EGI-ACE: HPC as a Service on CLOUDIFIN

Using udocker for EPOCH (PIC) simulations Demo

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EGI-ACE Project Final Review

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Introduction

- The study was focused on the implementation of virtual clusters on OpenStack endowed with MPI capabilities and low latency interconnects, and the investigation of the scaling performances of the EPOCH* code when running on this infrastructure.
- EPOCH is used at ELI-NP for plasma physics simulations.
- The results and demo were obtained on CLOUDIFIN OpenStack site.
- We deployed virtual clusters by using the InfiniBand SR-IOV interfaces and created Virtual Functions on the compute nodes. Then we configured Ubuntu based flavor VMs and performed various tests and benchmarks.

Extendable PIC (Particle in Cell) Open Collaboration, T D Arber et al 2015 Plasma Phys. Control. Fusion 57 113001]

1. EPOCH using uDocker
- *VM with Ubuntu 20.04, Mellanox OFED, OpenMPI-4.0.6*
- *uDocker container with Ubuntu 20.04, OpenMPI-4.1.1, Epoch-4.17.16*
- *NFS over Infiniband sharing the udocker project*

2. EPOCH on VM
- *VM with Ubuntu 20.04, Mellanox OFED, OpenMPI-4.1.1, Epoch-4.17.16*

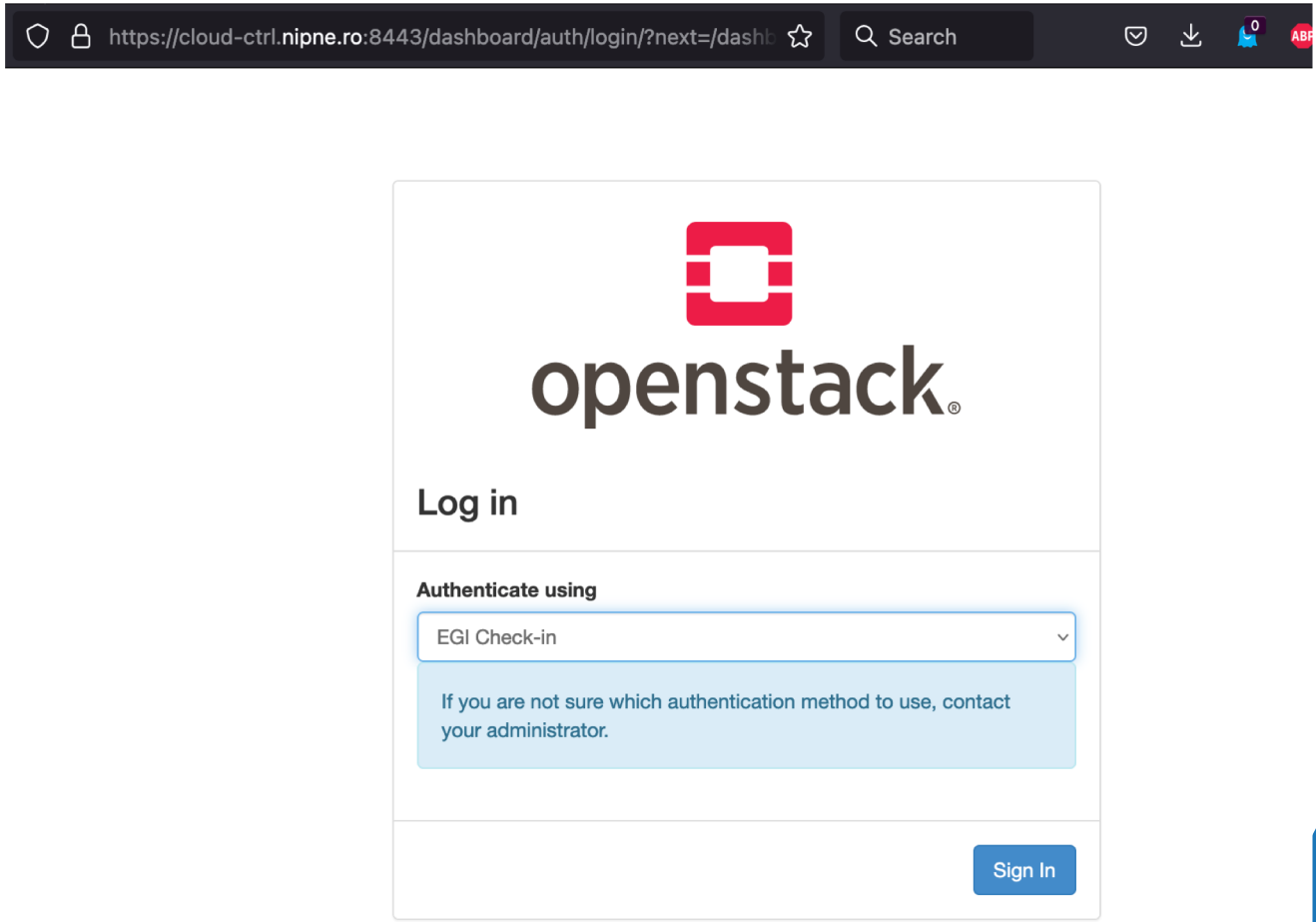
EPOCH code was compiled with mpif90 (*MPI fortran wrapper*) from OpenMPI-4.1.1
The simulations were run on 3 VMs each with 40 cores

OpenStack Horizon Dashboard

Login to the OpenStack dashboard with your EGI Check-in credentials

- All the OpenStack features available are reachable at https://cloud-ctrl.nipne.ro:8443/dashboard
- Federated access with EGI Check-in (used in the demo)
- Keystone credentials (using a username and password)

User is verified and authorized, then can initiate the launching of VMs.



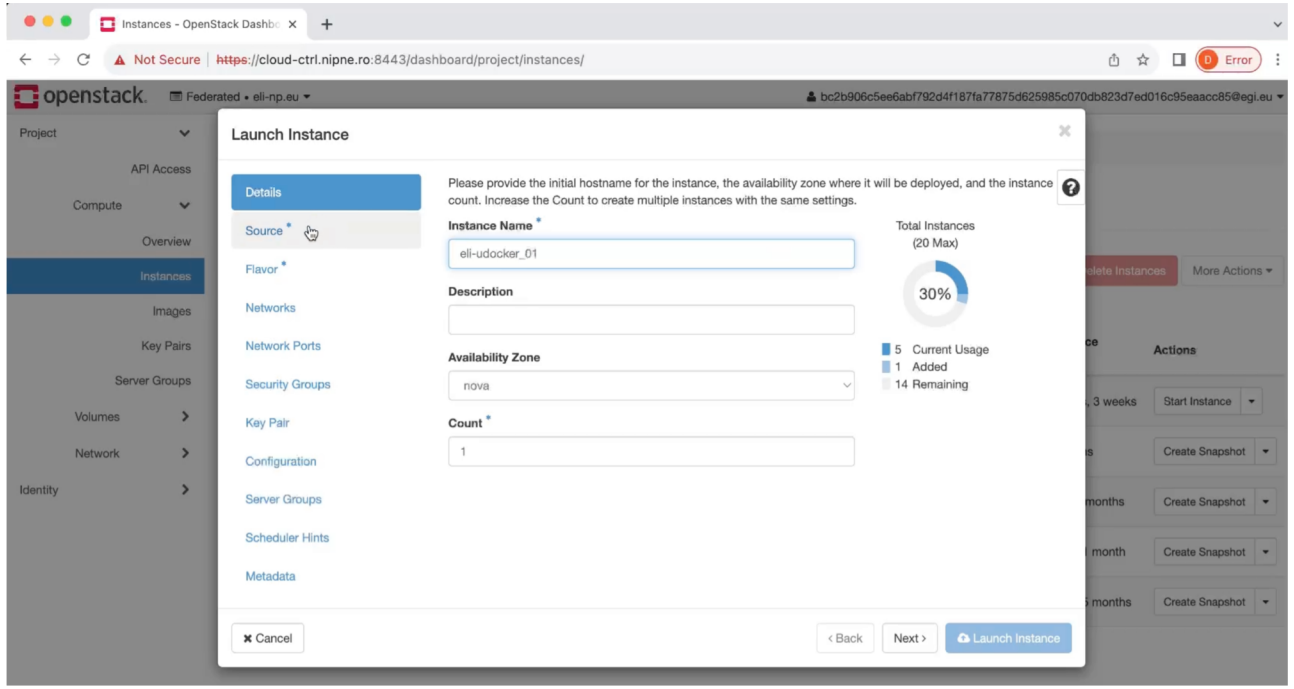
OpenStack Horizon Dashboard

Launching of VMs:

- hostnames used: *egi-udocker_0n* (n=1 for headnode, n=2,3 for computing nodes)
- VM with Ubuntu 20.04, Mellanox OFED, OpenMPI-4.0.6; uDocker container with Ubuntu 20.04, OpenMPI-4.1.1, Epoch-4.17.16
- flavor *elinp.xlarge*: 40 cores, 128G RAM, 80G disk

Access VM console remotely using integrated VNC protocol.

Execute mpi command for *epoch* simulations.



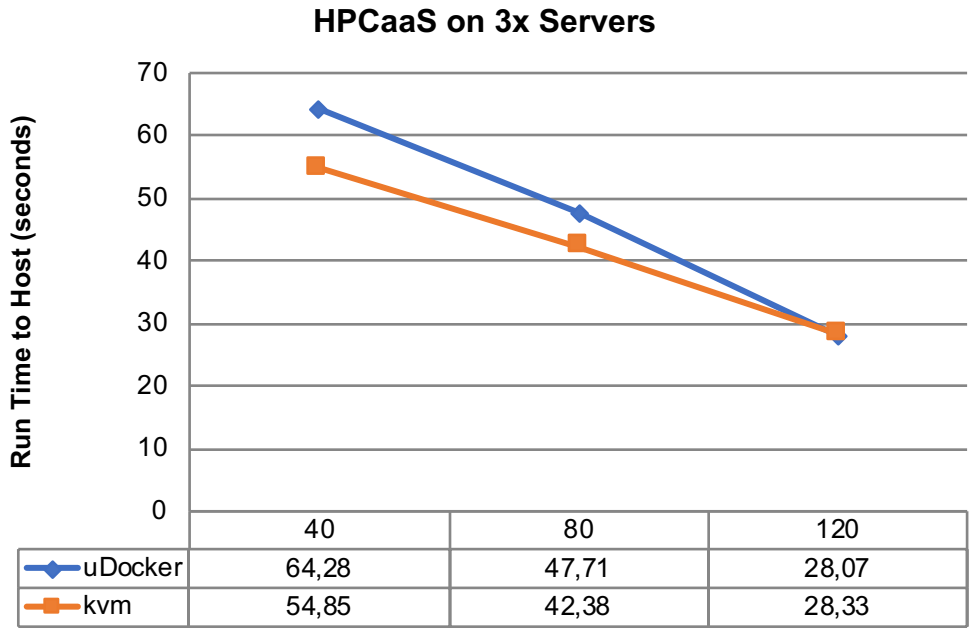
EPOCH MPI Simulations with udocker

The command used to run Epoch using OpenMPI on a HPC cluster with uDocker is:

```
mpiexec --hostfile cluster
        $HOME/udocker-1.3.10/udocker/udocker    run  -e
        LD_LIBRARY_PATH=/usr/lib
        --hostenv
        --hostauth
        --user=$USER
        --workdir=/opt/egi ubuntu
        /opt/egi/epoch2d/bin/epoch2d
```

Next > Demo

Comparison of simulation times



	40	80	120
uDocker	64,28	47,71	28,07
kvm	54,85	42,38	28,33

uDocker vs VM epoch simulations show no significant difference when running on 120 cores

Thank you!

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