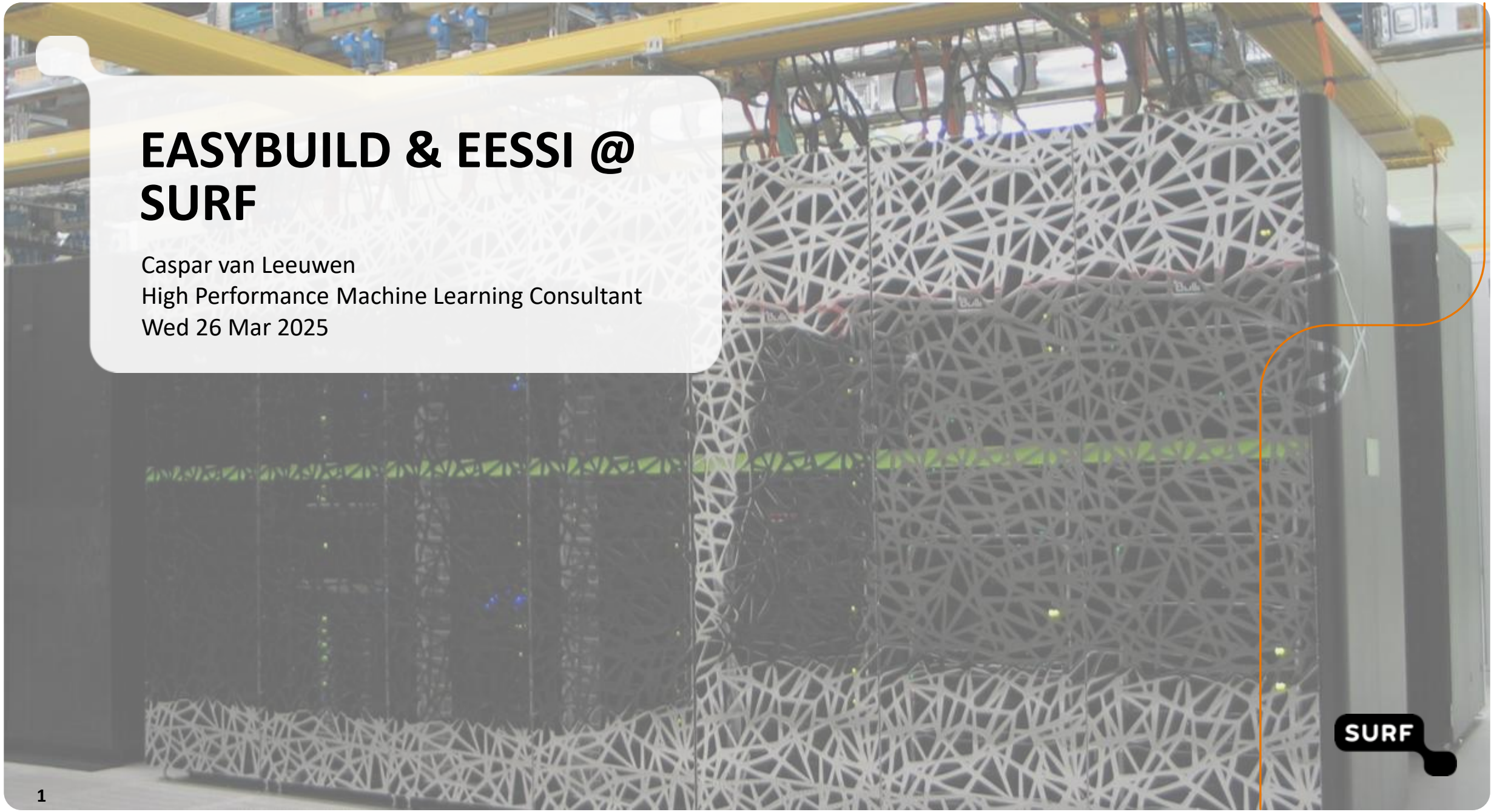

EASYBUILD & EESSI @ SURF

Caspar van Leeuwen
High Performance Machine Learning Consultant
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SURF

IT Cooperative of Dutch Education and Research

- Computing (HPC, HTC, grid, cloud)
- Storage & Data management (object store, tape, PID)
- Networking (Dutch National Research and Education Network)
- Procurement & contracting
- Identity & access management

Content

- The past
- The present
- The future

The past

- November 2016: EasyBuild 3.0.0 released with RPATH support
- Mid 2017: first (publicly available) installations @ SURF through EasyBuild
- Start 2019: EasyBuild becomes the default installation method. Manual installation only by *rare* exception!
- Initially build everything with foss & intel toolchains
- Since Snellius (2021): foss-only
  - More build issues with intel, too time consuming for little benefit

The present: Snellius

General-purpose HPC system

- Phase 1 (Q3 2021, Q4 2022)
  - 600 AMD Rome 7H12 CPU nodes
  - 72 Intel Ice Lake + A100 GPU nodes
- Phase 2 (Q3 2023)
  - 800 AMD Genoa 9654 CPU nodes
- Phase 3 (Q2 2024)
  - 88 AMD Genoa 9334 + H100 GPU nodes
- Total: 230k CPU cores, 640 GPUs, 38 PFLOPS

Variant symlink setup

Architecture-specific symlink: `/sw/arch`

- Points to one of these:

```
$ ls -al /gpfs/admin/_hpc/sw/arch
…
drwxrwxr-x  6 jenkins jenkins 8192 Dec 19 15:07 AMD-ZEN2
drwxrwxr-x  6 jenkins jenkins 4096 Oct  3 13:17 AMD-ZEN4
drwxrwxr-x  5 jenkins jenkins 4096 Oct  3 13:09 AMD-ZEN4-H100
drwxrwxr-x  6 jenkins jenkins 4096 Oct  3 13:15 INTEL-AVX512
```

Variant symlink setup

We don’t export submission environment in batch jobs, but even if you do, it resolves to the correct executable:

```
int1 $ module load GROMACS/2024.3-foss-2024a
int1 $ which gmx_mpi
/sw/arch/RHEL9/EB_production/2024/software/GROMACS/2024.3-foss-2024a/bin/gmx_mpi
int1 $ realpath $(which gmx_mpi)
/gpfs/admin/_hpc/sw/arch/AMD-ZEN2/RHEL9/EB_production/2024/software/GROMACS/2024.3-foss-2024a/bin/gmx_mpi
int1 $ srun -p genoa realpath $(which gmx_mpi)
/gpfs/admin/_hpc/sw/arch/AMD-ZEN4/RHEL9/EB_production/2024/software/GROMACS/2024.3-foss-2024a/bin/gmx_mpi
```

How we manage 4 optimizations

Semi-automated builds by Jenkins, based on a buildlist, e.g.

Site-specific customizations are done through hooks, rather than customizing EasyConfigs / EasyBlocks

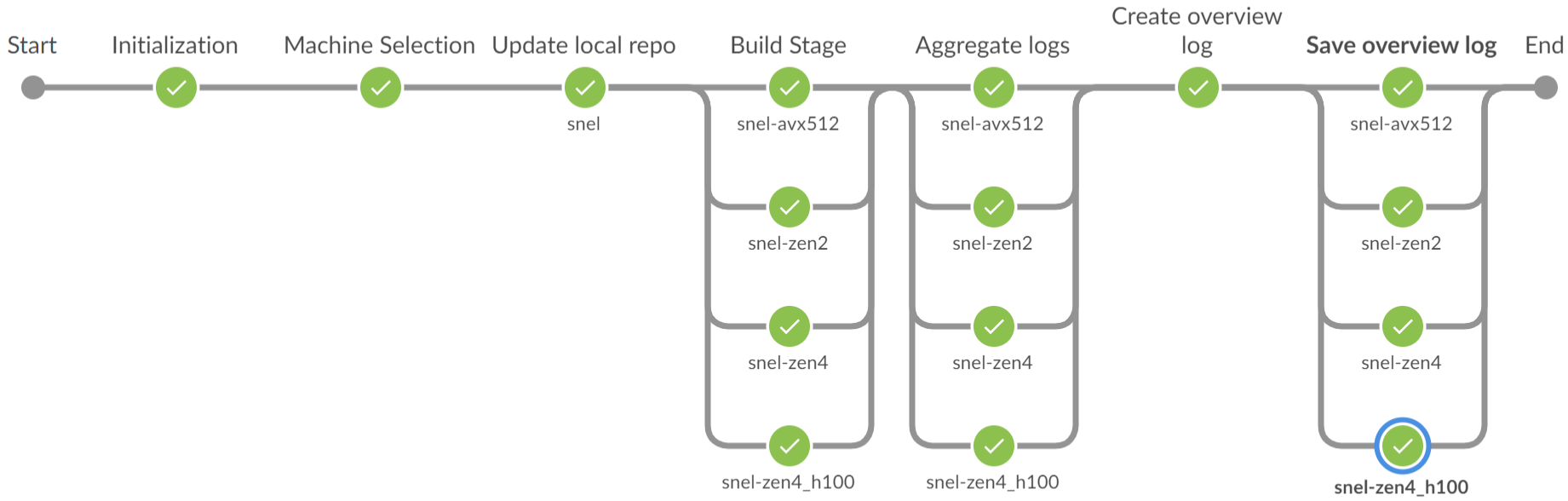
```
### Basic Compilers ####
GCCcore-13.3.0.eb
intel-compilers-2024.2.0.eb --accept-eula-for=Intel-oneAPI --from-pr=20903
Clang-18.1.8-GCCcore-13.3.0.eb --from-pr=21117

##### MPI Libraries ###
OpenMPI-5.0.3-GCC-13.3.0.eb --hooks=/sw/eb/easyconfigs-surf/hooks/mpi_hook.py --include-
easyblocks=/sw/eb/easyblocks-surf/openmpi.py --from-commit=a6c22ba28a69f0c42724a72243f92aa27fc6459c
impi-2021.13.0-intel-compilers-2024.2.0.eb --accept-eula-for=Intel-oneAPI --hooks=/sw/eb/easyconfigs-
surf/hooks/mpi_hook.py --from-pr=20919
MPICH-4.2.2-GCC-13.3.0.eb --from-pr=21442 --hooks=/sw/eb/easyconfigs-surf/hooks/mpi_hook.py
mpi4py-4.0.1-gompi-2024a.eb --from-pr=21662

##### Libraries ####
pybind11-2.12.0-GCC-13.3.0.eb --from-pr=20829
libcint-6.1.2-gfbf-2024a.eb --from-pr=21545
libpng-1.6.43-GCCcore-13.3.0.eb
libxml2-2.12.7-GCCcore-13.3.0.eb  --hook=/sw/eb/easyconfigs-surf/hooks/libxml2_hook.py
```

EasyConfigProduction < 2197 | Pipeline | Changes | Tests | Artifacts | Logout

Branch: –
Commit: –

4m 44s
a day ago

Changes by Benjamin Czaja
Started by user Benjamin Czaja



Save overview log / snel-zen4_h100 - 19s

✓	overview_logfile — Restore files previously stashed	<1s
✓	srun -p gpu_sw_h100 -N 1 --ntasks-per-node=1 -c 64 --gpus-per-node=4 -t 5:00 cp overview_summary.log ${JENKINS_LOGPATH_REAL}/overview_summary.log — Shell Script	16s

Managing OS upgrades

OS upgrades have caused issues in the past, requiring rebuilds

- One solution was to pro-actively just rebuild the entire stack, on the new OS
- OS-specific prefix allows building new stack while keeping old stack
- Update `MODULEPATH` to new prefix after upgrade to ‘flip the switch’

```
int1 $ realpath $(which gmx_mpi)
/gpfs/admin/_hpc/sw/arch/AMD-ZEN2/RHEL9/EB_production/2024/software/GROMACS/2024.3-foss-2024a/bin/gmx_mpi
```

- But: strategy not used anymore on RHEL8 to RHEL9 upgrade
  - ReFrame tests didn’t signal many issues
  - There were *some* issues in the end (e.g. OpenSSL related), but not many, and all handled on the fly after the upgrade

User installations

Wrapper *eblocalinstall:*

- EASYBUILD_INSTALLPATH = ~/.local/easybuild/…
- EASYBUILD_OPTARCH = <lowest_common_denominator>

Snellius software policy

We update our software stack once per year. Typically:

- based on 202Xa ← Currently considering to add 202Xb, but toolchains-only
- released around Q3 or Q4
- O(400) packages

Only honor sofware installation requests if:

- … is versioned
- … has an official release within last 2 years
- Max. 2 versions per software per year

Though we may allow exceptions (but don't tell our users ☺)

https://servicedesk.surf.nl/wiki/spaces/WIKI/pages/30660267/Software+policy+Snellius

Snellius software policy

Yearly software stacks available through meta-modules (that set `MODULEPATH`)

- Clear what is still supported
- Confronts users with how old things are that they are using…

```
$ module av
------------------------ /sw/noarch/environment --------------------------
2022    2023    2024    EESSI/2023.06
```

Full support: additional installations + resolve issues with existing installations

Limited support: resolve issues with existing installations

Deprecated: if it still works for you, we won't stop you from using it…

Older stacks (2020, 2021) are still there if you know where to look (but don't tell our users ☺)

Software testing

Local set of ReFrame tests

- Run periodically through Jenkins
- Run before / after maintenance

EESSI test suite[1]

- Based on ReFrame
- Run periodically through cronjob

[1] https://www.eessi.io/docs/test-suite/

The future

- Main Snellius software environment based on EESSI
  - Already the case on SURF Experimental Technologies Platform
- Provide site installations (proprietary software, other things not in EESSI) on top through the `EESSI-extend` module[1]
  - Initially on local filesystem
  - Long term, through CVMFS (‘software.surf.nl’) with whitelisting for SURF-internal systems
  - Build and deployed by eessi-bot[2]
- Integrate / deduplicate local ReFrame test suite & EESSI test suite

[1] https://www.eessi.io/docs/using_eessi/building_on_eessi/#building-software-on-top-of-eessi-with-easybuild
[2] https://www.eessi.io/docs/bot/

The future

Advantages for EESSI-based software environment

- More synergy / shared effort with other HPC teams: current yearly updates very time consuming!
- Less build effort when new system or phase gets deployed
- Uniform software stack across SURF systems (Snellius, SURF Research Cloud & Spider cluster)
- Better build automation (no more jenkins, triggered from the GitHub repository that holds the build list)
- User-space builds through `EESSI-extend` also optimized per architecture (but transparant to the user)
- Shared effort in test development for EESSI test suite

The future

Potential disadvantages / Risks for EESSI-based software environment

- (How) do we provide support on software that we did not build/deploy ourselves?
  - Active involvement in EESSI to build knowledge & experience
  - EESSI *community* can *also* provide support, and has much more knowledge!
- Risk: EESSI disappears / is no longer maintained
  - Mitigation: ‘software.eessi.io’ build on top of EESSI => easy to (re)build full stack
  - The more sites adopt EESSI as primary solution, the smaller the risk!

The future

Potential disadvantages / Risks for EESSI-based software environment

- Risk: EESSI infrastructure (Stratum 0 / 1) is unavailable
  - Mitigation: private Stratum 1 hosts full copy of the SW stack (+ better performance!)
- Risk: EESSI does not support the hardware architecture I care about
  - Mitigation: provide build infrastructure for EESSI

The future

So if it's EESSI, EESSI, EESSI, is there a future for EasyBuild?

- Yes! EasyBuild is a *key* technology in EESSI facilitating both the builds in the repository as well as the user-local builds!
- It may even create additional adoption
  - First, communities adopt EESSI to get easy access to software they care about
  - Then, they decide they want extra software, newer versions, etc => Motivation to dive into EasyBuild
  - I *actually* see this happening in my discussions on EESSI I had with developers from geosciences & radio-astronomy communities