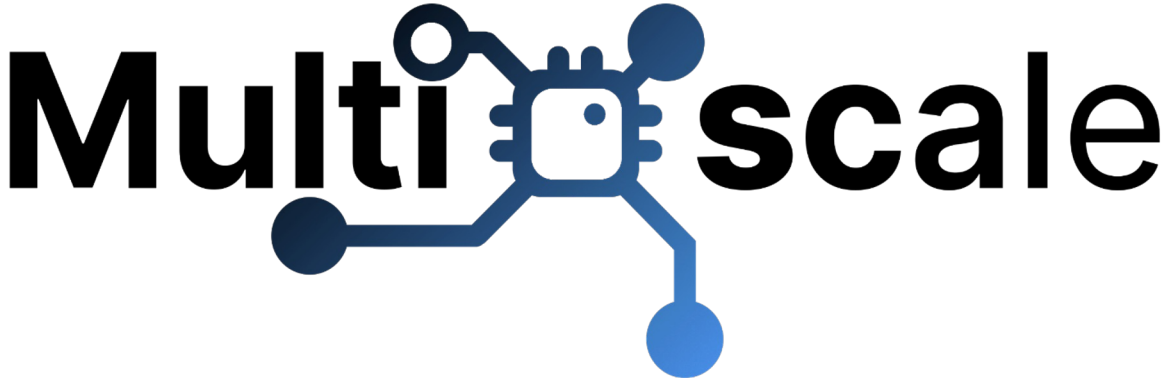


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**EuroHPC Centre of Excellence**

# MultiXscale kickoff meeting - Overview of technical work packages (WP1, WP5, WP6)

*Caspar van Leeuwen (SURF) - lead WP1*

*Kenneth Hoste (Ghent University) - lead WP5*

*Alan O'Cais (University of Barcelona) - lead WP6*

**23 March 2023**

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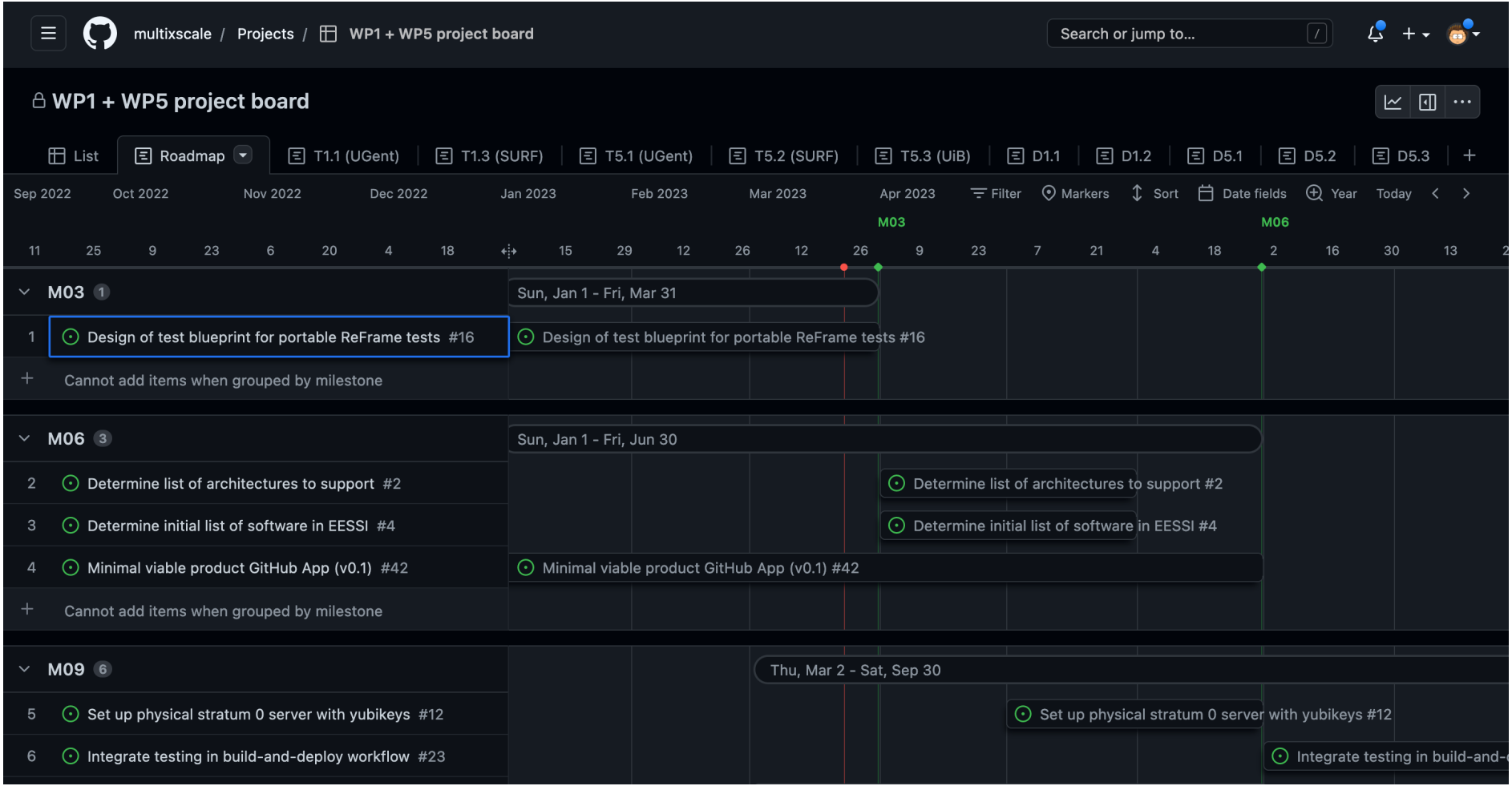
# MultiXscale technical WPs

- WP1: Developing a Central Platform for Scientific Software on Emerging Exascale Technologies - Lead: SURF (Caspar)
- WP5: Building, Supporting and Maintaining a Central Shared Stack of Optimized Scientific Software Installations - Lead: UGent (Kenneth)
- WP6: Community outreach, education, and training - Lead: UB (Alan)

# Organization/planning WP1+5+6

**How will we organize ourselves + plan our work?**

- Monthly sync meeting for WP1+WP5+WP6 (2nd Tuesday at 10:00 CE(S)T)
  - Notes in wiki of MultiXscale/meetings GitHub repo
- Project board in MultiXscale GitHub repo (currently only for WP1+WP5)
  - Track progress (task-based roadmap)
  - Easy overview when creating deliverables (deliverable-based roadmap)
  - Creating tickets in other repo's (EESSI, …) is fine, but have to be linked in issues in WP1_5 repo to maintain single overview of all work done!


multixscale / Projects / WP1 + WP5 project board
Search or jump to...
WP1 + WP5 project board
List
Roadmap
T1.1 (UGent)
T1.3 (SURF)
T5.1 (UGent)
T5.2 (SURF)
T5.3 (UiB)
D1.1
D1.2
D5.1
D5.2
D5.3
Sep 2022
Oct 2022
Nov 2022
Dec 2022
Jan 2023
Feb 2023
Mar 2023
Apr 2023
Filter
Markers
Sort
Date fields
Year
Today
M03
M06
11 25 9 23 6 20 4 18 15 29 12 26 12 26 9 23 7 21 4 18 2 16 30 13
M03 1
Sun, Jan 1 - Fri, Mar 31
1 Design of test blueprint for portable ReFrame tests #16
Design of test blueprint for portable ReFrame tests #16
Cannot add items when grouped by milestone
M06 3
Sun, Jan 1 - Fri, Jun 30
2 Determine list of architectures to support #2
Determine list of architectures to support #2
3 Determine initial list of software in EESSI #4
Determine initial list of software in EESSI #4
4 Minimal viable product GitHub App (v0.1) #42
Minimal viable product GitHub App (v0.1) #42
Cannot add items when grouped by milestone
M09 6
Thu, Mar 2 - Sat, Sep 30
5 Set up physical stratum 0 server with yubikeys #12
Set up physical stratum 0 server with yubikeys #12
6 Integrate testing in build-and-deploy workflow #23
Integrate testing in build-and-

# Organization/planning WP1+5+6

**MultiXscale Slack for easy day-to-day communication**

- Slack is a ”way of life” for most people involved in technical WPs
- Significantly lowers the threshold to reaching out to others for questions, etc.
- Communication via Slack should be considered ***asynchronous*** (just like email)
- Don’t expect an instant reply from anyone, at any time
- Messages in Slack will eventually disappear due to free plan (only last 90 days)
- ***Important and official communication should still be done via email!***

# WP1: Stabilize and extend EESSI

**First year** tasks:

- **T1.1 (UGent, M1-24): Providing a stable, optimized, shared scientific software stack with support for established system architectures**
- T1.2 (UG, M10-30): Extending support of the shared software stack to emerging system architectures
- **T1.3 (SURF, M1-30): Design and creation of a software test suite and facilitating CI for software developers**

# WP1: Stabilize and extend EESSI

**First year** deliverables/milestones:

- **D1.1 (M12, UG): Report on shared software stack prototype (T1.1, T1.2)**
- **D1.2 (M12, SURF): Plan for the design of a portable test suite (T1.3)**
- **MS 2 (M12, SURF): Shared software stack support for at least 1 accelerator (WP1 through WP5)**

# T1.1 Goals + status (M1-M24)

**Summary: Making EESSI ready for production use**

- Set up CernVM-FS infrastructure (ongoing) [#12, #14]
- NVIDIA GPU support (ongoing) [#1]
- Formalize & implement policy for updates (to start, currently manual) [#15]
- Determine initial list of software (for Milestone 2) (to start) [#4]
- Determine list of architecture support (for Milestone 2) (to start) [#2]
- Build software for initial list & architectures (to start) [#3]
- Performance evaluation of software (to start) [#7]

# T1.2 Goals + status (M10-M30)

**Summary: Extending support in EESSI for emerging system architectures**

- ARM CPU support (ongoing) [#32]
- AMD GPU support (to start) [#31]
- Intel GPU support (?) (todo) [#33]

# T1.3 Goals + status (M1-M30)

**Summary: Create a test suite for EESSI**

- Create blueprint for portable test (ongoing with GROMACS) [#16]
- Implement low level tests (ongoing) [#30]
- Implement tests for WP2, WP3, WP4 software (to start) [#18 ,#20]
- Collect & visualize performance metrics (to start) [#9]
- Support WP2, WP3, WP4 in using EESSI in CI (to start) [#21]
- Explore solutions for ‘portable’ performance monitoring (to start) [#17]

  (challenge: what is expected performance on an unknown system?)

# WP5: Support + maintain EESSI

**First year** tasks:

- **T5.1 (UGent, M1-M12) Setting up a support portal**
- T5.2 (SURF, M10-M30) Monitoring and testing of the central shared software stack
- **T5.3 (UiB, M1-M12) Facilitating community contributions to the central software stack**

# WP5: Support + maintain EESSI

**First year** deliverables/milestones:

- **D5.1 (M12, UiB): Community contribution policy and GitHub App**
- **D5.2 (M12, UGent): Support portal**
- **MS 2 (M12, SURF): Shared software stack support for at least 1 accelerator (WP1 through WP5)**

# T5.1 Goals + status (M1-M12)

**Summary: Create support portal for EESSI**

- Define initial level of support for EESSI (to start) [#24]
- Compare alternatives for support portal (ongoing) [#25]
- Set up and document support portal (to start) [#26]
- Create form or templates for reporting issues (to start) [#34]
- Set up periodic rotation for 1st-line support (to start) [#27]
- **D5.2 Report on support portal (alternatives, motivated selection, …)** [#28]

# T5.2 Goals + status (M10-M30)

**Summary: Monitoring + testing of EESSI** (using test suite developed in T1.3)

- Decide on schedule for periodic testing (what, where, when) (to start) [#35]
- Set up infrastructure for doing periodic testing (on-premise, cloud, …) (to start) [#36]
- Set up (automated) periodic functional tests - does it (still) run? (to start) [#49]
- Set up periodic correctness tests - does it produce correct results? (to start) [#38]
- Set up periodic performance tests - does it (still) perform well? (to start) [#39]
- Set up dashboard to present testing results (to start) [#10]
- **D5.3 Report on testing provided software** [#40]

# T5.3 Goals + status (M1-M12)

**Summary: Bot that automates workflow to add software to EESSI**

- GitHub App (bot) to automate workflow to add software to EESSI (ongoing) [#41]
  - M06: Minimal viable product v0.1: build-and-deploy workflow, enables contributions [#42]
  - M09: v0.5: integrate testing in workflow + improved status overview in PRs [#43]
  - M12: v1.0: stable version, incl. dashboard with overview of all bot instances [#44]
- Set up infrastructure to build/test/deploy software in EESSI using bot (ongoing) [#45]
- Define contribution policy + checklist of requirements for contributions (to start) [#46]
- Document semi-automated workflow to contribute to EESSI (to start) [#47]
- **D5.1 Community contribution policy and GitHub App** [#48]

# WP6: Training

*Community outreach, education, and training*

**First year** tasks:

- **T6.1 (NIC, M3-12): Awareness raising in the community**
- T6.2 (UiB, M6-24): Infrastructure to support training activities
- T6.3 (UB, M6-48): Generating and providing training content

# WP6: Training

*Community outreach, education, and training*

**First year** deliverables/milestones:

- D6.1 (M12, UB): Guidelines for Community Outreach, Education, and Training
- MS4 (M21, UB): First training event supported by the Ambassador Program WP 1+5+6

# T6.1 Goals + status (M3-M12)

**Awareness raising in the community**

Create “elevator pitch” to engage community *(only running activity)*

- Lead by NIC/HPCnow!
- Intended to be presented at a number of CECAM workshops to raise awareness

Prepare guidelines for Community Outreach, Education and Training

- Due in M12
- Created a similar deliverable for E-CAM which can be used as a starting point
- Will include information on uploading content to Lhumos (the project training portal)

# T6.2 Goals + status (M6-M24)

**Infrastructure to support training activities**

Technical infrastructure: on-demand cloud based resources for training events

- Access to resources guaranteed for 2023 (and longer via Azure/AWS sponsorship)
- Magic Castle as the platform (Slurm + JupyterHub)
    - Will need vendor platforms for specialised hardware

Organizational infrastructure: create Ambassador program for CECAM

+ HPC National Competence Centers (train-the-trainer)

- May be able to leverage CASTIEL-2 here
- No longer any budget for instructor training (!)

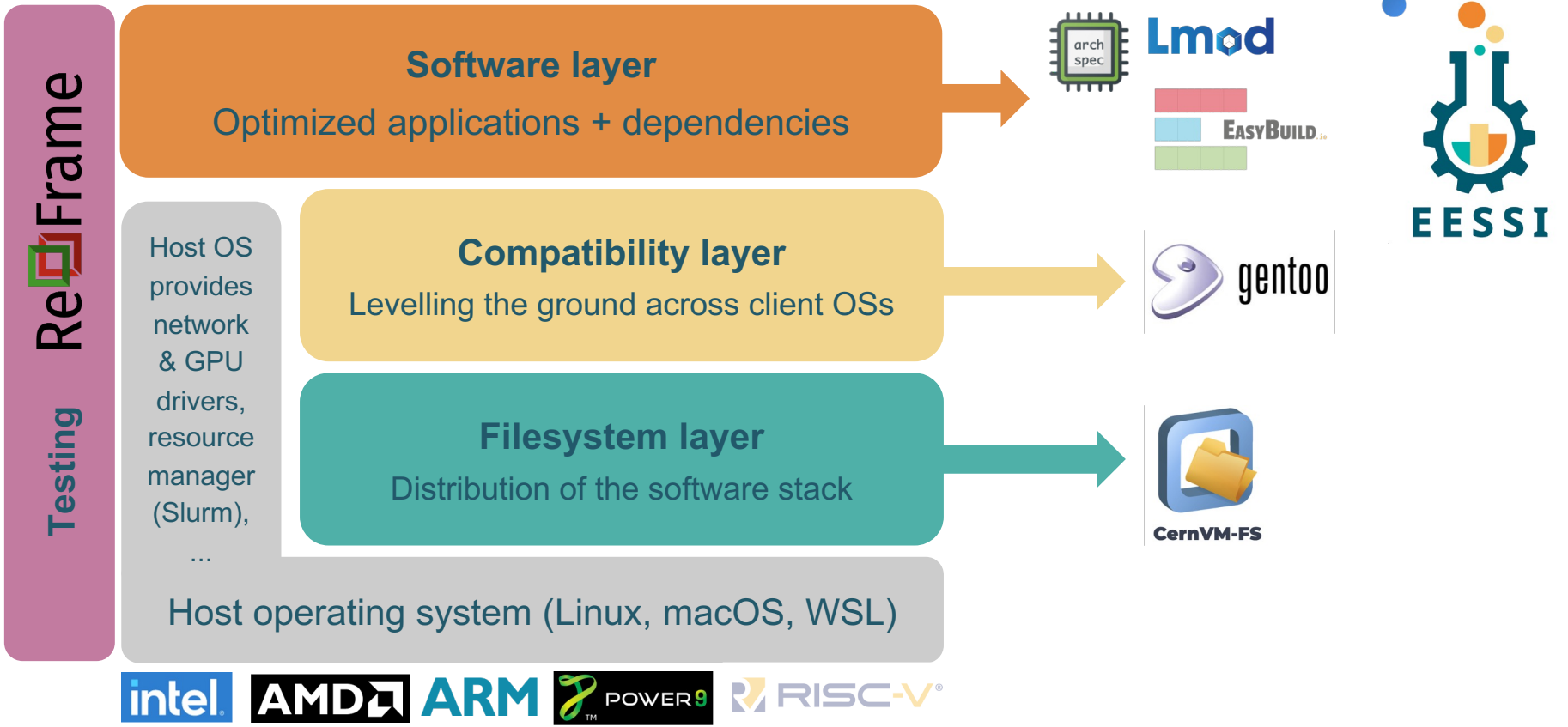
# T6.3 Goals + status (M6-M48)

**Generating and providing training content**

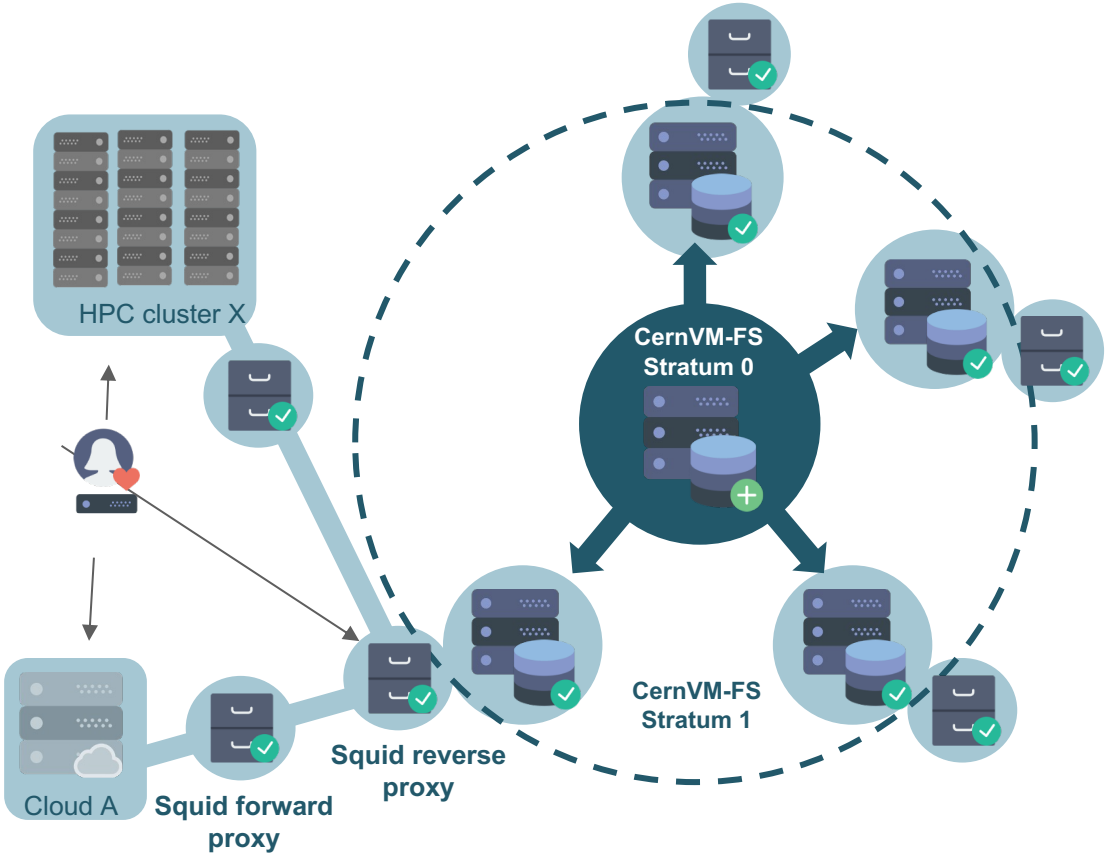
Ideas for training sessions:

- EESSI as an end-user (to start, based on EESSI documentation + EESSI demos)
  - Physical event, could be at HPC Knowledge Meeting 2023 (Barcelona, 17-18 May 2023)
- Providing EESSI as hosting site (sysadmin training) (to start)
  - Virtual event (to maximize interest/participation) - 2023Q4?
- Application-training for CoE applications
- EESSI as an application developer
- Contribution an application/library to EESSI
- EESSI test suite: usage + contributing

# High-level overview of EESSI



# EESSI as a shared software stack




CernVM-FS

cvmfs.readthedocs.io

EESSI

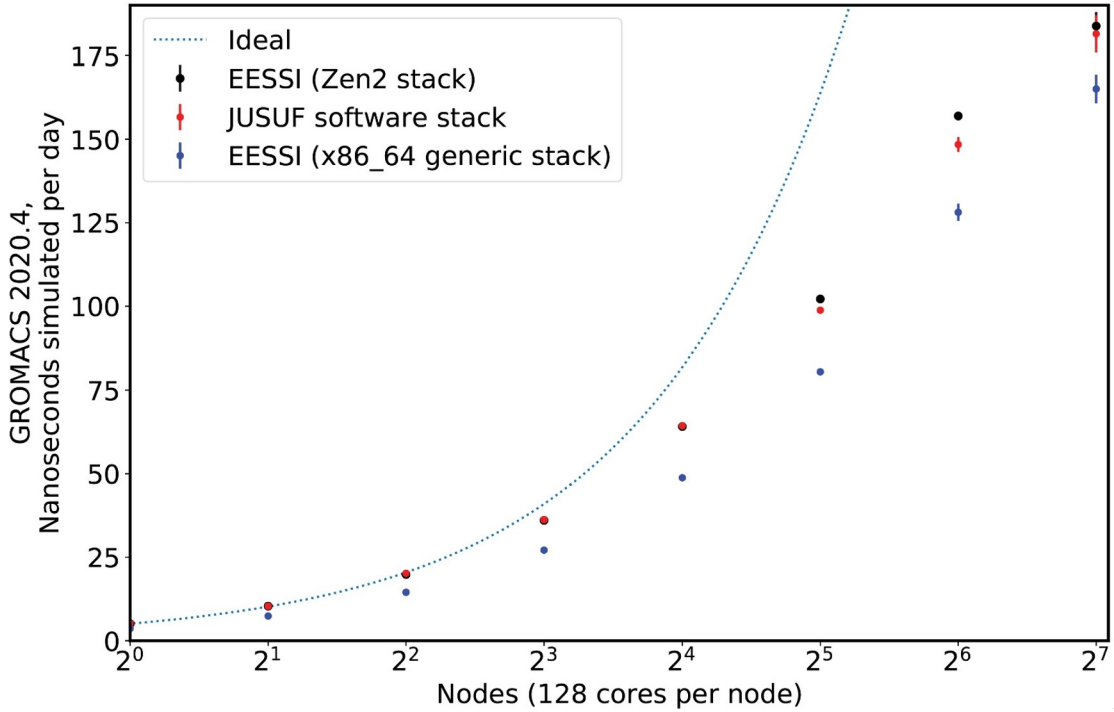
- Global distribution of software installations
- Centrally managed software stack
- Redundant network of “mirrors”
- Multiple levels of caching
- **Same software stack everywhere**:

  laptops, HPC clusters, cloud VMs, …

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

# EESSI paper (open access)

doi.org/10.1002/spe.3075




Paper includes proof-of-concept performance evaluation compared to system software stack, performed at JUSUF @ JSC using GROMACS 2020.4, up to 16,384 cores (CPU-only)

# EESSI demo: GROMACS


- See also https://eessi.github.io/docs/using_eessi/eessi_demos
- Also demos available for Bioconductor, OpenFOAM, TensorFlow

```
$ source /cvmfs/pilot.eessi-hpc.org/latest/init/bash
...
Environment set up to use EESSI pilot software stack, have fun!


$ module avail GROMACS
------ /cvmfs/pilot.eessi-hpc.org/versions/2021.12/software/linux/aarch64/graviton2/modules/all -------

      GROMACS/2020.1-foss-2020a-Python-3.8.2            GROMACS/2020.4-foss-2020a-Python-3.8.2 (D)


$ cd eessi-demo/GROMACS; ./run.sh

...
```

# MultiXscale

Web page: https://www.multixscale.eu

Facebook: MultiXscale

Twitter: @MultiXscale

Co-funded by the European Union

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