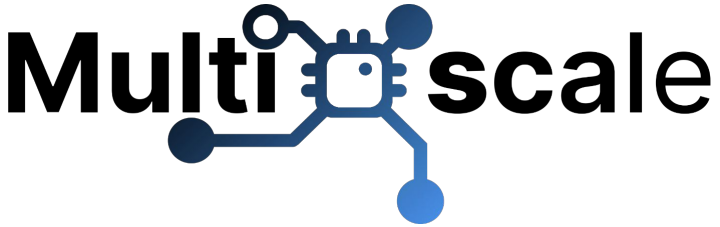
EESSI

EUROPEAN ENVIRONMENT FOR SCIENTIFIC SOFTWARE INSTALLATIONS




Co-funded by the European Union


# MultiXscale

## An EuroHPC Centre of Excellence

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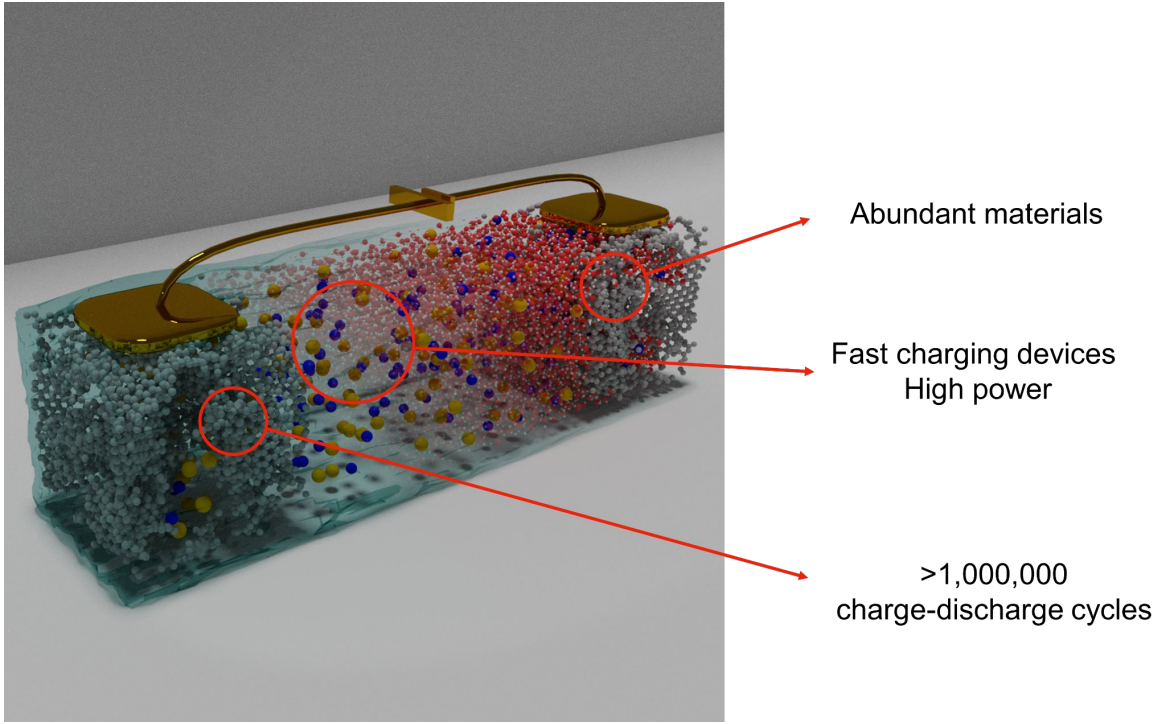
# What is MultiXscale?

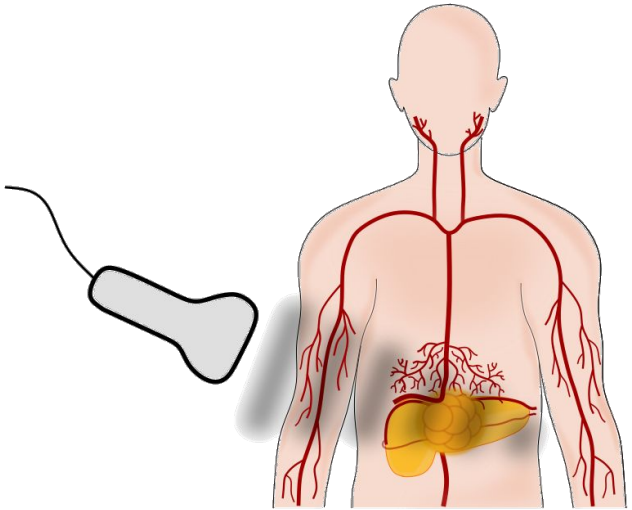
- Collaboration between scientific partners (CECAM nodes) who deliver **3 pilot use cases**, and technical partners (EESSI members) who provide the tools to allow application software to be seamlessly used on any available hardware
- MultiXscale targets improving the
  - **Productivity** of scientists who develop and/or use open source codes
  - **Performance** of those codes on EuroHPC hardware (and beyond)
  - **Portability** of the codes and workflows from laptop to server to cloud to HPC
- The focus of MultiXscale is multi-scale modelling and leveraging the opportunities that EuroHPC offers
- Advances the transition towards use of exascale resources for the community

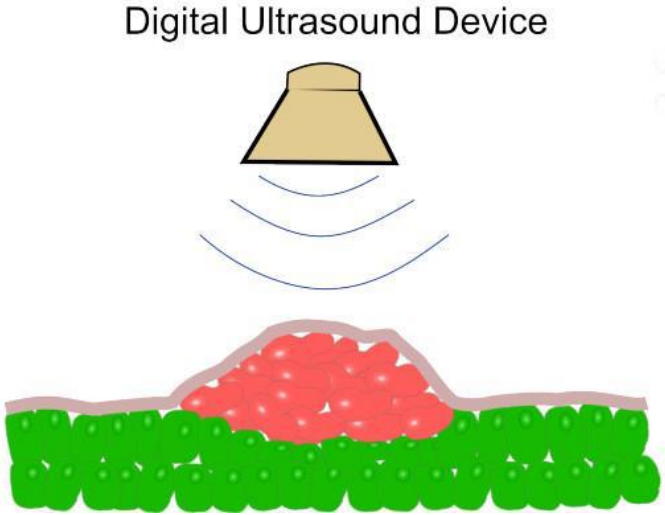
# Pilot: Batteries for sustainable energy

- Carbon/carbon supercapacitors are energy storage devices which are particularly attractive for their superior power density.
- Predicting materials with enhanced performance requires extremely large scales.



# Pilot: Biomedical Applications






- Create an accurate “digital twin” for the ultrasound process
- Use the digital twin to improve protocols: controlled testing and rational optimization of ultrasound parameters, such as frequency and amplitude

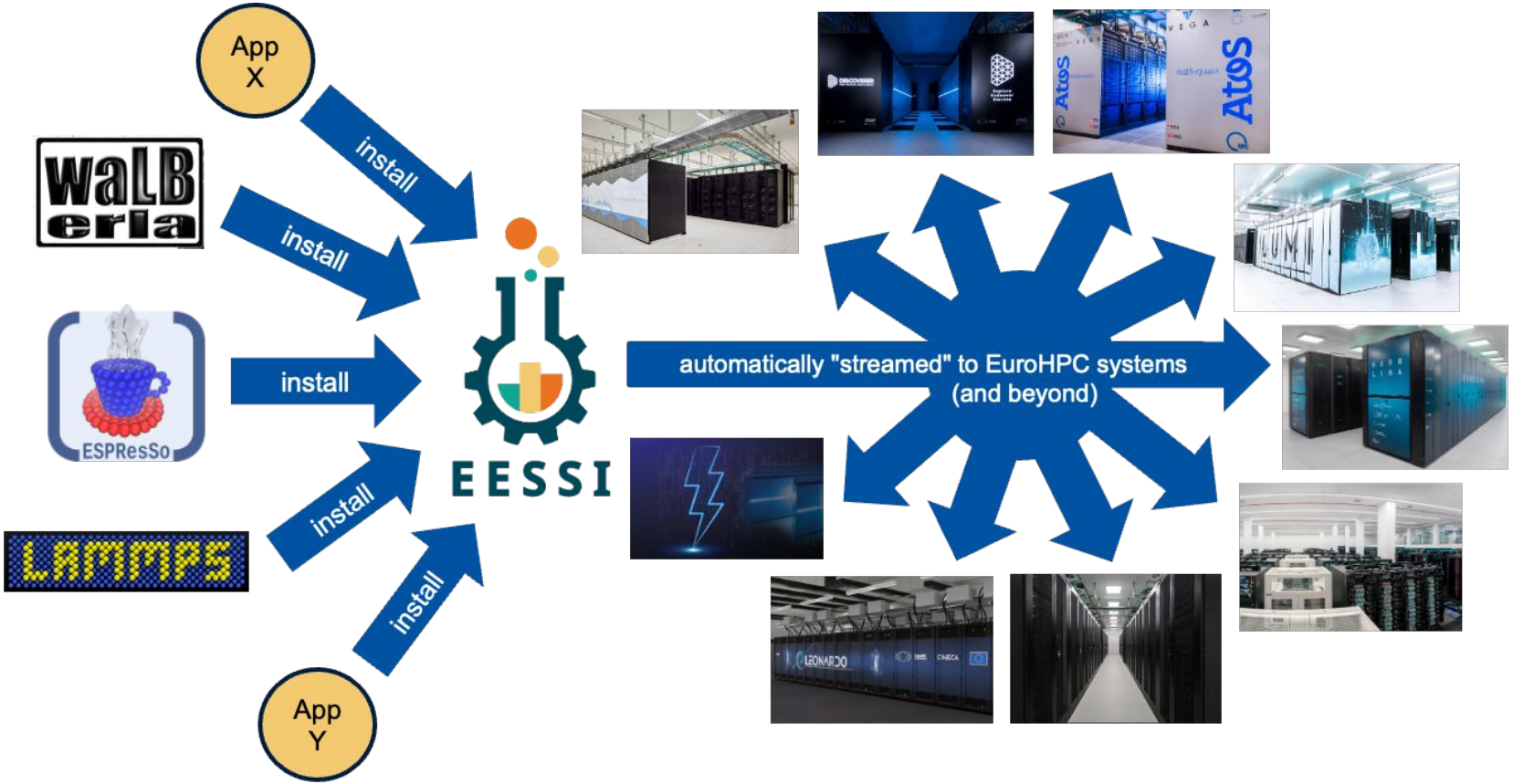
# Pilot: Design of innovative helicopters for civil applications

- An extremely complex task which requires proper modelling of the fluid flows around the helicopter body and detailed understanding of the mechanical forces sustained during flight operations.
- Coupling between aerodynamic and structural modelling is limited by the high computational cost associated to high-fidelity fluid dynamics methodologies, especially once applied to moving bodies, as in the case of helicopter rotors.

# Scientific motivation requiring technical innovations

- Each pilot is dealing with phenomena that manifest at multiple scales, and as a result each utilizes multiple methods and a variety of software applications
- The challenge is **coupling** these together, and making sure they can take advantage of large scale resources
- In Europe, the largest scale resources are to be found (for free!) in **EuroHPC**
- Having access to resources is not enough, we need to get the scientific workflows there and make it as easy as possible for the scientists to use

# EESSI as a shared software stack



# EESSI-extend: building on top of EESSI with EasyBuild

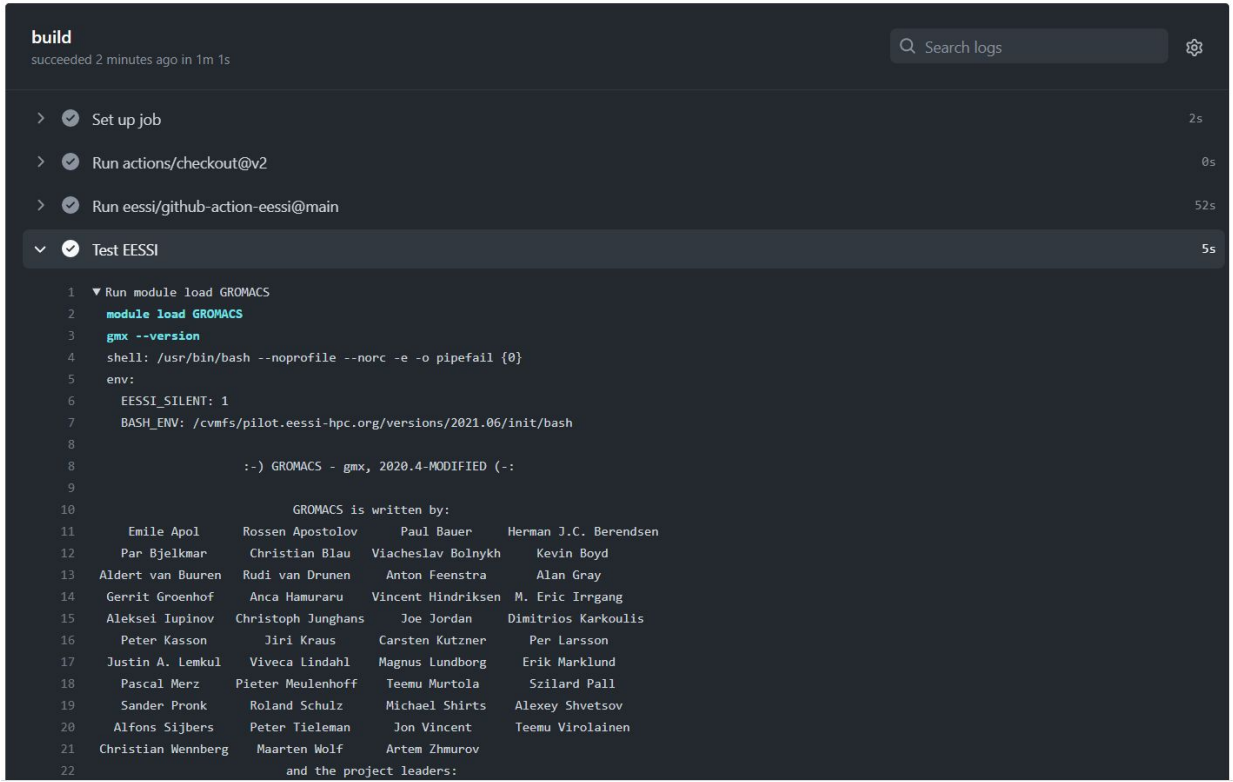
- EESSI provides base installations
- We can install on top of the EESSI software stack with EasyBuild

```
$ module load EESSI-extend/2023.06-easybuild

-- Using /tmp/$USER as a temporary working directory for installations, you can override this
by setting the environment variable WORKING_DIR and reloading the module (e.g., /dev/shm is a
common option)

Configuring for use of EESSI_USER_INSTALL under /home/ec2-user/eessi

-- To create installations for EESSI, you _must_ have write permissions to
/home/ec2-user/eessi/versions/2023.06/software/linux/x86_64/amd/zen4

-- You may wish to configure a sources directory for EasyBuild (for example, via setting the
environment variable EASYBUILD_SOURCEPATH) to allow you to reuse existing sources for packages.
```

# Leveraging EESSI in CI environments


- EESSI can be used in CI environments like:
  - GitHub: github.com/marketplace/actions/eessi
  - GitLab: gitlab.com/explore/catalog/eessi/gitlab-eessi
- EESSI can provide:
  - Different compilers to test your software with
  - Required dependencies for your software
  - Additional tools like ReFrame, performance analysis tools, …
- Other than CernVM-FS to get access to EESSI, no software installations required!
  - Everything that is actually needed is pulled in on-demand by CernVM-FS
- Significantly facilitates also running CI tests in other contexts (laptop, HPC, …)

# Leveraging EESSI GitHub Action




https://github.com/EESSI/github-action-eessi/actions/runs/11183032689/job/31090668500



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# Leveraging EESSI in CI environments


We have an EESSI GitHub Action that provides EESSI+`direnv`:

See it in action in the `github-eessi-action` repository:

github.com/EESSI/github-action-eessi

github.com/EESSI/github-action-eessi/blob/main/.github/workflows/tensorflow-usage.yml

```yaml
name: ubuntu_tensorflow
on: [push, pull_request]
jobs:
 build:
   runs-on: ubuntu-latest
   steps:
   - uses: actions/checkout@v3
   - uses: eessi/github-action-eessi@v3
     with:
       eessi_stack_version: '2023.06'
   - name: Test EESSI
     shell: bash
     run: |
       module load TensorFlow
       python -c 'import tensorflow; print(tensorflow.__version__)'
```



Alan

# Putting things together


- Can create an EasyBuild recipe which uses `**`--software-commit`**` and git repository sources
- Use EESSI to build and test via EasyBuild in CI
- Simplest case has all dependencies existing in EESSI
- In GitHub, can build for Arm and x86_64 for free
- *Future work: `**`buildenv`**` module with exported RPATH wrappers so method can also work more easily work without EasyBuild*



Alan

# MultiXscale

Co-funded by the European Union

EuroHPC Joint Undertaking

**Web page:** multixscale.eu

**Facebook:** MultiXscale

**Twitter:** @MultiXscale

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