.**

Now as a Developer let’s test our workflow



● Deployed

install

Reminder of current deployment

Application : myid_minimal_workflow

Environment : Environment

Ressources installed

Output properties

No output properties or attributes

Deployed at Thu, Sep 8, 2022 5:01 PM

Duration 3 minutes

Workflows

exec_job

Workflow Inputs

user_id *

vault_id *

oid *

target_path *

source_path *

num_nodes

Select the “exec_job” workflow and fill inputs:

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source_path **is the path to a directory where the PyCOMPSs job produces results and which is uploaded to the data catalogue by the DLS. Typically use some directory in your home, like /home/nct01/<user_id>/data/results . This directory SHOULD exist before running the workflow.**

num_nodes **is the number of compute nodes used to run the PyCOMPSs job. Use “2” for this input.**

Now as a Developer let's test our workflow

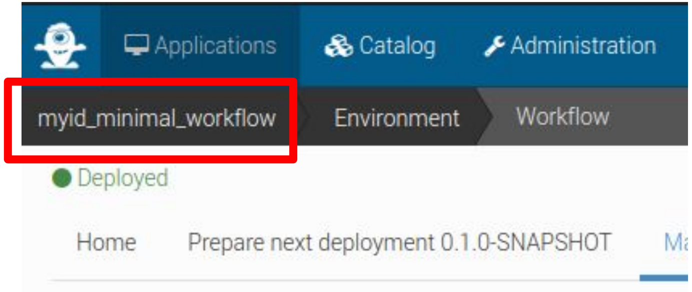
Finally, click on the "Launch" button to run the workflow.

You can follow the workflow execution exactly like we did for the workflow deployment (workflow & logs tabs).

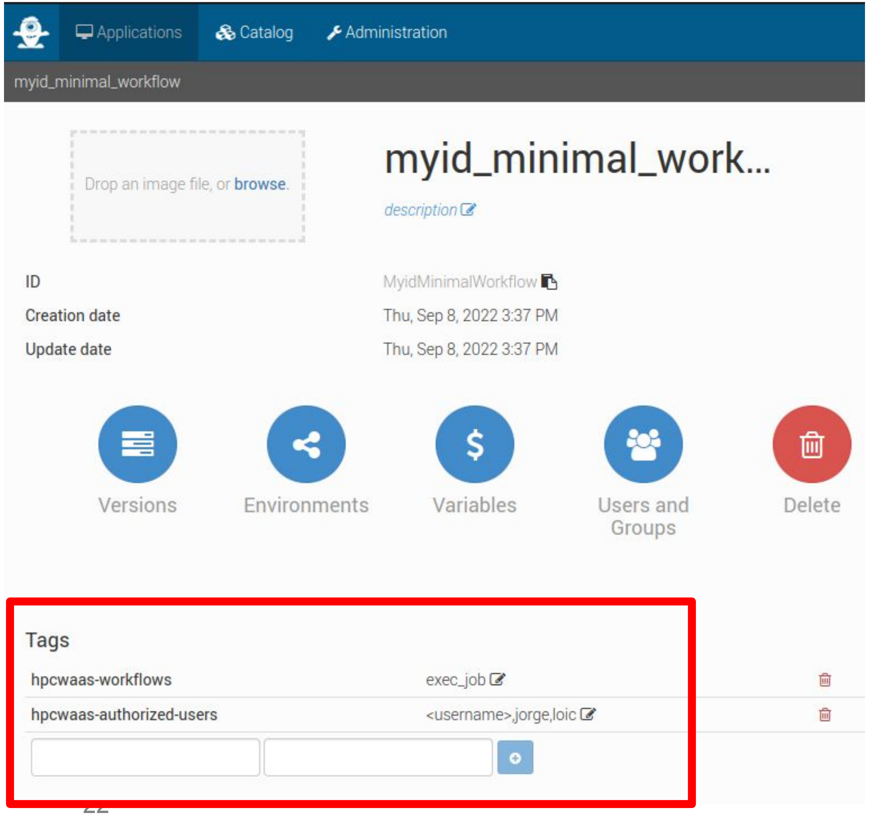
Expose your workflow to the HPCWaaS API

Once you tested that everything works properly, you could choose to expose your workflow to end-users.

Go back to the main page of your application by clicking on its name on the top left corner



Expose your workflow to the HPCWaaS API



ID	MyidMinimalWorkflow
Creation date	Thu, Sep 8, 2022 3:37 PM
Update date	Thu, Sep 8, 2022 3:37 PM

Tags

hpcwaas-workflows	exec_job
hpcwaas-authorized-users	<username>,jorge,loic

Use the tags section to configure the way the HPCWaaS API will interact with your application.

hpcwaas-workflows is a comma-separated list of workflows of your application that should be exposed to the API. In the case of the minimal workflow use “exec_job” as value.

hpcwaas-authorized-users is a comma-separated list of users that are authorized to use this workflow. If this tag is not set every authenticated user can access your workflow. To keep things readable please specify at least your username here.

Now we are done with the Developer role, let’s switch to the end-user role

Interacting with the HPCWaaS API with the CLI

For the end-user the first thing to do is normally to generate an SSH keypair just like you did on slide 6.

You can do it again or just use the one you previously generated.

Let list available workflows

```
./waas --api_url https://eflows4hpc.bsc.es/waas -u <user>:<password> workflows list
```

As a result you will get various information about workflows. The most important one is the Workflow ID as it uniquely identifies a workflow and allow to trigger an execution.

Trigger an execution on a given workflow

```
./waas --api_url https://eflows4hpc.bsc.es/waas -u <user>:<password> workflows
trigger -f -i user_id=<username> -i vault_id=<SSH_KEYPAIR_ID> -i
oid=2c2463377aac4aa59381c6b06fe800f3 -i
target_path=/home/nct01/<username>/data/inputs -i
source_path=/home/nct01/<username>/data/results -i num_nodes=2 <workflow_id>
```

Remember that target_path & source_path SHOULD EXIST before running the workflow.

Monitor a workflow an execution

The -f flag on the “trigger” command allows to follow the execution by regularly refreshing its status from the HPCWaaS API.

Another way to do it is to use the “execution status” command on the Execution ID returned by the “trigger” command.

```
./waas --api_url https://eflows4hpc.bsc.es/waas -u <user>:<password> executions
status <Execution_ID>
```

“execution status” command also have its own -f flag

Cancel a workflow an execution

Cancelling a running execution can be done using the “executions cancel” command

```
./waas --api_url https://eflows4hpc.bsc.es/waas -u <user>:<password> executions
cancel <Execution_ID>
```

That’s all folks!

eFlows4HPC

Enabling dynamic and Intelligent workflows
in the future EuroHPC ecosystem

www.eFlows4HPC.eu

@eFlows4HPC   in eFlows4HPC Project

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