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DIRECTIE ICT
AFDELING INFRASTRUCTUUR

Multiscale

ICT-commissie 31 maart 2023

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HPC @ UGENT

https://www.ugent.be/hpc

HPC: High-Performance Computing (a.k.a. supercomputing)

Task HPC-UGent team: centralized hardware + services for *scientific computing* (since 2009)

Currently 9 team members, ~2 FTE for user support

9 Tier-2 clusters + Tier-1 cluster “Hortense”
=> over 800 servers in total (excl. Tier-1 extension)

Over 2,800 VSC accounts (UGent only)

Over 2,500 helpdesk tickets per year related to HPC-UGent services & infrastructure,

incl. ~375 software installation requests (statistics from 2022)

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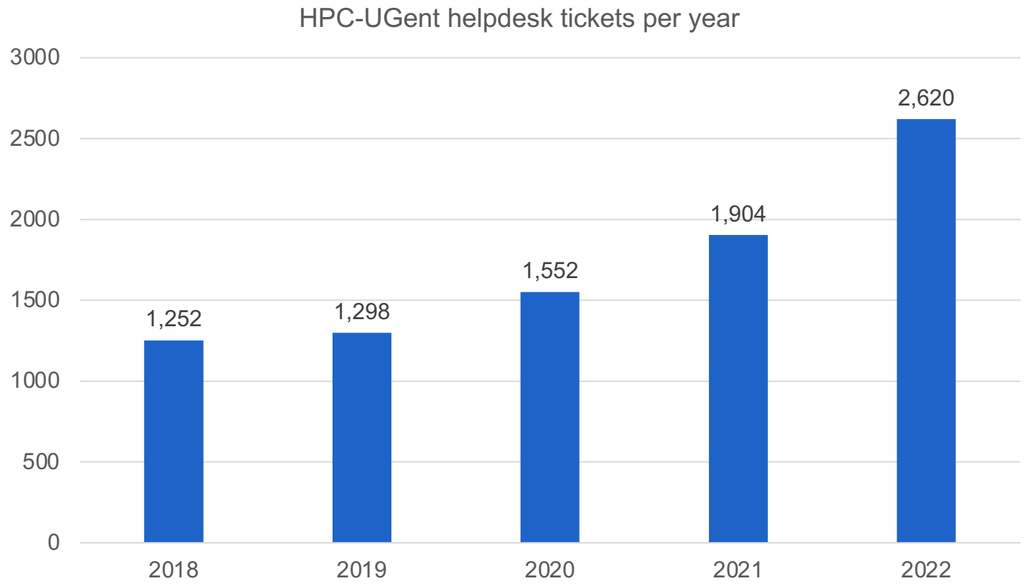
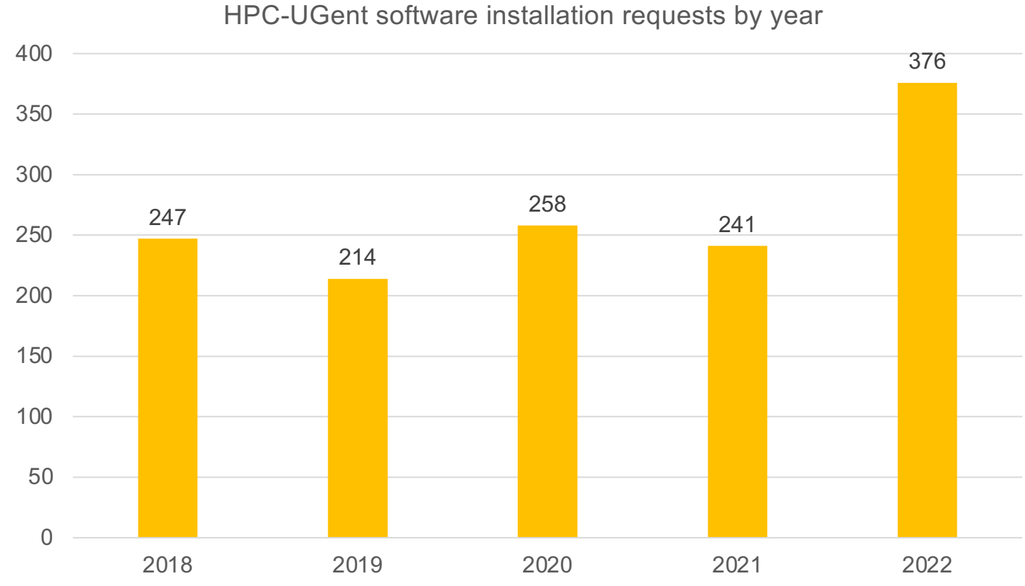
INCREASING DEMAND FOR HPC SUPPORT

We see an increasing demand for support by end users of the HPC-UGent infrastructure





Increase can only be *partially* explained by advent of Tier-1 Hortense in 2022

Researchers from more and more scientific domains are using the HPC infrastructure

Scientific software stack is quickly becoming more diverse, more complex, …

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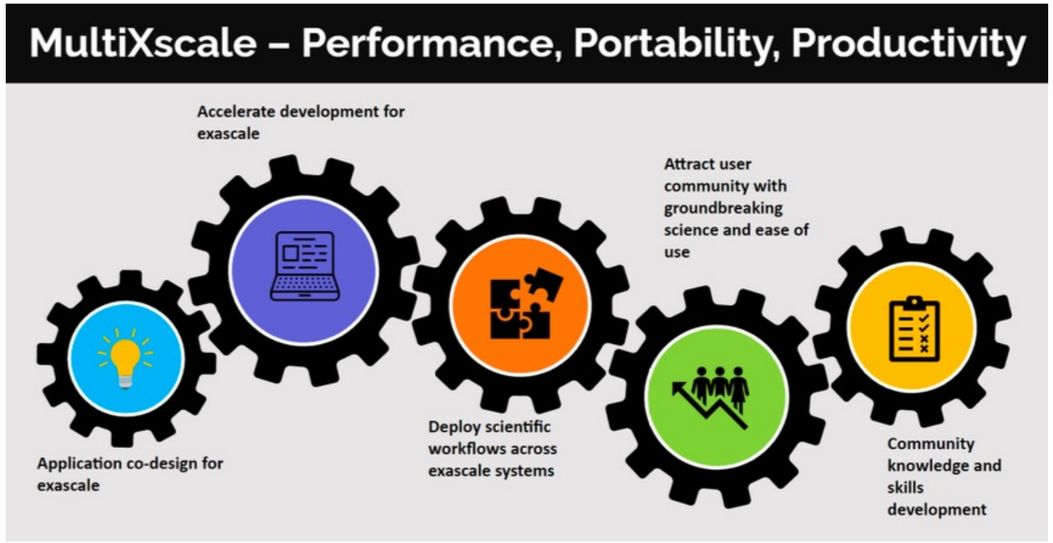
MULTIXSCALE: A EUROHPC COE

EuroHPC Centre of Excellence (CoE) in exascale-oriented application co-design and delivery for multiscale simulations

Total funding: € 6,000,000 (2023-2027)

16 partners, incl. UGent (via HPC team)

Funding for UGent: € 500,000 (~1 FTE)
(50/50 funding by EU + Flemish government)



MULTIXSCALE: A EUROHPC COE

There are two main aspects in the MultiXscale project:

- **Services to facilitate development and deployment of scientific software**
- Development of software for efficient large-scale multiscale simulations

The HPC-UGent team is involved in the service-oriented (technical) work packages:

- WP1: Developing a Central Platform for Scientific Software on Emerging Exascale Technologies
- WP5: Building, Supporting and Maintaining a Central Shared Stack of Optimized Scientific Software Installations

MultiXscale is supporting the grass-roots EESSI project

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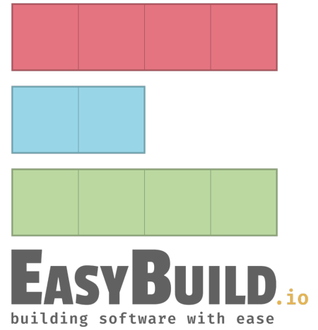
EESSI
EUROPEAN ENVIRONMENT FOR SCIENTIFIC SOFTWARE INSTALLATIONS

FROM EASYBUILD TO EESSI

https://easybuild.io



EasyBuild is tool that *automates* the installation (from source) of scientific software on HPC systems.

It was created in 2009 by Stijn De Weirdt (tech lead HPC-UGent), to make installation of scientific software *feasible* for a small support team.

We released it open source software in 2012, which kickstarted the EasyBuild community.

Today EasyBuild is used, developed, maintained, and supported by a worldwide community of experts in installing (scientific) software on HPC systems.

- ~3,000 contributions to EasyBuild per year
- Close to 400 unique contributors (~120 per year)
- Over 20 maintainers (incl. VSC, JSC, SURF, Digital Research Alliance of Canada, …)

EasyBuild User Meeting 2020 in Barcelona

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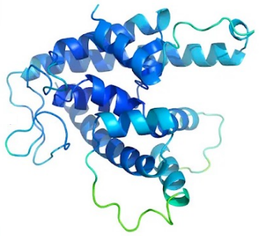
EXAMPLE: ALPHAFOLD



AlphaFold (AI software to predict 3D structure of proteins) was released as open source software in July'21 – *"most important achievement in AI, ever" (quote Forbes)*

Originates from Google's DeepMind team (who also did AlphaGo, AlphaZero, etc.)

Quick and massive interest from UGent research groups, multiple installation requests in a week.

Complex installation procedure, several "difficult" dependencies (TensorFlow, jax, …), only works well on GPU hardware, …

Supported in EasyBuild since Aug'21, thanks to combined effort by several HPC sites.

Now it's quick and easy to install AlphaFold, without compromising on performance…

https://www.youtube.com/watch?v=jP9Qg1yBGcs

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EASYBUILD: A SUCCESS STORY

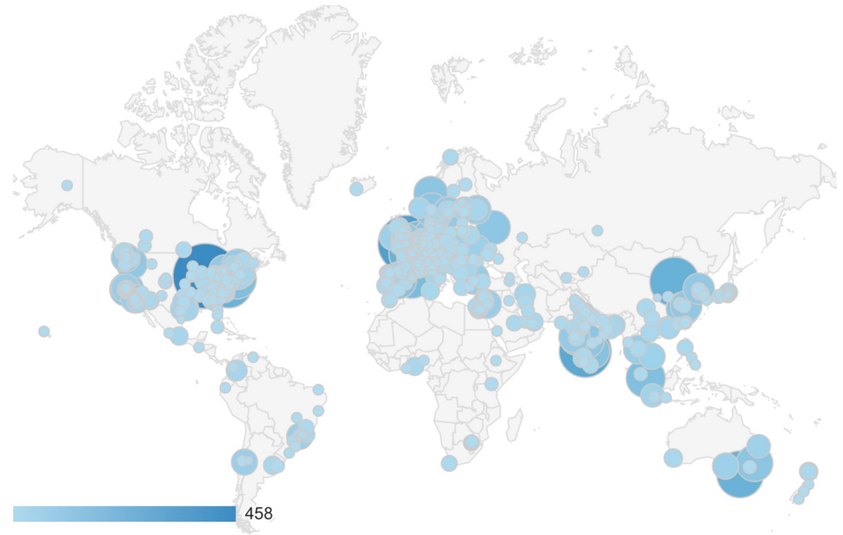
EasyBuild enables to quickly tackle software installation requests from researchers, and facilitates maintaining a huge central software stack on the HPC-UGent + VSC clusters.

Supports the installation of ~3,000 different (scientific) software packages (excl. versions)

Used by 100s of HPC sites, including JSC, CSCS, LUMI, Digital Research Alliance of Canada, …

Platform for collaboration with experts from around the world.

Has put Ghent University on the map in the HPC community.



COMPUTING LANDSCAPE IS CHANGING

Increasing diversity in hardware

CPUs: Intel era has ended => AMD, Arm (Fugaku, …), soon also RISC-V in HPC?

GPUs are here to stay: now mostly NVIDIA, but soon also AMD, Intel, …

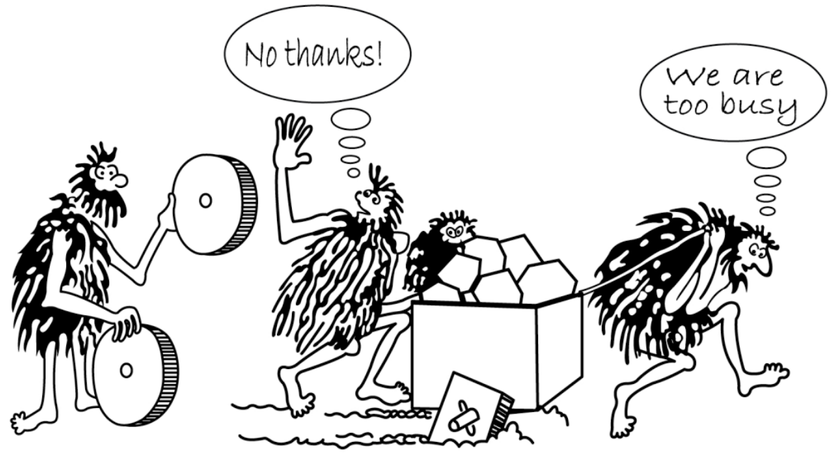
Expansion of computational science to other domains: AI, bioinformatics, …

⇒ Increasing demand for more and different software packages to install

More complex software, deeper software stacks (more dependencies), …

In strong contrast: available manpower in HPC support teams

NEED FOR MORE COLLABORATION



EasyBuild enables collaboration on installing scientific software across HPC sites, but it is not enough anymore…

HPC sites still struggle with software installation problems, due to lack of manpower and expertise, system-specific aspects, new scientific software emerging, …

Problem is getting worse due to increasing diversity/complexity in hardware/software

RISE OF EESSI

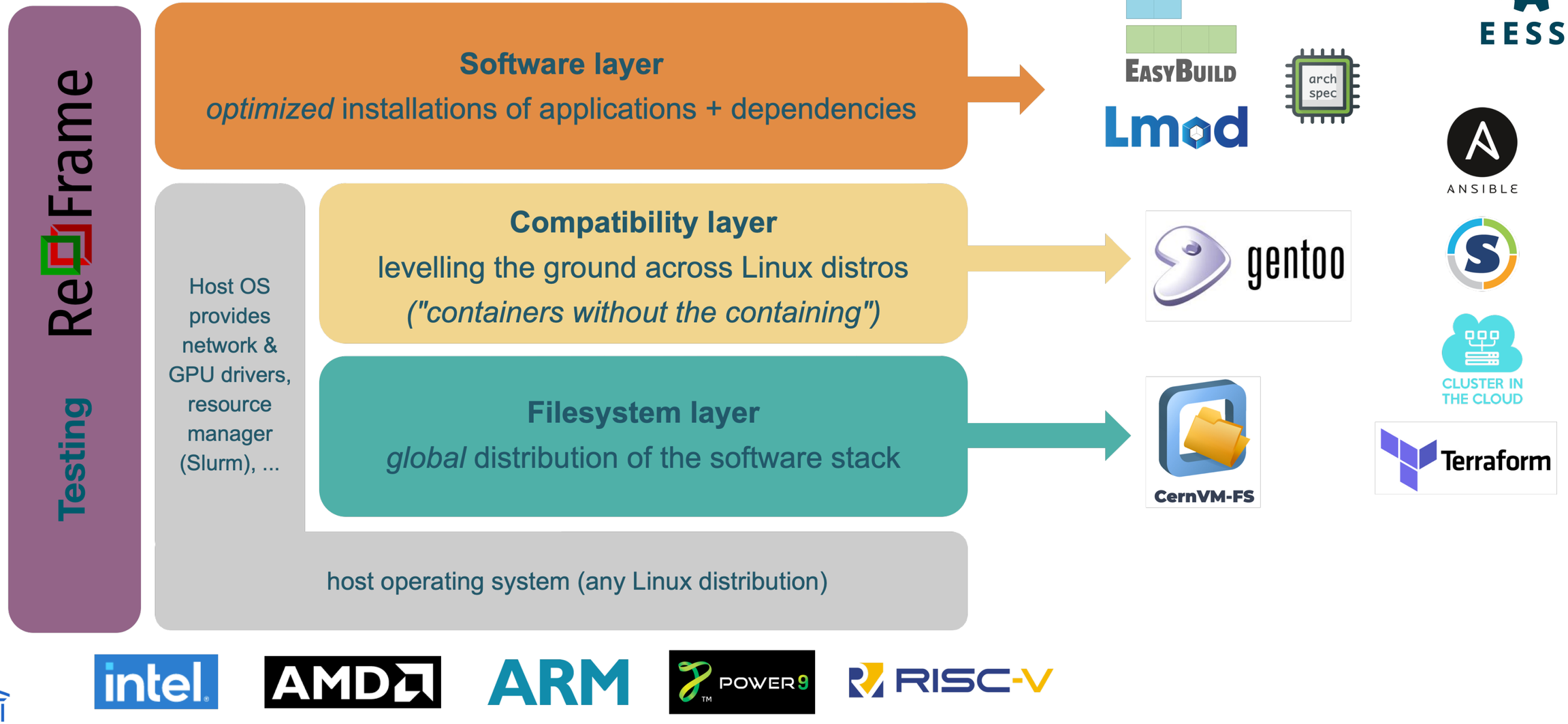
Early 2020, we were invited to TU Delft (via Dell, thanks to EasyBuild) to join a meeting between Dutch universities on collaborating (more) to tackle the problem of software installation on HPC systems.

We agreed to kickstart a project to work together, inspired by the shared software stack of the ComputeCanada consortium.

No funding available initially, so only as a side project, no strong commitments…

Several (virtual) meetings quickly led to a proof-of-concept setup of the **European Environment for Scientific Software Installation (EESSI)**.

EESSI IN A NUTSHELL



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SUPPORTING EESSI VIA MULTIXSCALE

There is a lot of interest from HPC sites to collaborate on EESSI,
but it can only become production-ready if **dedicated manpower** is available.

Open access paper on EESSI was published in Feb'22: https://doi.org/10.1002/spe.3075

Project proposal for EuroHPC Centre-of-Excellence "MultiXscale" submitted in April'22.

MultiXscale was accepted for funding in context of EuroHPC JU in Aug'22.

Service-related work packages in MultiXscale will make EESSI ready for production.

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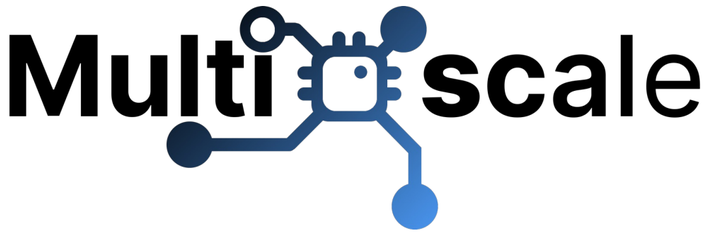


https://www.multixscale.eu

MULTIXSCALE: OUR INVOLVEMENT

HPC-UGent is mainly involved in the technical work packages (WP1 + WP5)

- Actively involved in WP1:

  Developing a Central Platform for Scientific Software on Emerging Exascale Technologies

- Lead for WP5:

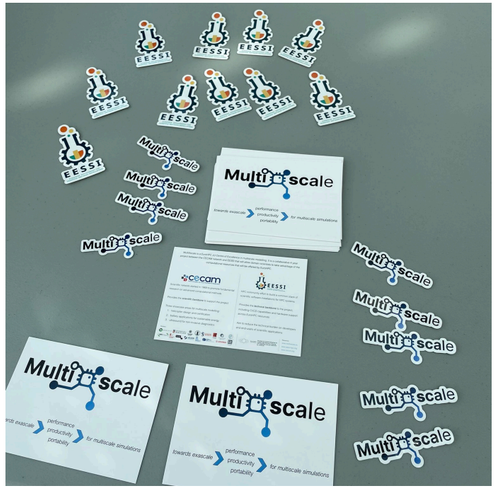
  Building, Supporting and Maintaining a Central Shared Stack of Optimized Scientific Software Installations

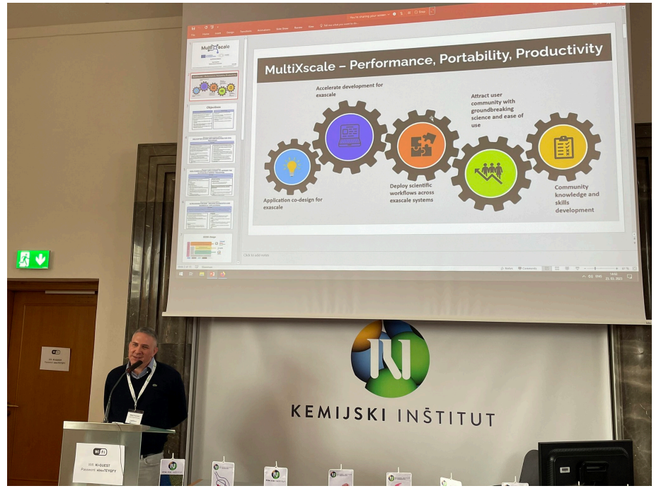
Funding for UGent: € 500,000 (2023-2027)
(50/50 funding by EU + Flemish government)

~1 FTE for HPC-UGent
=> hiring process for additional junior team member is ongoing (hopefully to start May 2023)

MULTIXSCALE KICKOFF MEETING

- MultiXscale kick-off meeting took place in Ljubljana 23+24 March 2023
- Doubled as first MultiXscale General Assembly meeting (to discuss project planning, etc.)
- Preceded by press conference to present the MultiXscale project,
  which was an item on the national news in Slovenia (see https://vimeo.com/810503122)





MULTIXSCALE GA IN 2024

- Possible that next MultiXscale General Assembly meeting will be hosted in Ghent
- Could be in conjunction with EuroHPC Summit 2024 (which will probably be in Brussels)

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