E4S

Trilinos Users Group Meeting 2022, Wednesday, Oct. 26, 2022, 10:30am MDT/9:30am PDT

https://trilinos.github.io/trilinos_user-developer_group_meeting_2022.html

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https://e4s.io/talks/E4S_TUG22.pdf

E4S: Extreme-scale Scientific Software Stack

- E4S is a community effort to provide open-source software packages for developing, deploying and running scientific applications on HPC platforms.
- E4S has built a comprehensive, coherent software stack that enables application developers to productively develop highly parallel applications that effectively target diverse exascale architectures.
- E4S provides a curated, Spack based software distribution of 100+ HPC and AI/ML packages (e.g., TensorFlow, PyTorch).
- With E4S Spack binary build caches, E4S supports both bare-metal and containerized deployment for GPU based platforms.
  - X86_64, ppc64le (IBM Power 9), aarch64 (ARM64) with support for GPUs from NVIDIA, AMD, and Intel
  - HPC and AI/ML packages are optimized for GPUs and CPUs.
- Container images on DockerHub and E4S website of pre-built binaries of ECP ST products.
- Base images and full featured containers (with GPU support).
- Commercial support for E4S through ParaTools, Inc. for installation, maintaining an issue tracker, and ECP AD engagement.
  - https://dashboard.e4s.io https://e4s.io/talks/E4S_Support_Sep22.pdf
- E4S for commercial cloud platforms: AWS image supports multiple MPI implementations and containers with remote desktop (DCV).
  - Intel MPI, NVHPC, MVAPICH2, MPICH, OpenMPI
- e4s-cl container launch tool allows binary distribution of applications by substituting MPI in the containerized app with the system MPI.
- Quarterly releases: E4S 22.08 released on August 31, 2022: https://e4s.io/E4S_22.08.pdf

E4S: Extreme-scale Scientific Software Stack

- Curated, Spack based software distribution
- Spack binary build caches for bare-metal installs with 90,000+ binaries
- Container images on DockerHub and E4S website of pre-built binaries of ECP ST products
- Base images and full featured containers (with GPU support)
- GitHub recipes for creating custom images from base images
- GitLab integration for building E4S images
- E4S validation test suite on GitHub
- e4s-cl container launcher tool for MPI substitution in applications
- E4S VirtualBox image with support for container runtimes
  - Docker
  - Singularity
  - Shifter
  - Charliecloud
- AWS and GCP images to deploy E4S

https://e4s.io

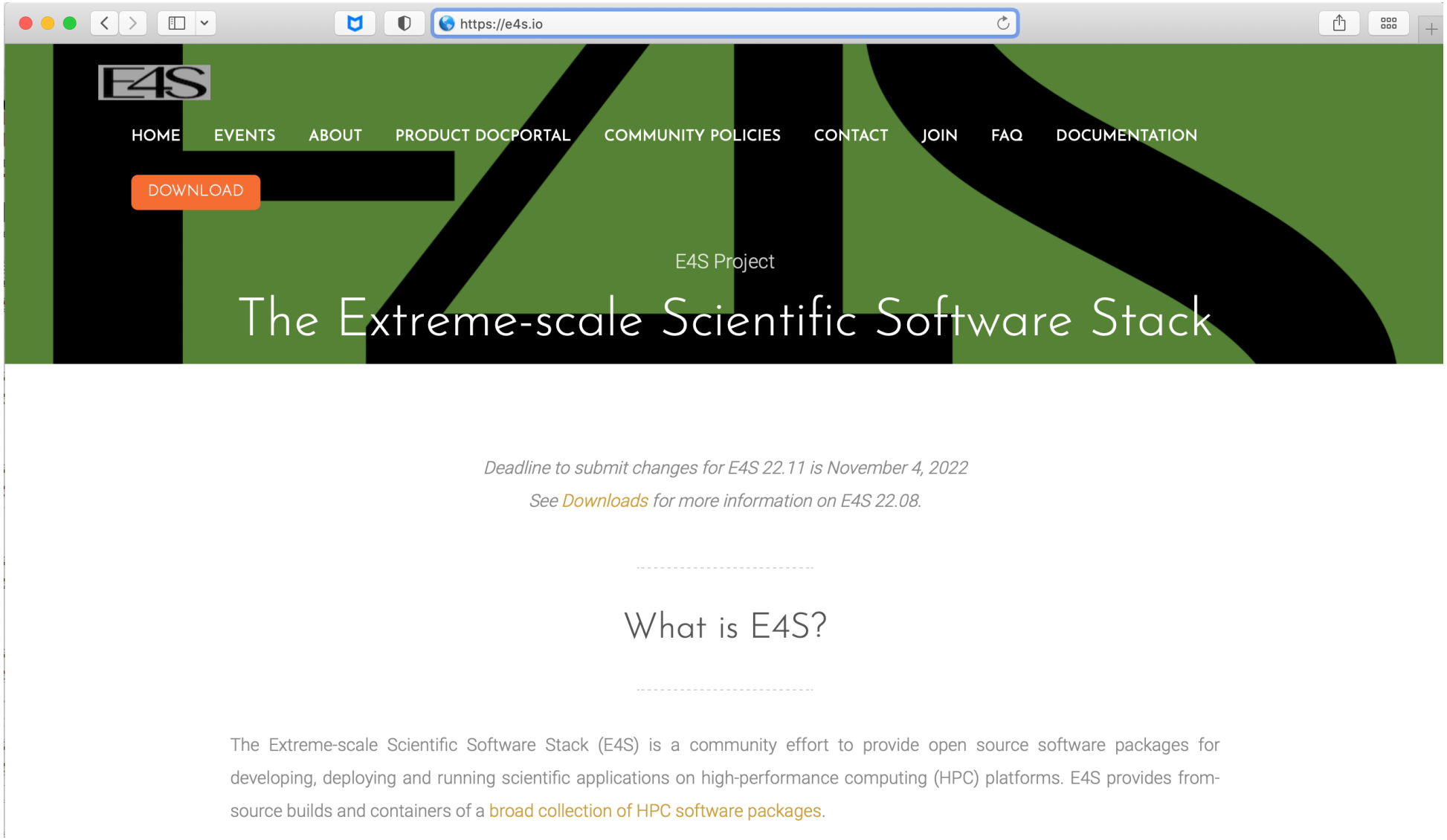
Extreme-scale Scientific Software Stack (E4S)

- E4S: HPC Software Ecosystem – a curated software portfolio
- A **Spack-based** distribution of software tested for interoperability and portability to multiple architectures with support for GPUs from NVIDIA, AMD, and Intel in a single distribution
- Available from **source**, **containers**, **cloud, binary caches**
- Leverages and enhances SDK interoperability thrust
- Not a commercial product – an open resource for all
- Oct 2018: E4S 0.1 - 24 full, 24 partial release products
- Jan 2019: E4S 0.2 - 37 full, 10 partial release products
- Nov 2019: E4S 1.0 - 50 full, 5 partial release products
- Feb 2020: E4S 1.1 - 61 full release products
- Nov 2020: E4S 1.2 (aka, 20.10) - 67 full release products
- Feb 2021: E4S 21.02 - 67 full release, 4 partial release
- May 2021: E4S 21.05 - 76 full release products
- Aug 2021: E4S 21.08 - 88 full release products
- Nov 2021: E4S 21.11 - 91 full release products
- Feb 2022: E4S 22.02 – 100 full release products
- May 2022: E4S 22.05 – 101 full release products
- August 2022: E4S 22.08 – 102 full release products

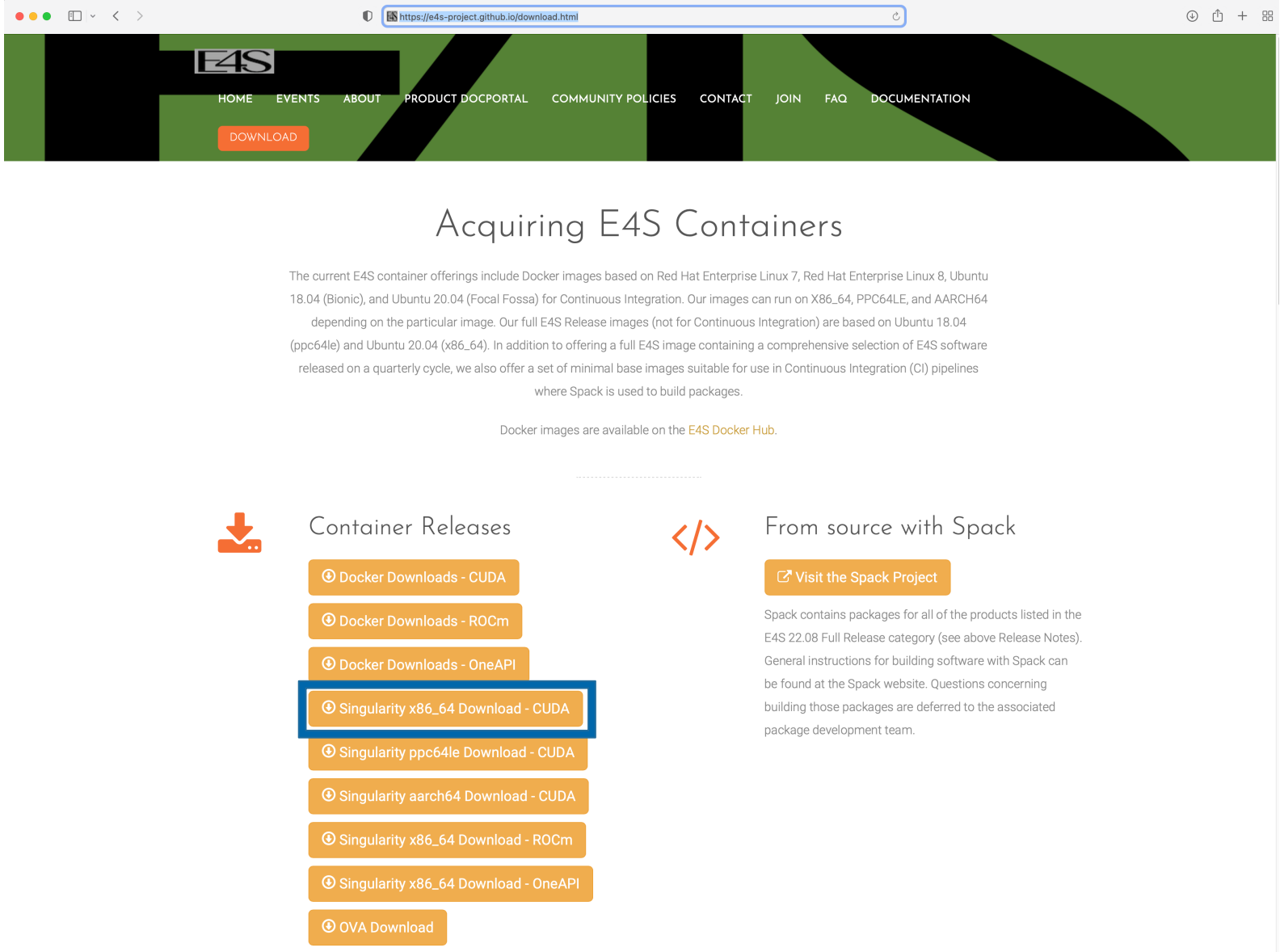
https://e4s.io

Also include other products .e.g.,
AI: PyTorch, TensorFlow (CUDA, ROCm)
Co-Design: AMReX, Cabana, MFEM

E4S Download from https://e4s.io



Download E4S 22.08 GPU Container Images: NVIDIA, AMD, Intel



- Separate full featured Singularity images for 3 GPU architectures
- GPU full featured images for
  - x86_64 (Intel, AMD, NVIDIA)
  - ppc64le (NVIDIA)
  - aarch64 (NVIDIA) NEW!
- Full featured images available on Dockerhub
- 100+ products on 3 architectures

https://e4s.io

Download E4S 22.05 GPU Container Images: NVIDIA, AMD, Intel

Note on Container Images

Container images contain binary versions of the Full Release packages listed above. Full-featured GPU-enabled container images are available from Dockerhub:

```
# docker pull ecpe4s/e4s-cuda:22.08
```

```
# docker pull ecpe4s/e4s-rocm:22.08
```

```
# docker pull ecpe4s/e4s-oneapi:22.08
```

E4S Full GPU Images

These images contain a full Spack-based deployment of E4S, including GPU-enabled packages for NVIDIA, AMD, or Intel GPUs.

These images also contain TensorFlow, PyTorch, and TAU.

AMD ROCm (x86_64)

ecpe4s/e4s-rocm:22.08 docker

e4s-rocm-22.08.sif mirror 1

NVIDIA CUDA (x86_64, ppc64le, aarch64)

ecpe4s/e4s-cuda:22.08 docker

e4s-cuda-x86_64-22.08.sif mirror 1

e4s-cuda-ppc64le-22.08.sif mirror 1

e4s-cuda-aarch64-22.08.sif mirror 1

Intel OneAPI (x86_64)

ecpe4s/e4s-oneapi:22.08 docker

e4s-oneapi-22.08.sif mirror 1

https://e4s.io

E4S 22.08 Full Featured and Base Images

E4S Full GPU Images

These images contain a full Spack-based deployment of E4S, including GPU-enabled packages for NVIDIA, AMD, or Intel GPUs.

These images also contain TensorFlow, PyTorch, and TAU.

AMD ROCm (x86_64)

ecpe4s/e4s-rocm:22.08 docker

e4s-rocm-22.08.sif mirror 1

NVIDIA CUDA (x86_64, ppc64le, aarch64)

ecpe4s/e4s-cuda:22.08 docker

e4s-cuda-x86_64-22.08.sif mirror 1

e4s-cuda-ppc64le-22.08.sif mirror 1

e4s-cuda-aarch64-22.08.sif mirror 1

Intel OneAPI (x86_64)

ecpe4s/e4s-oneapi:22.08 docker

e4s-oneapi-22.08.sif mirror 1

GPU Base Images

These images come with MPICH, CMake, and the relevant GPU SDK -- either AMD ROCm, NVIDIA CUDA Toolkit and NVHPC, or Intel OneAPI.

NVIDIA Multi-Arch (X86_64, PPC64LE, AARCH64)

ecpe4s/e4s-base-cuda:22.08 docker

e4s-base-cuda-x86_64-22.08.sif mirror 1

e4s-base-cuda-aarch64-22.08.sif mirror 1

e4s-base-cuda-ppc64le-22.08.sif mirror 1

ROCM X86_64

ecpe4s/e4s-base-rocm:22.08 docker

e4s-base-rocm-22.08.sif mirror 1

Intel OneAPI X86_64

ecpe4s/e4s-base-oneapi:22.08 docker

e4s-base-oneapi-22.08.sif mirror 1

22.08 Release: 102 Official Products + dependencies (gcc, cuda, x86_64)

```
 1: adios2              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/adios2-2.8.3-ifkuulgk4fcrwgcizlflfquna2x5ofay
 2: alquimia            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/alquimia-1.0.9-2lrac7o4ffv4rqt4h2vgzjud3tkjwkrd
 3: aml                 /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/aml-0.2.0-pwiapieu4qrmlv64dvz6ztnlryomtxov
 4: amrex               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/amrex-22.08-2k6mn7x6c6bn37e4qqhcjjpof5l663ec
 5: arborx              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/arborx-1.2-hpqevuvvjoqfpgt3334czuut4secym7u
 6: archer              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/archer-2.0.0-ubhbdonoquovu6i6yh6byf5vkjqdst2s
 7: argobots            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/argobots-main-62s4jy7ijfzur2pw2rzadwo5ixgnizjl
 8: ascent              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/ascent-0.8.0-k6pkjgeaxjbtjnqv4qalvfi76a3tecyn
 9: axom                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/axom-0.6.1-adc6pqaau33eh47lt62cd7gx6qv3qebj
10: bolt                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/bolt-2.0-t3nxvx37r4r4b4v6o4tmjplwxosamm65
11: bricks              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/bricks-r0.1-75cmpltjkrkwrjklzkss7khajjf72lco
12: butterflypack       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/butterflypack-2.1.1-q5eimvsxo5jzoyxlaq7mrkoe7l5o3y2n
13: cabana              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/cabana-0.5.0-uzm7qvptohoxhz3fpxqbob2sq4a5bbli
14: caliper             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/caliper-2.8.0-v4tnqpfc5dcnxslg4ltuqkhxcr6aydfa
15: chai                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/chai-2022.03.0-v4q3jdzv5zvmq4x2gswjxscqonewm43j
16: conduit             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/conduit-0.8.3-zphidjxhjkiwukbg4sdftgsrjbfov5y3
17: darshan-runtime     /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/darshan-runtime-3.4.0-caydqukivwqaecivrajoj5nusrqzgl7t
18: datatransferkit     /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/datatransferkit-3.1-rc3-blednv72j7co7xf7j3wspaswy6jtxbwy
19: dyninst             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/dyninst-12.2.0-3dwen3nn22mkqjsivikdd43rrl4vehvz
20: faodel              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/faodel-1.2108.1-kqkwty5hn4cvjrgbvutzgk3p45tb5sdc
21: flecsi              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/flecsi-2.1.0-jdt5s7vqugxnqcco3hiqyqdtc6p3jlp3
22: flit                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/flit-2.1.0-hh43s4mmqrw3p7zj2hlkylklgr3tggf5
23: flux-sched          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/flux-sched-0.23.0-qod4dtvrvmat3npnpwysrpebxjexsxhr
24: fortrilinos         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/fortrilinos-2.0.0-6lceq2wyliv7xqkif2es47bpgm3ztvxj
25: gasnet              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/gasnet-2022.3.0-mjam365qep6iiqr36s454x4psmgrkwp6
26: geopm               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/geopm-1.1.0-vzi6bqaktmcahuvu66oozto2wtoe27la
27: ginkgo              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/ginkgo-1.4.0-7iqzf3oxknmk2iv3i74eu4d44otnqh37
28: globalarrays        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/globalarrays-5.8-2qdtkpndvwvqylybsfxps2px3ansltxn
29: gotcha              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/gotcha-1.0.3-a2gy4enms44svpeek5vzlvnalx3pr6ia
30: gptune              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/gptune-3.0.0-db3njgcxugdun5d452wiw7goxw4hhykx
31: h5bench             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/h5bench-1.2-hul73s3xtl2srumekg7cuo2bb533fmot
32: hdf5                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/hdf5-1.13.2-doki3exhfk6ofx2gum2nv6fdjs3lab4s
33: hdf5-vol-async       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/hdf5-vol-async-1.2-34dt32yinsj52cwxykv6jzcpbnejdptf
34: heffte              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/heffte-2.2.0-goupv4n2hgxdtezc3g6r7isf4h5jvsm3
35: hpctoolkit          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/hpctoolkit-2022.05.15-xjug5nhvocxzdrbooncuk3te6t3rw7wa
36: hpx                 /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/hpx-1.8.1-lrb5wsjktqgsswclupnaayb2ohq3ptkw
37: hypre               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/hypre-2.25.0-4nmvphj2dtfh7uisr44f7oftptmenl3l
38: kokkos              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/kokkos-3.6.01-7vuflt6v5ahimf6e3noa6o67kx5ut3ns
39: kokkos-kernels      /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/kokkos-kernels-3.6.00-uihsqkd6swloqua3hdkxe6kr5oaolkxz
40: lammps              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/lammps-20220623-5cqu3suoycin5fgoz4cvc3qzq7elqqif
41: legion              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/legion-21.03.0-y36c4daichtlrjq3zlarfzdcenlndktb
42: libnrm              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/libnrm-0.1.0-tj463dbbvyerlzhtesccp525byjmug5n
43: libquo              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/libquo-1.3.1-zihxwoeobknjaj3bmaybfaoqn3jwfvso
44: loki                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/loki-0.1.7-rgel6sujgugxzqvtddd2jibhuw7dmhai
45: magma               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/magma-2.6.2-zw7i6ultwjuxsyztuyijjx72fle7ytil
46: mercury             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mercury-2.1.0-ubcppuuys2e6mbwe26kg5rerwuzfrqno
47: metall              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/metall-0.21-vi6z32g7zotumjtcgonykfhje35z4lmr
48: mfem                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mfem-4.4.0-bcbkjggyj26nvx7ojhxyats3mbm57ycl
49: mpark-variant       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mpark-variant-1.4.0-fokhy42s3yd7uh75qo43ifjnzchsbr3g
50: mpich               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mpich-4.0.2-yurg3uwktdw4kw76r5djfsnjdzdmp6cm
51: mpifileutils        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mpifileutils-0.11.1-6dj2vqlpw5qydyq7v52ubu55op3ajpq7
```

- NVHPC 22.7 with CUDA 11.7
- Support for A100 and V100 GPUs
- TensorFlow v2.9.1 and
- PyTorch v1.12.1 optimized for GPUs

22.08 Release: 102 Official Products + dependencies (gcc, cuda, x86_64) (contd.)

```
 52: netlib-scalapack  /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/netlib-scalapack-2.2.0-25vd6rfq4ufuesofo57jysj5x53nxu74
 53: nccmp             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/nccmp-1.9.0.1-ftszrnqzc2cygoqrtioee6h3fjx6w6yv
 54: nco               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/nco-5.0.1-rlffrqp2xzm4uvdwqqodtn3exrr2dlnd
 55: nrm               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/nrm-0.1.0-uwg666h4ka32lj2bxmc4nj36liyil3zq
 56: omega-h           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/omega-h-9.34.1-27heb5almci24q7zg7mfn2mdqq6562va
 57: openmpi           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/openmpi-4.1.4-7co3hc3hfgfszjffum3fu7c3q23ozqy4
 58: openpmd-api       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/openpmd-api-0.14.5-pj2hi5r2m5wubpacflddd3tivqjwunbi
 59: papi              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/papi-6.0.0.1-yjnzh45s2nzeeb553xpx5qxinm73jdgz
 60: papyrus           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/papyrus-1.0.2-ae7pqcjs72utsbtgq6x3q4e5tqzpgocb
 61: parallel-netcdf   /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/parallel-netcdf-1.12.2-v7h7r3hqjw6vakzqj6uarb465ss4oj6v
 62: paraview          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/paraview-5.10.1-lf7udp3dnwkptjh5mxr4xotc4wuf2jfm
 63: parsec            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/parsec-3.0.2012-7hbcudupjmlfcgihhtfp7pe2moszdvcl
 64: pdt               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/pdt-3.25.1-22x4lgxduh2ejs477htndgxuiha5uo2s
 65: petsc             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/petsc-3.17.4-ywonj5xmzv4nsjahsg5oww6f246t7r62
 66: phist             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/phist-1.9.5-ey2e2xjqrkogucncqlcaiay5pi5yqnpo
 67: plasma            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/plasma-21.8.29-q4m6euppnulfmxi5aufltyd3kgdhvtts
 68: plumed            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/plumed-2.8.0-z265gsvzvb43xn42lajf6d3fa6k6jpn2
 69: precice           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/precice-2.5.0-mojal5qfjqzzseifja5xdulyeukdzjml
 70: pruners-ninja     /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/pruners-ninja-1.0.1-okgyfnztj2rfcyitth4n4oexghk445hr
 71: pumi              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/pumi-2.2.7-whec6o6kj7qpo53s2yyqch5xda5akdgp
 72: py-cinemasci      /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/py-cinemasci-1.7.0-n3pshnjlwj5mdpp4m3w5xc42h3cufci3
 73: py-jupyterhub     /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/py-jupyterhub-1.4.1-odbpt2k2xolyk4qnfeti6pyjlrxm7n2a
 74: py-libensemble    /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/py-libensemble-0.9.2-2zefvm7ymmap5i66nie5ocfq7a7ewz7v
 75: py-parsl          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/py-parsl-1.1.0-w6buwwgyvx7qk3d66an6nzhlh2d7fe3f
 76: py-radical-saga   /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/py-radical-saga-1.16.0-qkvjgejq5dwb7x2245wgah6h7yobzvto
 77: qthreads          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/qthreads-1.16-vujctsewvsjga2drshoekdnvl4l6cp6d
 78: raja              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/raja-2022.03.0-shzxmdu6mmyuwlxfwsa6k54njfu34r23
 79: rempi             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/rempi-1.1.0-3fg5re7uwjzb33j7dq2mathtmosmmisq
 80: scr               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/scr-3.0-7wiky6bzgzdc3tjt5ifb2mjqohp2yfs7
 81: slate             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/slate-2022.06.00-7cfrzgha7dslzh7b5z5ut5al5msxt3gr
 82: slepc             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/slepc-3.17.2-5r2ldqn5hlnnwqv32yp7esc7whvkx32r
 83: stc               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/stc-0.9.0-qhahav5nnvg5l2nrp4duimrhao6baxem
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 88: sz                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/sz-2.1.12.2-akue3hil6zq2zzenppezg45bbqt3i5yn
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 90: tau               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/tau-2.31.1-eaz3ll4c7te7unzirnnprsaoaweooqjc
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 92: turbine           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/turbine-1.3.0-rjsro3aodby6kmnjjrttzzztm6rqz2kp
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 94: umpire            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/umpire-2022.03.1-jd62ya4tnh57jsg6mnya646hxcsfhadm
 95: unifyfs           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/unifyfs-0.9.2-pacjxtgkc7jmvfkolj4iyo77n2xxxgh6
 96: upcxx             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/upcxx-2022.3.0-rafoonfubm2nlnwdwftgq4zmr2vcbg36
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```

- Trilinos v13.4.0
- NVHPC 22.7 with CUDA 11.7
- Support for A100 and V100 GPUs
- TensorFlow v2.9.1 and
- PyTorch v1.12.1 optimized for GPUs

- Also, support for ROCm 5.2.0 optimized for MI250X and MI100
- Intel oneAPI 2022.1.0

22.08 Release: 102 Official Products + dependencies (gcc, cuda, ppc64le)

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  7: argobots              /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/argobots-main-ilx5nitwe7gaacifewubp2dvxc2uskuq
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 10: bolt                  /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/bolt-2.0-bl5ig6en3zunbu5tfnvxqw62jknumnas
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 18: dyninst               /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/dyninst-12.2.0-kwpzzbzicwsphaf7ocdpgt6baguqdpf3
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 27: globalarrays          /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/globalarrays-5.8-wettvecurrakqb5ffsjlcbzig47kkqtv
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 39: lammps                /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/lammps-20220623-id74dp3jg7thpobmyrtxqfu6zhbtofh7
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```

- NVHPC 22.7 with CUDA 11.7
- Support for NVIDIA GPUs
- TensorFlow v2.5.1 and
- PyTorch v1.9.0a0

22.08 Release: 102 Official Products + dependencies (gcc, cuda, ppc64le) (contd.)

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 94: umpire             /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/umpire-2022.03.1-6uumqt5rw72uqrg5lybqtbgezjhjzz6a
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 96: upcxx              /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/upcxx-2022.3.0-xpvexkttgp576asxt2cgenlwaczxryy2
 97: veloc              /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/veloc-1.5-cnqwbrkslgu5lfrdon73qqde2znaep7n
 98: vtk-m              /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/vtk-m-1.8.0-msm4mqdhfqgywx45juamwyi6j5nybqxh
 99: wannier90          /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/wannier90-3.1.0-3wohurtflidtoz2yv4uepvrivr6iiy2k
100: warpx              /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/warpx-22.08-asny47ruhqvuyjfemc276zo36n3lbhhu
101: yaksa              /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/yaksa-0.2-6rybbzhpmv4clemvrcncyqjndnhwf436
102: zfp                /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/zfp-0.5.5-mk5enpglkfouqzvc6vhy74fnooyzv5yi
```

- Trilinos v13.4.0 for ppc64le
- NVHPC 22.7 with CUDA 11.7
- Support for NVIDIA GPUs
- TensorFlow v2.5.1 and
- PyTorch v1.9.0a0

22.08 Release: 101 Official Products + dependencies (gcc, cuda, aarch64) NEW!

1:	adios2	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/adios2-2.8.3-rgr2vbgswebchs6ymdould42fwjxiwe7
2:	alquimia	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/alquimia-1.0.9-teodmopfaqz7viav2ctczfjipeeoqtwv
3:	aml	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/aml-0.2.0-tim3isvremvkujg7y6ckvtsuwwhxhmao
4:	amrex	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/amrex-22.08-ealqug3ntw5f3nozkqpzcoabc5oztwri
5:	arborx	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/arborx-1.2-ae4n4db4ckqozmkicvwandpd2x5xlbfd
6:	archer	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/archer-2.0.0-4scivwwlzlr7nu63lpln443twh746xmg
7:	argobots	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/argobots-main-bmuh5lsksx7l6xu7bsm5ayofvw6mlo4k
8:	ascent	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/ascent-0.8.0-fcvvqoquxxw7ri4fvblgyuiaqsiafm7g
9:	axom	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/axom-0.6.1-uu7v4ibgwt3eteszxc2krn5uypjl5nvh
10:	bolt	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/bolt-2.0-pgzaq5aullwxnjchzyums74qyut37jtk
11:	butterflypack	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/butterflypack-2.1.1-rejgtjnhcctlbov7brawhxev7cilubtv
12:	cabana	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/cabana-0.5.0-edh3x7tosealn3sadyl4gr6piouv4t2r
13:	caliper	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/caliper-2.8.0-go7uhpm6qqy5i2brnbty3qgbeaqd2njf
14:	chai	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/chai-2022.03.0-hrlbfqdziweoefpukxwfe43azyato6mw
15:	conduit	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/conduit-0.8.3-gwiudnpzdrwvcumatfmnytjk44bjaqym
16:	darshan-runtime	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/darshan-runtime-3.4.0-rklgx5hbnq3vgylaw6s34fpwyq4iqrlc
17:	datatransferkit	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/datatransferkit-3.1-rc3-harz4dlj2z3lzr4hhkhc5zzqplkytwja
18:	dyninst	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/dyninst-12.2.0-jfrrwtqtsonluclyhbks4rqugtjenawk
19:	exaworks	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/exaworks-0.1.0-o7dcje73ldpwobqf5ohytnmxu257c7ld
20:	faodel	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/faodel-1.2108.1-i6rm7nvhaoet4hrc5y5aeczuxqqfpyff
21:	flecsi	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/flecsi-2.1.0-pm4xvjbvv2vpdfpbmsv2hfn2wtv2stqn
22:	flit	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/flit-2.1.0-wzxaiopjcpxurdhrlfkujkl2qit2w5em
23:	flux-sched	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/flux-sched-0.23.0-7qdi2ps6373qjamcn4ntdpu54pq6k5tp
24:	fortrilinos	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/fortrilinos-2.0.0-ti6atcwvdvwax7aml345tadljktq52vg
25:	gasnet	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/gasnet-2022.3.0-mbkku2iucn7jhg6kupah4flwiehaj3vj
26:	ginkgo	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/ginkgo-1.4.0-2o45765ui46nivg3i46io7lwohdyq2rj
27:	globalarrays	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/globalarrays-5.8-vmsjflq4ebhorerizfakwwqmwqvbx4cm
28:	gotcha	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/gotcha-1.0.3-jqzmqv4n5mt7pmugchp7s35dpnzbyrd4
29:	gptune	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/gptune-3.0.0-hhmgrhop7dlqrkt4m5yj2ceq7fyaa6dj
30:	h5bench	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/h5bench-1.2-xqv6sfmaa4ad5sirfymaxx2t62dgydd5
31:	hdf5	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/hdf5-1.13.2-ewffjmwghvsll6naya3k36yoyt3777qk
32:	hdf5-vol-async	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/hdf5-vol-async-1.2-zzbuohnrofqgelyvk4t7xytufpqh4b4h
33:	heffte	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/heffte-2.2.0-wmrpm672x3e6v5acq7hetopxsmezx26g
34:	hpctoolkit	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/hpctoolkit-2022.05.15-rzz2eknpgsvpnhlp3ize2xh7zz22dnuz
35:	hypre	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/hypre-2.25.0-s754pjqu24ohc3uwmcf37gu3blvcwtxd
36:	kokkos	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/kokkos-3.6.01-cvv2233fqh7pnzt3xd3gxrg6enihak6g
37:	kokkos-kernels	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/kokkos-kernels-3.6.00-znn2n5ppc7bo7xsncfnaz3eq56tp74nu
38:	lammps	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/lammps-20220623-r7quv3v5tusjyaeoprh6w4cklsuv5hfw
39:	legion	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/legion-21.03.0-xqvx3m7gdhd43ybpj75n63c7yjrqelwb
40:	libnrm	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/libnrm-0.1.0-f7s5tgfcurkdcgwuzu4zbn2znfct6t6t
41:	libquo	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/libquo-1.3.1-xm3d4gimqssduwhdecszuhtzsfzxgymo
42:	loki	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/loki-0.1.7-q5dtcfozzf4p7pycx4gtlqkvvglrworn
43:	magma	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/magma-2.6.2-4u3gt62dtczmlvv2c7nt5qpru6yzmmze
44:	mercury	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/mercury-2.1.0-fv5bxqdvqb3lv57s77xw3pmmjlk45gcq
45:	metall	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/metall-0.21-op6ltaipplev2llrmqet3e5frtyp73y7
46:	mfem	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/mfem-4.4.0-uvizvyebucxiqhbq4y7twveiqfydtzsi
47:	mpark-variant	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/mpark-variant-1.4.0-hhfriafnm45uljscabscmahuhfclvmql
48:	mpich	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/mpich-4.0.2-q3ba3kgzkdsuc2cl2eii665iltbk4pd4
49:	mpifileutils	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/mpifileutils-0.11.1-guvx7all5mej2j4oujhkxu7taauznrry
50:	netlib-scalapack	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/netlib-scalapack-2.2.0-ogqhecw42emxrrcrn57leamqxhlwiv22
51:	nccmp	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/nccmp-1.9.0.1-pxiqx2mvs4tb2l67ln46nnmhwqai7bg2

- NVHPC 22.7 with CUDA 11.7
- Support for NVIDIA GPUs
- PyTorch v1.12.1

22.08 Release: 101 Official Products + dependencies (gcc, cuda, aarch64) NEW!

```
 52: nco              /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/nco-5.0.1-gbbbpvjdasvadznrpqr2ibtt2hjrudrj
 53: nrm              /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/nrm-0.1.0-y2u765zdsxaoxbyyj5ii27exgpkhusu5
 54: omega-h          /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/omega-h-9.34.1-k67w4q7kmvuzr4x45wavdpwdwql25hcg
 55: openmpi          /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/openmpi-4.1.4-atoxcgheeantzvq7qalgzwbz3axezzi4
 56: openpmd-api      /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/openpmd-api-0.14.5-lng5ww566gno2cdlptitqxiec6xdclr2
 57: papi             /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/papi-6.0.0.1-srlrzt2prj2k47kzlgtg7555nelbxi7n
 58: papyrus          /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/papyrus-1.0.2-6yzifukoakiquambm32owcilw36yoekz
 59: parallel-netcdf  /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/parallel-netcdf-1.12.2-7vjruqq222uvddu2vca275dill3e2a3p
 60: paraview         /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/paraview-5.10.1-w2tl34cwojcu5urjayyxwkpmymflogth
 61: parsec           /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/parsec-3.0.2012-ebkp56dh3hqmi3fqtfldtgzd5e32op2e
 62: pdt              /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/pdt-3.25.1-abjcjdc5w2hdvhib27b3xguyfzeo3hhh
 63: petsc            /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/petsc-3.17.4-yepzel5qjzwm6kupg4ua5pqbx5l2rgmu
 64: plasma           /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/plasma-21.8.29-dxlxswgsrzxzcxgmj2w32bxg5gcptivy
 65: plumed           /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/plumed-2.8.0-37hrtcs6kr6dwt42iwe7tsg2ve4dlkly
 66: precice          /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/precice-2.5.0-f6igne52tjfjt5kafhr7w47i5juuo7j4
 67: pruners-ninja    /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/pruners-ninja-1.0.1-fp7k4jxfd74dgghwpqdmjtu2lvmiw2bt
 68: pumi             /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/pumi-2.2.7-osovfu2vcsvra4orfhk4sscov4okv2ue
 69: py-cinemasci     /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/py-cinemasci-1.7.0-mvzka5s67jkk343hwl3xyuh2zz7eq3jx
 70: py-jupyterhub    /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/py-jupyterhub-1.4.1-6dieq54hv4td7sgrcmti24bdjazl6xpc
 71: py-libensemble   /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/py-libensemble-0.9.2-ounmseonelaqueazjhfaaqlxxi6t6vbj
 72: py-opentuner     /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/py-opentuner-0.8.7-rsdlieu2al6g25lrlumqvj3dcb6cxphr
 73: py-parsl         /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/py-parsl-1.1.0-j2ramnsdu4zz5s7bchf7buhns6e5nwvn
 74: py-radical-pilot /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/py-radical-pilot-1.16.0-5l3efsvga3ot2bmdm26katk7z274tmxk
 75: py-radical-saga  /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/py-radical-saga-1.16.0-bsdgy53odz7xbpken65baalnff2npdg5
 76: qthreads         /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/qthreads-1.16-3nh4xmtaptpkqmzmjln5cshnkkkk4pzd
 77: raja             /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/raja-2022.03.0-6eskyhbk5jl7vor6pjqic656wfcj6xok
 78: rempi            /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/rempi-1.1.0-c2nci6esacmv2i3wv7zbafj24jqmkfa7
 79: scr              /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/scr-3.0-44nhq57qlgxrmgezeud4mbgo7qvuglmt
 80: slate            /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/slate-2022.06.00-k6jdbfottjj5ujw25d6fkix7hxadytyp
 81: slepc            /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/slepc-3.17.2-36xj5xq2ojbj5sjxbmxopmgk6vxuwrrs
 82: stc              /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/stc-0.9.0-jfdjo25gl6cyost5hi5mpg3qfubzn4wk
 83: strumpack        /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/strumpack-6.3.1-olxykkpasg23rbjor3dwi6tkdfmiuoww
 84: sundials         /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/sundials-6.2.0-4qldezzkrgss7pnozdzkcoxqhup5i4yd
 85: superlu-dist     /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/superlu-dist-7.2.0-53kdsn33u5jeh6hq2eimwrkef5amrgnj
 86: swig             /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/swig-4.0.2-fortran-fdu2szubut42nxivrzggo47ahwfji4j6
 87: sz               /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/sz-2.1.12.2-sovcw4kcmxxs2oz6sh2jeyimocik6gr4
 88: tasmanian        /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/tasmanian-7.7-jodfk74drvk6kunjwz5jzw7ifj6odnzg
 89: tau              /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/tau-2.31.1-ydbuxabngrbidmlxnj7e2enuztdwwjk2
 90: trilinos         /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/trilinos-13.4.0-eqvhpdov6elszekkzyovcobzw6hv6jzw
 91: turbine          /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/turbine-1.3.0-3vou37d6rrodyhmwivlu7gb33fywipbs
 92: umap             /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/umap-2.1.0-ikhuysi655ghcdyrtx4a65rtmcibntjz
 93: umpire           /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/umpire-2022.03.1-cuudeezgk33ysguxr4sc3ovn6lodqhnf
 94: unifyfs          /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/unifyfs-0.9.2-z3kx3p5l45rezwho2lqktfswztbsrlmw
 95: upcxx            /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/upcxx-2022.3.0-ozqrl36zdacykfwohpw2ubzbbfflnw7z
 96: veloc            /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/veloc-1.5-vunhtbm5se6sc4e4mrr66xn6d456f2cr
 97: vtk-m            /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/vtk-m-1.8.0-yrweg65332slls5onxv7jr4oppgqagh3
 98: wannier90        /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/wannier90-3.1.0-76cc4klulcfmdukwav3teatt3jrgsolm
 99: warpx            /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/warpx-22.08-luvfurdkag5cz2yg7btywfupbtrijqhz
100: yaksa            /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/yaksa-0.2-ouc72jlxh5sgfrigmtvvyd2llimnfhir
101: zfp              /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/zfp-0.5.5-ztprlcezlhtvnntskofecuze3hkqkax6
```

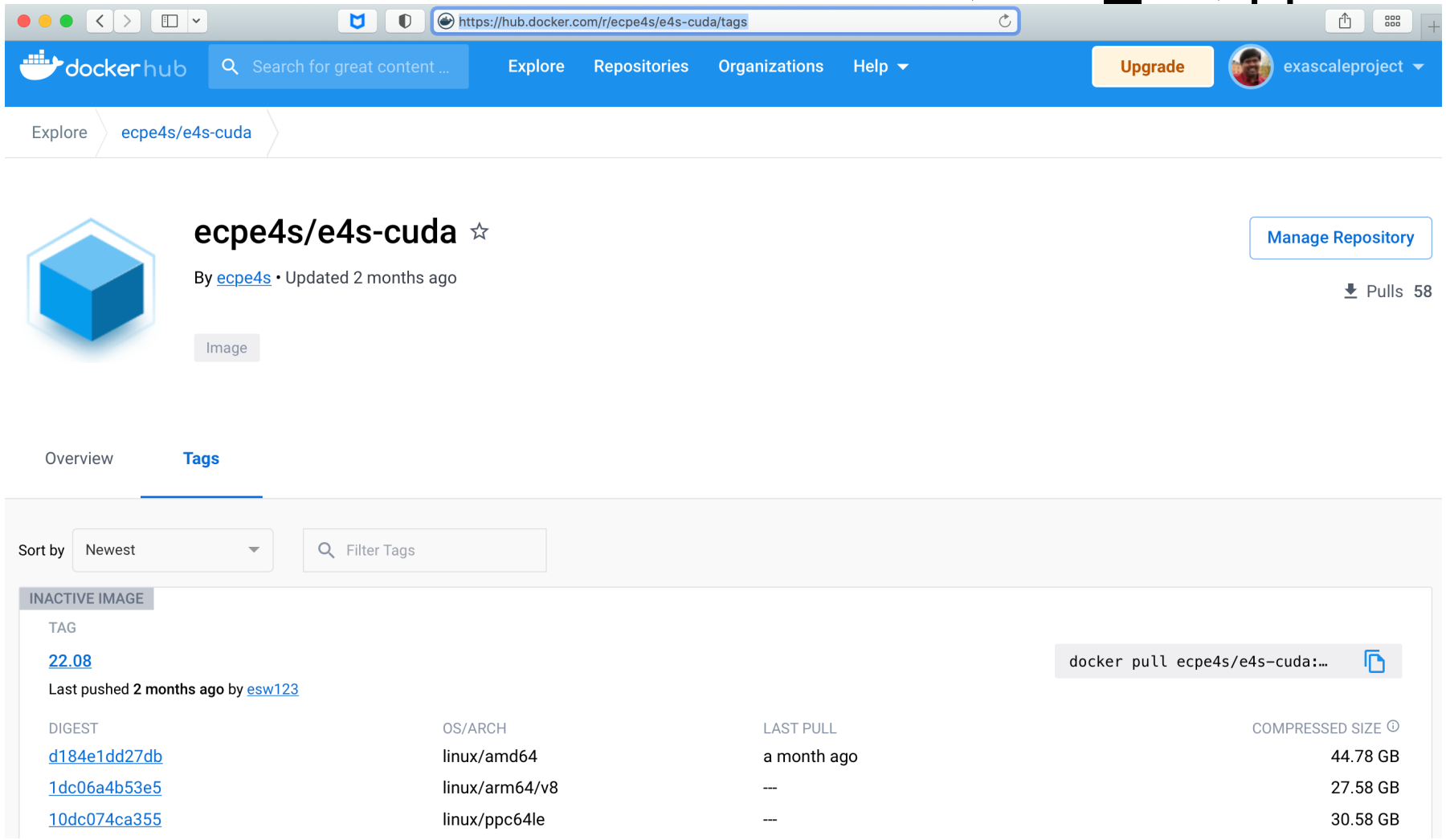
- Trilinos v13.4.0 for aarch64
- NVHPC 22.7 with CUDA 11.7
- Support for NVIDIA GPUs
- PyTorch v1.12.1

E4S 22.08: Trilinos Spack configuration +cuda cuda_arch=80

```
Singularity> spack find trilinos +cuda cuda_arch=80
==> 1 installed package
-- linux-ubuntu20.04-x86_64 / gcc@9.4.0 --------------------------
trilinos@13.4.0
Singularity> spack find -dl -v trilinos +cuda cuda_arch=80
==> 1 installed package
-- linux-ubuntu20.04-x86_64 / gcc@9.4.0 --------------------------
lxifibt trilinos@13.4.0~adelus~adios2+amesos+amesos2+anasazi+aztec~basker+belos+boost~chaco~complex+cuda~cuda_rdc~debug~dtk+epetra+epetraext~epetraextbtf~
epetraextexperimental~epetraextgraphreorderings~exodus+explicit_template_instantiation~float+fortran~gtest~hdf5~hypre+ifpack+ifpack2+intrepid+intrepid2~ip
o+isorropia+kokkos~mesquite+minitensor+ml+mpi+muelu~mumps+nox~openmp~panzer+phalanx+piro~python~rocm~rocm_rdc+rol+rythmos+sacado~scorec+shards+shared+shyl
u+stk+stokhos+stratimikos~strumpack~suite-sparse~superlu+superlu-dist+teko+tempus+thyra+tpetra+trilinoscouplings~uvm+wrapper~x11+zoltan+zoltan2 build_type
=RelWithDebInfo cuda_arch=80 cxxstd=14 gotype=long_long
57jswcn     boost@1.79.0~atomic~chrono~clanglibcpp~container~context~contract~coroutine~date_time~debug+exception~fiber~filesystem+graph~graph_parallel~ic
u~iostreams~json~locale~log+math+mpi+multithreaded~nowide~numpy~pic~program_options~python~random~regex~serialization+shared~signals~singlethreaded+stackt
race~system~taggedlayout~test~thread~timer~type_erasure~versionedlayout~wave cxxstd=98 patches=a440f96,b8569d7 visibility=hidden
yurg3uw         mpich@4.0.2~argobots~cuda+fortran+hwloc+hydra+libxml2+pci~rocm+romio~slurm~two_level_namespace~vci~verbs~wrapperrpath datatype-engine=auto
 device=ch4 netmod=ofi patches=d4c0e99 pmi=pmi
2meaymk             findutils@4.9.0 patches=440b954
poo3xn4             hwloc@2.8.0~cairo+cuda~gl~libudev+libxml2~netloc~nvml~oneapi-level-zero~opencl+pci~rocm+shared
slt5lpw                 cuda@11.4.4~allow-unsupported-compilers~dev
q4psrtu                 libpciaccess@0.16
4o7qnns                     libtool@2.4.7
qr7lniy                         m4@1.4.19+sigsegv patches=9dc5fbd,bfdffa7
n2fjcg5                             diffutils@3.8
c75f7vl                                 libiconv@1.16 libs=shared,static
xu34agk                             libsigsegv@2.13
jodzku6                     pkgconf@1.8.0
kgquruf                     util-macros@1.19.3
wmzytwr                 libxml2@2.9.13~python
odpuh4q                     xz@5.2.5+pic libs=shared,static
2jmcbiq                     zlib@1.2.12+optimize+pic+shared patches=0d38234
sfi4ust                 ncurses@6.3~symlinks+termlib abi=none
cfy25dm             libfabric@1.14.1~debug~kdreg fabrics=rxm,sockets,tcp,udp
3cws7on             yaksa@0.2~cuda~rocm
bqg7jkg                 autoconf@2.69 patches=35c4492,7793209,a49dd5b
nkpm5ba                     perl@5.34.1+cpanm+shared+threads
5ddr2oz                         berkeley-db@18.1.40+cxx~docs+stl patches=b231fcc
sy4wi34                         bzip2@1.0.8~debug~pic+shared
uv6hph5                         gdbm@1.19
xv7r2sl                             readline@8.1.2
clt6yw4                 automake@1.16.5
hhokobj                 python@3.8.13+bz2+ctypes+dbm~debug+libxml2+lzma~nis~optimizations+pic+pyexpat+pythoncmd+readline+shared+sqlite3+ssl~tix~tkinter~uc
s4+uuid+zlib patches=0d98e93,4c24573,f2fd060
```

- Trilinos 13.4.0
- CUDA 11.4.4
- cuda_arch=80 (for A100)

E4S 22.08 Release: NVIDIA GPU, x86_64, ppc64le, and aarch64



- 100+ E4S Products
- Dockerhub
- Support for NVIDIA
  - ppc64le, x86_64, and aarch64 in a single image

% docker pull ecpe4s/e4s-cuda

E4S bare-metal installation spack.yaml recipe

https://github.com/E4S-Project/e4s/blob/master/environments/21.11/spack-x86_64.yaml

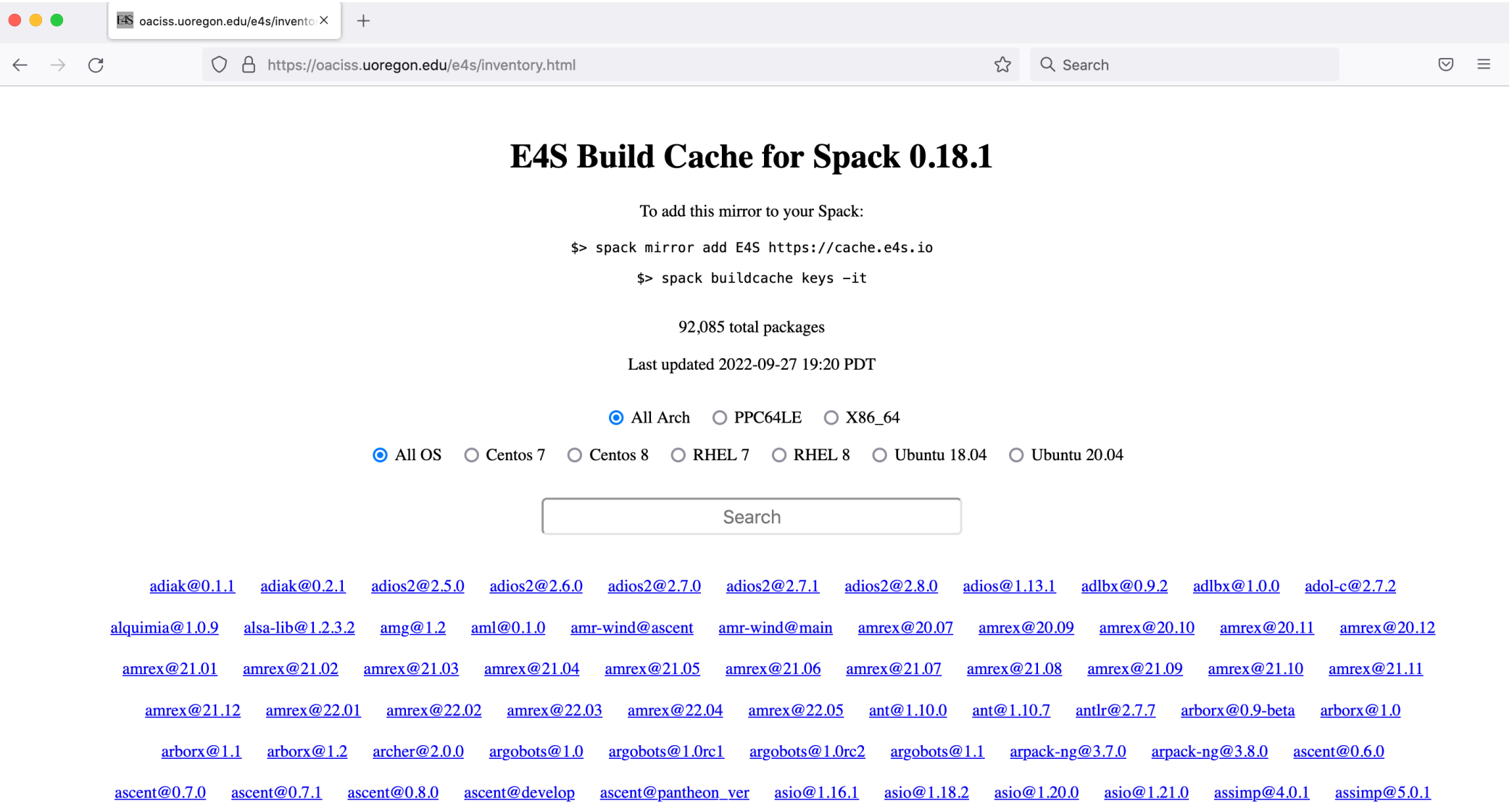
```
30      elfutils:
31        variants: +bzip2 ~nls +xz
32      fftw:
33        variants: +openmp
34      hdf5:
35        variants: +fortran +hl +shared api=v18
36        version:
37        - 1.12.1
38      libfabric:
39        variants: fabrics=sockets,tcp,udp,rxm
40      libunwind:
41        variants: +pic +xz
42      mesa:
43        variants: ~llvm
44      mesa18:
45        variants: ~llvm
46      mpich:
47        variants: ~wrapperrpath
48      ncurses:
49        variants: +termlib
50      openblas:

52      trilinos:
53        variants: +amesos +amesos2 +anasazi +aztec +belos +boost +epetra +epetraext
54          +ifpack +ifpack2 +intrepid +intrepid2 +isorropia +kokkos +ml +minitensor +muelu
55          +nox +piro +phalanx +rol +rythmos +sacado +stk +shards +shylu +stokhos +stratimikos
56          +teko +tempus +tpetra +trilinoscouplings +zoltan +zoltan2 +superlu-dist gotype=long_long

58        variants: +pic
59
60    definitions:
61    - cuda_specs:
62      - amrex@21.11 +cuda cuda_arch=80
63      - caliper@2.7.0 +cuda cuda_arch=80
64      - chai@2.4.0 ~benchmarks ~tests +cuda cuda_arch=80 ^umpire ~shared
65      - flecsi@2.1.0 +cuda cuda_arch=80
66      - ginkgo@1.4.0 +cuda cuda_arch=80
67      - heffte@2.2.0 +cuda cuda_arch=80
68      - hpx@1.7.1 +cuda cuda_arch=80
69      - hypre@2.23.0 +cuda cuda_arch=80
70      - kokkos@3.4.01 +wrapper +cuda cuda_arch=80
71      - kokkos-kernels@3.4.01 +cuda cuda_arch=80 ^kokkos +wrapper +cuda cuda_arch=80
72      - magma@2.6.1 +cuda cuda_arch=80
73      - mfem@4.3.0 +cuda cuda_arch=80
74      - parsec@3.0.2012 +cuda cuda_arch=80
75      - petsc@3.16.1 +cuda cuda_arch=80
76      - raja@0.14.0 +cuda cuda_arch=80
77      - slate@2021.05.02 +cuda cuda_arch=80
78      - slepc@3.16.0 +cuda cuda_arch=80
79      - strumpack@6.1.0 ~slate +cuda cuda_arch=80
80      - sundials@5.8.0 +cuda cuda_arch=80
81      - superlu-dist@7.1.1 +cuda cuda_arch=80
82      - tasmanian@7.7 +cuda cuda_arch=80
83      - trilinos@13.2.0 +cuda cuda_arch=80
84      - umpire@6.0.0 ~shared +cuda cuda_arch=80
85      - upcxx@2021.9.0 +cuda
86      - vtk-m@1.6.0 +cuda cuda_arch=80
87      - zfp@0.5.5 +cuda cuda_arch=80
```

- Trilinos variants
- Built with CUDA

E4S: Spack Build Cache at U. Oregon to speed up installation



- 92,000+ binaries
- S3 mirror
- No need to build from source code!

- https://oaciss.uoregon.edu/e4s/inventory.html

E4S Frank build statistics, monitoring failure of jobs

Summary

Period Beginning: 2021-09-22 07:48:34.025+00

Period Ending: 2021-11-24 20:25:43.62+00

Number of Jobs: 193014

Number of Failed Jobs, all types: 9669

Number of Failed Jobs, system failures only: 876

Node Descriptions

- UO Frank Node Descriptions

Shortcuts

- Job Times, Last 4 Hours
- Job Times, Overview, All
- Job Times, Detailed, All
- Runner System Failures, by Runner, Last 4 Hours
- Runner System Failures, by Runner, All
- Runner System Failures, by Type, Last 4 Hours
- Runner System Failures, by Type, all
- Runner System Failures, Last 20

Job Times, Last 4 Hours

name	total_runtime	avg_runtime	n	pct_uo	pct_aws
rebuild	23:14:32.5	00:11:49.088983	118	100%	0%
generate	01:41:42.054	00:02:02.04108	50	100%	0%
service	00:52:17.515	00:00:51.434672	61	97%	3%

Job Times, Overview

name	total_runtime	avg_runtime	n	pct_uo	pct_aws
rebuild	16605:48:23.241	00:06:16.086963	158955	60%	40%
generate	2320:23:16.259	00:08:33.202449	16277	67%	33%
service	305:14:02.474	00:01:02.215065	17662	81%	19%
other	00:49:16.909	00:00:24.640908	120	98%	2%

Job Times, Detailed

name	total_runtime	avg_runtime	n	pct_uo	pct_aws
rebuild	16605:48:23.241	00:06:16.086963	158955	60%	40%
e4s-pr-generate	1203:50:57.253	00:22:00.090543	3283	66%	34%
radiuss-pr-generate	370:30:59.29	00:06:57.483346	3195	65%	35%
e4s-develop-generate	201:14:29.111	00:22:44.348608	531	85%	15%
rebuild-index	188:27:27.859	00:02:44.871898	4115	86%	14%
data-vis-sdk-pr-generate	144:55:12.951	00:02:41.022516	3240	64%	36%
build_systems-pr-generate	134:54:25.661	00:02:26.284838	3320	66%	34%
e4s-on-power-pr-generate	111:39:57.649	00:26:41.584259	251	95%	0%
cleanup	59:17:42.459	00:00:51.83644	4118	84%	16%
no-specs-to-rebuild	57:28:52.156	00:00:21.946352	9429	77%	23%
radiuss-develop-generate	55:23:44.022	00:06:25.733118	517	82%	18%
tutorial-pr-generate	48:41:52.415	00:03:45.627304	777	52%	48%
data-vis-sdk-develop-generate	20:32:30.767	00:02:23.038234	517	80%	20%
build_systems-develop-generate	19:14:09.214	00:02:13.171565	520	83%	17%
tutorial-develop-generate	05:35:00.044	00:02:48.907933	119	58%	42%
e4s-on-power-develop-generate	03:49:57.882	00:32:51.126	7	71%	0%
other	00:49:16.909	00:00:24.640908	120	98%	2%

Runner System Failures, by Runner, Last 4 Hours

runner	n_jobs	n_system_failures	system_failure_rate	facility
empty				

Runner System Failures, by Runner

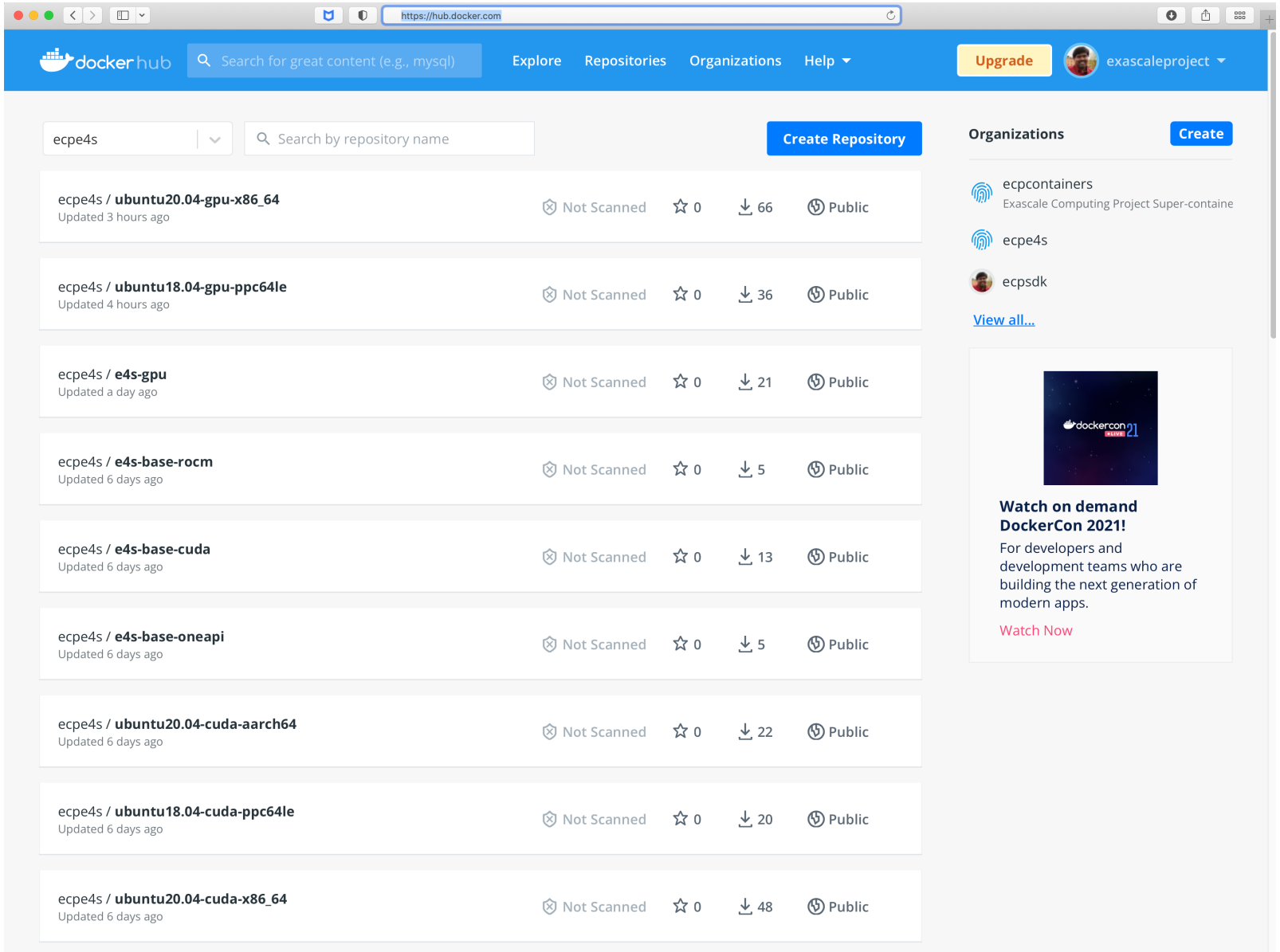
runner	n_jobs	n_system_failures	pct_system_failures	facility
large-x86-pub-gitlab-runner-64fcfb66b-w2gnl	41727	50	0.12%	AWS
large-x86-pub-gitlab-runner-64fcfb66b-28pd5	16326	277	1.70%	AWS
medium-x86-pub-gitlab-runner-5b4ddf9758-bxjvf	4002	110	2.75%	AWS
xlarge-x86-pub-gitlab-runner-7c58cc9d47-k87vf	3870	120	3.10%	AWS
medium-x86-pub-gitlab-runner-5b4ddf9758-n62pg	3272	4	0.12%	AWS
xlarge-x86-pub-gitlab-runner-7c58cc9d47-6rh2n	1802	106	5.88%	AWS
medium-x86-pub-gitlab-runner-5b4ddf9758-9qjtp	1400	114	8.14%	AWS
huge-x86-pub-gitlab-runner-658c9ff576-h7czw	174	1	0.57%	AWS
uo-jupiter	26154	0	0.00%	UO
uo-instinct	21024	0	0.00%	UO
uo-illyad	17826	0	0.00%	UO
uo-godzilla	13993	43	0.31%	UO
uo-gilgamesh	12620	0	0.00%	UO
uo-delphi	12444	5	0.04%	UO
uo-saturn	5887	4	0.07%	UO
uo-eagle	3369	1	0.03%	UO
uo-vina	3207	0	0.00%	UO
uo-minotaur	1815	12	0.66%	UO
uo-centaur	1671	29	1.74%	UO
uo-typhon	13	0	0.00%	UO
uo-medusa	9	0	0.00%	UO

Runner System Failures, by Type, Last 4 Hours

failure_type	n	n_aws	n_uo	percent
empty				

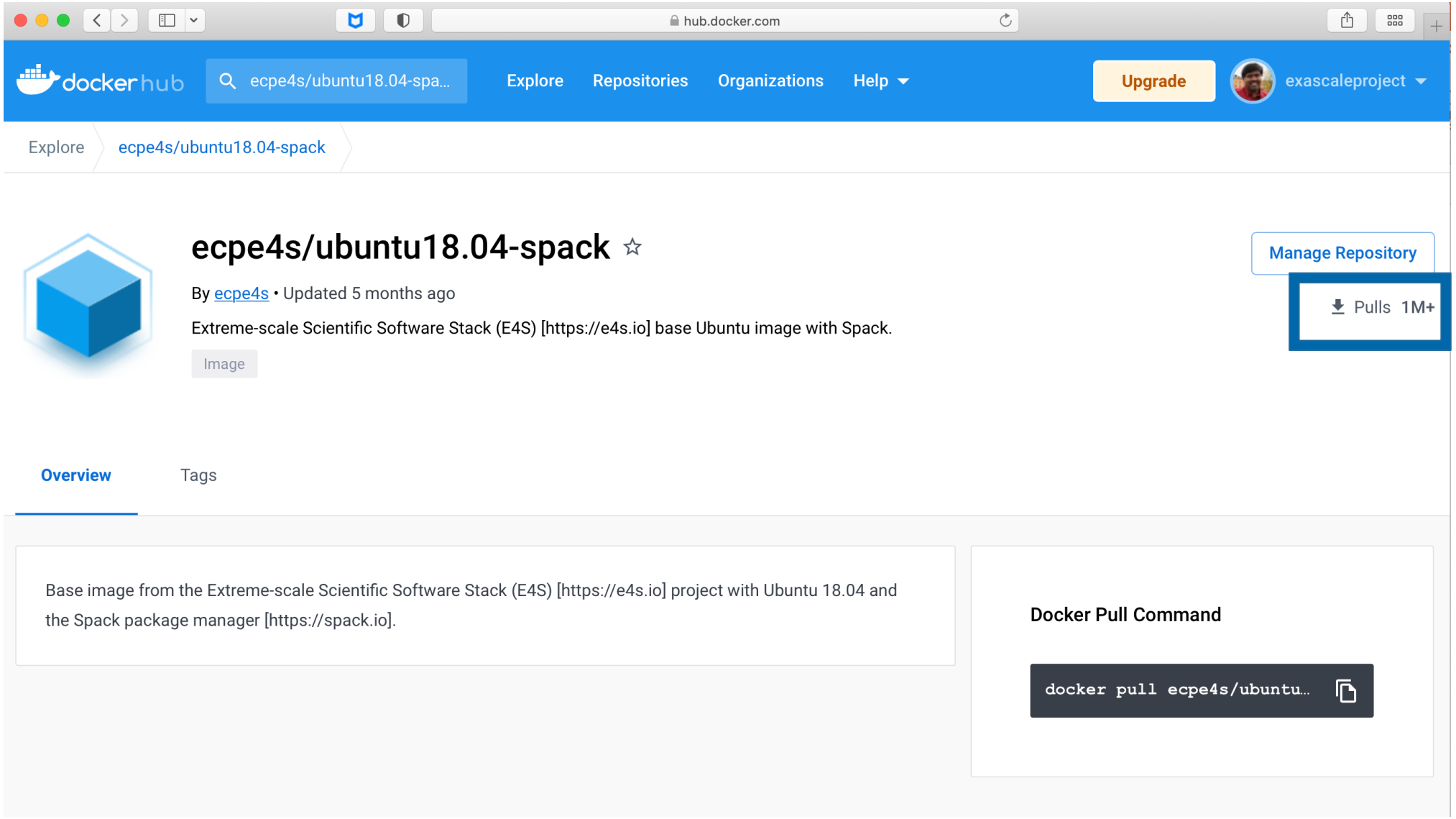
- https://stats.e4s.io

E4S Base Container Images for x86_64, ppc64le, and aarch64



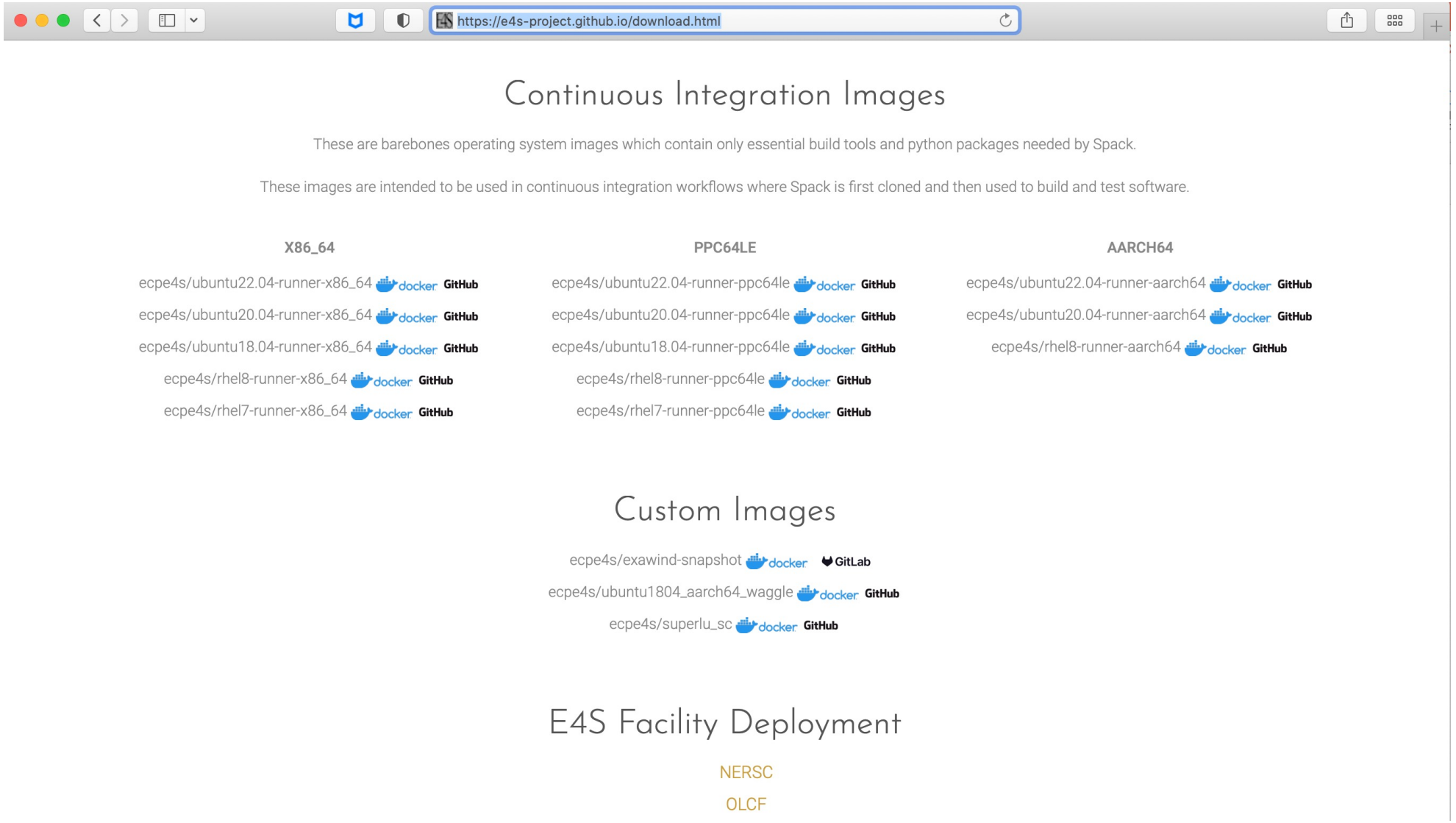
- Hub.docker.com
- ecpe4s
- Platforms:
  - x86_64
  - Ppc64le
  - aarch64
- GPU runtimes:
  - CUDA
  - ROCm
  - oneAPI

E4S Base Container Images for x86_64 with Spack (no GPU)

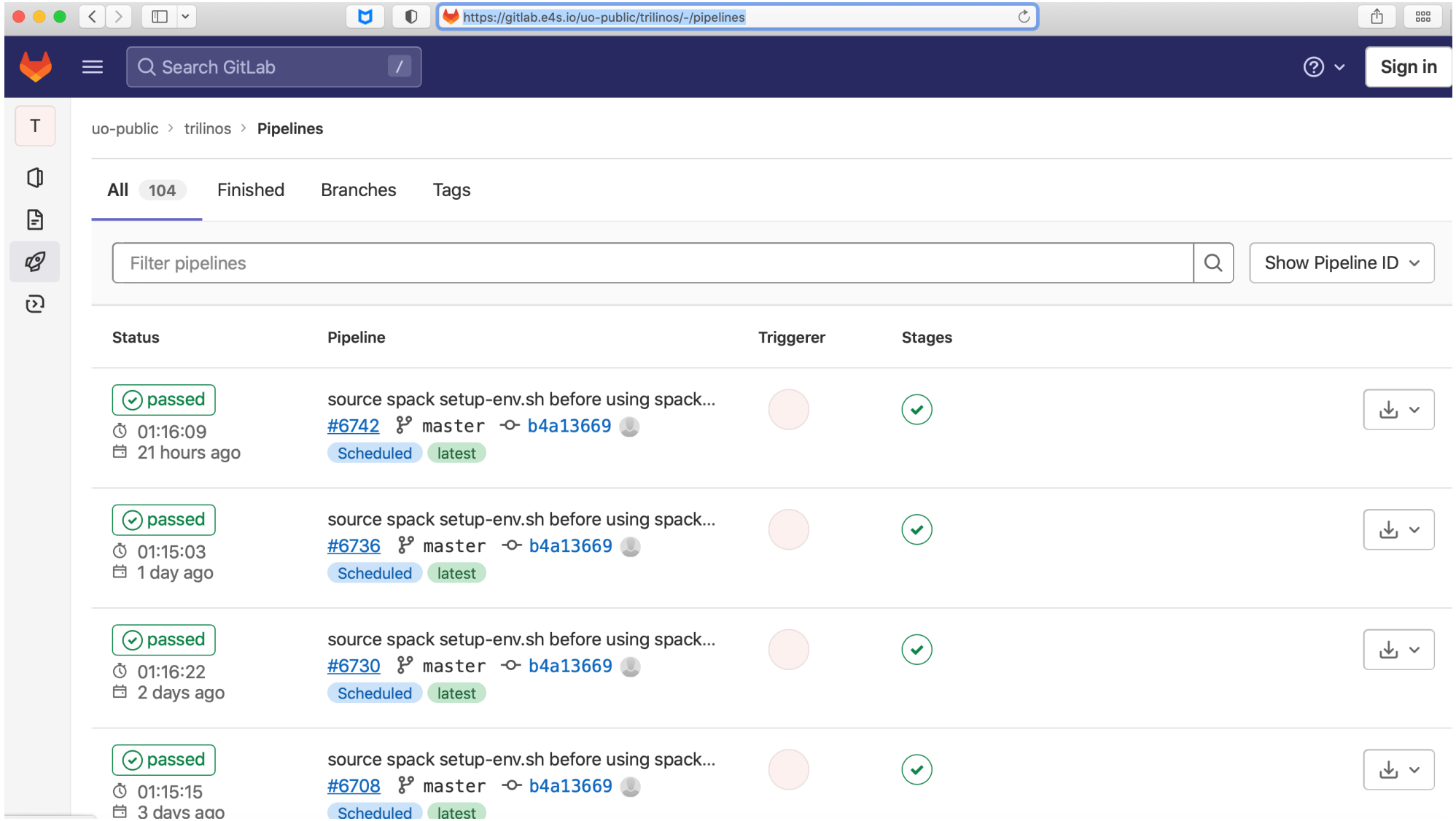


- Popular Ubuntu18.04
- 1M+ downloads!

E4S 22.08 Cloud, CI, and Custom images

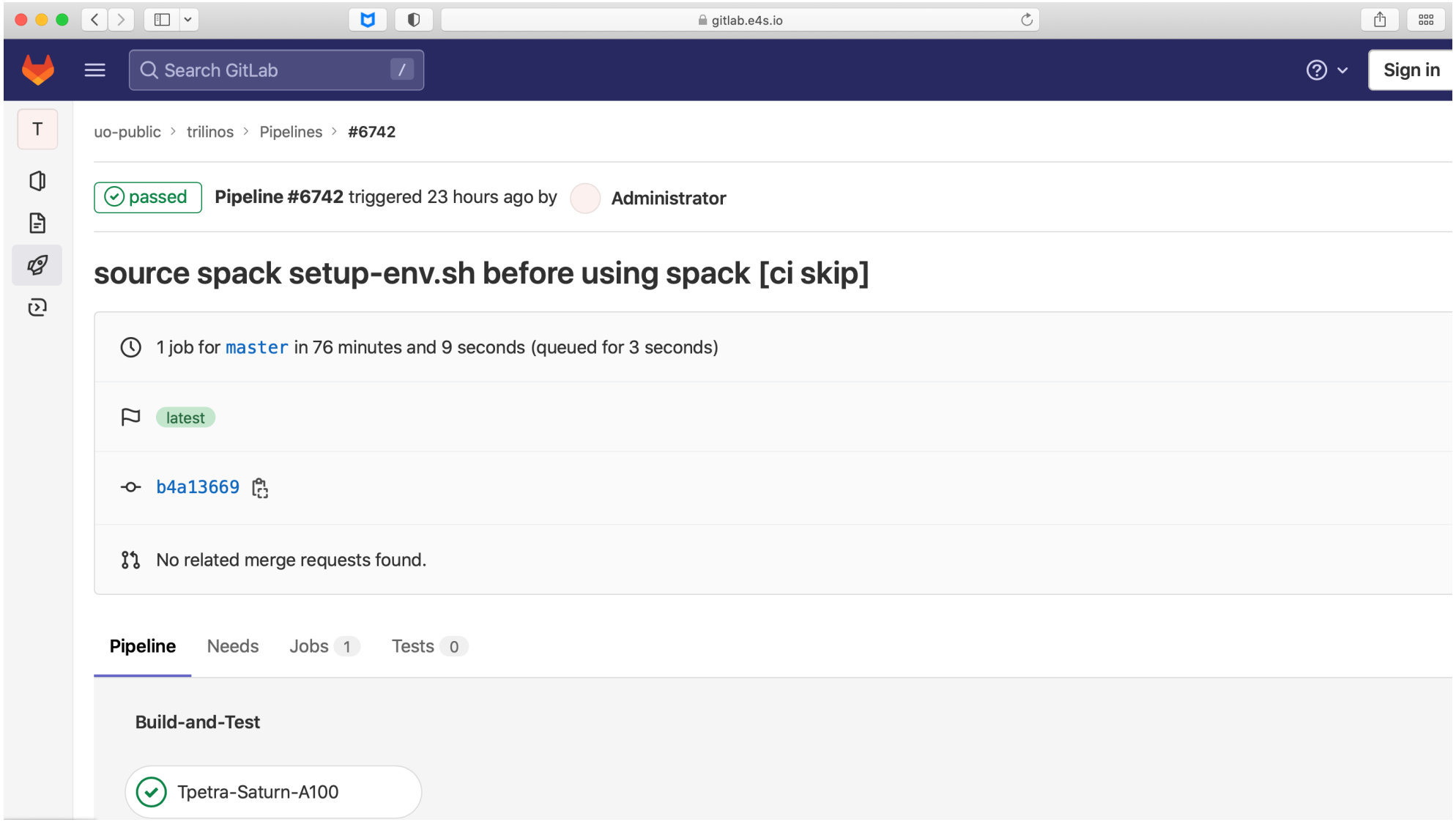


E4S GitLab Nightly Testing of Trilinos at U. Oregon on Frank*



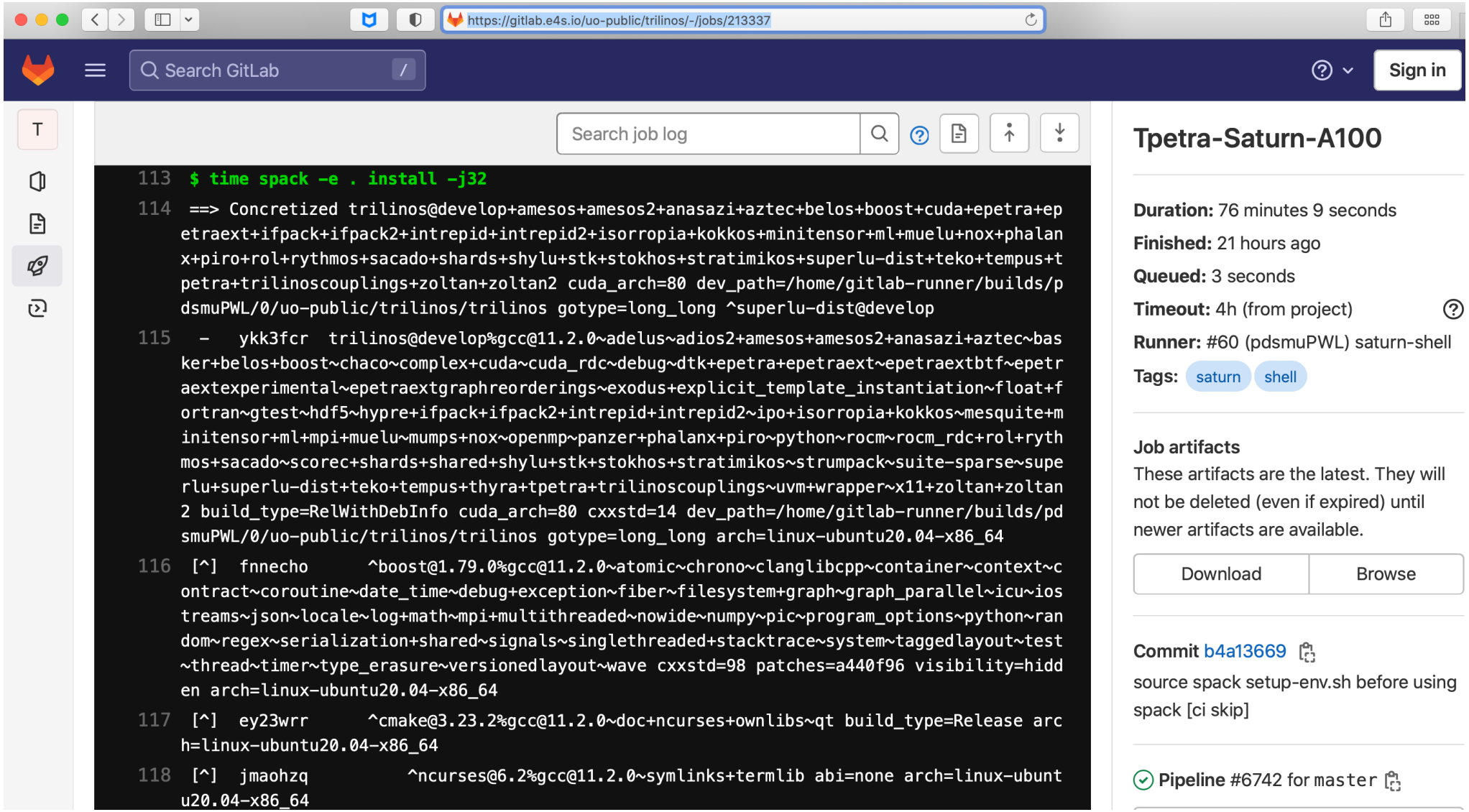
* https://oaciss.uoregon.edu/frank

E4S GitLab Testing of Trilinos@develop on A100 (CUDA)



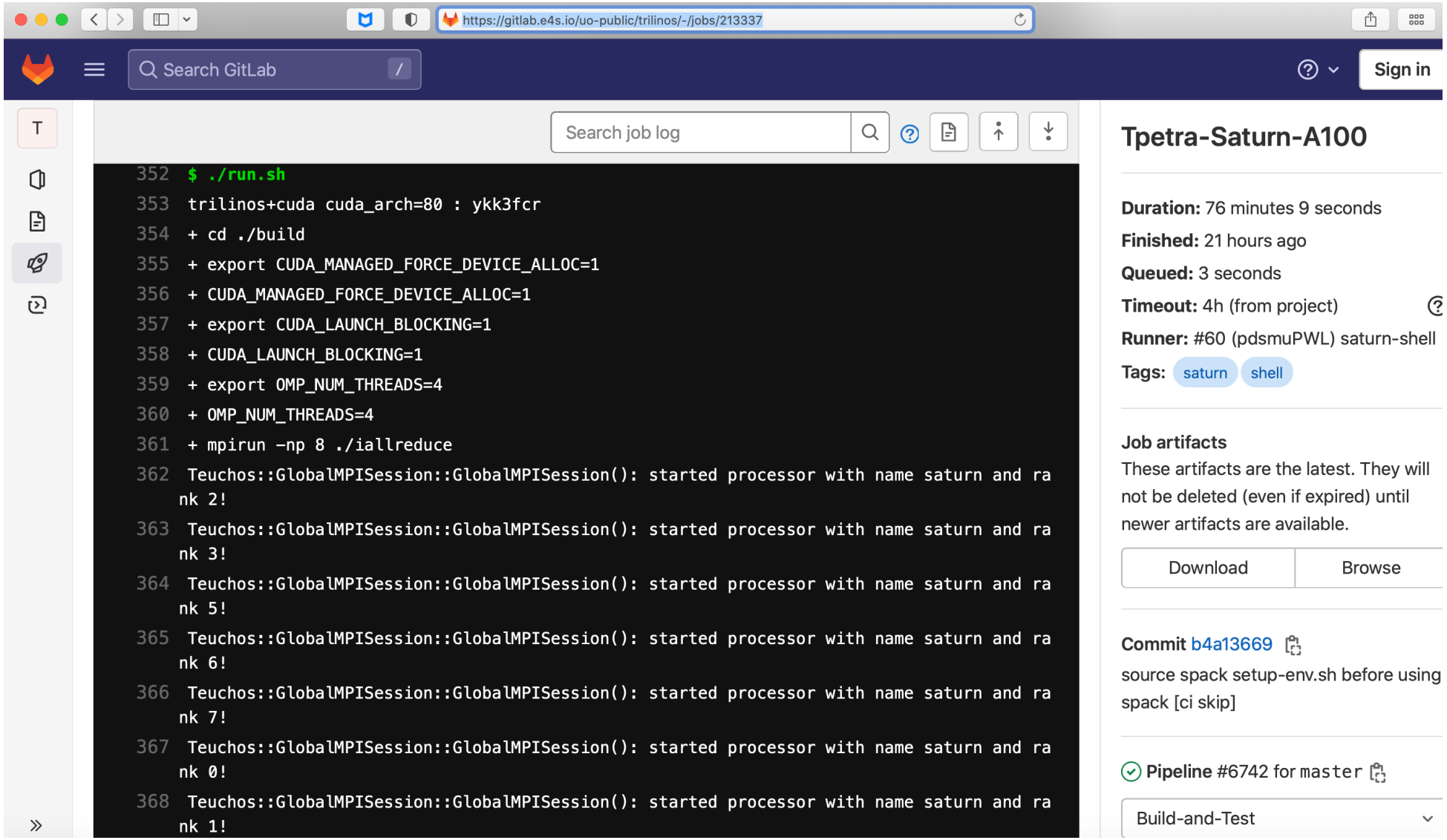
https://gitlab.e4s.io/uo-public/trilinos

E4S GitLab Building Trilinos@develop using CUDA

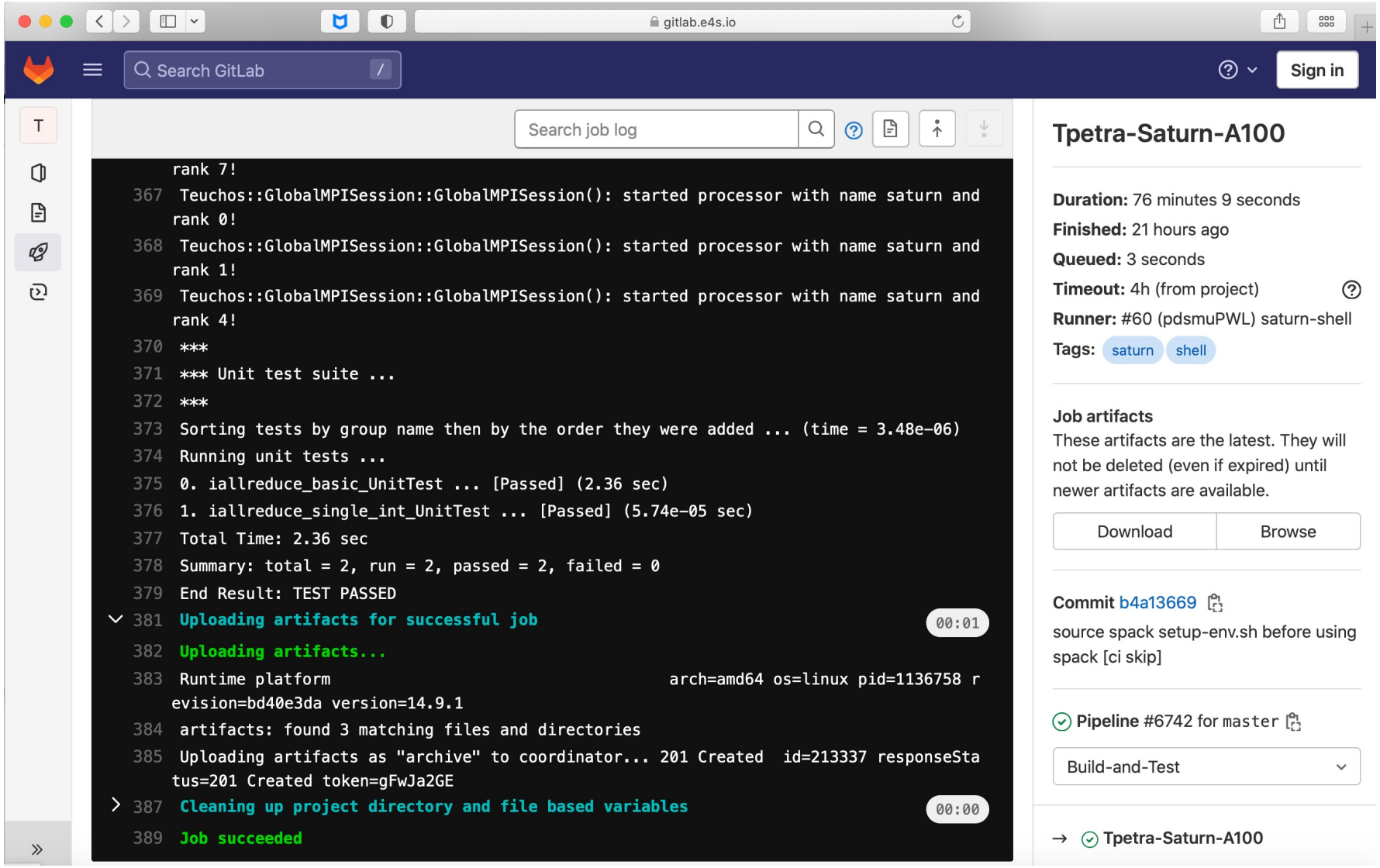


https://gitlab.e4s.io/uo-public/trilinos

E4S GitLab: Running Trilinos Tpetra Testcase on A100



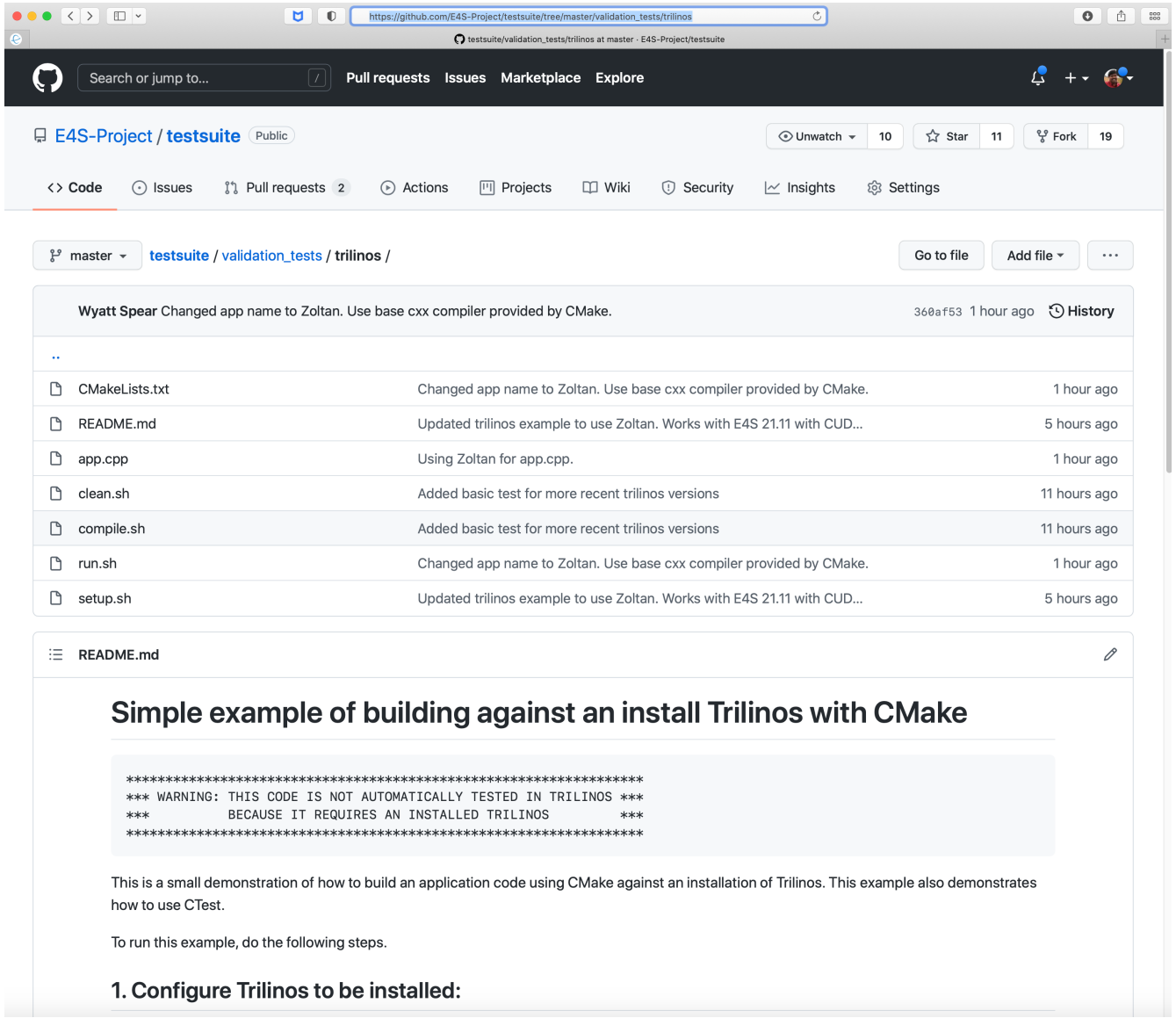
E4S GitLab: Running Trilinos Tpetra Testcase on A100



Notifies developers on failure

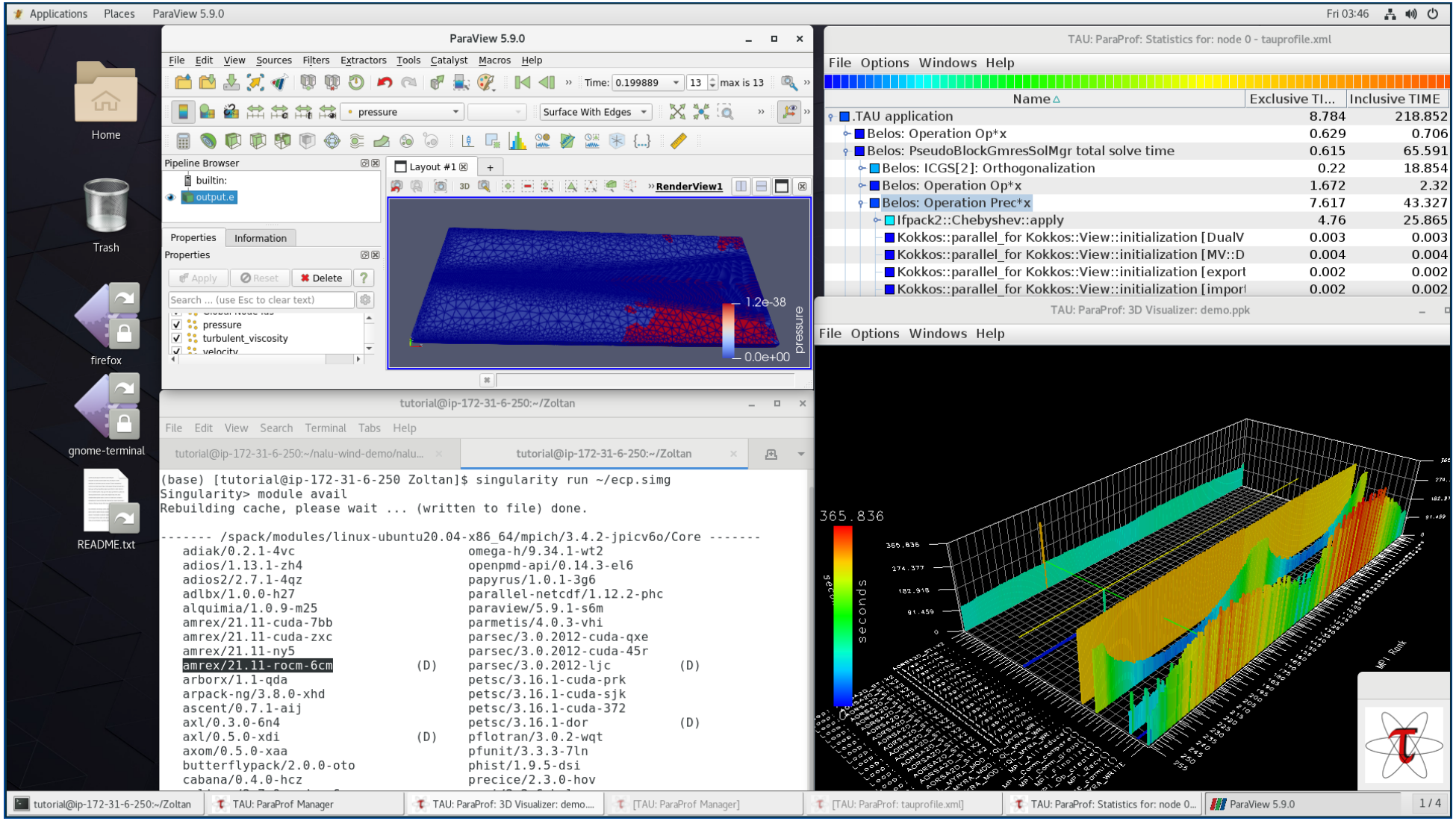
E4S Validation Test Suite: Trilinos

- Provides automated build and run tests
- Validate container environments and products



- git clone https://github.com/E4S-Project/testsuite.git

E4S 22.08 AWS image: US-West2 (OR) ami-0d7295416d1c63e3a



E4S 22.08 AWS

- Intel oneAPI
- CUDA
- NVHPC
- ROCm
- AWS DCV
- Spack Build Cache
- ECP: Nalu-Wind
- Trilinos 13.4.0
- OpenFOAM
- ParaView
- TAU
- Docker
- Shifter
- Charliecloud
- E4S Singularity…

e4s-cl: A tool to simplify the launch of MPI jobs in E4S containers

- E4S containers support replacement of MPI libraries using MPICH ABI compatibility layer and Wi4MPI [CEA] for OpenMPI replacement.
- Applications binaries built using E4S can be launched with Singularity using MPI library substitution for efficient inter-node communications.
- e4s-cl is a new tool that simplifies the launch and MPI replacement.
  - e4s-cl init --backend [singularity|shifter|docker] --image <file> --source <startup_cmds.sh>
  - e4s-cl mpirun -np <N> <command>
- Usage:

. /opt/intel/oneapi/setvars.sh

e4s-cl init --backend singularity --image ~/images/e4s-gpu-x86.sif --source ~/source.sh

cat ~/source.sh

```
. /spack/share/spack/setup-env.sh
spack load trilinos+cuda cuda_arch=80
```

e4s-cl mpirun -np 4 ./a.out

https://github.com/E4S-Project/e4s-cl

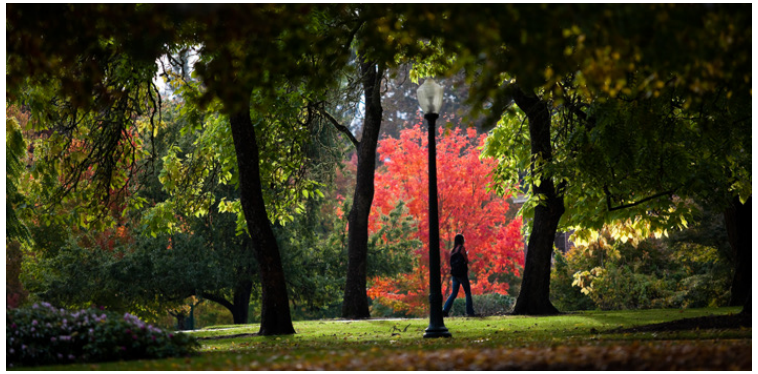
E4S Summary

What E4S is not	• What E4S is
A closed system taking contributions only from DOE software development teams.	Extensible, open architecture software ecosystem accepting contributions from US and international teams. Framework for collaborative open-source product integration.
A monolithic, take-it-or-leave-it software behemoth.	A full collection of compatible software capabilities **and** A manifest of a la carte selectable software capabilities.
A commercial product.	Vehicle for delivering high-quality reusable software products in collaboration with others.
A simple packaging of existing software.	The conduit for future leading edge HPC software targeting scalable next-generation computing platforms. A hierarchical software framework to enhance (via SDKs) software interoperability and quality expectations.

Vision for E4S Now and in the Future

- E4S has emerged as a new top-level component in the DOE HPC community, enabling fundamentally new relationships
- E4S has similar potential for new interactions with other US agencies, US industry and international collaborators. NSF and UK are examples
- The E4S portfolio can expand to include new domains (ML/AI), lower—level components (OS), and more.
- E4S can provide better (increased quality), faster (timely delivery of leading-edge capabilities) and cheaper (assisting product teams)

Performance Research Laboratory, University of Oregon, Eugene



www.uoregon.edu

Thank you

https://www.exascaleproject.org

This research was supported by the Exascale Computing Project (17-SC-20-SC), a joint project of the U.S. Department of Energy's Office of Science and National Nuclear Security Administration, responsible for delivering a capable exascale ecosystem, including software, applications, and hardware technology, to support the nation's exascale computing imperative.

Thank you to all collaborators in the ECP and broader computational science communities. The work discussed in this presentation represents creative contributions of many people who are passionately working toward next-generation computational science.