

# **EESSI** meeting

August 5th 2021

https://github.com/EESSI/meetings/wiki

# Agenda



- 1. Quick introduction by new people
- EESSI-related meetings in last month [Kenneth, Alan]
- 3. Progress update per EESSI layer [Kenneth]
- 2021.06 version of pilot repository [Kenneth]
- 5. AWS/Azure sponsorship update [Kenneth, Alan, Henk-Jan]
- 6. AWS/Arm hackthon [Christian]
- 7. Q&A

# Quick introduction by new people



#### New people on the call: feel free to introduce yourself!

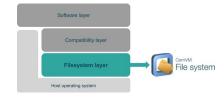
- Who are you, where do you work, on what?
- Why are you interested in the EESSI project?
- Are you planning to actively contribute,
   and if so, to which aspect(s) of the project?

# **EESSI-related meetings**



- July 13th: Monthly CernVM-FS coordination meeting (Bob?)
  - "interesting news" regarding corruption issue on in-place updates (<u>CVM-2001</u>)
- July 15th: kickoff meeting regarding Azure sponsorship for EESSI incl. RUG + SURF (Alan, Bob)
  - Subscription will be handled through <u>SURF Research Cloud</u>
  - Contacts are Ivar Janmaat and Martin Brandt
  - Will get access to a sub-subscription once Martin is back from vacation
  - Monthly coordination meeting every 3rd Friday at 3pm CEST (starting Sept'21)

# Progress update: filesystem layer



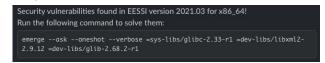
- Support for "direct I/O files" was implemented by CernVM-FS developers
  - See <a href="https://github.com/cvmfs/cvmfs/pull/2746">https://github.com/cvmfs/cvmfs/pull/2746</a> (not in latest CernVM-FS release yet)
  - Files can be marked to *not* be included in client kernel cache
  - Allows for in-place updates of stuff like glibc in compat layer with trouble client-side
  - Only when clients opt-in to accessing specific files via direct I/O?
  - o cvmfs server publish -dto mark files in transaction with direct I/O bit

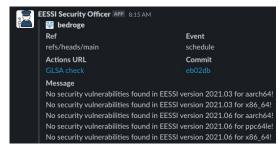
No changes/updates to EESSI filesystem layer in last couple of weeks (summer vacation)

# Progress update: compatibility layer



- Security officer bot is regularly checking whether security updates are needed
  - Semi-daily check, reports via private channel in Slack
  - Mentions command to run to update packages
  - Still requires significant amount of credits in GitHub Actions...
  - Security updates installed in 2021.03 compat layer on July 13th (glibc, glib, libxml2)





- Should ReFrame tests for compat layer be run daily via a cron in GitHub Actions?
  - o Currently only run when changes are merged in compatibility-layer GitHub repo...
  - o cfr. <a href="https://github.com/EESSI/compatibility-layer/pull/120">https://github.com/EESSI/compatibility-layer/pull/120</a>



# Progress update: software layer



- Some progress on getting software layer in 2021.06 in place, but got stuck on Java...
  - Java is installed as a binary package
  - Picks up libc.so from host OS, should be from compat layer!
  - glibc version in compat layer is now recent enough for that to cause trouble...
  - See <a href="https://github.com/EESSI/software-layer/issues/123">https://github.com/EESSI/software-layer/issues/123</a>
  - Requires use of patchelf to fix RPATH in Java installation, like ComputeCanada does
  - Or use Java from compat layer instead? (probably not a good idea)
- Init script doesn't correctly fall back to x86\_64/generic when it should (issue #124)
- Improved ReFrame tests for GROMACS (<u>PR #115</u>) and TensorFlow/Horovod (<u>PR #122</u>)

# **EESSI** pilot repository

# NOT FOR PRODUCTION USE!



#### https://eessi.github.io/docs/pilot

#### 2021.06 version of pilot software stack

#### Current status:

Compatibility layer in place for x86\_64 + aarch64 + ppc64le

#### To do:

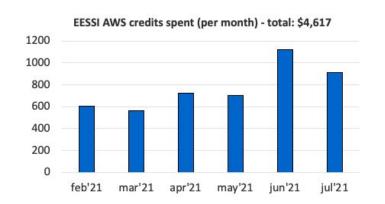
- Install software (work-in-progress)
  - Target CPUs:
    - {aarch64,x86\_64,ppc64le}/generic
    - intel/{haswell,skylake\_avx512}, amd/zen2, aarch64/graviton2, ppc64le/power9le
  - Bioconductor (R), GROMACS, OpenFOAM, TensorFlow, Spark, IPython, Horovod, QuantumESPRESSO, ...
- Provide init scripts
- GPU installations: on hold (cfr. discussion with NVIDIA on CUDA, meeting to be planned)

# Usage of sponsored AWS credits

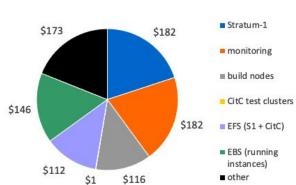
EESSI

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GERTFUR ROTTAME HERDELALANDES

- Sponsored credits (\$25,000) are being put to good use!
- Ask in #aws-resources Slack channel to get access!
- In July '21: ~\$910 worth of credits spent
- on Stratum-1, monitoring node, build nodes, ...
- ~\$4,617 worth of credits spent in total









# Azure sponsorship



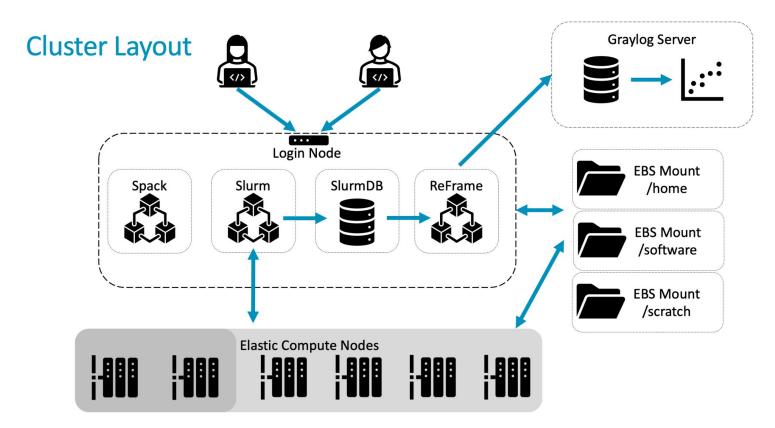


- Access to provides Azure credits needs to be set up with SURF
  - Will be looked into after summer vacation breaks...
- Monthly follow-up meetings planned with Azure + SURF
  - every 3rd Friday at 3pm CEST (starting Sept'21)

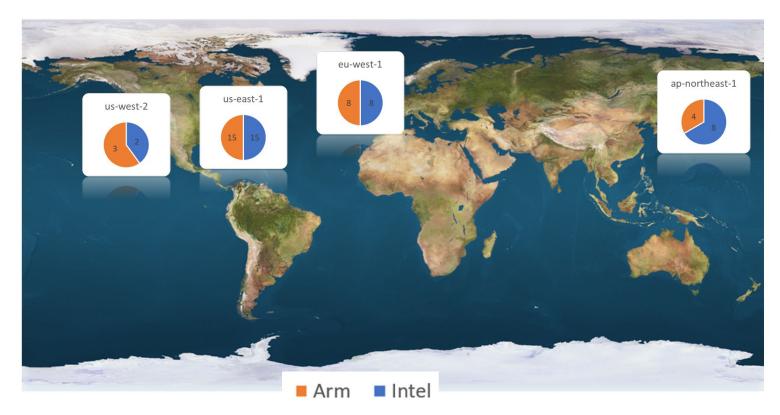
### AWS / Arm hackathon

- Collaboration between ARM HPC Usergroup (AHUG) and AWS
- Supported by the open-source groups from: \$THE\_OTHER\_TOOL (Spack) and ReFrame
- Hackathon started on Monday morning and went until Friday Afternoon
  - 17h time-zone difference (Australia to US westcoast)
  - > 30 teams, > 50 mentors (Spack, ReFrame, AWS, ARM, NVIDIA)
  - Three toolchains (gcc, nvhpc, arm)
- Self-paced workshop: <a href="https://cloud-hpc-hackathon.workshop.aws">https://cloud-hpc-hackathon.workshop.aws</a>

# AWS / Arm hackathon - Cluster Layout

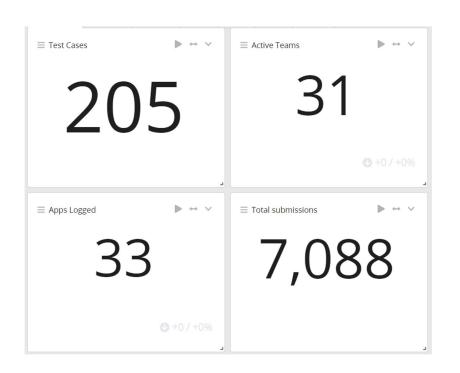


### AWS / Arm hackathon - Cluster Distribution

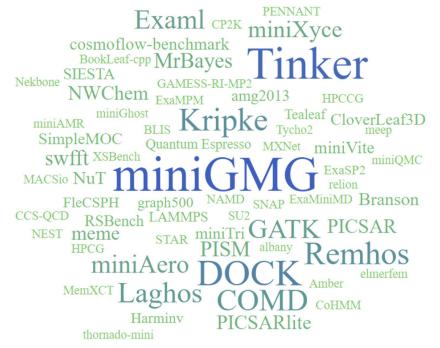


### AWS / Arm hackathon - Stats Overview

#### **Graylog Overview**



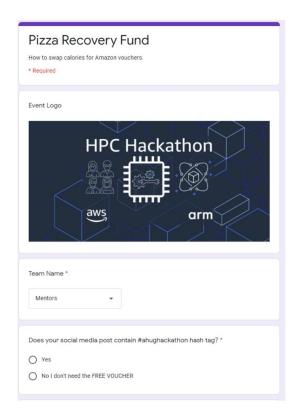
#### App Impact



### AWS / Arm hackathon - Pizza!

Virtual Pizza Eating: #pizzawednesday





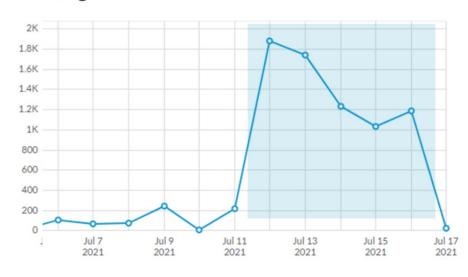
### AWS / Arm hackathon - Slack stats

#### **Active Users:**



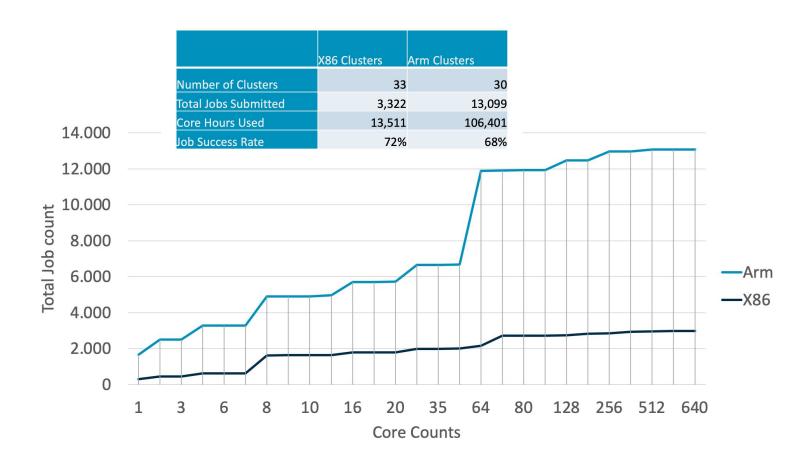
Total Members: 183

#### Messages Sent:



Total Messages: ~8k

### AWS / Arm hackathon - SLURM Stats



# AWS / Arm hackathon - App Porting per Compiler

|              | C5n (X86) |       | C6gn (Arm) |     | m)    |
|--------------|-----------|-------|------------|-----|-------|
|              | GCC       | NVHPC | ACFL       | GCC | NVHPC |
| CloverLeaf   | Х         | Χ     | Χ          | Χ   | X     |
| CloverLeaf3D | Х         | Χ     | Χ          | Х   | X     |
| CoMD         | Х         | Χ     | Χ          | Χ   | X     |
| ExaML        | Х         |       | Χ          | Х   |       |
| FlecSPH      | Х         | Χ     |            | Х   | X     |
| GATK         | Х         |       | Χ          | Х   |       |
| Kripke       | Х         |       | Χ          | Χ   | X     |
| MiniGMG      | Х         |       | Χ          | X   |       |
| MiniXyce     | Х         |       | Χ          | Х   | X     |
| MrBayes      | Х         |       | Χ          | X   |       |
| NWChem       | Х         |       | Χ          | Х   |       |
| PICSAR       | Х         |       | Χ          | Х   | X     |
| PICSARlite   | Х         |       | Χ          | Х   | X     |
| RSbench      | Х         | X     |            |     |       |
| Remhos       | Х         | Χ     | Χ          | Χ   | Χ     |
| SIESTA       | Χ         |       |            | X   |       |

|                     | C5n | (X86) | C6gn (Arm) |     |       |  |
|---------------------|-----|-------|------------|-----|-------|--|
|                     | GCC | NVHPC | ACFL       | GCC | NVHPC |  |
| SWFFT               | X   |       | Χ          | Χ   | X     |  |
| SimpleMOC           |     |       | X          | X   | X     |  |
| amg2013             |     |       | X          | X   | X     |  |
| branson             |     |       | X          | X   | X     |  |
| cosmoflow           | Х   |       |            | Χ   |       |  |
| cosmoflow-benchmark | Х   |       |            |     |       |  |
| dock                | Х   | Х     | Χ          | Χ   | Χ     |  |
| laghos              |     |       | X          | X   | X     |  |
| meme                | Х   | X     | X          | X   | X     |  |
| miniAero            |     |       | X          | X   |       |  |
| miniTri             |     |       | Χ          | Χ   | Χ     |  |
| miniVite            | X   | Х     | X          | X   | X     |  |
| nut                 |     |       | Χ          | Χ   | Χ     |  |
| pism                |     |       | X          | X   |       |  |
| tinker              |     |       | X          | X   | X     |  |

# AWS / Arm hackathon - Example App

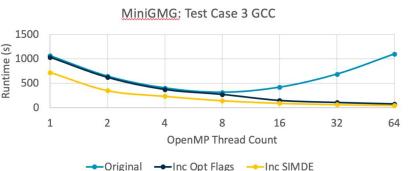
### MiniGMG (Wolfpack)

Geometric MultiGrid Mini-App

- Benchmarked:
  - 4 Test cases
  - C6gn: ACFL + GCC
  - C5n: GCC
- Identified huge OpenMP overhead
- Optimisations:
  - Compiler flags
    - '-O3' => '-Ofast'
  - Application flags
    - '-D\_\_PREFETCH\_NEXT\_PLANE\_FROM\_DRAM'
    - '-D\_\_FUSION\_RESIDUAL\_RESTRICTION'
  - Replaced Intel vector intrinsics with SIMDE
- Spack PR with changes
  - https://github.com/spack/spack/pull/24926







### AWS / Arm hackathon - Tentative Conclusion

- Event went well hiding AWS setup from participants
  - ssh into ParallelCluster
  - Some confusion about the time to scale up a node
  - We had to redo the setup the night before still worked
- End-To-End scope smaller scope might be easier next time
  - Teams build app, created ReFrame testcase, tinkered with optimization
- Next time (Christian's thoughts):
  - Focus on either building or testing
  - in-person/virtual hybrid?

### AWS / Arm hackathon - More info

- Announcement blog post: <a href="https://aws.amazon.com/blogs/hpc/aws-arm-hpc-hackathon-2021">https://aws.amazon.com/blogs/hpc/aws-arm-hpc-hackathon-2021</a>
- Introductory video: <a href="https://www.youtube.com/watch?v=NrsZvFsdxuq">https://www.youtube.com/watch?v=NrsZvFsdxuq</a>
- Application Scaling talk by Jeff Hammond:
   <a href="https://www.youtube.com/watch?v=Hfrc\_Pqm0oY">https://www.youtube.com/watch?v=Hfrc\_Pqm0oY</a>
- GitHub repo: <a href="https://github.com/arm-hpc-user-group/Cloud-HPC-Hackathon-2021">https://github.com/arm-hpc-user-group/Cloud-HPC-Hackathon-2021</a>
  - ReFrame tests in <u>Applications</u> subdirectory
- Self-paced workshop: <a href="https://cloud-hpc-hackathon.workshop.aws">https://cloud-hpc-hackathon.workshop.aws</a>

### Coming soon...



- Acceptance notification of submission of paper on EESSI
  - Special issue "New Trends in HPC: Software Systems and Applications" in

"Software: Practice and Experience" journal

- Original dates:
  - Notification: July 31, 2021 (but no news yet so far...)
  - Revision due: Aug 20, 2021
  - Notification of final acceptance: Sept 20, 2021
  - Final revised paper due: October 15, 2021
- Feedback on S4 project NeIC proposal
  - "Scientific Software Stacks as a Service (S4)", ~100PMs over 2 years
  - o Partners: Uolceland, UoEstonia, Sigma2 (NO), SNIC/Umeå (SE), CERN, CSCS, UGent, RUG
  - o 11 project applications were sent, <a href="https://neic.no/news/2021/03/18/open-call-applications">https://neic.no/news/2021/03/18/open-call-applications</a>
  - Acceptance notification expected in Sept'21