EESSI

EUROPEAN ENVIRONMENT FOR SCIENTIFIC SOFTWARE INSTALLATIONS

Kenneth Hoste (HPC-UGent, Belgium)

13 Sept 2022

CernVM workshop @ Amsterdam

whoami

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@kehoste (Twitter)

EasyBuild Slack

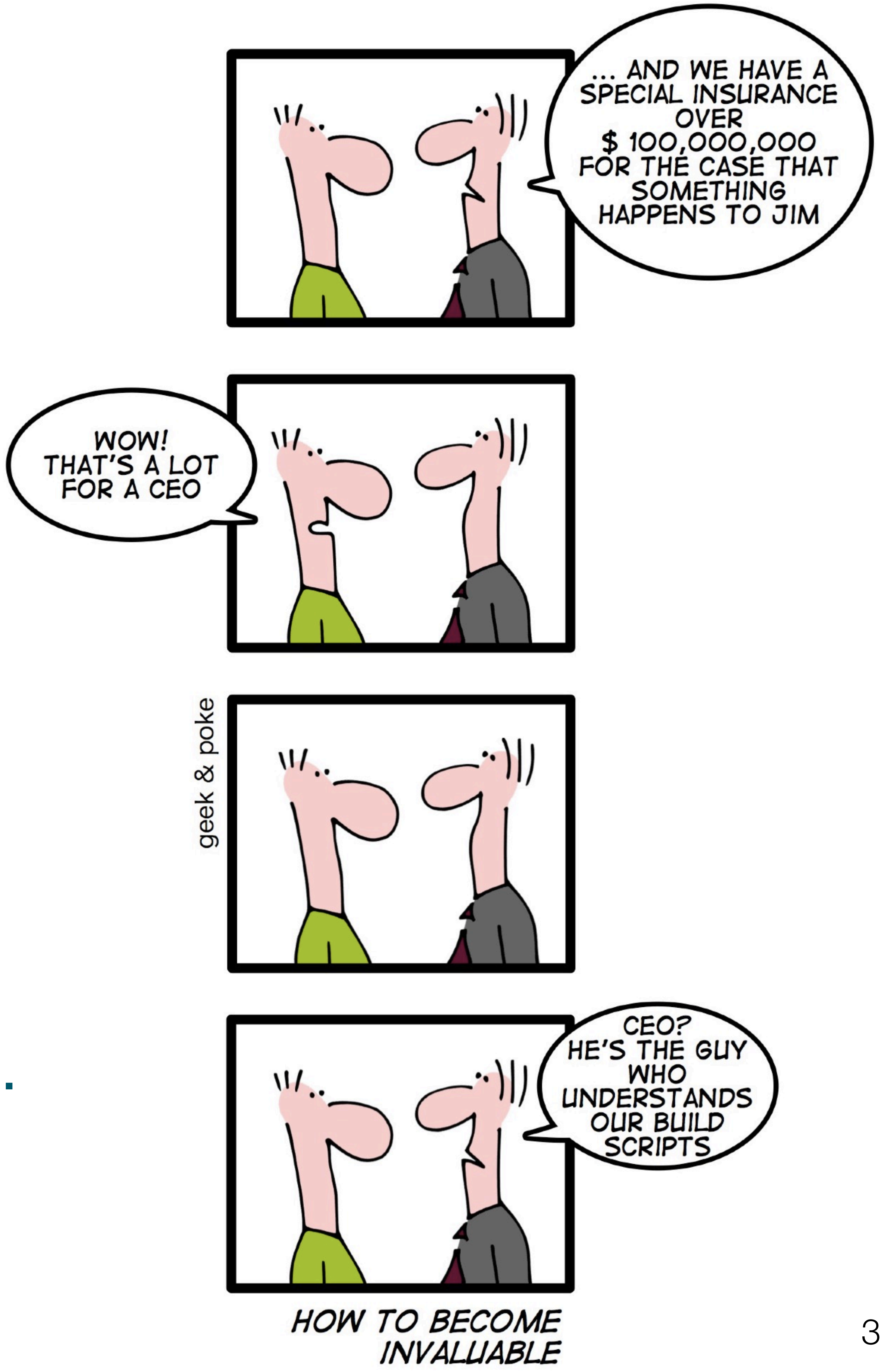
LinkedIn

- Computer scientist with Masters + PhD from Ghent University (BE)
- Joined HPC team at Ghent University in October 2010
- Main tasks: user support, incl. installation of scientific software
- Inherited maintenance of EasyBuild in 2011
- Slowly also became **EasyBuild lead developer & release manager** ...
- I like beer, loud music, FOSS, stickers, dad jokes
- I don't like C++ compiler errors, CMake, SCons, Bazel, TensorFlow, OpenFOAM, ...

Getting Scientific Software Installed

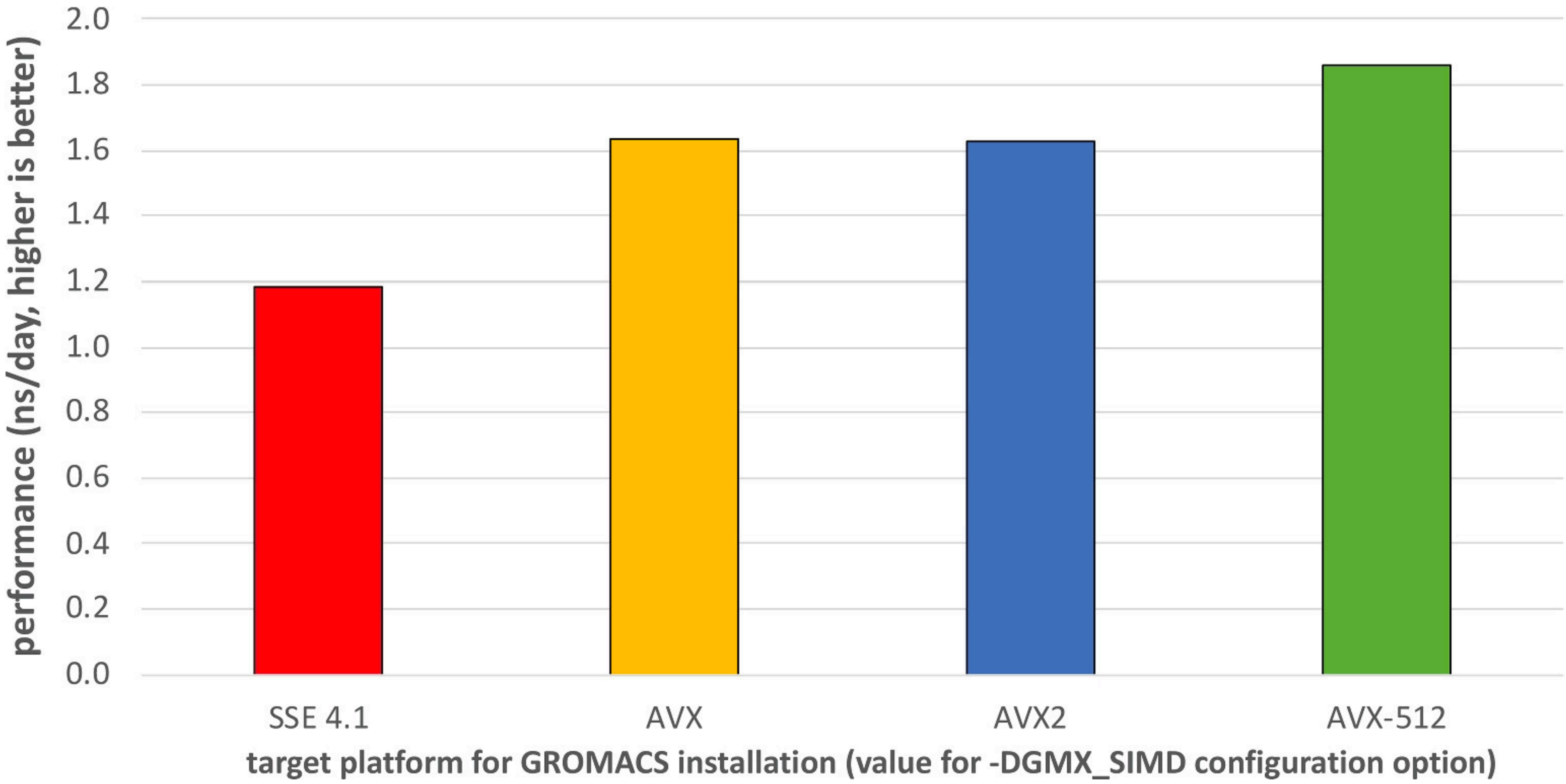
Installing scientific software is (still) a tremendous problem for High Performance Computing (HPC) sites all around the world.

- Ideally built from source - performance is key!
- Tedious, time-consuming, frustrating,
  sometimes simply not worth the (manual) effort...
- **Huge burden on researchers & HPC support teams**
- Installation requests are ~15% of HPC-UGent helpdesk tickets,
  but they consume ***way*** more than 15% of our user support time...
- Very little collaboration among HPC sites (until recently)


... AND WE HAVE A SPECIAL INSURANCE OVER $ 100,000,000 FOR THE CASE THAT SOMETHING HAPPENS TO JIM
WOW! THAT'S A LOT FOR A CEO
geek & poke
CEO? HE'S THE GUY WHO UNDERSTANDS OUR BUILD SCRIPTS
HOW TO BECOME INVALUABLE

http://geekandpoke.typepad.com/geekandpoke/2010/05/how-to-become-invaluable.html

Don’t sacrifice performance for “mobility of compute”



- Performance evaluation of GROMACS with different binaries on an Intel Cascade Lake system
- Impact of target ISA on GROMACS: **57% speedup** on a system that support AVX-512 instructions!
- When using containers (and CernVM-FS?) performance is often sacrificed for "mobility of compute"...

(all technical details in EESSI paper, see doi.org/10.1002/spe.3075)

easybuild to the rescue

easybuild.io

docs.easybuild.io

youtube.com/c/easybuilders

twitter.com/easy_build

easybuild.io/tutorial

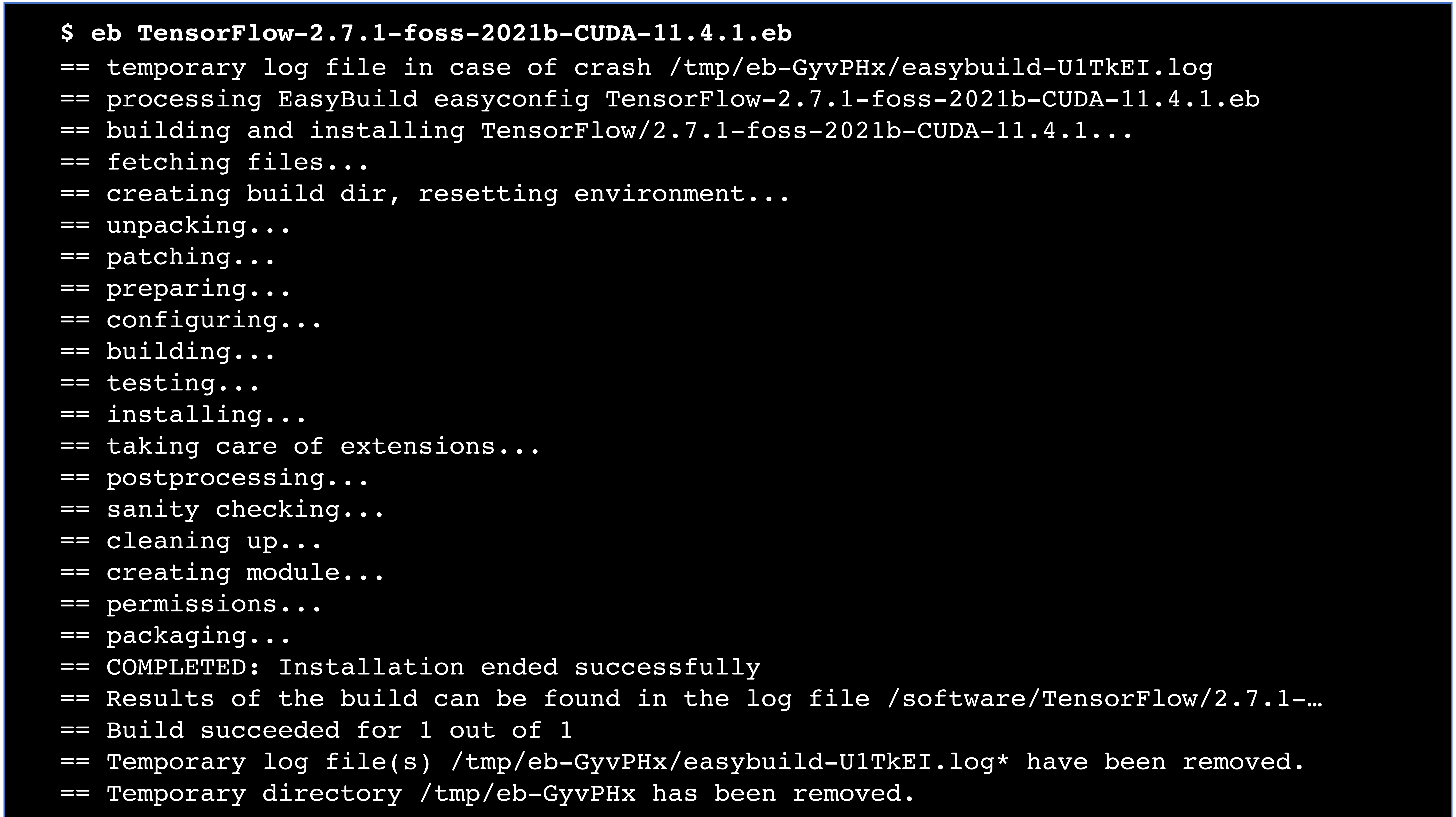
easybuild.io/eum

easybuild.io/tech-talks

- **Tool to make installation of scientific software easier** (preferably from source)
- Created in 2009, available as open source software (GPLv2) since 2012 via GitHub + PyPI
- Focus on Linux & HPC systems, specific attention to ***performance*** of installed software
- By default: optimise for CPU microarchitecture of system on which software is being compiled
- Implemented in Python, supports both Python 2.7 and 3.5+
- Integrates with environment modules tool (Tcl-based Environment Modules + Lmod)
- Supports different compiler toolchains + over 2,700 software packages (excl. extensions)
- Created by HPC-UGent team, now supported & developed by a **worldwide community**...

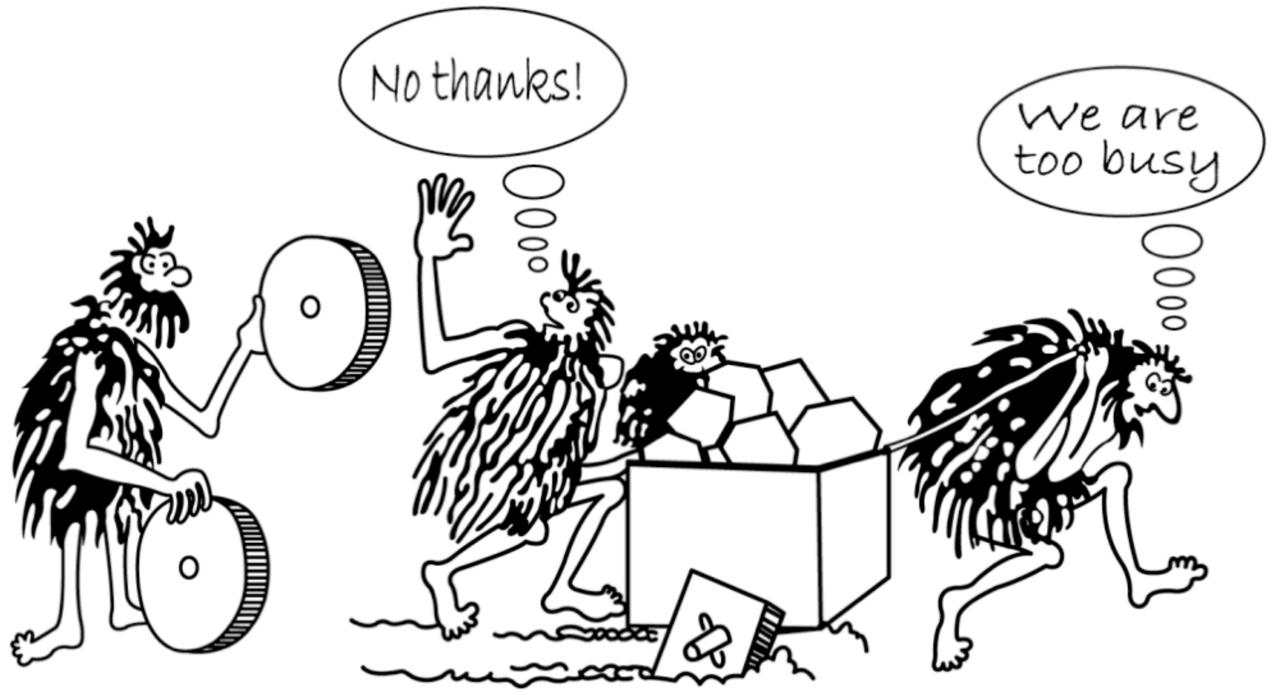
Installing TensorFlow from source, with ease

easybuild.io



```
$ eb TensorFlow-2.7.1-foss-2021b-CUDA-11.4.1.eb
== temporary log file in case of crash /tmp/eb-GyvPHx/easybuild-U1TkEI.log
== processing EasyBuild easyconfig TensorFlow-2.7.1-foss-2021b-CUDA-11.4.1.eb
== building and installing TensorFlow/2.7.1-foss-2021b-CUDA-11.4.1...
== fetching files...
== creating build dir, resetting environment...
== unpacking...
== patching...
== preparing...
== configuring...
== building...
== testing...
== installing...
== taking care of extensions...
== postprocessing...
== sanity checking...
== cleaning up...
== creating module...
== permissions...
== packaging...
== COMPLETED: Installation ended successfully
== Results of the build can be found in the log file /software/TensorFlow/2.7.1-…
== Build succeeded for 1 out of 1
== Temporary log file(s) /tmp/eb-GyvPHx/easybuild-U1TkEI.log* have been removed.
== Temporary directory /tmp/eb-GyvPHx has been removed.
```

Landscape of computational science is changing



- **Explosion of available scientific software applications**
    - Broader scope in terms of scientific domains (bioinformatics, AI, ...)
    - Fuelled by recent shifts in scientific community
        - Pressure to publish code along with research articles + popularity of GitHub
        - Wider adoption of HPC across scientific domains (GPUs in bioinformatics, ...)
- **Increasing interest in using cloud infrastructure** (both private and commercial)
- **Increasing variety in processor (micro)architectures**
    - Intel + AMD, Arm, POWER, soon also RISC-V? (cfr. European Processor Initiative, ...)
    - In addition, GPUs (NVIDIA, AMD, soon Intel?) and other accelerators (TPUs, IPUs, ...)
- **In strong contrast: available manpower in HPC support teams...**

It is time to take the next step…

- EasyBuild helps a lot with managing scientific software stacks, but it's not enough anymore...
- **HPC sites are *still* losing way too much time in getting scientific software installed**
  - Installation requests for new software often require significant investment & expertise
  - Problems occur due to site-specific differences in system setup & configuration
  - Small details (OS packages, disk partitioning, ...) can cause trouble
- **Situation is getting *worse*, not better**: more software, increasing variety in hardware, ...
- **There is a lot of potential for more extensive collaboration beyond installing software**
  - Ensuring correctness of installations w.r.t. scientific results they produce
  - Evaluating performance of provided installations + performance monitoring
  - ReFrame developed by CSCS is definitely a step in the right direction!

Introducing EESSI…

- *European Environment for Scientific Software Installations*
- Collaborative project, by and for the computational science community
- **Shared central stack of (optimised) scientific software installations**
- Uniform way of providing software to users, regardless of system they use
- Should work regardless of OS and system architecture (HPC, cloud, laptop,…)
- Focus on **performance**, automation, testing, collaboration

EESSI

EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS

www.eessi-hpc.org

eessi.github.io/docs (try out pilot repository!)

Goals of EESSI, and how we can achieve them

CernVM-FS

Global distribution of scientific software installations, transparent for end users

“Netflix for scientific software”

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gentoo

Abstraction from OS, one software stack (per type of CPU) to rule them all

“Containers without the containing”

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Provide optimised software installations for specific CPUs
+ automatically select best suitable

Don’t sacrifice performance for mobility of compute!

easybuild Lmod arch spec

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Abstraction from OS, one software stack (per type of CPU) to rule them all

“Containers without the containing”

Provide optimised software installations for specific CPUs + automatically select best suitable

Don’t sacrifice performance for mobility of compute!

Test provided software installations, monitor performance over time

Go (well) beyond just installing software: ensure correctness, performance, …

easybuild Lmod archspec

ReFrame

High-level overview of EESSI

Software layer

optimized installations of applications + dependencies

Compatibility layer

levelling the ground across Linux distros

("containers without the containing")

Filesystem layer

global distribution of the software stack

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

host operating system (any Linux distribution)

Testing

Heavily inspired by compute canada software stack

From zero to science in 3 steps

- Step 1: Get access to EESSI repository, either through:
  - system-wide CernVM-FS installation (requires admin privileges)
  - container with CernVM-FS + EESSI configuration pre-installed
- Step 2: Set up environment: source EESSI init script
- Step 3: Load module(s) and run!

eessi.github.io/docs/pilot

github.com/eessi/eessi-demo

```
# Assumption: EESSI is accessible (CernVM-FS is installed + EESSI configuration is in place)

# Step 2: set up environment (CPU architecture is detected automatically!)
$ source /cvmfs/pilot.eessi-hpc.org/latest/init/bash

# Step 3: load module(s) to activate software (check with ‘module avail’), and run!
[EESSI pilot 2021.12] $ module load GROMACS
[EESSI pilot 2021.12] $ gmx mdrun ...
```

Use cases

- A **uniform software stack** across HPC clusters, clouds, servers, and laptops
- Can be leveraged in **continuous integration** (CI) environments for software testing
- Significantly facilitates setting up **infrastructure for HPC training**
  - Using throwaway clusters in the cloud (Azure, AWS, …)
  - Participants can easily get access to same software environment "at home"
- **Enhanced collaboration** with software developers and application experts
  - Work towards "vetting" of scientific software installations included in EESSI
  - Relieve developers from burden of getting their software (properly) installed
- **Community software** and **portable workflows**

Current status of EESSI

EESSI

status.eessi-infra.org

- Started as an idea early 2020, effort kickstarted shortly after
- Monthly online meetings since mid 2020
- Currently an unfunded "side project", actively pursuing dedicated project funding...
- **Work-in-progress, proof-of-concept pilot repository available** - eessi.github.io/docs/pilot
  - Supports `x86_64` (Intel, AMD), `aarch64` (Arm 64-bit), `ppc64le` (POWER)
  - Included software: Bioconductor, GROMACS, OpenFOAM, R, TensorFlow, ...
  - Targets: Intel Haswell + Skylake, AMD Rome + Milan, AWS Graviton2 + 3, POWER9 (partial),
    + `generic` fallback for `aarch64` (Raspberry Pi!), `ppc64le`, `x86_64`
- Sponsored credits provided by both AWS and Azure to support development
- Actively developing monitoring, tooling, test suite, GPU support, contribution workflow, etc.

Future work

- **Make EESSI ready for production use**
  - Switch to eessi.io domain (more neutral, EESSI is not specific to HPC)
  - New Stratum-0 (dedicated hardware + Yubikey) + Stratum-1 servers (managed by small team?)
  - Follow up on (impact of) necessary security updates in compatibility layer (glibc, …)
  - Stabilise support for NVIDIA GPUs + implement bot to automatically build/deploy more software
  - Include more scientific software (all open source software that EasyBuild supports?)
- **Add support for RISC-V CPUs** (`riscv64`)
  - CernVM-FS already works on RISC-V (?), Gentoo Prefix bootstrapping works (cfr. GSoC project)
  - Next steps: build EESSI compat layer + see which scientific software works on top
- Also support other types of GPUs: AMD, Intel, …

Funding via MultiXscale EuroHPC project

- EuroHPC Centre of Excellence:
  Exascale-oriented application co-design and delivery for multiscale simulations

- Total funding: € 6,000,000 (2023-2027, 16 partners incl. HPC-UGent)

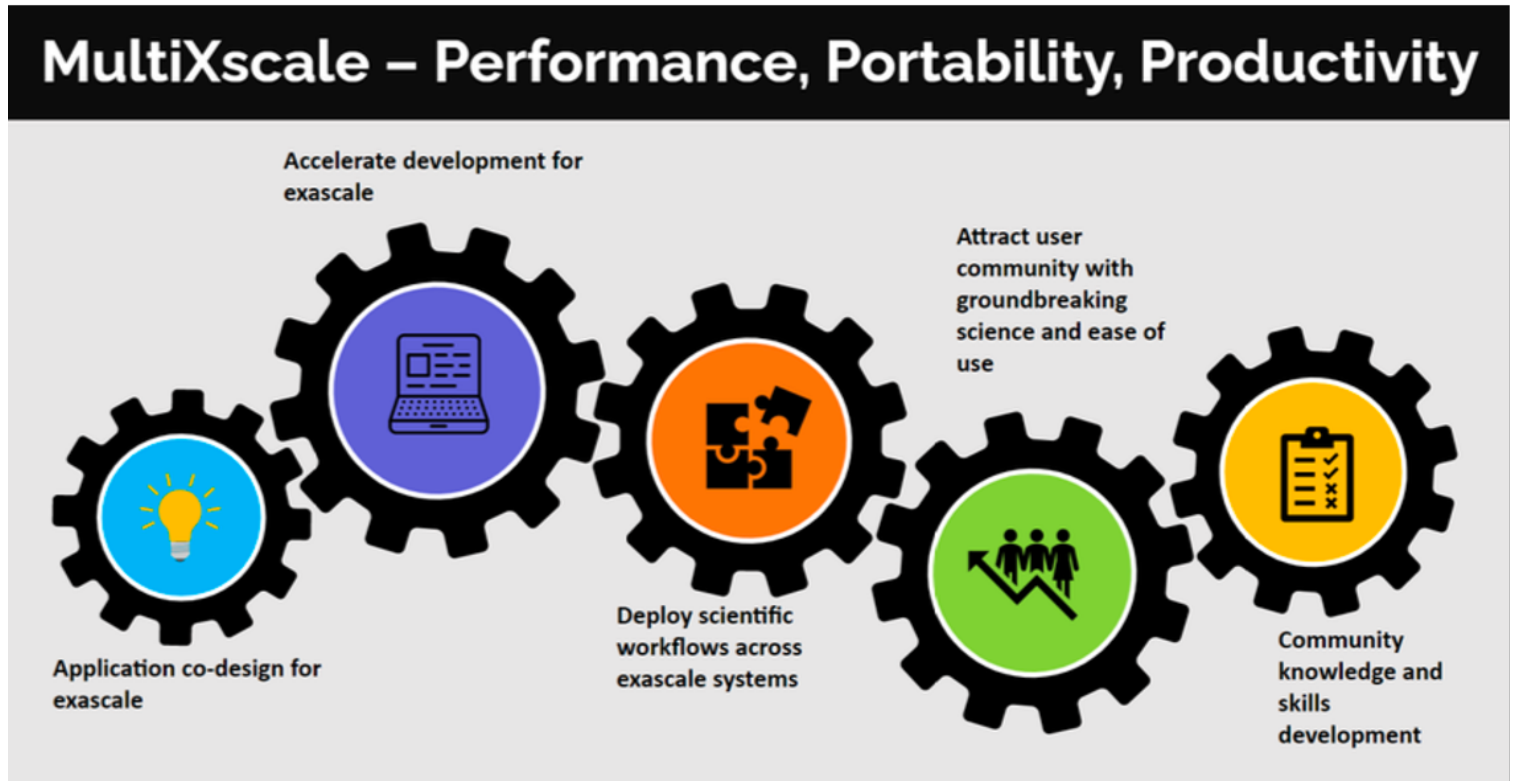
- Two aspects:

  - **Services to facilitate development and deployment of scientific software** =>

  - Development of software for efficient large-scale multiscale simulations

- Project proposal was accepted for funding, currently working towards grant agreement

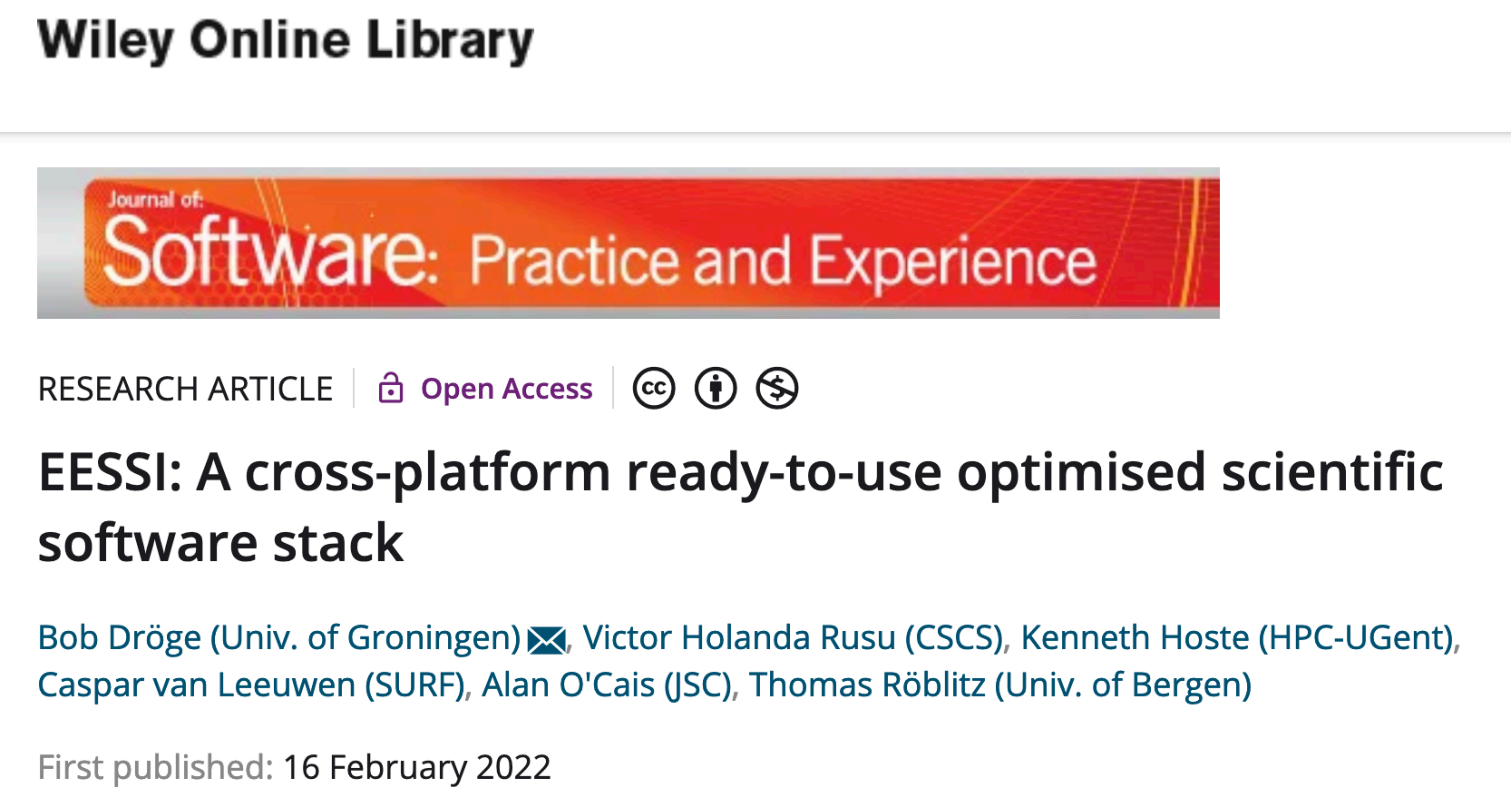
- Expected timeframe: Feb’23 - Jan’28


MultiXscale – Performance, Portability, Productivity
Accelerate development for exascale
Attract user community with groundbreaking science and ease of use
Application co-design for exascale
Deploy scientific workflows across exascale systems
Community knowledge and skills development

EESSI paper (open access)

doi.org/10.1002/spe.3075

Detailed overview of motivation, project goals, design, challenges & limitations, use cases, etc.



Wiley Online Library

Journal of: Software: Practice and Experience

RESEARCH ARTICLE | Open Access

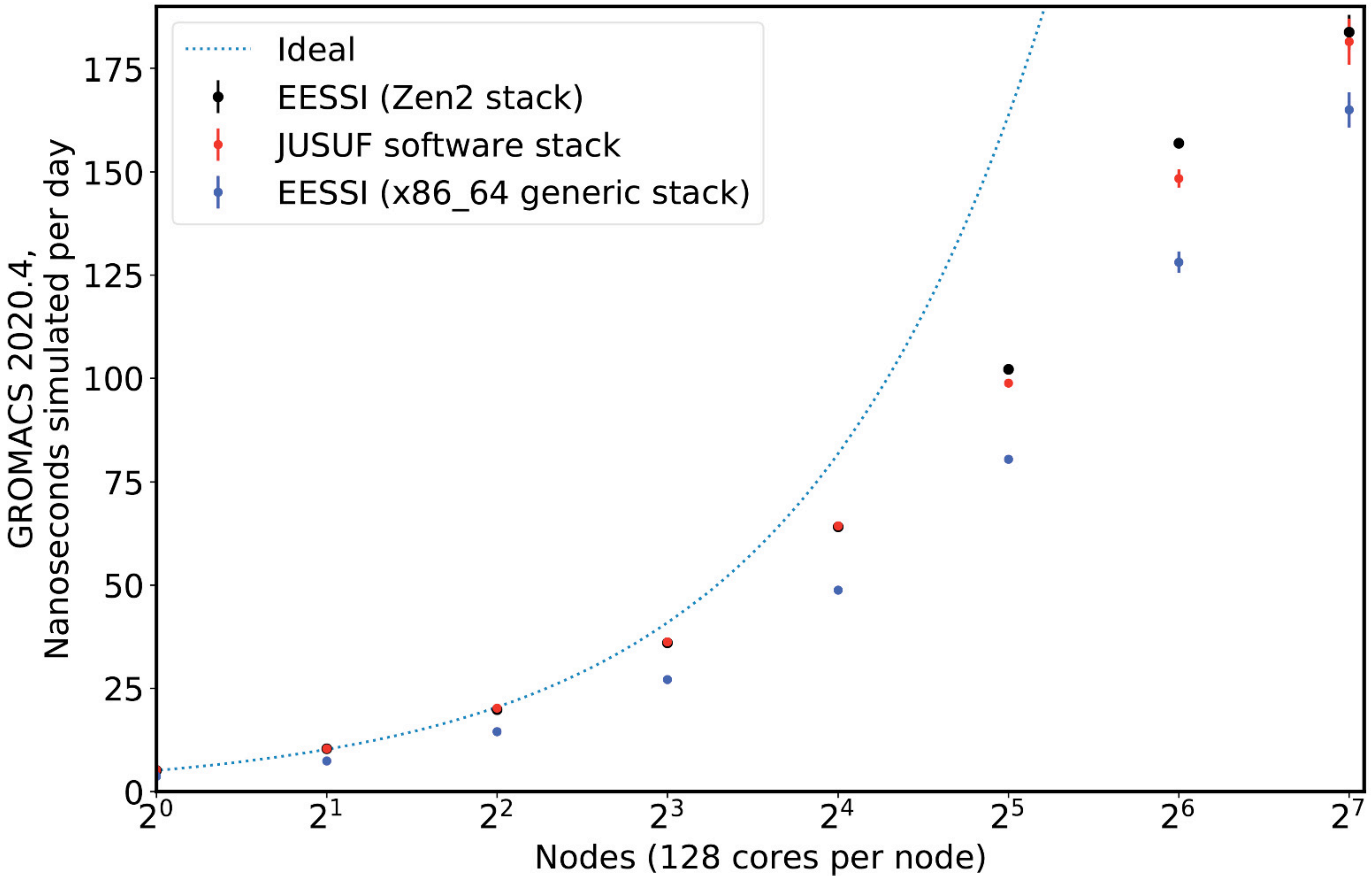
EESSI: A cross-platform ready-to-use optimised scientific software stack

Bob Dröge (Univ. of Groningen), Victor Holanda Rusu (CSCS), Kenneth Hoste (HPC-UGent), Caspar van Leeuwen (SURF), Alan O'Cais (JSC), Thomas Röblitz (Univ. of Bergen)

First published: 16 February 2022

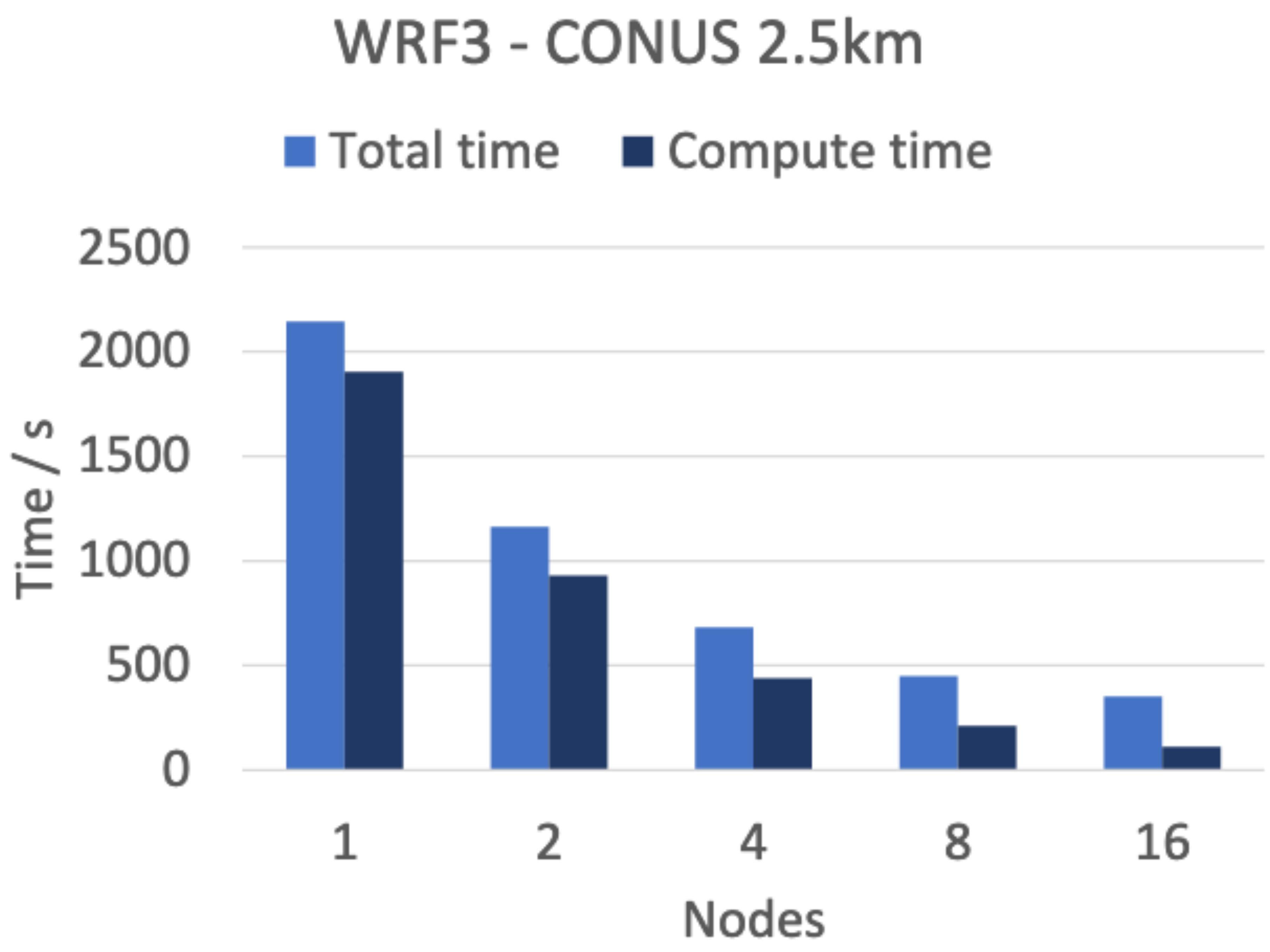
Large-scale GROMACS run via EESSI on JUSUF (JSC)

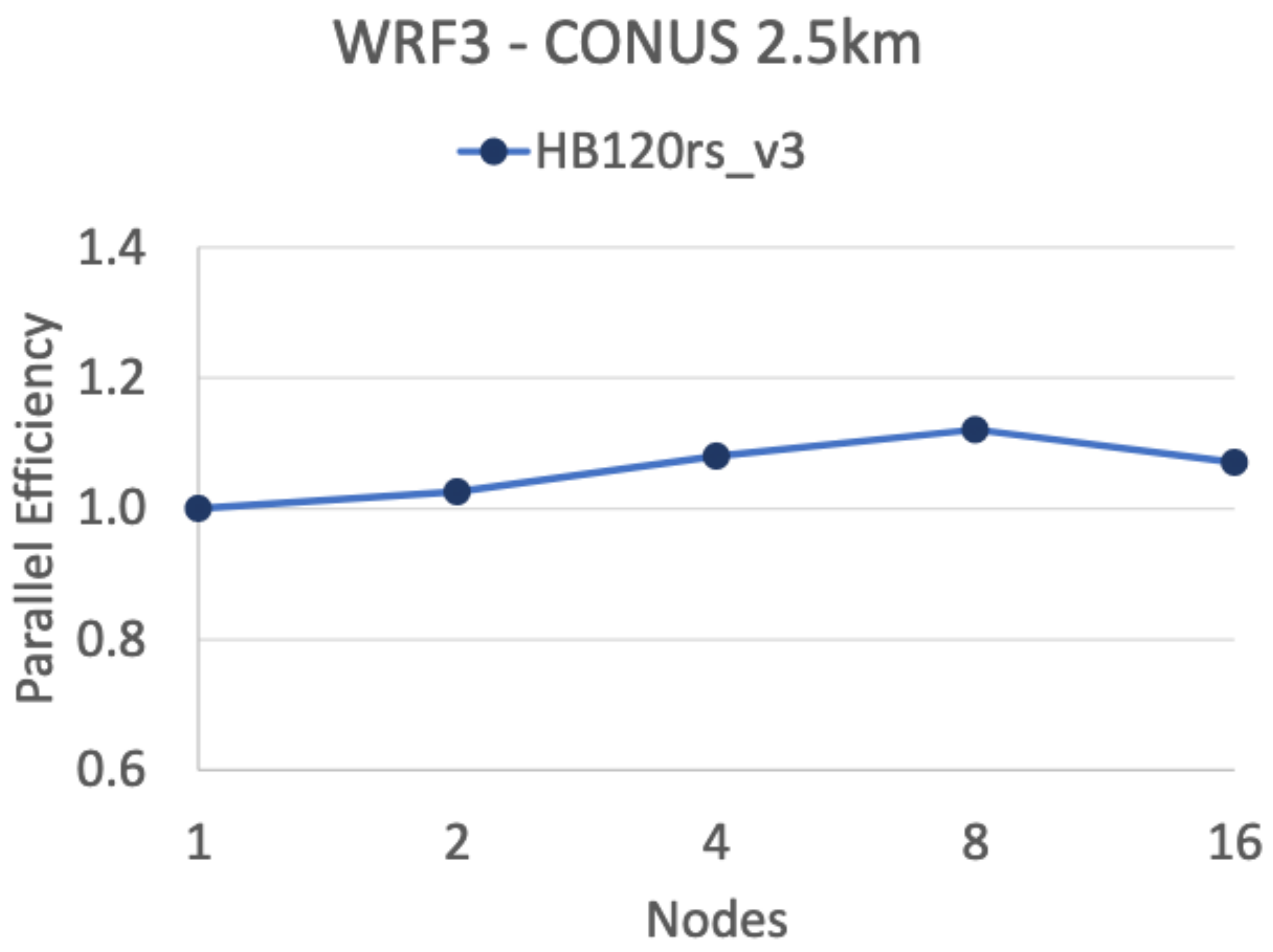
doi.org/10.1002/spe.3075



- 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)

Running WRF in Azure via EESSI





- Performance experiment by Hugo Meiland & Davide Vanzo (Microsoft Azure), for their EUM'22 talk "Leveraging EESSI for WRF simulations at scale on Azure HPC"
- WRF v3.9.1.1 with `foss/2020a` on `HB120rs_v3` (120 cores, AMD EPYC 7V13, HDR Infiniband)
- Essentially using EESSI pilot repository as is, no changes needed to leverage fast interconnect!

EESSI Community Meeting

- After dozens of online meetings, finally a physical (hybrid) community meeting! \o/
- **Wed-Fri 14-16 2022 in Amsterdam**
- Venue: meeting room at restaurant Polder, across the street from Amsterdam Science Park
- Agenda: mix of presentations (introductory & beyond) + hackathon/discussion sessions
- Live streaming of all presentations via the (brand new) EESSI YouTube channel
- All info via https://eessi.github.io/docs/meetings/2022-09-amsterdam
- **If you would like to attend one or multiple days, let me know!**

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eessi-hpc.org

eessi.github.io/docs

github.com/EESSI

Join our mailing list & Slack channel

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Twitter: @eessi_hpc

Status page: status.eessi-infra.org

Paper: doi.org/10.1002/spe.3075

EESSI-related talks at EUM'22:

Getting started - WRF in Azure - Adding software

Monthly online meetings, open to anyone interested

(first Thursday, 14:00 CE(S)T)