



doitnow
HPC Services

EUM2026: DoITNowgroup site talk

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A global HPC Services Company

Servicing HPC customers world-wide

- 100% independent capital (Self-funded company)
- **150+ HPC experts** at your service
- **30+ years of experience** in the EMEA HPC Market
- **200+ clients through all industry verticals** (Aereospace, Automotive, Chemical, Energy, FSI, Life Sciences, Manufacturing, Oil & Gas)
- Services managed
 - 12k+ users/year**
 - 150+ clusters/year**
 - 200+ Training sessions/year**
- Installation services
 - 5 clusters in the Top 500**

Do IT Now Team

EMEA:

France (Montpellier) – (22 people)

Germany (Munich) – (2 people)

Italy (Torino, Maranello) – (60 people)

Spain (Barcellona) – (41 people)

APAC:

New Zealand (Auckland) – (11 people)

USA: 3 people

BRASIL: 4 people

Total 150+ people

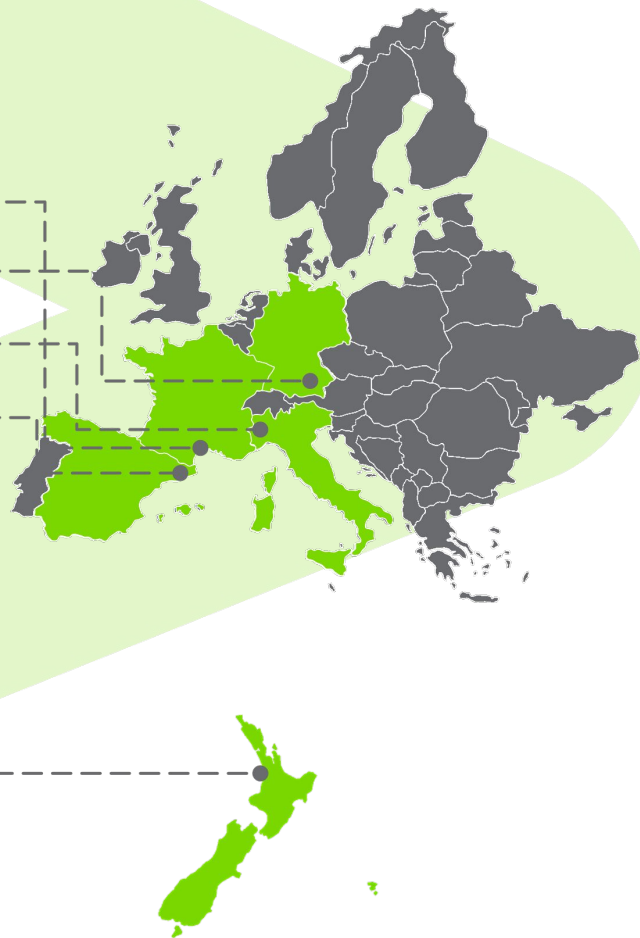
France - Montpellier

Germany - Munich

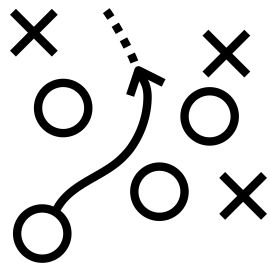
Italy - Turin

Spain - Barcelona

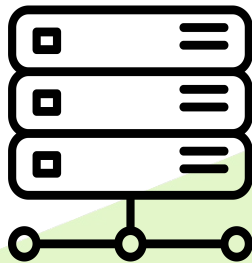
New Zealand - Auckland



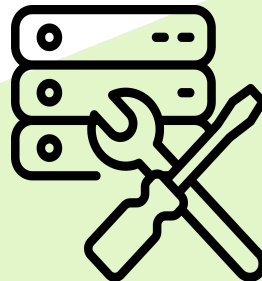
What we offer?



CONSULTING



INSTALLATION



SUPPORT



R&D-as-a-Service

We actively contribute to and integrate EESSI



- Centre of Excellence for multiscale simulations, powered by EESSI



- Bringing EESSI into web-based HPC portals for seamless user access and experience

ODD meets EESSI: Potential use cases

1. Training

- Offer continuous formation without being limited by environments



2. Deploying applications

- Avoiding dependences of containers and or continuous installations



3. Sharing software

- Improve collaboration and scientific software development and sharing between centers



Training



1. Setup Environment

Prepare a cluster structure

We can prepare a basic cluster environment with cloud providers (Aws, Azure...)



2. Prepare OOD

Automatized installation

With automatized installers for Open OnDemand we can deploy and launch over base cluster



3. Software Access

Enable use of Software

Enabling EESSI access for the compute nodes allows us to have access to the scientific software from the OOD apps

Deploying applications

Home / My Interactive Sessions / Jupyter Notebook EESSI

Interactive Apps

Desktops

- Classiq
- Desktop XFCE-GNOME
- Desktop w.Container

GUIs

- Avogadro2
- DIA
- MATLAB
- ParaView

Jupyter Notebook EESSI

This app will launch a Jupyter Notebook server on one or more nodes.

Account:

Number of hours:

I would like to receive an email when the session starts

Launch

* The Jupyter Notebook EESSI session data for this session can be accessed under the data root directory.

```
GNU nano 2.9.8                                     template/script.sh.erb

#!/usr/bin/env bash

# Benchmark Info
echo "TIMING - Starting main script at: $(date)"

# Set working directory to home directory
cd "${HOME}"

#
# Start Jupyter Notebook Server
#

# Purge the module environment to avoid conflicts
module purge

# Prepare EESSI
source /cvmfs/software.eessi.io/versions/2023.06/init/bash

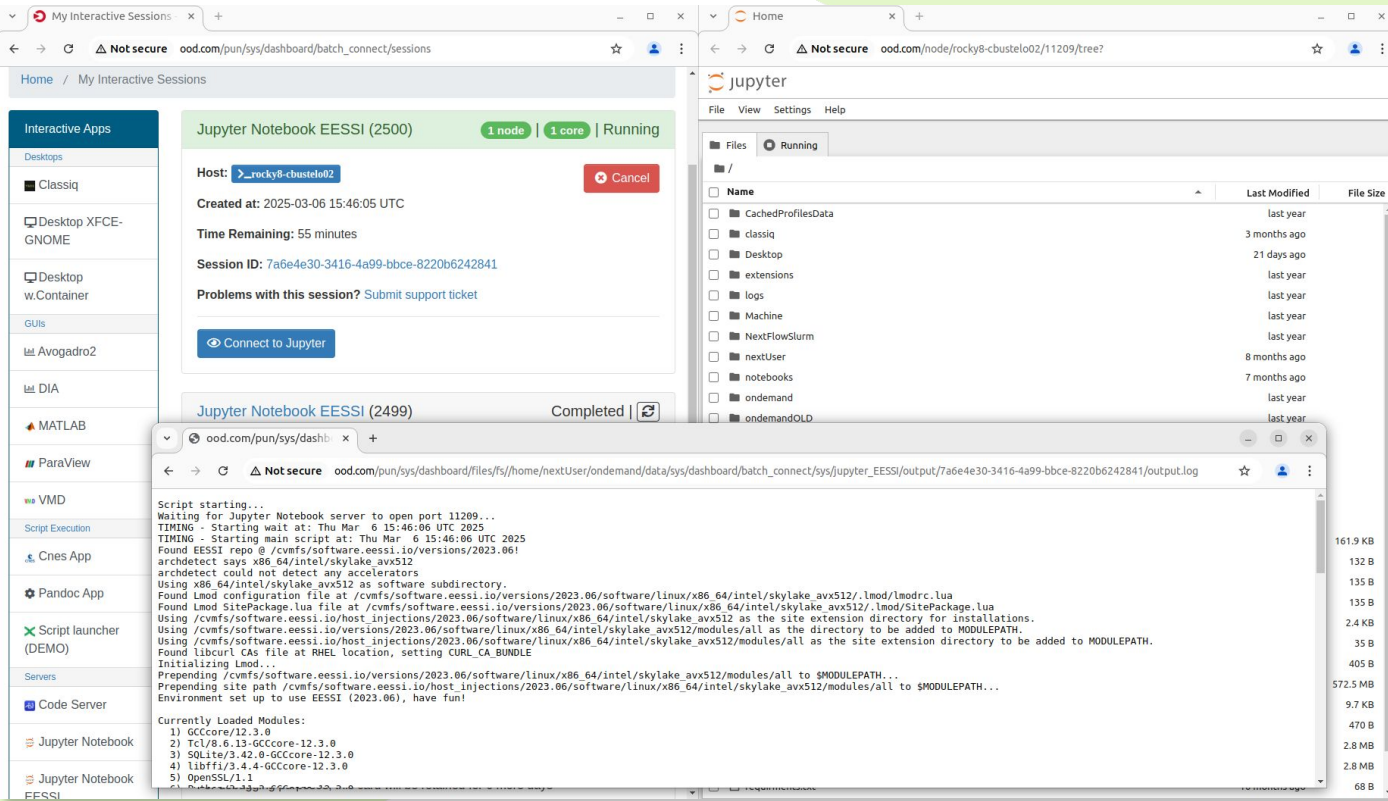
# Load the module
module load JupyterNotebook

# List loaded modules
module list

# Benchmark Info
echo "TIMING - Starting jupyter at: $(date)"

# Launch the Jupyter Notebook Server
#set -x
jupyter notebook --config="${CONFIG_FILE}" <%= context.extra_jupyter_args %>
```

Deploying applications



The screenshot displays a web dashboard for interactive sessions. On the left, a sidebar lists various applications like Desktops, Desktop XFCE-GNOME, Desktop w.Container, GUIS, Avogadro2, DIA, MATLAB, ParaView, VMD, Script Execution, Cnes App, Pandoc App, Xcrt launcher (DEMO), Servers, and Code Server. The main area shows a 'Jupyter Notebook EESSI (2500)' session that is 'Running' on '1 node | 1 core'. It provides details such as the host 'rocky8-cbustelo02', creation time '2025-03-06 15:46:05 UTC', and a 'Time Remaining' of '55 minutes'. A 'Connect to Jupyter' button is visible. Below this, a 'Jupyter Notebook EESSI (2499)' session is shown as 'Completed'.

Overlaid on the dashboard is a terminal window showing the output of a Jupyter Notebook script. The log includes the following text:

```
Script starting...
Waiting for Jupyter Notebook server to open port 11209...
TIMING - Starting wait at: Thu Mar 6 15:46:06 UTC 2025
TIMING - Starting main script at: Thu Mar 6 15:46:06 UTC 2025
Found EESSI repo @ /cvmfs/software.eessi.io/versions/2023.06!
archdetect says x86_64/intel/skylake_avx512
archdetect could not detect any accelerators
Using x86_64/intel/skylake_avx512 as software subdirectory.
Found Lmod configuration file at /cvmfs/software.eessi.io/versions/2023.06/software/linux/x86_64/intel/skylake_avx512/lmod/lmodrc.lua
Found Lmod SitePackage.lua file at /cvmfs/software.eessi.io/versions/2023.06/software/linux/x86_64/intel/skylake_avx512/lmod/SitePackage.lua
Using /cvmfs/software.eessi.io/host_injections/2023.06/software/linux/x86_64/intel/skylake_avx512 as the site extension directory for installations.
Using /cvmfs/software.eessi.io/versions/2023.06/software/linux/x86_64/intel/skylake_avx512/modules/all as the directory to be added to MODULEPATH.
Using /cvmfs/software.eessi.io/host_injections/2023.06/software/linux/x86_64/intel/skylake_avx512/modules/all as the site extension directory to be added to MODULEPATH.
Found libcurl CAS file at RHEL location, setting CURL_CA_BUNDLE
Initializing Lmod...
Prepending /cvmfs/software.eessi.io/versions/2023.06/software/linux/x86_64/intel/skylake_avx512/modules/all to $MODULEPATH...
Prepending site path /cvmfs/software.eessi.io/host_injections/2023.06/software/linux/x86_64/intel/skylake_avx512/modules/all to $MODULEPATH...
Environment set up to use EESSI (2023.06), have fun!

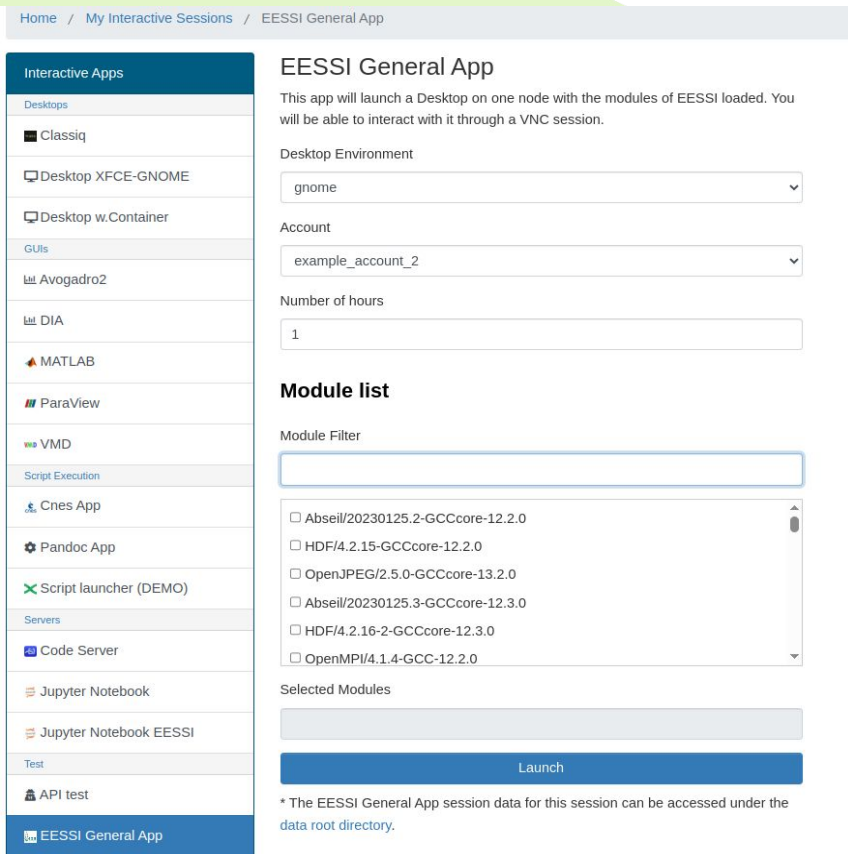
Currently Loaded Modules:
  1) GCCcore/12.3.0
  2) Tcl/8.6.13-GCCcore-12.3.0
  3) SQLite/3.42.0-GCCcore-12.3.0
  4) libffi/3.4.4-GCCcore-12.3.0
  5) OpenSSL/1.1
```

On the right side of the terminal window, a file list is visible with columns for Name, Last Modified, and File Size:

Name	Last Modified	File Size
CacheProfilesData	last year	
classiq	3 months ago	
Desktop	21 days ago	
extensions	last year	
logs	last year	
Machine	last year	
NextFlowSlurm	last year	
nextUser	8 months ago	
notebooks	7 months ago	
ondemand	last year	
ondemandOLD	last year	

Sharing Software

- Web Desktop based application
- Modules field to select software needed by the user
- Selected modules unwritable field to check the selected ones
- Search mechanism to find specific modules



Home / My Interactive Sessions / EESSI General App

Interactive Apps

- Desktops
 - Classiq
 - Desktop XFCE-GNOME
 - Desktop w.Container
- GUIs
 - Avogadro2
 - DIA
 - MATLAB
 - ParaView
 - VMD
- Script Execution
 - Cnes App
 - Pandoc App
 - Script launcher (DEMO)
- Servers
 - Code Server
 - Jupyter Notebook
 - Jupyter Notebook EESSI
- Test
 - API test
- EESSI General App**

EESSI General App

This app will launch a Desktop on one node with the modules of EESSI loaded. You will be able to interact with it through a VNC session.

Desktop Environment
gnome

Account
example_account_2

Number of hours
1

Module list

Module Filter

- Abseil/20230125.2-GCCcore-12.2.0
- HDF/4.2.15-GCCcore-12.2.0
- OpenJPEG/2.5.0-GCCcore-13.2.0
- Abseil/20230125.3-GCCcore-12.3.0
- HDF/4.2.16-2-GCCcore-12.3.0
- OpenMPI/4.1.4-GCC-12.2.0

Selected Modules

Launch

* The EESSI General App session data for this session can be accessed under the data root directory.

Sharing software

- Adding software to the EESSI stack also grant access from all the other

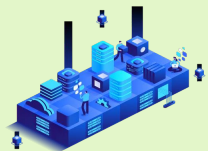
OPEN
 + **EESSI**

integrations

- Accessible via this App simplifying the sharing between centers



HPC CENTER A



OPEN

 **nDemand**

HPC CENTER B



EESSI
EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS



OPEN

 **nDemand**

HPC CENTER C

General customer support

- R&D groups or departments with its own computational resources
- Support cluster post installation
- Small/medium size clusters
- A lot of **scientific applications**
- Very **heterogeneous infrastructure**
 - Different microarchitectures
 - Different kind of GPUs

EasyBuild benefits

- Guaranty: Tested applications at some extend. A HPC expert community behind.
- Reproducibility
 - Compiler, libraries, and required dependencies are mostly controlled by EasyBuild.
 - Fixed software versions for compiler, libraries, (build) dependencies, etc.
- Performance:
 - Building software from source
 - Software is optimized for the processor architecture of build host (by default).



Microarchitecture support needed

Final user wants:

Specify the module application/version to run



System configuration provides the right microarchitecture

Microarchitecture support: detection

- Archspec
 - Similar approach to one used in [EESSI software-layer-scripts](#)
 - [Distro](#) package to detect OS version

```
$ clush -w @all /shared/easybuild/extra/bin/software_subdir.py
n14: rockylinux/8.10/amd/zen5
n13: rockylinux/8.10/amd/zen4
n12: rockylinux/8.10/intel/skylake_avx512
n10: rockylinux/8.10/intel/broadwell
n05: rockylinux/8.10/intel/broadwell
n08: rockylinux/8.10/intel/broadwell
n11: rockylinux/8.10/intel/skylake_avx512
n04: rockylinux/8.10/intel/sandybridge
n07: rockylinux/8.10/intel/broadwell
n03: rockylinux/8.10/intel/sandybridge
n01: rockylinux/8.10/intel/sandybridge
```

Microarchitecture support: Cluster manager integration

- Local easybuild user devoted to general EasyBuild software installation.
- `easybuild-links.service`: systemd service to create a internode common path that **simlinks** or **bindmount** the corresponding microarchitecture path.

```
$ ls -alrt /eb/x86_64
lrwxrwxrwx 1 root root 59 Mar  5 12:13 /eb/x86_64 ->
/shared/easybuild/software/rockylinux/9.5/amd/zen5
```

- Node `/etc/profile:ml use /eb/${uname -i}/modules/all`

Microarchitecture support: login node

- A login node used to be a virtual machine with limited resources
- easybuild-links.service: specific for the login node (maintaining MODULEPATH: /eb/\${uname -i})
- Hook on LMod SitePackage.lua to avoid module loading

```
local function load_hook(t)
    local advice = "which has been compiled on a different microarch. "
    advice = advice .. "In order to be able to use the module, you will need "
    advice = advice .. "to run an interactive session with salloc or submit a
job\n"
    LmodError("\nYou requested to load ", simpleName, " ", advice)
end
```

Architecture support: GPU

- NVIDIA GPUs: **CUDA compute capability** (sm_75,sm_80,...)

- For specific applications install **a version per gpu arch**:

```
eb PyTorch-2.9.1-foss-2024a-CUDA-12.6.0.eb --cuda-compute-capabilities=9.0  
--try-amend=versionsuffix="-CUDA-12.6.0/$(nvptx-arch) "  
nvptx-arch, amdgpu-arch: clang-tools
```

- Default module depending on local node setting:

```
modules/all/PyTorch/2.9.1-foss-2024a-CUDA-12.6.0/.modulerc.lua
```

```
local function read_file(path)  
    local f = io.open(path, "rb")  
    if not f then return nil end  
    local content = f:read(5)  
    f:close()  
    return content  
end  
module_version(read_file("/defaults/DEFAULTGPU") or "", "default")
```

Conclusions

- Experience from participation in R&D projects let us provides better services to our costumers improving user experience:
 - EESSI+OOD = users reach reproducible software via a web interface.
 - Easybuild ensures microarchitecutre optimization - the same module runs optimised transparently to the user.



doitnow

HPC Services

Questions?

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