



# OOD Meets ESSI:

**Accessing and Distributing  
Scientific Software with Ease**

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R&D - Do IT Now

Arturo Gimeno  
Support - Do IT Now



# A global HPC Services Company

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Servicing HPC customers world-wide

- 100% independent capital (Self-funded company)
- **140+ HPC experts** at your service
- **30+ years of experience** in the EMEA HPC Market
- **200+ clients through all industry verticals** (Aerospace, 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)

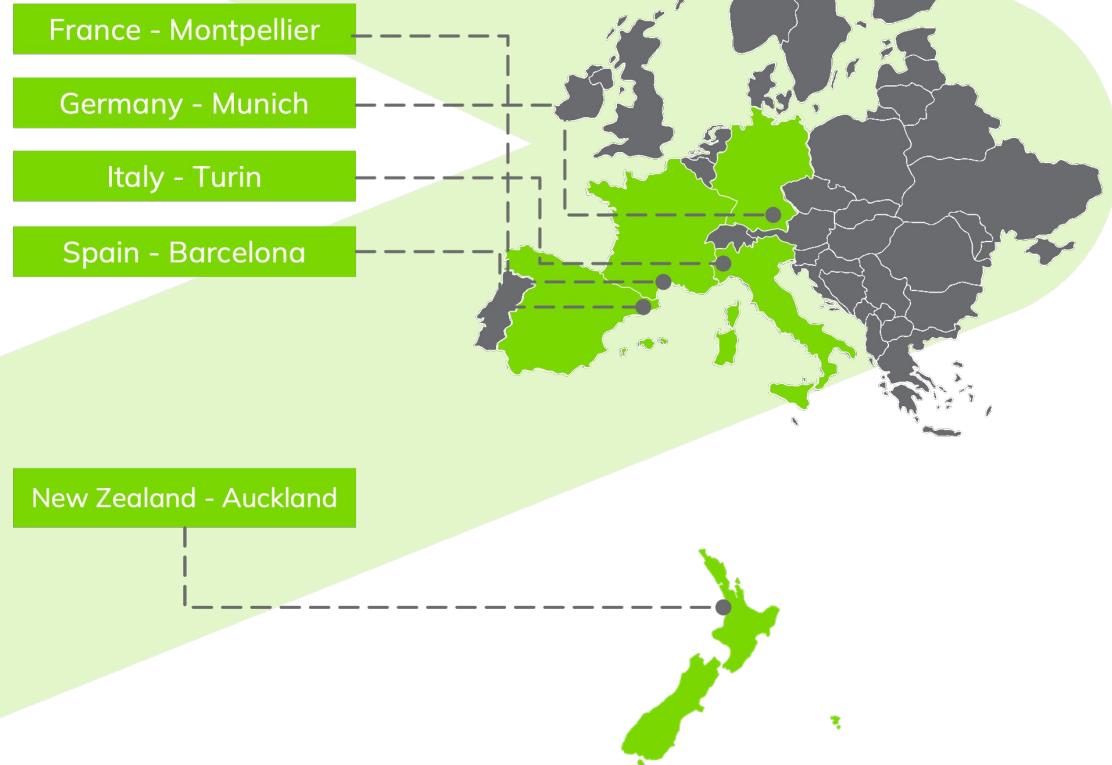
### APAC:

- New Zealand (Auckland) – (11 people)

### USA: 3 people

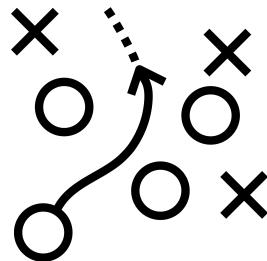
### BRASIL: 4 people

**Total 140+ people**

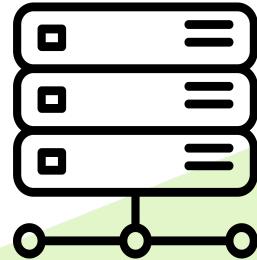


## What we offer?

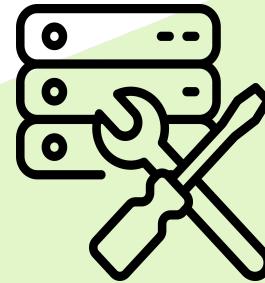
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CONSULTING



INSTALLATION



SUPPORT



R&D-as-a-Service

# Open OnDemand & EESSI

**OPEN**

## 1. **OnDemand:**

- Make HPC resources more accessible for everyone + Point of gathering of multiple types of resources.

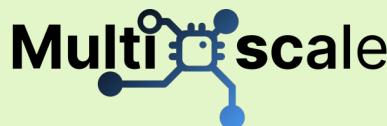
## 2. **EESSI:**

- EESSI is a shared repository of optimized scientific software installations

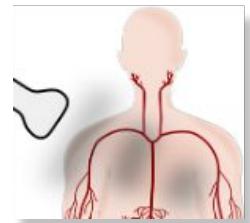
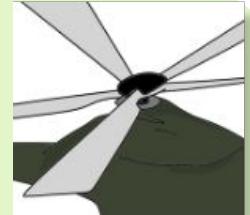


# MultiXscale Centre-of-Excellence in a nutshell

- 4-year project (started in Jan 2023), ~€6M budget
- Collaboration between EESSI and CECAM (total of 16 partners)
  - EESSI primarily addresses technical aspects
  - CECAM network provides scientific expertise
- Scientific target: multiscale simulations with 3 key use cases
  - Helicopter design and certification for civil transport
  - Battery applications to support the sustainable energy transition
  - Ultrasound for non-invasive diagnostics and biomedical applications



<https://multixscale.eu>

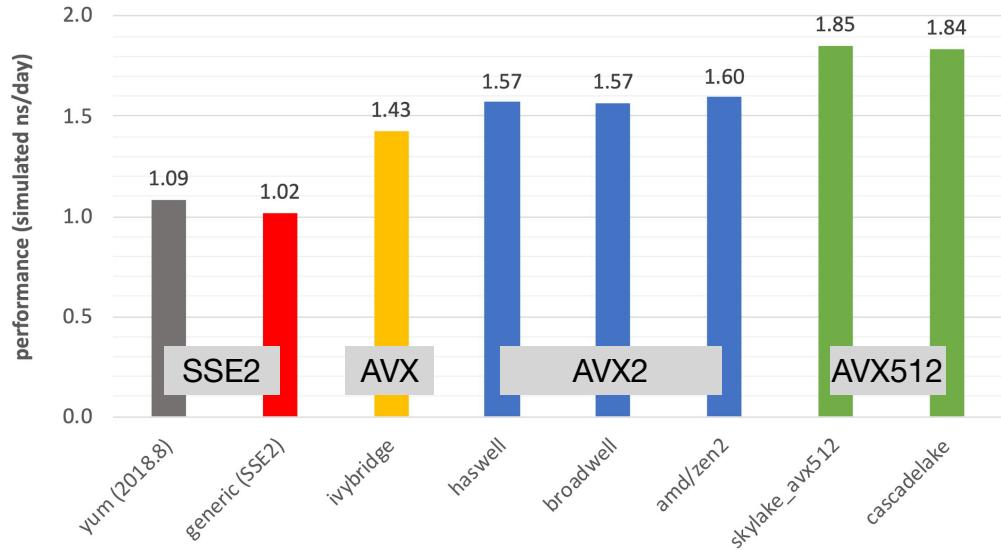


## The changing landscape of scientific computing

- **Explosion of available scientific software applications** (bioinformatics, AI boom, ...)
- Increasing interest in **cloud** for scientific computing (flexibility!)
- **Increasing variety in processor (micro)architectures** beyond Intel & AMD:
  - Arm is already here (see Fugaku, JUPITER, ...), RISC-V is coming (soon?)
- In strong contrast: available (wo)manpower in **HPC support teams** is (**still**) limited...

# Optimized scientific software installations

- Software should be optimized for the system it will run on (keep the P in HPC!)
- Impact on performance is often significant for scientific software!
- Example: GROMACS 2020.1  
(PRACE benchmark, Test Case B)
- Metric: (simulated) ns/day,  
higher is better
- Test system: dual-socket  
Intel Xeon Gold 6420  
(Cascade Lake, 2x18 cores)
- Performance of different GROMACS binaries,  
on exact same hardware/OS



What if you no longer have to install  
**a broad range of scientific software**  
from scratch on every laptop, HPC cluster,  
or cloud instance you use or maintain,  
**without compromising on performance?**



## EESSI in a nutshell

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- European Environment for Scientific Software Installations (**EESSI**)
- **Shared repository of (optimized!) scientific software installations**
- Uniform way of providing software to users, regardless of the system they use!
- Should work on any Linux OS (+ WSL, macOS via Lima) and system architecture
- From laptops and personal workstations to HPC clusters and cloud
- Support for different CPU (micro)architectures, interconnects, GPUs, etc.
- **Focus on performance, automation, testing, collaboration**

## Major goals of EESSI

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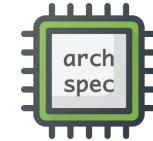
- Avoid duplicate work (for researchers, HPC support teams, sysadmins, ...)
  - Tools that automate software installation process (EasyBuild, Spack) are not sufficient anymore
  - Go beyond sharing build recipes, work towards a shared software stack
- Providing a truly uniform software stack
  - Use the (exact) same software environment everywhere
  - Without sacrificing performance for “mobility of compute” (like is typically done with containers/conda)
- Facilitate HPC training, development of (scientific) software, ...



Host OS provides network & GPU drivers, resource manager (Slurm), ...

### Software layer

Optimized applications + dependencies



### Compatibility layer

Levelling the ground across client OSs



### Filesystem layer

Distribution of the software stack

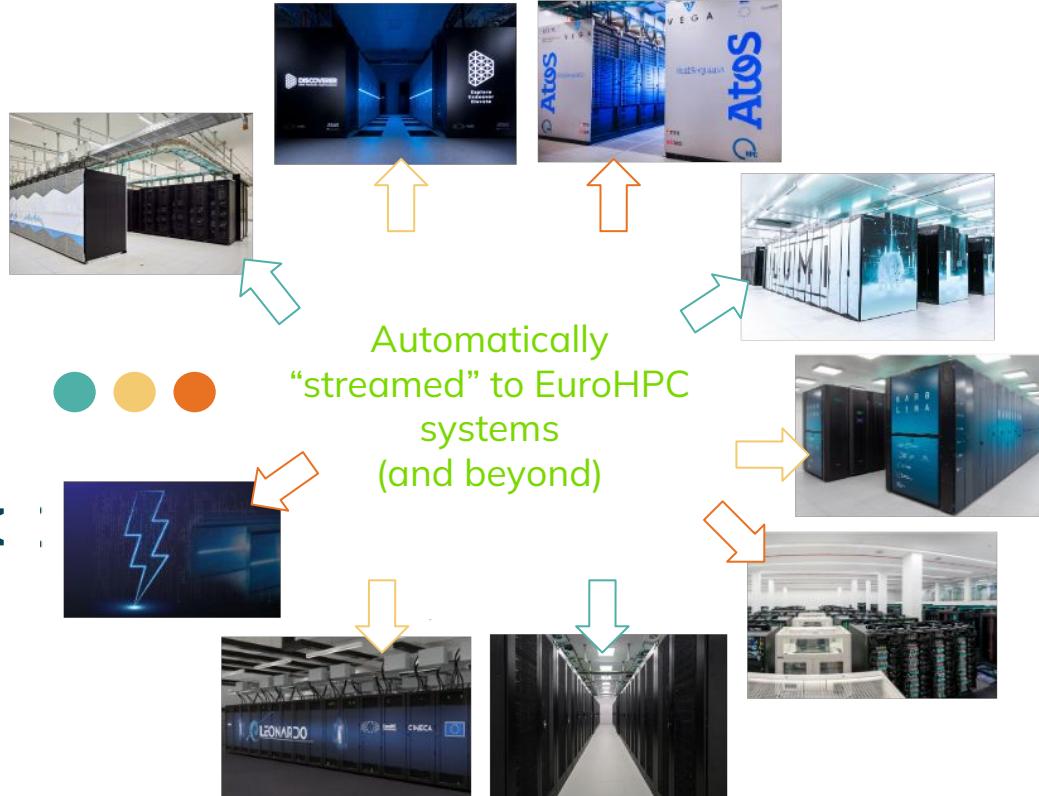


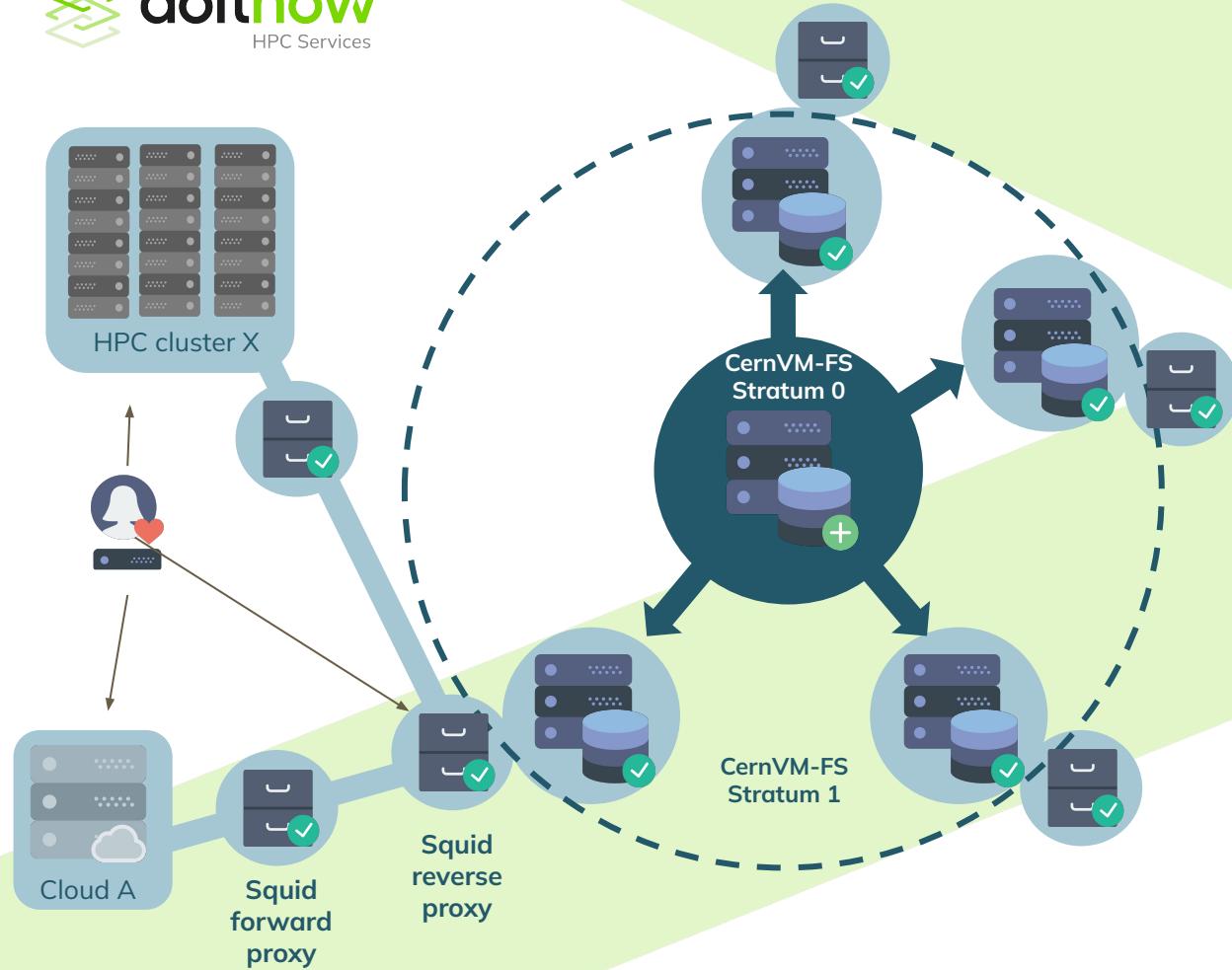
CernVM-FS

Host operating system



**EESSI**  
EUROPEAN ENVIRONMENT FOR  
SCIENTIFIC SOFTWARE INSTALLATIONS





### CernVM-FS

[cvmfs.readthedocs.io](https://cvmfs.readthedocs.io)



[github.com/EESSI/filesystem-layer](https://github.com/EESSI/filesystem-layer)

- Global distribution of software installations
- Centrally managed software stack
- Redundant network of “mirrors”
- Multiple levels of caching
- **Same software stack everywhere:**  
laptops, HPC clusters, cloud VMs, ...

# EESSI user experience

```
$ source /cvmfs/software.eessi.io/versions/2023.06/init/bash
archdetect says x86_64/intel/haswell
archdetect could not detect any accelerators
Using x86_64/intel/haswell as software subdirectory.
{EESSI 2023.06} $ module load GROMACS/2024.4-foss-2023b
{EESSI 2023.06} $ gmx --version
:-) GROMACS - gmx, 2024.4-EasyBuild_4.9.4 (-:
```



Local client cache



Mirror server



Central server

## Supported system architectures

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- Different generations of x86\_64 (Intel, AMD) and Arm 64-bit CPUs; RISC-V is WIP
  - Including A64FX (Deucalion, WIP) & NVIDIA Grace (JUPITER, coming soon)
  - Also works on laptops, in virtual machines in the cloud, on Raspberry Pi boards, etc.
- Different accelerators: NVIDIA GPUs (today) + AMD GPUs (soon)
  - For now, only software installations for AMD Rome (Zen2) + NVIDIA A100 are available
- Various interconnects like Infiniband, via “fat” MPI libraries
  - Support for injecting a vendor-provided MPI library is available
- Goal is to support system architecture of all (current & future) EuroHPC systems



**doitnow**  
HPC Services

Reviewers



EESSI/staging



Open PR



Stratum 0  
server

Deploy in  
EESSI repo  
(automated)



Contributors



Create PR

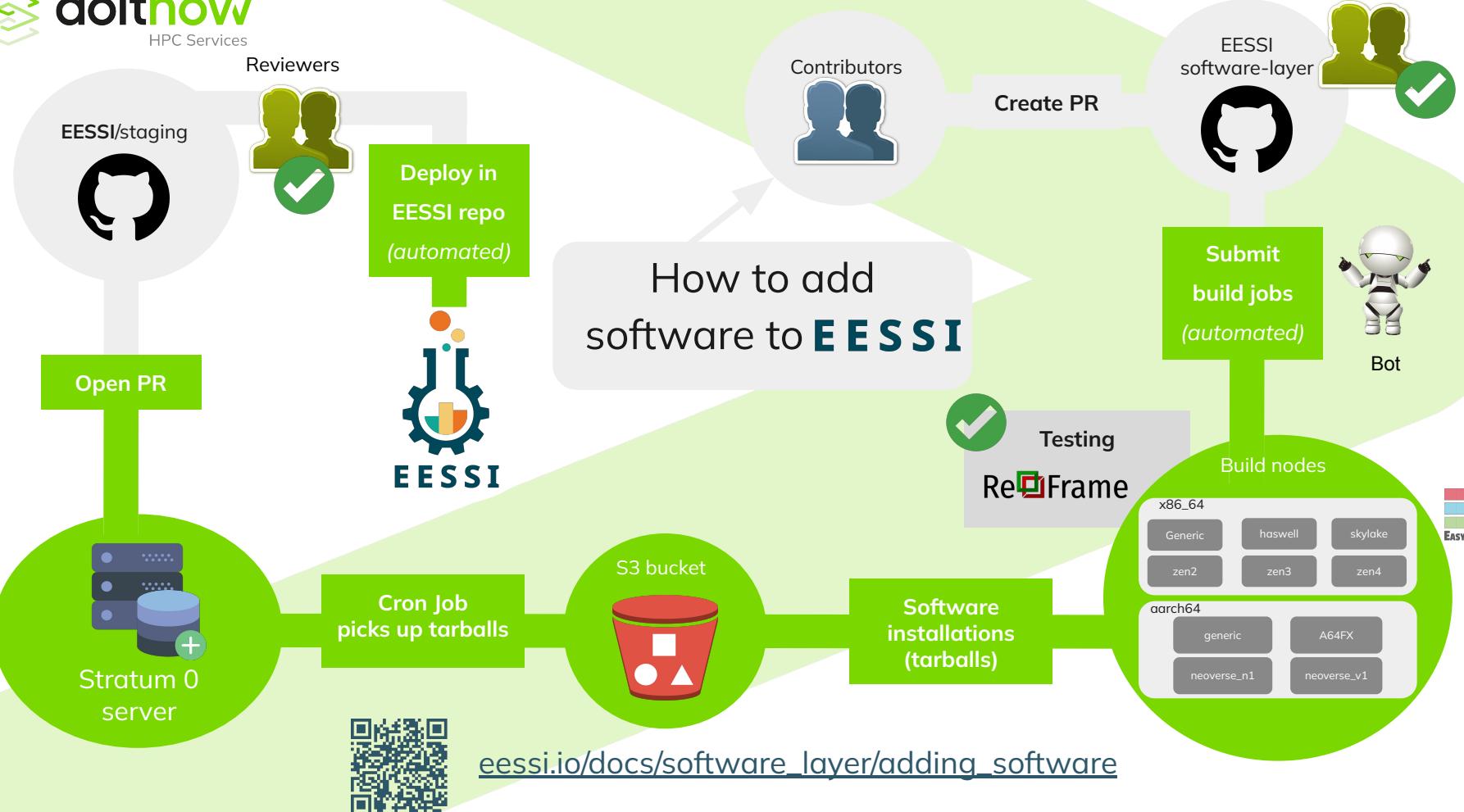
EESSI  
software-layer



Reviewers



## How to add software to **EESSI**





## How about integration?

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**OPEN**  **onDemand**

The text "OPEN" is in a white, sans-serif font inside a black rounded rectangle. To its right is the "onDemand" logo, which consists of a red play button icon followed by the word "onDemand" in a large, bold, black, sans-serif font.

## Potential use cases

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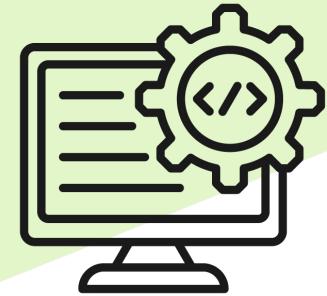
### 1. Training

- Offer continuous formation without being limited by environments



### 2. Deploying

- Avoiding dependences of containers and or continuous installations



### 3. Sharing software

- Improve collaboration and scientific software development and sharing between centers



# Training

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OPEN

- **OnDemand** project → Training?
  - User training for learn how to work with OOD
  - Sysadmin training for learn how to manage and solve problems
  
- Currently using the cluster of the client
  - Problems in case of full installation
  - Difficult to have full control of the environment
  - Sometimes not enough resources for big trainings



# Training



## 1. Setup Environment

Prepare a cluster structure

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



ANSIBLE  
Playbooks

## 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

## Training

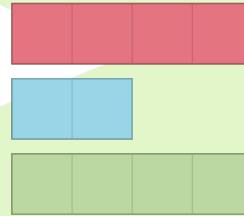
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- Avoid having local cluster and give access to everyone every different training .
- Avoid having configured clusters on the cloud unused.
- No dependencies on the current status of the client cluster



# Deploying

- New applications on the portal means:
  - Prepare Application in OOD Server
  - Installation of Software on the compute nodes
- Compute nodes:
  - Classical installation
  - EasyBuild Modules
  - Containers and Images



**EASYBUILD**.io  
building software with ease



# Deploying

[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

example\_account\_2

Number of hours

4

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
#!/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

My Interactive Sessions

Not secure ood.com/pun/sys/dashboard/batch\_connect/sessions

Home / My Interactive Sessions

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 EESSI
- Jupyter Notebook EESSI
- Jupyter Notebook EESSI

Host: >rocky8-cbustelo02

Created at: 2025-03-06 15:46:05 UTC

Time Remaining: 55 minutes

Session ID: 7a6e4e30-3416-4a99-bbce-8220b6242841

Problems with this session? Submit support ticket

Connect to Jupyter

Home

Not secure ood.com/node/rocky8-cbustelo02/11209/tree?

jupyter

File View Settings Help

Files Running

Name	Last Modified	File Size
CachedProfilesData	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	

ood.com/pun/sys/dashboard/files/fs/home/nextUser/ondemand/data/sys/dashboard/batch\_connect/sys/jupyter\_EESSI/output/7a6e4e30-3416-4a99-bbce-8220b6242841/output.log

Script starting...

```

Waiting for Jupyter Notebook server to open port 12099...
TIMEOUT - Starting waiting for Thu Mar 06 15:46:06 UTC 2025
TIMEOUT - Starting main script at: Thu Mar 06 15:46:06 UTC 2025
Found EESSI repodata/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 /cmvms/software.eessi.io/versions/2023.06/software/linux/x86_64/intel/skylake_avx512/lmod/lmodrc.lua
Found Lmod SitePackage.lua file at /cmvms/software.eessi.io/versions/2023.06/software/linux/x86_64/intel/skylake_avx512/lmod/SitePackage.lua
Using /cmvms/software.eessi.io/host_injections/2023.06/software/linux/x86_64/intel/skylake_avx512 as the site extension directory for installations.
Using /cmvms/software.eessi.io/versions/2023.06/software/linux/x86_64/intel/skylake_avx512/modules/all as the directory to be added to MODULEPATH.
Using /cmvms/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 Lmod file at RHEL location, setting CURL_CA_BUNDLE
Initializing Lmod...
Prepending /cmvms/software.eessi.io/versions/2023.06/software/linux/x86_64/intel/skylake_avx512/modules/all to $MODULEPATH...
Prepending site path /cmvms/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

## Sharing Software

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- How can we take advantage of **EESSI**'s OPEN ability to share software from **OnDemand** in the most user-friendly way?
- What can **OnDemand** do to help **EESSI** software sharing?



# Sharing Software

- VNC 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
<b>EESSI General App</b>

**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**

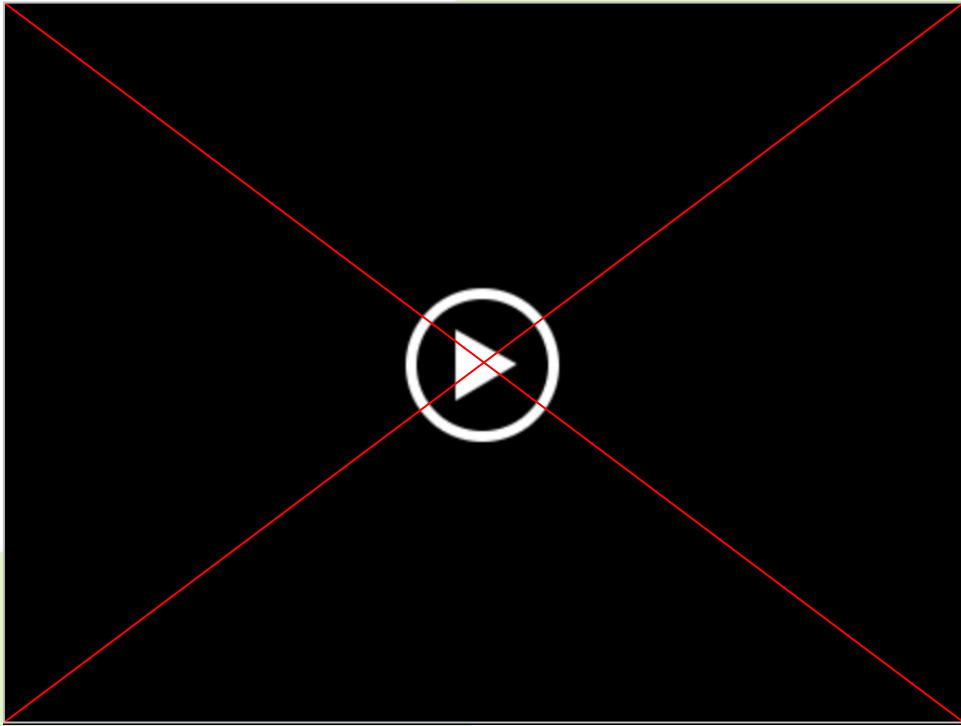
Module Filter

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

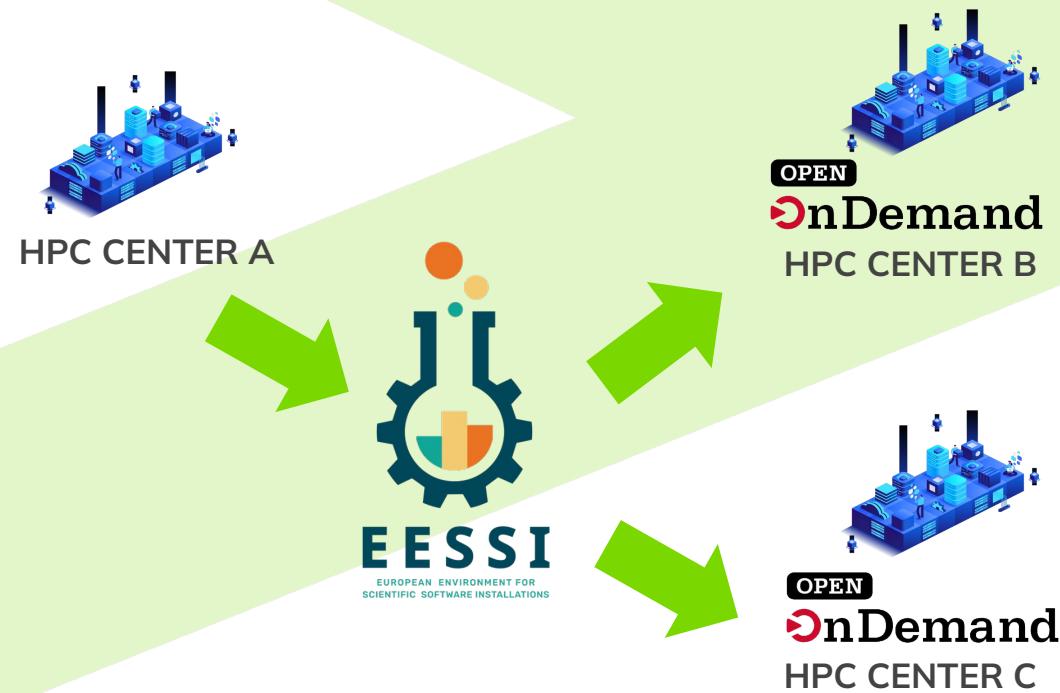
\* The EESSI General App session data for this session can be accessed under the data root directory.



## Sharing Software

- Adding software to the EESSI stack also grants access from all the other integrations
- OPEN**  
 **OnDemand** + **EESSI**

- Accessible via this App simplifying the sharing between centers





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