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OOD Meets EESSI:

Accessing and Distributing Scientific Software with Ease

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R&D - Do IT Now

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Support - Do IT Now

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A global HPC Services Company

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** (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

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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

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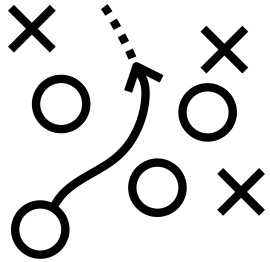
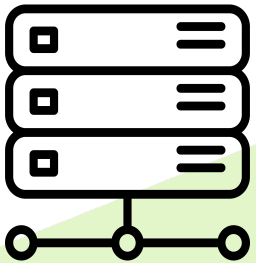
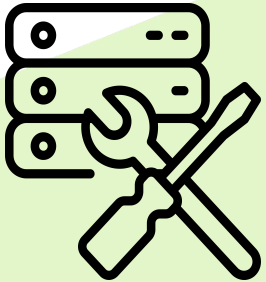
What we offer?



CONSULTING



INSTALLATION



SUPPORT

R&D-as-a-Service

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Open Ondemand & EESSI

1. OPEN 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

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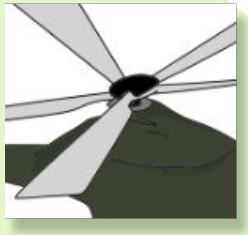
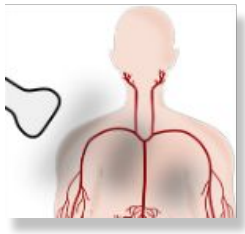
MultiXscale Centre-of-Excellence in a nutshell

- 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





MultiXscale

https://multixscale.eu

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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...**

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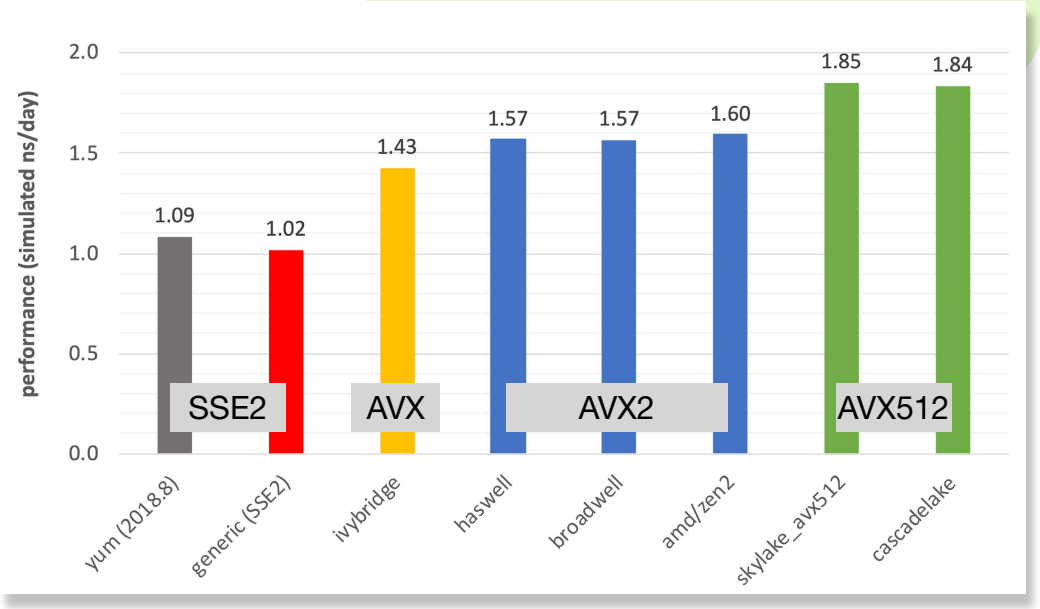
Optimized scientific software installations

- 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



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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?

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EESSI in a nutshell

- 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**

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Major goals of EESSI

- 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, …

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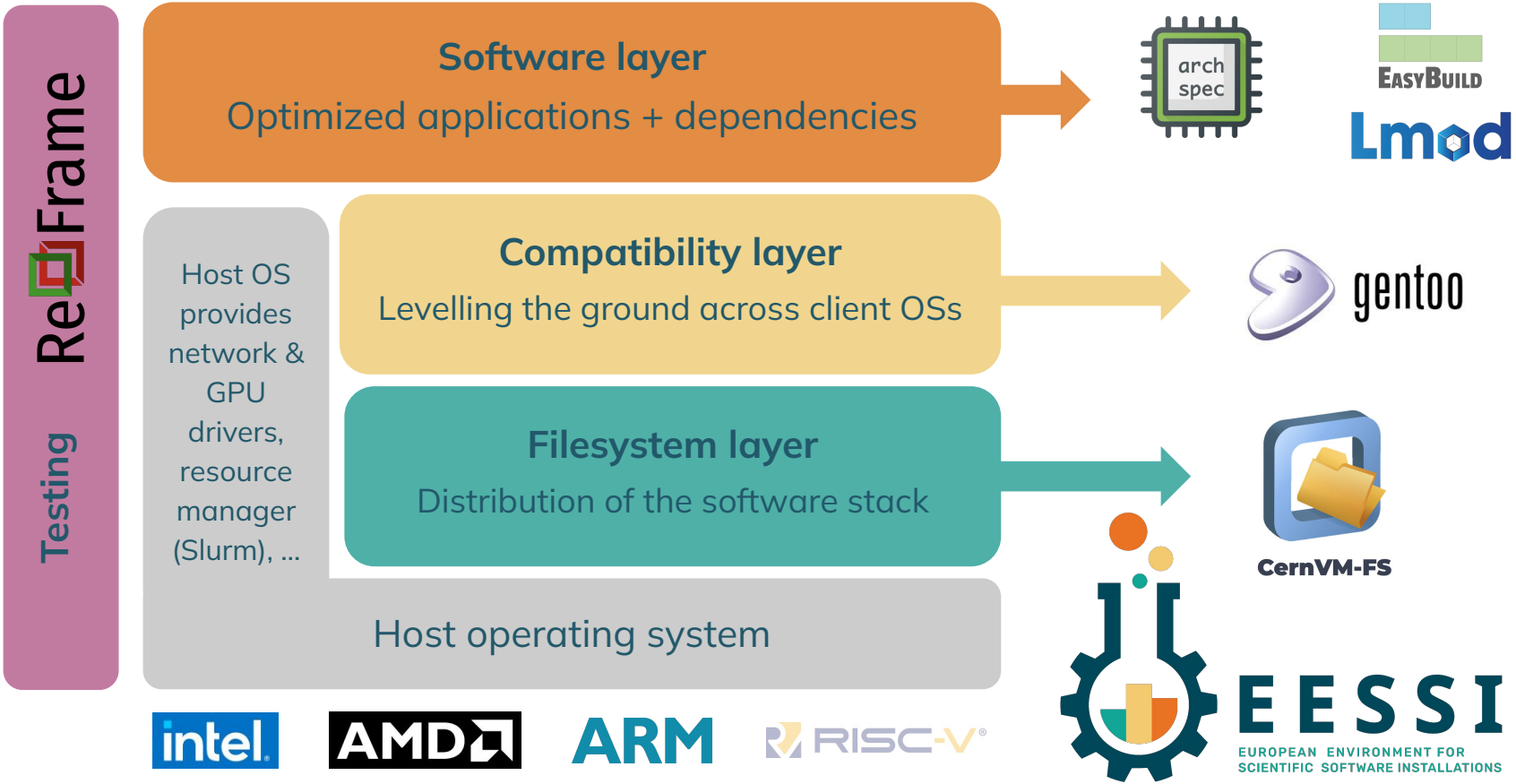

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App X

Install

Install

Install

Install

Install

App Y

waLBerla

ESPResSo

LAMMPS

EESSI

Automatically
“streamed” to EuroHPC
systems
(and beyond)

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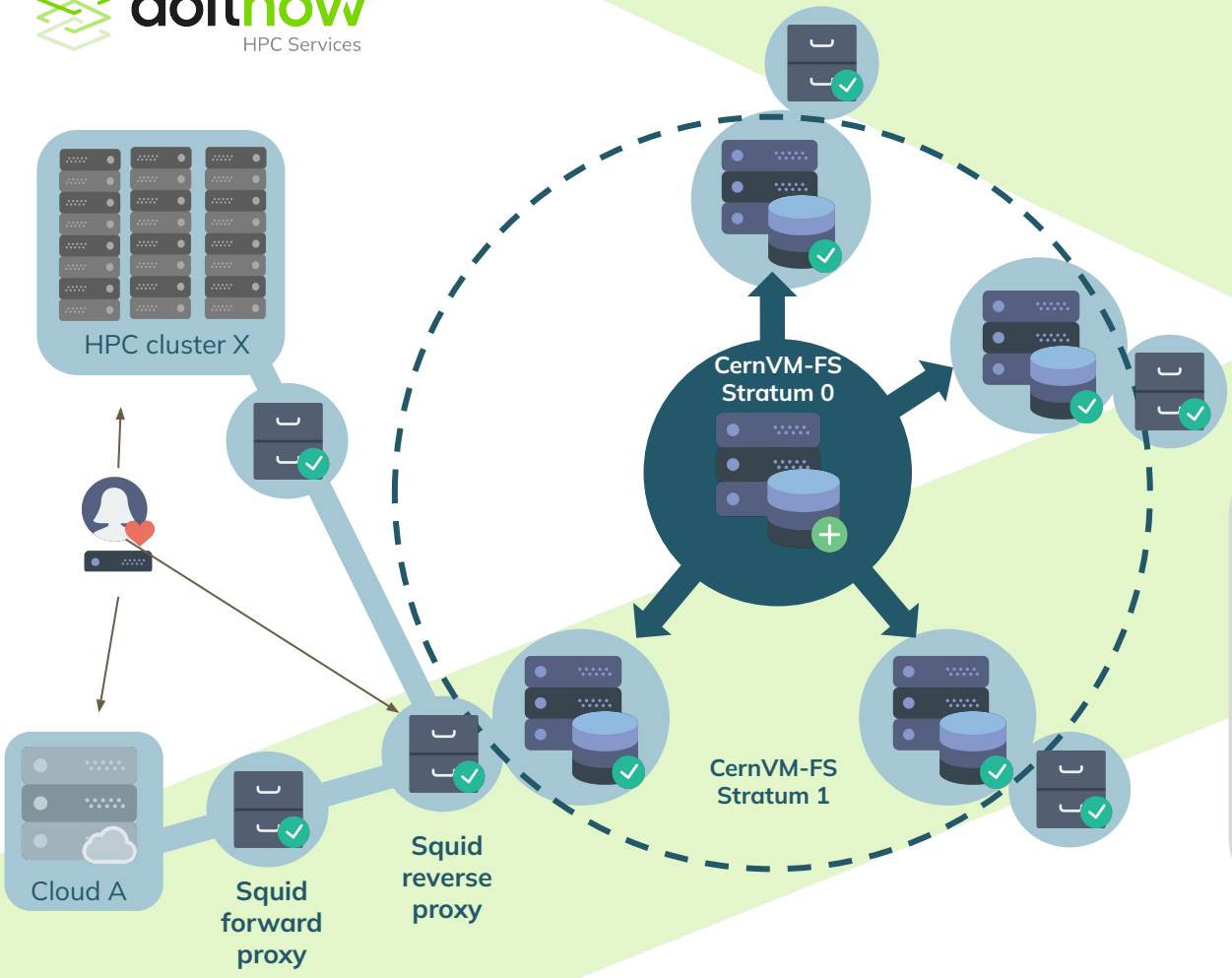

CernVM-FS

cvmfs.readthedocs.io

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, …

(icons via https://www.flaticon.com/authors/smashicons)

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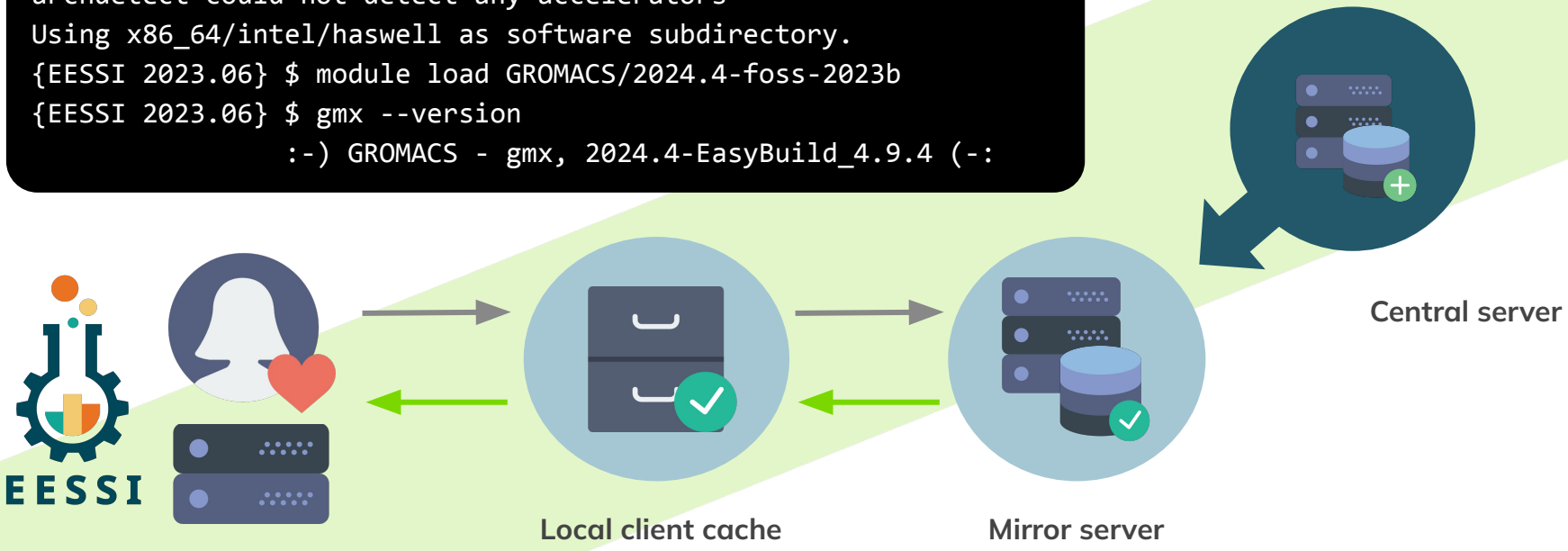
EESSI user experience

```
$ 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 (-:
```



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Supported system architectures

- 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

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How to add software to EESSI

Contributors

Create PR

EESSI software-layer

Reviewers

Reviewers

EESSI/staging

Deploy in EESSI repo *(automated)*

EESSI

Submit build jobs *(automated)*

Bot

Open PR

Testing

ReFrame

Build nodes

x86_64

Generic | haswell | skylake | zen2 | zen3 | zen4

aarch64

generic | A64FX | neoverse_n1 | neoverse_v1

EasyBuild

Stratum 0 server

Cron Job picks up tarballs

S3 bucket

Software installations (tarballs)

eessi.io/docs/software_layer/adding_software

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How about integration?

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Potential use cases

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

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Training

- 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

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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

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Training

- 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

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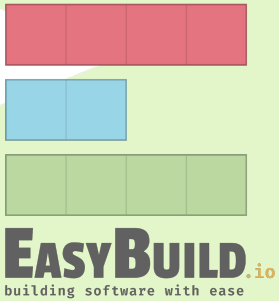
Deploying

- 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

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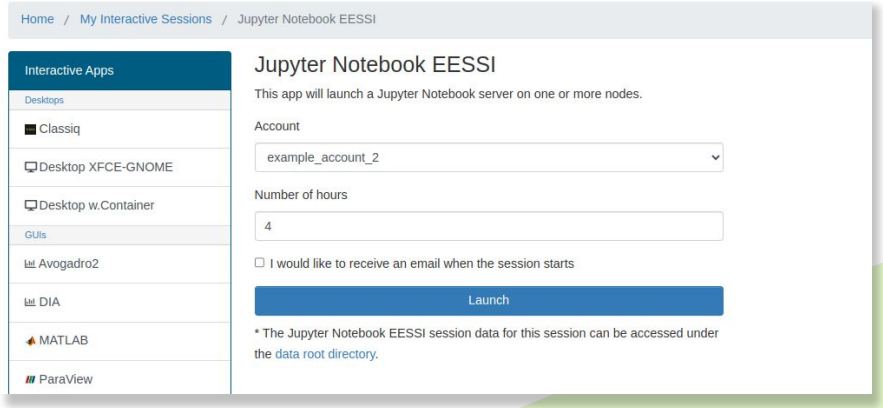
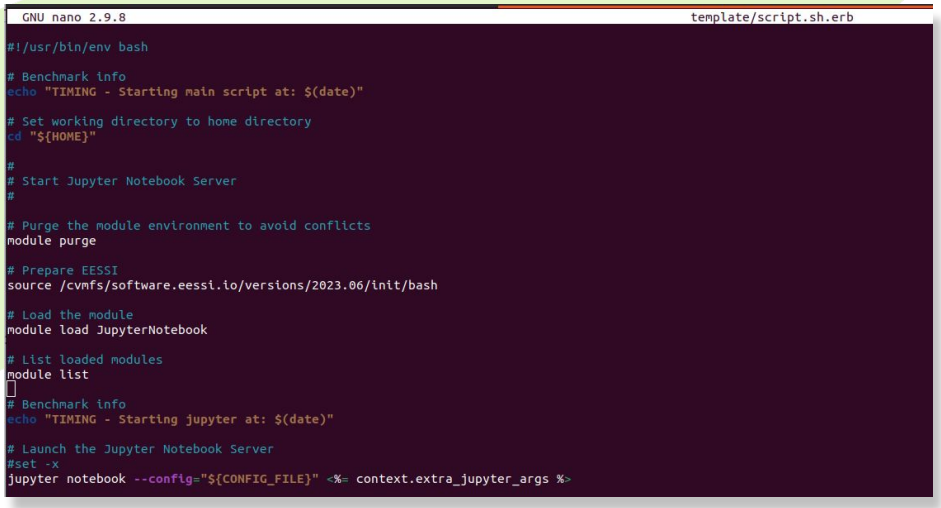
Deploying





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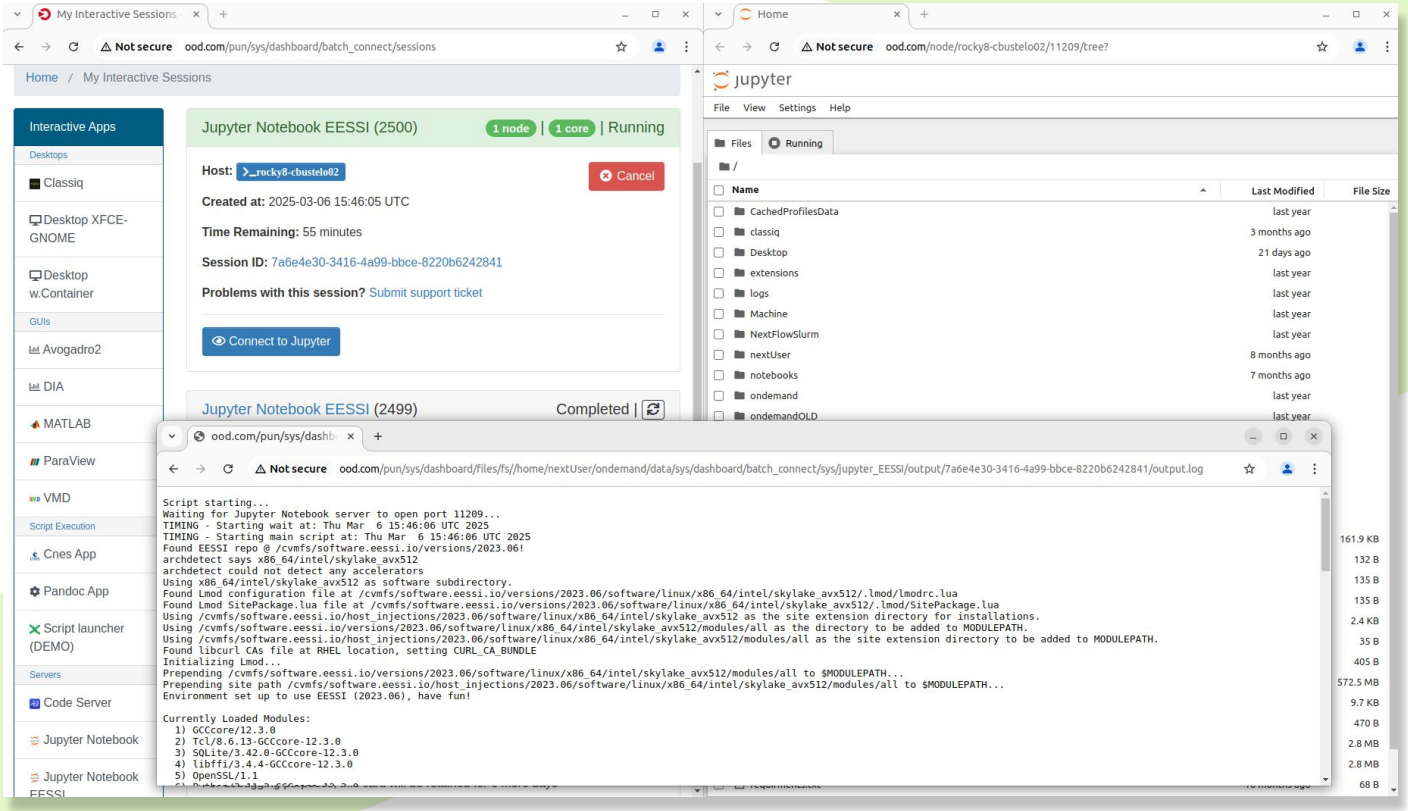
Deploying



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Sharing Software

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

- What can OPEN OnDemand do to help EESSI software sharing?

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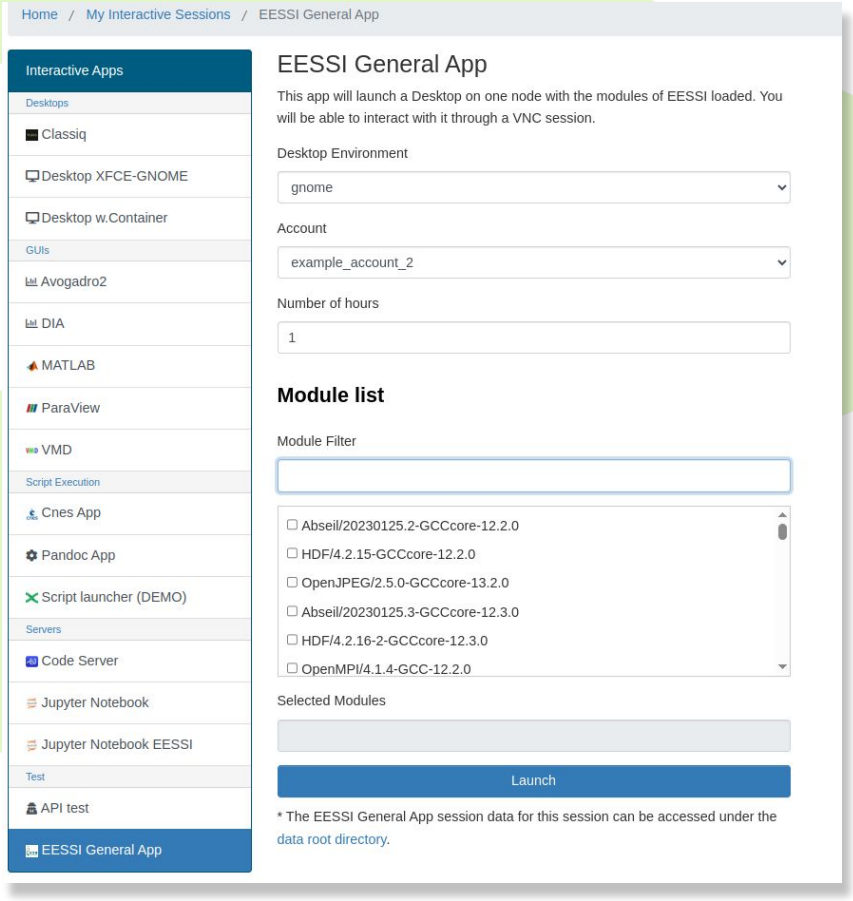
Sharing Software

- 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



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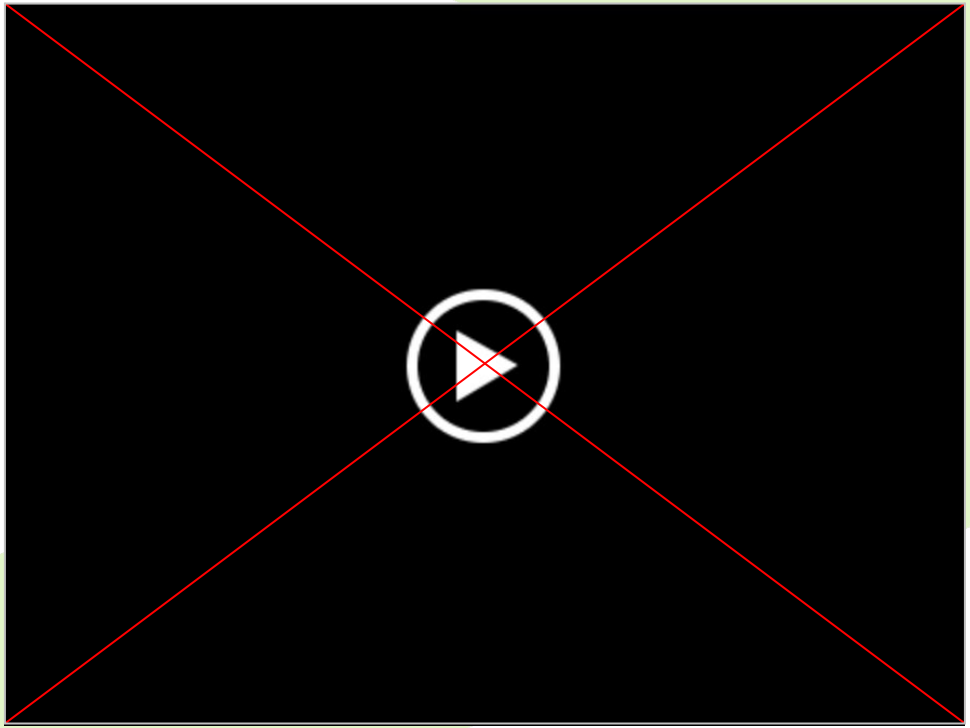

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Sharing Software

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

OPEN OnDemand + EESSI

integrations

- Accessible via this App simplifying the sharing between centers

HPC CENTER A

EESSI
EUROPEAN ENVIRONMENT FOR SCIENTIFIC SOFTWARE INSTALLATIONS

OPEN OnDemand
HPC CENTER B

OPEN OnDemand
HPC CENTER C

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