What is E4S?

E4S at NERSC 2022 workshop:
https://www.nersc.gov/users/training/events/e4s-at-nersc-2022/
Thursday, August 25, 2022

https://e4s.io/talks/E4S_at_NERSC_Shende_1.pptx

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E4S: Extreme-scale Scientific Software Stack

- Curated, Spack based software distribution
- Spack binary build caches for bare-metal installs
  - x86_64, ppc64le (IBM Power 9), and aarch64 (ARM64)
- 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 using MPICH ABI
- 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

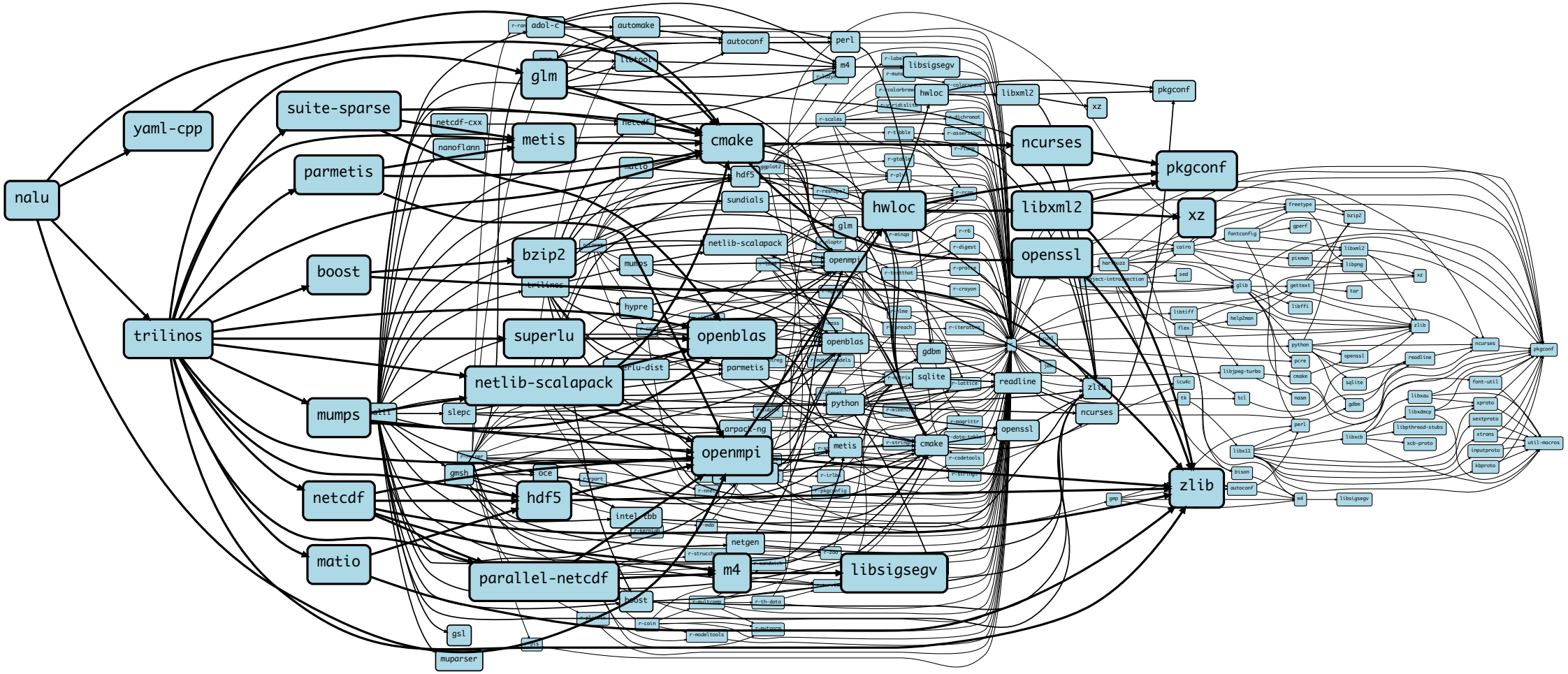
https://e4s.io

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

Spack

- E4S uses the Spack package manager for software delivery
- Spack provides the ability to specify versions of software packages that are and are not interoperable.
- Spack is a build layer for not only E4S software, but also a large collection of software tools and libraries outside of ECP ST.
- Spack supports achieving and maintaining interoperability between ST software packages.
- https://spack.io

Scientific software is becoming extremely complex

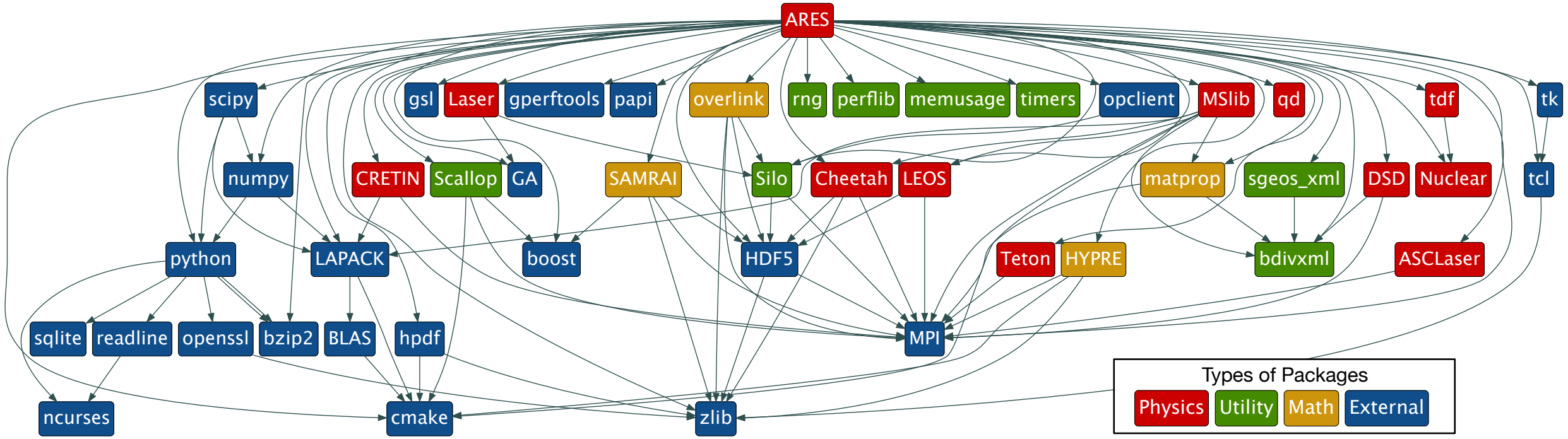


Nalu: Generalized Unstructured Mass Mixer: Parallel Mining Machine

deal.ii: C++ Finite Element Library

Flow

Even proprietary codes are based on many open source libraries



- Half of this DAG is external (blue); *more* than half of it is open source
- Nearly *all* of it needs to be built specially for HPC to get the best performance

The Exascale Computing Project is building an entire *ecosystem*

15+ applications x **80+ software packages** x **5+ target architectures/platforms**
Xeon Power KNL
NVIDIA ARM Laptops?

x **Up to 7 compilers**
Intel GCC Clang XL
PGI Cray NAG

x **10+ Programming Models**
OpenMPI MPICH MVAPICH OpenMP CUDA
OpenACC Dharma Legion RAJA Kokkos

x **2-3 versions of each package + external dependencies**

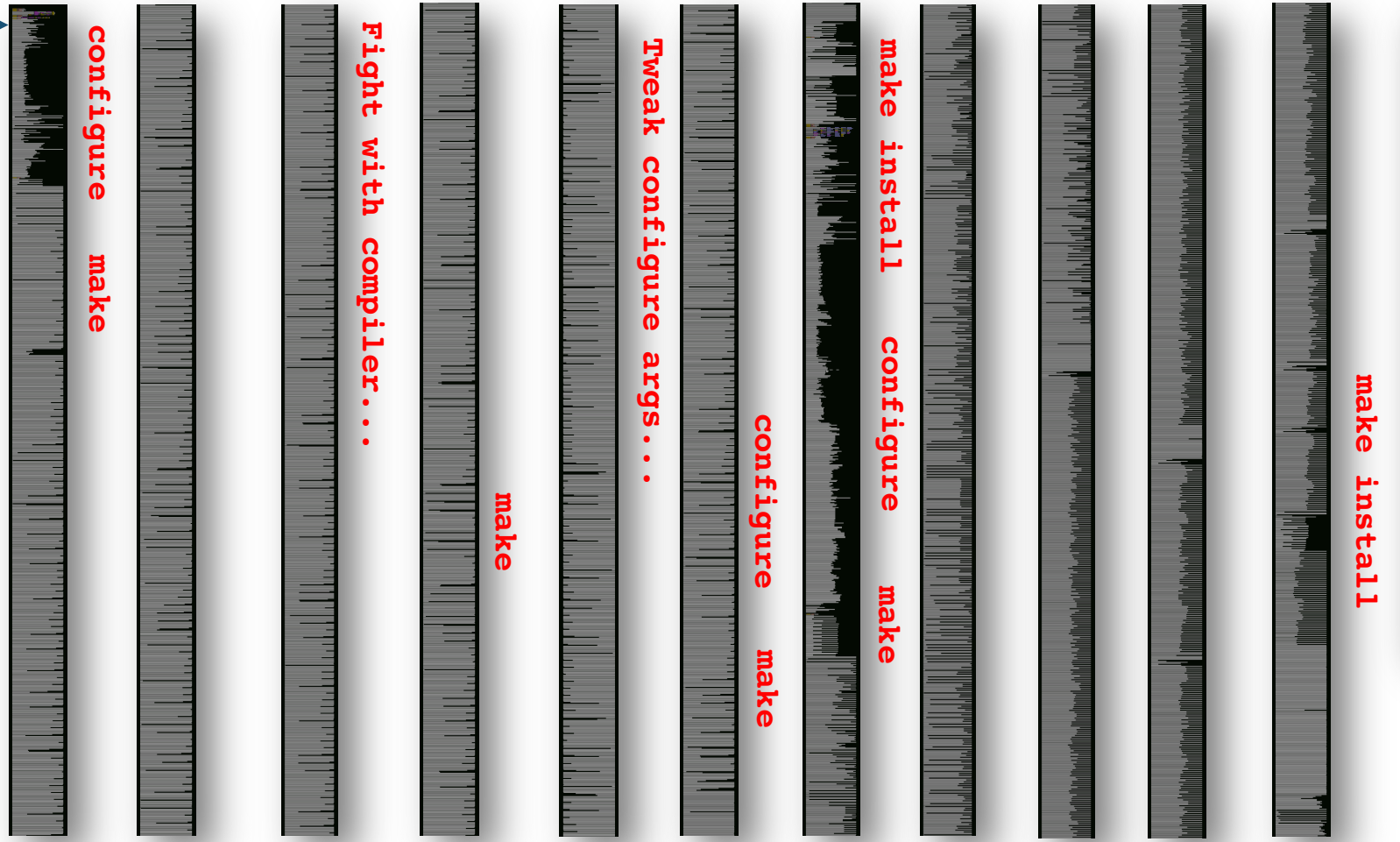
= up to **1,260,000** combinations!

- Every application has its own stack of dependencies.
- Developers, users, and facilities dedicate (many) FTEs to building & porting.
- Often trade reuse and usability for performance.

We must make it easier to rely on others' software!

How to install software on a supercomputer

1. Download all 16 tarballs you need
2. Start building!



3. Run code
4. **Segfault!?**
5. Start over…

What about modules?

- Most supercomputers deploy some form of *environment modules*
  - TCL modules (dates back to 1995) and Lmod (from TACC) are the most popular

```
$ gcc
- bash: gcc: command not found

$ module load gcc/7.0.1
$ gcc –dumpversion
7.0.1
```

- Modules don't handle installation!
  - They only modify your environment (things like PATH, LD_LIBRARY_PATH, etc.)
- Someone (likely a team of people) has already installed gcc for you!
  - Also, you can *only* `module load` the things they've installed

Spack is a flexible package manager for HPC

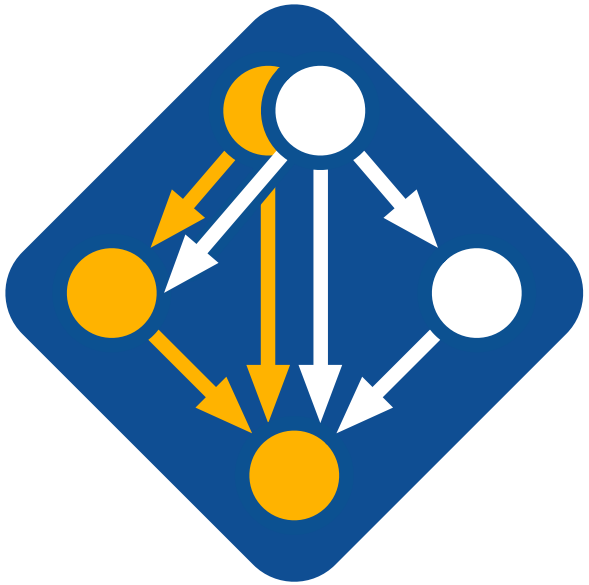
- How to install Spack (works out of the box):

```
$ git clone https://github.com/spack/spack
$ . spack/share/spack/setup-env.sh
```

- How to install a package:

```
$ spack install tau
```

- TAU and its dependencies are installed within the Spack directory.
- Unlike typical package managers, Spack can also install many variants of the same build.
  - Different compilers
  - Different MPI implementations
  - Different build options



Visit spack.io

github.com/spack/spack

@spackpm

Spack provides the *spec* syntax to describe custom configurations

```
$ git clone https://github.com/spack/spack
$ . spack/share/spack/setup-env.sh
$ spack compiler find                                   # set up compilers
$ spack external find                                   # set up external packages
```

```
$ spack install tau                                     unconstrained
$ spack install tau@2.31                                @ custom version
$ spack install tau@2.31 %gcc@9.3.0                     % custom compiler
$ spack install tau@2.31 %gcc@9.3.0 +rocm               +/- build option
$ spack install tau@2.31 %gcc@9.3.0 +mpi ^mvapich2@2.3~wrapperrpath   ^ dependency information
```

- Each expression is a ***spec*** for a particular configuration
  - Each clause adds a constraint to the spec
  - Constraints are optional – specify only what you need.
  - Customize install on the command line!
- Spec syntax is recursive
  - Full control over the combinatorial build space

`spack find` shows what is installed

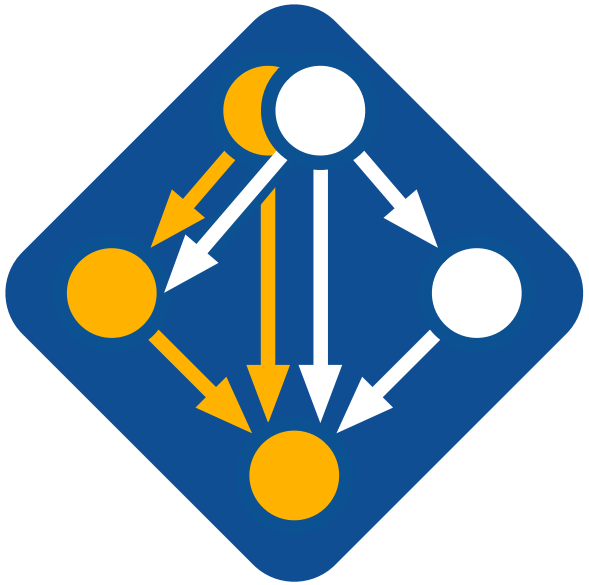
Terminal — ssh crusher — 198×57

```
[sameer@login2.crusher ~]$ spack find
==> 702 installed packages
-- cray-sles15-zen3 / gcc@11.2.0 ---------------------------------
adiak@0.2.1                     gdbm@1.19                       libxkbcommon@1.4.0              pmix@4.1.2                      py-nest-asyncio@1.5.4           py-warlock@1.3.3
adios@1.13.1                    gdk-pixbuf@2.42.6               libxkbcommon@1.4.0              precice@2.4.0                   py-netifaces@0.10.5             py-warpx@22.05
adios2@2.8.0                    gettext@0.21                    libxkbfile@1.0.9                protobuf@3.18.0                 py-networkx@2.7.1               py-warpx@22.05
adlbx@1.0.0                     ginkgo@1.4.0                    libxml2@2.9.13                  pugixml@1.11.4                  py-notebook@6.4.5               py-warpx@22.05
adol-c@2.7.2                    ginkgo@1.4.0                    libxrandr@1.5.0                 pumi@2.2.7                      py-notebook@6.4.5               py-wcwidth@0.2.5
aml@0.1.0                       git@2.35.2                      libxrender@0.9.10               py-alembic@1.5.5                py-ntplib@0.4.0                 py-webencodings@0.5.1
amrex@22.05                     glib@2.72.1                     libxt@1.1.5                     py-anyio@3.5.0                  py-numexpr@2.7.3                py-websocket-client@1.2.1
amrex@22.05                     glib@2.72.1                     libxtst@1.2.2                   py-apache-libcloud@1.2.1        py-numexpr@2.7.3                py-wheel@0.37.0
ant@1.10.7                      globalarrays@5.8                libyaml@0.2.5                   py-argon2-cffi@21.3.0           py-numpy@1.21.5                 py-wheel@0.37.0
antlr@2.7.7                     glproto@1.4.17                  libyogrt@1.27                   py-argon2-cffi-bindings@21.2.0  py-numpy@1.22.3                 py-widgetsnbextension@3.6.0
arborx@1.1                      gmake@4.3                       libzmq@4.3.4                    py-astroid@2.11.4               py-oauthlib@3.1.1               py-wrapt@1.13.3
arborx@1.2                      gmp@6.2.1                       llvm@8.0.0                      py-asttokens@2.0.5              py-opentuner@0.8.7              py-ytopt-autotune@1.1.0
arborx@1.2                      gmp@6.2.1                       llvm@12.0.1                     py-async-generator@1.10         py-packaging@21.3               py-zipp@3.6.0
archer@2.0.0                    gobject-introspection@1.56.1    llvm-amdgpu@5.1.0               py-attrs@21.4.0                 py-pamela@1.0.0                 py-zope-event@4.5.0
argobots@1.1                    googletest@1.8.1                llvm-openmp-ompt@tr6_forwards   py-autograd@1.3                 py-pandas@1.4.2                 py-zope-interface@5.4.0
arpack-ng@3.8.0                 googletest@1.10.0               lua@5.3.5                       py-babel@2.9.1                  py-pandas@1.4.2                 pygmo@2.18.0
asio@1.16.1                     gotcha@1.0.3                    lua-luaposix@35.0               py-backcall@0.2.0               py-pandocfilters@1.5.0          python@3.8.13
asio@1.21.0                     gperf@3.1                       lwgrp@1.0.5                     py-bcrypt@3.2.0                 py-paramiko@2.7.1               python@3.8.13
assimp@5.2.3                    gperftools@2.9.1                lz4@1.9.3                       py-beniget@0.4.1                py-paramz@0.9.5                 qhull@2020.2
at-spi2-atk@2.38.0              gptune@3.0.0                    lzo@2.10                        py-black@22.1.0                 py-parse@1.18.0                 qt@5.15.4
at-spi2-core@2.40.1             graphlib@3.0.0                  m4@1.4.19                       py-bleach@4.1.0                 py-parsl@1.1.0                  qthreads@1.16
atk@2.36.0                      graphviz@2.49.0                 magma@2.6.2                     py-blinker@1.4                  py-parso@0.8.2                  raja@0.14.0
autoconf@2.69                   gsl@2.7.1                       mbedtls@2.28.0                  py-bottleneck@1.3.2             py-pathspec@0.9.0               raja@0.14.0
autoconf-archive@2022.02.11     harfbuzz@4.2.1                  med@4.0.0                       py-bottleneck@1.3.2             py-patsy@0.5.2                  randrproto@1.5.0
automake@1.15.1                 harfbuzz@4.2.1                  memkind@1.13.0                  py-certifi@2021.10.8            py-periodictable@1.5.0          rankstr@0.1.0
automake@1.16.5                 hdf5@1.8.22                     mercury@2.1.0                   py-certipy@0.1.3                py-petsc4py@3.17.1              readline@8.1
axl@0.3.0                       hdf5@1.10.7                     mercury@2.1.0                   py-cffi@1.15.0                  py-pexpect@4.8.0                recordproto@1.14.2
axl@0.5.0                       hdf5@1.12.2                     mesa@21.3.8                     py-charset-normalizer@2.0.12    py-pickleshare@0.7.5            redset@0.1.0
axom@0.6.1                      heffte@2.2.0                    meson@0.62.1                    py-cinemasci@1.7.0              py-picmistandard@0.0.19         renderproto@0.11.1
bdftopcf@1.0.5                  heffte@2.2.0                    meson@0.62.1                    py-click@8.0.3                  py-pika@0.13.0                  rocblas@5.1.0
berkeley-db@18.1.40             help2man@1.47.16                metall@0.20                     py-cloudpickle@1.6.0            py-pillow@9.0.0                 rocfft@5.1.0
binutils@2.38                   hip@5.1.0                       metis@5.1.0                     py-colorama@0.4.4               py-pip@21.3.1                   rocminfo@5.1.0
bison@3.8.2                     hipblas@5.1.0                   mfem@4.4.0                      py-configspace@0.4.20           py-pip@21.3.1                   rocprim@5.1.0
blaspp@2021.04.01               hipify-clang@5.1.0              mfem@4.4.0                      py-cppheaderparser@2.7.4        py-pkgconfig@1.5.5              rocrand@5.1.0
blaspp@2021.04.01               hipsparse@5.1.0                 mkfontdir@1.0.7                 py-cppy@1.1.0                   py-platformdirs@2.4.0           rocsolver@5.1.0
blt@0.4.1                       hpctoolkit@2022.04.15           mkfontscale@1.1.2               py-cryptography@3.2.1           py-ply@3.11                     rocsparse@5.1.0
blt@0.4.1                       hpcviewer@2022.03               mmg@5.6.0                       py-cryptography@3.4.8           py-poetry-core@1.0.8            rocthrust@5.1.0
bolt@2.0                        hpx@1.7.1                       mochi-margo@0.9.9               py-cycler@0.11.0                py-prometheus-client@0.12.0     ruby@3.1.0
boost@1.76.0                    hpx@1.7.1                       mount-point-attributes@master   py-cython@0.29.24               py-prompt-toolkit@3.0.29        ruby-hpricot@0.8.6
boost@1.79.0                    hsa-rocr-dev@5.1.0              mpark-variant@1.4.0             py-cython@3.0.0a9               py-psutil@5.8.0                 ruby-mustache@1.1.1
boost@1.79.0                    hsakmt-roct@5.1.0               mpc@1.2.1                       py-debugpy@1.5.1                py-ptyprocess@0.7.0             ruby-rdiscount@2.2.0.2
boost@1.79.0                    hwloc@2.7.1                     mpfr@4.1.0                      py-decorator@5.1.1              py-pure-eval@0.2.2              ruby-ronn@0.7.3
boost@1.79.0                    hypre@2.24.0                    mpfr@4.1.0                      py-defusedxml@0.7.1             py-py@1.11.0                    rust@1.60.0
boost@1.79.0                    icu4c@67.1                      mpich@4.0.2                     py-deprecation@2.1.0            py-pyaml@21.8.3                 rust@1.60.0
boost@1.79.0                    icu4c@67.1                      mpifileutils@0.11.1             py-dill@0.3.4                   py-pybind11@2.8.1               scotch@7.0.1
boost@1.79.0                    inputproto@2.3.2                mrnet@5.0.1-3                   py-docutils@0.18.1              py-pycairo@1.20.0               sed@4.2.2
boost@1.79.0                    intel-tbb@2020.3                munge@0.5.14                    py-entrypoints@0.4              py-pycparser@2.20               shared-mime-info@1.9
boost@1.79.0                    intel-xed@2022.04.17            muparser@2.2.6.1                py-executing@0.8.2              py-pyelftools@0.26              shuffile@0.1.0
butterflypack@2.1.1             intltool@0.51.0                 nasm@2.15.05                    py-filelock@3.5.0               py-pygments@2.10.0              slate@2021.05.02
bzip2@1.0.8                     jansson@2.13.1                  nccmp@1.9.0.1                   py-flit@3.6.0                   py-pyjwt@2.1.0                  slepc@3.17.1
c-blosc@1.21.1                  jq@1.6                          nco@5.0.1                       py-flit-core@3.6.0              py-pyjwt@2.1.0                  slepc@3.17.1
cabana@0.4.0                    json-c@0.15                     ncurses@6.2                     py-fn-py@0.5.2                  py-pylint@2.13.5                slepc@3.17.1
```

- All the versions coexist!
  - Multiple versions of same package are ok.
- Packages are installed to automatically find correct dependencies.
- Binaries work *regardless of user's environment*.
- Spack also generates module files.
  - Don't *have* to use them.

The Spack community is growing rapidly

- **Spack simplifies HPC software for:**
  - Users
  - Developers
  - Cluster installations
  - The largest HPC facilities
- **Spack is central to ECP's software strategy**
  - Enable software reuse for developers and users
  - Allow the facilities to consume the entire ECP stack
- **The roadmap is packed with new features:**
  - Building the ECP software distribution
  - Better workflows for building containers
  - Stacks for facilities
  - Chains for rapid dev workflow
  - Optimized binaries
  - Better dependency resolution

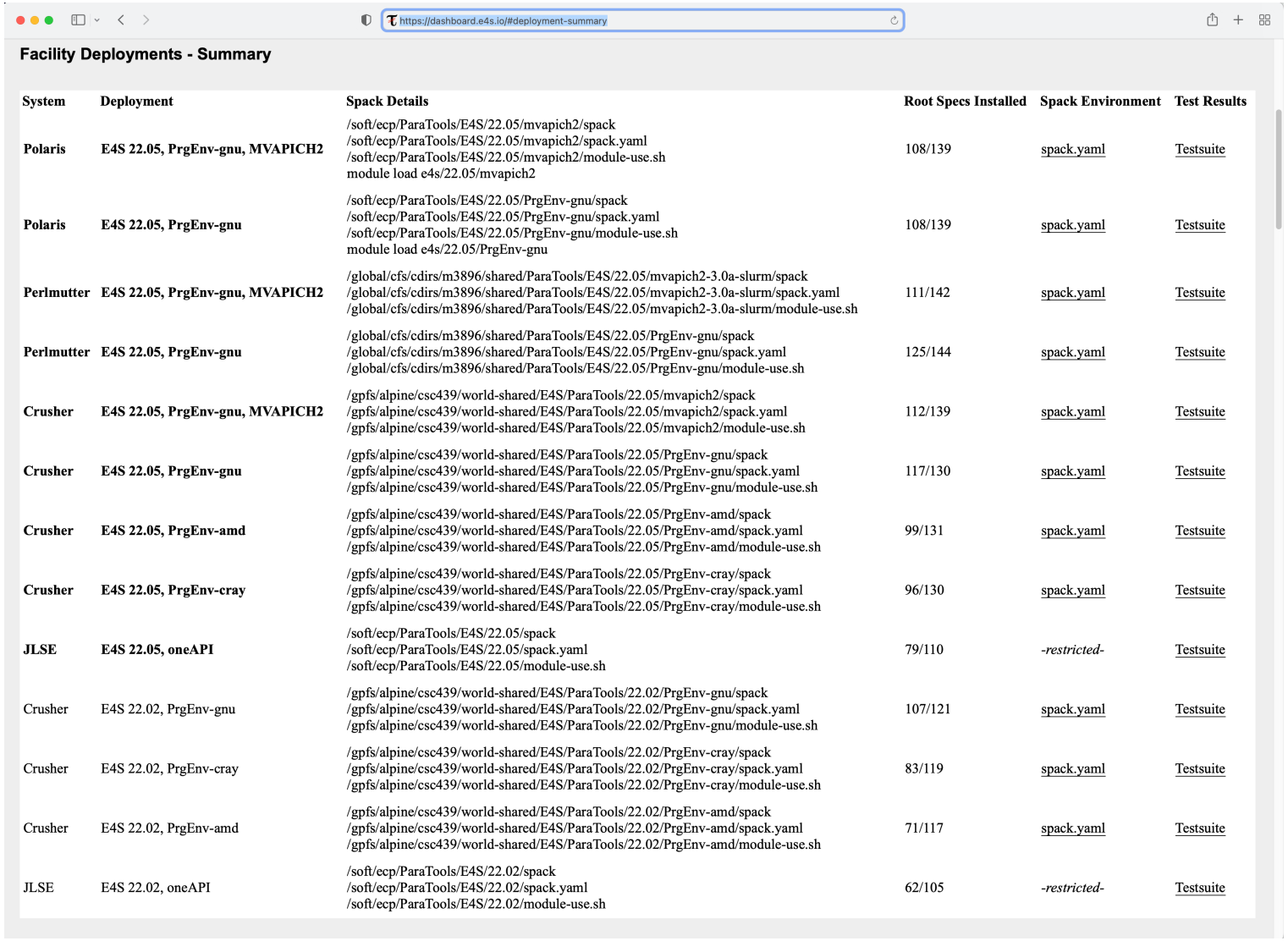


Visit spack.io

github.com/spack/spack

@spackpm

Facility Deployment: https://dashboard.e4s.io



Facility Deployments - Summary

System	Deployment	Spack Details	Root Specs Installed	Spack Environment	Test Results
Polaris	**E4S 22.05, PrgEnv-gnu, MVAPICH2**	/soft/ecp/ParaTools/E4S/22.05/mvapich2/spack /soft/ecp/ParaTools/E4S/22.05/mvapich2/spack.yaml /soft/ecp/ParaTools/E4S/22.05/mvapich2/module-use.sh module load e4s/22.05/mvapich2	108/139	spack.yaml	Testsuite
Polaris	**E4S 22.05, PrgEnv-gnu**	/soft/ecp/ParaTools/E4S/22.05/PrgEnv-gnu/spack /soft/ecp/ParaTools/E4S/22.05/PrgEnv-gnu/spack.yaml /soft/ecp/ParaTools/E4S/22.05/PrgEnv-gnu/module-use.sh module load e4s/22.05/PrgEnv-gnu	108/139	spack.yaml	Testsuite
Perlmutter	**E4S 22.05, PrgEnv-gnu, MVAPICH2**	/global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a-slurm/spack /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a-slurm/spack.yaml /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a-slurm/module-use.sh	111/142	spack.yaml	Testsuite
Perlmutter	**E4S 22.05, PrgEnv-gnu**	/global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack.yaml /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/module-use.sh	125/144	spack.yaml	Testsuite
Crusher	**E4S 22.05, PrgEnv-gnu, MVAPICH2**	/gpfs/alpine/csc439/world-shared/E4S/ParaTools/22.05/mvapich2/spack /gpfs/alpine/csc439/world-shared/E4S/ParaTools/22.05/mvapich2/spack.yaml /gpfs/alpine/csc439/world-shared/E4S/ParaTools/22.05/mvapich2/module-use.sh	112/139	spack.yaml	Testsuite
Crusher	**E4S 22.05, PrgEnv-gnu**	/gpfs/alpine/csc439/world-shared/E4S/ParaTools/22.05/PrgEnv-gnu/spack /gpfs/alpine/csc439/world-shared/E4S/ParaTools/22.05/PrgEnv-gnu/spack.yaml /gpfs/alpine/csc439/world-shared/E4S/ParaTools/22.05/PrgEnv-gnu/module-use.sh	117/130	spack.yaml	Testsuite
Crusher	**E4S 22.05, PrgEnv-amd**	/gpfs/alpine/csc439/world-shared/E4S/ParaTools/22.05/PrgEnv-amd/spack /gpfs/alpine/csc439/world-shared/E4S/ParaTools/22.05/PrgEnv-amd/spack.yaml /gpfs/alpine/csc439/world-shared/E4S/ParaTools/22.05/PrgEnv-amd/module-use.sh	99/131	spack.yaml	Testsuite
Crusher	**E4S 22.05, PrgEnv-cray**	/gpfs/alpine/csc439/world-shared/E4S/ParaTools/22.05/PrgEnv-cray/spack /gpfs/alpine/csc439/world-shared/E4S/ParaTools/22.05/PrgEnv-cray/spack.yaml /gpfs/alpine/csc439/world-shared/E4S/ParaTools/22.05/PrgEnv-cray/module-use.sh	96/130	spack.yaml	Testsuite
JLSE	**E4S 22.05, oneAPI**	/soft/ecp/ParaTools/E4S/22.05/spack /soft/ecp/ParaTools/E4S/22.05/spack.yaml /soft/ecp/ParaTools/E4S/22.05/module-use.sh	79/110	*-restricted-*	Testsuite
Crusher	E4S 22.02, PrgEnv-gnu	/gpfs/alpine/csc439/world-shared/E4S/ParaTools/22.02/PrgEnv-gnu/spack /gpfs/alpine/csc439/world-shared/E4S/ParaTools/22.02/PrgEnv-gnu/spack.yaml /gpfs/alpine/csc439/world-shared/E4S/ParaTools/22.02/PrgEnv-gnu/module-use.sh	107/121	spack.yaml	Testsuite
Crusher	E4S 22.02, PrgEnv-cray	/gpfs/alpine/csc439/world-shared/E4S/ParaTools/22.02/PrgEnv-cray/spack /gpfs/alpine/csc439/world-shared/E4S/ParaTools/22.02/PrgEnv-cray/spack.yaml /gpfs/alpine/csc439/world-shared/E4S/ParaTools/22.02/PrgEnv-cray/module-use.sh	83/119	spack.yaml	Testsuite
Crusher	E4S 22.02, PrgEnv-amd	/gpfs/alpine/csc439/world-shared/E4S/ParaTools/22.02/PrgEnv-amd/spack /gpfs/alpine/csc439/world-shared/E4S/ParaTools/22.02/PrgEnv-amd/spack.yaml /gpfs/alpine/csc439/world-shared/E4S/ParaTools/22.02/PrgEnv-amd/module-use.sh	71/117	spack.yaml	Testsuite
JLSE	E4S 22.02, oneAPI	/soft/ecp/ParaTools/E4S/22.02/spack /soft/ecp/ParaTools/E4S/22.02/spack.yaml /soft/ecp/ParaTools/E4S/22.02/module-use.sh	62/105	*-restricted-*	Testsuite

Default modules for E4S on JLSE and Polaris at ALCF for all users:

```
% module avail e4s/22.05
```

E4S 22.05 on Perlmutter using PrgEnv-gnu

```
sameer@perlmutter:login13:~> module use $CFS/m3896/shared/modulefiles
sameer@perlmutter:login13:~> module avail e4s

------------------------------------- /global/cfs/cdirs/m3896/shared/modulefiles -------------------------------------
   e4s/mvapich2/22.05    e4s/PrgEnv-gnu/22.05

---------------------------- /global/common/software/nersc/pm-2022.05.0/extra_modulefiles ----------------------------
   e4s/spack-develop    e4s/21.11-lmod    e4s/21.11-tcl (D)    spack/e4s-22.02 (D)

  Where:
   D:  Default Module

Use "module spider" to find all possible modules and extensions.
Use "module keyword key1 key2 ..." to search for all possible modules matching any of the "keys".


sameer@perlmutter:login13:~> module load e4s/PrgEnv-gnu

Due to MODULEPATH changes, the following have been reloaded:
  1) cray-mpich/8.1.15

sameer@perlmutter:login13:~> spack find +cuda cuda_arch=80
==> 25 installed packages
-- cray-sles15-zen3 / gcc@11.2.0 ---------------------------------
adios2@2.8.0   chai@2.4.0    hypre@2.24.0          legion@21.03.0  raja@0.14.0       sundials@6.2.0      zfp@0.5.5
arborx@1.2     ginkgo@1.4.0  kokkos@3.6.00         magma@2.6.2     slate@2021.05.02  superlu-dist@7.2.0
caliper@2.7.0  heffte@2.2.0  kokkos@3.6.00         mfem@4.4.0      slepc@3.17.1      tasmanian@7.7
camp@0.2.2     hpx@1.7.1     kokkos-kernels@3.6.00 petsc@3.17.1    strumpack@6.3.1   umpire@6.0.0
sameer@perlmutter:login13:~> module avail nvhpc

----- /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/share/spack/lmod/cray-sles15-x86_64/Core -----
   nvhpc/22.3

------------------------------------ /opt/cray/pe/lmod/modulefiles/mix_compilers -------------------------------------
   nvhpc-mixed/21.3    nvhpc-mixed/21.11 (D)

---------------------------------------- /opt/cray/pe/lmod/modulefiles/core ----------------------------------------
   nvhpc/21.3    nvhpc/21.11 (D)    PrgEnv-nvhpc/8.3.2    PrgEnv-nvhpc/8.3.3 (D)

------------------------------------------------- /opt/modulefiles -------------------------------------------------
   nvhpc/21.3    nvhpc/21.11
```

Perlmutter @ NERSC: E4S 22.05 with SLURM and gcc@11.2.0

```
 1: adios2             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/adios2-2.8.0-kif4mquqytlh4cybngifuux4fn3ivrtd
 2: aml                /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/aml-0.1.0-5gdlj3ickdtb27qq6p2kopfpdoxmui3t
 3: amrex              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/amrex-22.05-ft3rksivlgipqauadvsh7gxuis4izq6m
 4: arborx             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/arborx-1.2-tc4i6d3k6piplycwtmy6shbq2wba4tbp
 5: archer             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/archer-2.0.0-pa33i3csxzhlsd5t5nfcw64taxxrw7tx
 6: argobots           /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/argobots-1.1-nsmph2wbkrus4zx4jemebzhabx7qgr7y
 7: axom               /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/axom-0.6.1-gdjebwss54lr2capdigtrhh5zt6xd4u3
 8: bolt               /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/bolt-2.0-7hf4fziabmplaj7hryhps5cozunhymyv
 9: butterflypack      /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/butterflypack-2.1.1-ooghq5wo5xszwmojoew4g74rscnzwmsg
10: cabana             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/cabana-0.4.0-l2bj6kvhvuxd3xabnrv3p272oqq2b65v
11: caliper            /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/caliper-2.7.0-svgn26f3u7qha5626zeftyf2mbrkkpis
12: chai               /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/chai-2.4.0-w6sv4m7r4r2hxawg63yrw5j55aikxqqx
13: charliecloud       /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/charliecloud-0.26-czgnnskv4k7rjfcjxv3ndy62lwk44skb
14: conduit            /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/conduit-0.8.3-wkjkgnso3xzjtj63gg3heby3kp72btef
15: darshan-runtime    /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/darshan-runtime-3.3.1-44lbnty4ftucbf7gowla26ztvdkovxvt
16: datatransferkit    /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/datatransferkit-3.1-rc3-ivroczm2xowtjvtyqoj5a5rk6o6tuec7
17: dyninst            /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/dyninst-12.1.0-wickbpnislxl6iztkpnnigte4jtiiych
18: faodel             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/faodel-1.2108.1-isf6laqpcman3qr73lk64d5jaacngw3j
19: flit               /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/flit-2.1.0-bhhseffdpfpuewy53ztrrqrv5k3vsnl2
20: fortrilinos        /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/fortrilinos-2.0.0-zlzgmeycesulqwzidlgwm2juplygs4kg
21: gasnet             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/gasnet-2022.3.0-bwmz3brqu4oqcttgs6ibkeztmxyqtxjm
22: ginkgo             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/ginkgo-1.4.0-qvk5kjo3gpqzxlsompq27ddbjd3irjtd
23: globalarrays       /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/globalarrays-5.8-rhohqdk3vg3icaoxtn6q46wia3zl3bwp
24: gotcha             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/gotcha-1.0.3-s2xkdnmdusbrxwuhssqvgrcsh7rnhucn
25: gptune             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/gptune-3.0.0-k4q6zkfhkctseol46lvbhek54ulwgrw6
26: hdf5               /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/hdf5-1.12.2-bubavnl5ec5lmfxd3ck3g4jtjtym7fsk
27: heffte             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/heffte-2.2.0-wgagrclzssnki6aqtmcrpqsr2jvkutjl
28: hpx                /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/hpx-1.7.1-xuw726mdztobnu7api6jowdhgcr6zgz4
29: hypre              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/hypre-2.24.0-2okdvy7gxanlhtwnvvum2uvo3ntjmwhr
30: kokkos             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/kokkos-3.6.00-7eud56psz6e63wkwkoi2722fq7n645vl
31: kokkos-kernels     /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/kokkos-kernels-3.6.00-lcqcx55m2chvnyizpfboscsivhialepe
32: lammps             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/lammps-20220107-uk7x4i2eio4yvgwk5e4rxws5coerrvpz
33: legion             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/legion-21.03.0-53f3b6ytkfwl5fnux5yz3uka3bl5cshr
34: libquo             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/libquo-1.3.1-5ju66szpfhrwpkbd6o2lwhhkitrnwy5v
35: magma              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/magma-2.6.2-zwuh6mm62fc5oe6ypvkmgajbizz4hkzq
36: mercury            /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/mercury-2.1.0-leykx65oexkkj6xh4fnt5glmzoq7tcho
37: metall             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/metall-0.20-ncgmfczomrownqbgxvinm4tz5exdfa7s
38: mfem               /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/mfem-4.4.0-iyvynznmxdoxacwoynhfbz5ru2clxvwe
```

Perlmutter @ NERSC: E4S 22.05 with SLURM and gcc@11.2.0

```
39: mpark-variant       /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/mpark-variant-1.4.0-uvr4bft4rni7i254ctevurkikuv36z6x
40: nccmp               /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/nccmp-1.9.0.1-pwjdebjxx7bk4glw573b4lekjfybuk5g
41: nco                 /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/nco-5.0.1-dtzaouk2bid2kqyijzqodu773x75sqvj
42: netlib-scalapack    /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/netlib-scalapack-2.2.0-dhiu327cln5fql3djmya2q56sudyuyve
43: nrm                 /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/nrm-0.1.0-7dphpnstxxwwtvqjfqtne2vm25syq5ok
44: omega-h             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/omega-h-9.34.1-mpoe4zlgqnls7hpavj6quk62luzom5lw
45: openmpi             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/openmpi-4.1.3-gw3a4bvon2tyeg55baaui7pvedk45c42
46: openpmd-api         /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/openpmd-api-0.14.4-dx3hlgyze2mdfuvlfouvjwgghkdzodgn
47: papi                /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/papi-6.0.0.1-o5pxe7ejjzala2y5bwreiv6utoldk4mz
48: papyrus             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/papyrus-1.0.2-twr7purknxy6ympux6xdqnfmlau5l5rq
49: parsec              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/parsec-3.0.2012-vuxyi7v3czbng3vicfoydu4j5s53he6n
50: pdt                 /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/pdt-3.25.1-4wzbhsadvu6upir6eowsqbymg2op3a5j
51: petsc               /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/petsc-3.17.1-v5gxr3udlpadu6b24sy5mdf73xfmynwb
52: plasma              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/plasma-21.8.29-6wzczv2jqnn23s7gc2ujfxq3yvzy4ckb
53: precice             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/precice-2.4.0-v7wscgidow3wlmn4chqgxow4kgjdhrqn
54: pumi                /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/pumi-2.2.7-ff2gzmwq5b4l7uvtfxcqechbdfbf2edf
55: py-cinemasci        /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/py-cinemasci-1.7.0-j7sbb2inxxr5piawm2wy4uhb4jfrbesf
56: py-jupyterhub       /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/py-jupyterhub-1.4.1-jsyxh242wzampidb5r355lx7bd4tixwb
57: py-libensemble      /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/py-libensemble-0.9.1-ppigxh7jxsypyupqilgt2vje4m3x3zyn
58: qthreads            /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/qthreads-1.16-s32g45lb5o62o7fmlkcbyb4rrzvp6pug
59: raja                /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/raja-0.14.0-ztcuu26vls3eibwdi6pfxw22qryfluki
60: scr                 /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/scr-3.0rc2-s3cjkoco7bok3bqzw44sjt54qwikzh7v
61: slate               /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/slate-2021.05.02-wkdnguku4cicegrntu4pu4p5j5u7o3b5
62: slepc               /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/slepc-3.17.1-t5dplaioot4kzutfmoegqpnka5voxw2n
63: strumpack           /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/strumpack-6.3.1-vdjhqejektpmxzu3kr2dnpj7anc32om6
64: sundials            /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/sundials-6.2.0-dn7ff7ianhsyvu7g2ybegqbfeapipteg
65: superlu-dist        /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/superlu-dist-7.2.0-h2asqfgiihip3kws2clrfz3yzkzqnv5p
66: swig                /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/swig-4.0.2-fortran-orersnc6ghyazliftwa6qvk2lhttpcxe
67: sz                  /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/sz-2.1.12-dkedzzkzogqrhlazcwrusoa67icas3nc
68: tasmanian           /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/tasmanian-7.7-55rvccldbgb53cwkprl2ybexdqvqkvxf
69: tau                 /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/tau-2.31.1-x75mktmygps6ew5mps7em4mvaauivgq3
70: trilinos            /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/trilinos-13.0.1-yft4mfqzoyqauhlh3mqbmc2jcmjsrwpw
71: umap                /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/umap-2.1.0-5ryuhmh3tefsqtfiv3dayyegjepxob2d
72: umpire              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/umpire-6.0.0-4wkonl77m7w53j554ak7juwxu26fbhrv
73: veloc               /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/veloc-1.5-3zk6uqg36fu7ctmqunrroof2bnykz3mr
74: zfp                 /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/zfp-0.5.5-jha3y22e7gajahbmut6qfwlq3fwvtie3
```

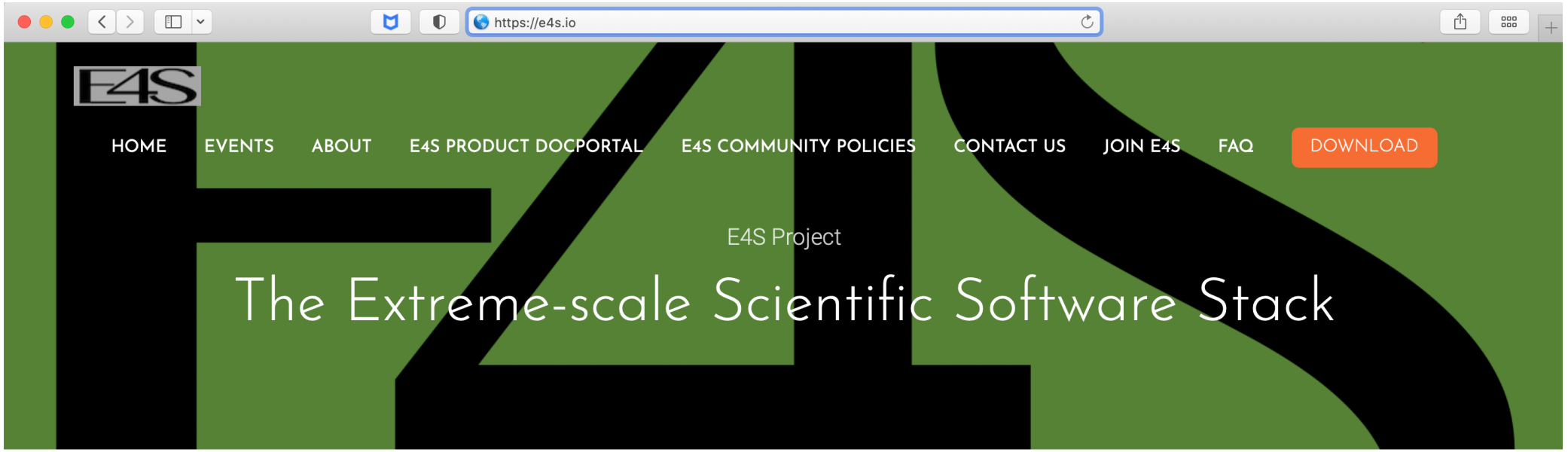
Perlmutter @ NERSC: E4S 22.05 with PrgEnv-gnu

```
 1: adios2              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/adios2-2.8.0-ebqgj4m7gva7iiulnloq2qfq2zj75wot
 2: aml                 /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/aml-0.1.0-5gdlj3ickdtb27qq6p2kopfpdoxmui3t
 3: amrex               /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/amrex-22.05-rkmj3qh35wjczpsgqz2kmiks5zvliooj
 4: arborx              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/arborx-1.2-dzq55sqp43ukm47m6tmqpwfjt5ccdp37
 5: archer              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/archer-2.0.0-pa33i3csxzhlsd5t5nfcw64taxxrw7tx
 6: argobots            /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/argobots-1.1-nsmph2wbkrus4zx4jemebzhabx7qgr7y
 7: axom                /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/axom-0.6.1-arx3rdkr6dcwtnnmbzvyuqyej3363qpm
 8: bolt                /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/bolt-2.0-7hf4fziabmplaj7hryhps5cozunhymyv
 9: butterflypack       /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/butterflypack-2.1.1-n5jtjakqydwx43iw5eb44qber623nxm3
10: cabana              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/cabana-0.4.0-ywmdbzwhmfsq4ozmaneglmhr5q6ap5v3
11: caliper             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/caliper-2.7.0-tenxvf32vmze54krfcuo5onpploexkdo
12: chai                /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/chai-2.4.0-aclkrr5ozppae3utmoaehmvud6kbsbex
13: charliecloud        /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/charliecloud-0.26-czgnnskv4k7rjfcjxv3ndy62lwk44skb
14: conduit             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/conduit-0.8.3-dinrfzrgynaiodrske75dv3fdo7oyvno
15: darshan-runtime     /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/darshan-runtime-3.3.1-imunxqtyb2b33h6ragdwj2wpcwtowvcp
16: datatransferkit     /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/datatransferkit-3.1-rc3-oom6wpuwop4fmhuhc7gdwhtojzihu6f4
17: dyninst             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/dyninst-12.1.0-7cz2lmh7lhsh27llesnxlehs4xb4ji2l
18: faodel              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/faodel-1.2108.1-e4gshfews4qmgec5vwkqv3tkfsmvfti6
19: flecsi              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/flecsi-1.4.2-mp3xmyaqwa5yyzerhem77n2z7rsesjio
20: flit                /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/flit-2.1.0-bhhseffdpfpuewy53ztrrqrv5k3vsnl2
21: flux-sched          /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/flux-sched-0.22.0-fvp6nkzgaaxgwh5ticecxegfa5pc2jou
22: fortrilinos         /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/fortrilinos-2.0.0-i4onp4upkkvd3rojciouceqs2crttlqa
23: gasnet              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/gasnet-2022.3.0-bwmz3brqu4oqcttgs6ibkeztmxyqtxjm
24: ginkgo              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/ginkgo-1.4.0-qvk5kjo3gpqzxlsompq27ddbjd3irjtd
25: globalarrays        /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/globalarrays-5.8-7fcamxiwkukxhmr4zuhm7dfdgnwwp2xj
26: gotcha              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/gotcha-1.0.3-s2xkdnmdusbrxwuhssqvgrcsh7rnhucn
27: gptune              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/gptune-3.0.0-k4q6zkfhkctseol46lvbhek54ulwgrw6
28: hdf5                /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/hdf5-1.12.2-nhriei2p4726tu72qalywexiza7hi6jw
29: heffte              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/heffte-2.2.0-xrarvwgyout4cm4ydpi37swbxvxwnt4l
30: hpctoolkit          /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/hpctoolkit-2022.04.15-ixt7dgumm32e3zuxgbztvisgho6z2h5f
31: hpx                 /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/hpx-1.7.1-cdmvjsvgg26p72tb3kbcktlag4a66kmw
32: hypre               /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/hypre-2.24.0-loubbk3bpkh6lnz53g6setwmx4pqsyx6
33: kokkos              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/kokkos-3.6.00-yq47xesrwau5hkvizotenpdq2gwscaf5
34: kokkos-kernels      /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/kokkos-kernels-3.6.00-vxyxliujcemrwkbg22jhm3kohbpz6bxr
35: lammps              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/lammps-20220107-dm2c3slvgxprezhhazhdm5swe64yelxh
36: legion              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/legion-21.03.0-53f3b6ytkfwl5fnux5yz3uka3bl5cshr
37: libquo              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/libquo-1.3.1-fl2s7e6im2fhajouta5xxkkp7w2pek6i
38: magma               /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/magma-2.6.2-zwuh6mm62fc5oe6ypvkmgajbizz4hkzq
39: mercury             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/mercury-2.1.0-nhzjaqz556sldnrog2dag5vdpqcf627u
40: metall              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/metall-0.20-skcxyx6dq5r6lfypnsywmxg5v7ed6h73
41: mfem                /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/mfem-4.4.0-lxsd7oqkkfgkqyglcvfrq235d6ain7yn
```

Perlmutter @ NERSC: E4S 22.05 with PrgEnv-gnu

```
42: mpark-variant       /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/mpark-variant-1.4.0-uvr4bft4rni7i254ctevurkikuv36z6x
43: mpifileutils        /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/mpifileutils-0.11.1-zs6fdx5wxdpuoilayjtj47rrtqckj2z4
44: nccmp               /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/nccmp-1.9.0.1-mfryg4t3s46zirshzvu4lz7gqeabhlmq
45: nco                 /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/nco-5.0.1-tk7gnyokee7zip6kp3vr46fx2vawak36
46: netlib-scalapack    /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/netlib-scalapack-2.2.0-dhiu327cln5fql3djmya2q56sudyuyve
47: nrm                 /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/nrm-0.1.0-7dphpnstxxwwtvqjfqtne2vm25syq5ok
48: omega-h             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/omega-h-9.34.1-bc76qpjlaqn4ttohy6fgav5u7v2zrqfy
49: openmpi             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/openmpi-4.1.3-gw3a4bvon2tyeg55baaui7pvedk45c42
50: openpmd-api         /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/openpmd-api-0.14.4-m6ohwjdwzjsytqf4spkvk2ygmlrqx4ns
51: papi                /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/papi-6.0.0.1-o5pxe7ejjzala2y5bwreiv6utoldk4mz
52: papyrus             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/papyrus-1.0.2-ggjpdneiuvyoizfwkiqlhedwjqxje47w
53: parallel-netcdf     /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/parallel-netcdf-1.12.2-zwbammyyjbbfunvurlbh3g7qvmq3mmkn
54: parsec              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/parsec-3.0.2012-xyu7xpkvn2c7hrx7vysha4da2cduwrgf
55: pdt                 /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/pdt-3.25.1-4wzbhsadvu6upir6eowsqbymg2op3a5j
56: petsc               /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/petsc-3.17.1-u7tsfkjnw3onz7fojsbywagkezuzyrss
57: phist               /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/phist-1.9.5-lq76cw473chjmuvevsjnwhfwdmlcdwdq
58: plasma              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/plasma-21.8.29-6wzczv2jqnn23s7gc2ujfxq3yvzy4ckb
59: precice             /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/precice-2.4.0-v2gv4iluyrsbuzhpqb5b446puffbpel6
60: pumi                /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/pumi-2.2.7-wr6bmv2lfpybzxw3sufv3m4irdbjevt7
61: py-cinemasci        /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/py-cinemasci-1.7.0-rucnpuzn73dvwvxzcslcdl3vf2a2utqp
62: py-jupyterhub       /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/py-jupyterhub-1.4.1-jsyxh242wzampidb5r355lx7bd4tixwb
63: py-libensemble      /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/py-libensemble-0.9.1-c7orlymeeivselyvwsinivq5ybtdks3u
64: qthreads            /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/qthreads-1.16-s32g45lb5o62o7fmlkcbyb4rrzvp6pug
65: raja                /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/raja-0.14.0-ztcuu26vls3eibwdi6pfxw22qryfluki
66: scr                 /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/scr-3.0rc2-tsd5ivq6fxy44zlg7cziasvd7sog4efp
67: slate               /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/slate-2021.05.02-3qul2vtqh24ixhwjg3xxznjluua6qa5r
68: slepc               /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/slepc-3.17.1-mbijafs75iqzjaft6nj3lbqcjz6aai5p
69: stc                 /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/stc-0.9.0-sm5urbkheg4rxnqof4bjf4j4yzgdneoc
70: strumpack           /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/strumpack-6.3.1-iapp37z5vat2tyejpv5zynflbhqhys2n
71: sundials            /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/sundials-6.2.0-kn5wm4foklvkm6oj6d4riyt275ygi5ul
72: superlu-dist        /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/superlu-dist-7.2.0-bsd63xtzha3klfkgm3wqklblc4swkinu
73: swig                /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/swig-4.0.2-fortran-orersnc6ghyazliftwa6qvk2lhttpcxe
74: sz                  /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/sz-2.1.12-dkedzzkzogqrhlazcwrusoa67icas3nc
75: tasmanian           /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/tasmanian-7.7-vizyvcrjtsqyd2epn6fjebkzjhtpzbwp
76: tau                 /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/tau-2.31.1-icww2pa2es56isc4gzgjmcnj5tbehajj
77: trilinos            /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/trilinos-13.0.1-rhk32i353nr3dyivggfy3g6kuhc4uklr
78: umap                /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/umap-2.1.0-5ryuhmh3tefsqtfiv3dayyegjepxob2d
79: umpire              /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/umpire-6.0.0-birc3ndlvj5ds6poer2djbreduxipxgx
80: veloc               /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/veloc-1.5-45ipct3s3i3htlbp6dg7sraipoz4pruh
81: zfp                 /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/zfp-0.5.5-jha3y22e7gajahbmut6qfwlq3fwvtie3
```

E4S Download from https://e4s.io



E4S 22.05 is now available!

See Downloads for more information.

What is E4S?

The Extreme-scale Scientific Software Stack (E4S) is a community effort to provide open source software packages for developing, deploying and running scientific applications on high-performance computing (HPC) platforms. E4S provides from-source builds and containers of a broad collection of HPC software packages.

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

Container Releases

- Docker Downloads - CUDA
- Docker Downloads - ROCm
- Docker Downloads - OneAPI
- Singularity x86_64 Download - CUDA
- Singularity ppc64le Download - CUDA
- Singularity x86_64 Download - ROCm
- Singularity x86_64 Download - OneAPI
- OVA Download

From source with Spack

Visit the Spack Project

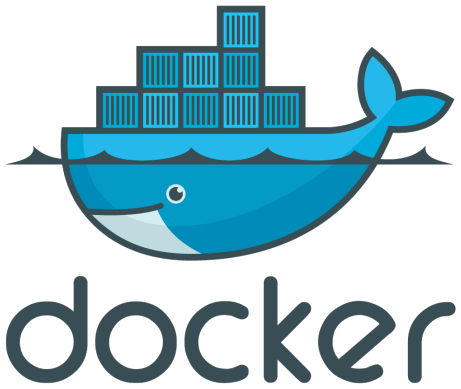
Spack contains packages for all of the products listed in the E4S 22.05 Full Release category (see above Release Notes). General instructions for building software with Spack can be found at the Spack website. Questions concerning building those packages are deferred to the associated package development team.

- Separate full featured Singularity images for 3 GPU architectures
- GPU base images for
  - x86_64 (Intel, AMD, NVIDIA)
  - ppc64le
  - aarch64

https://e4s.io

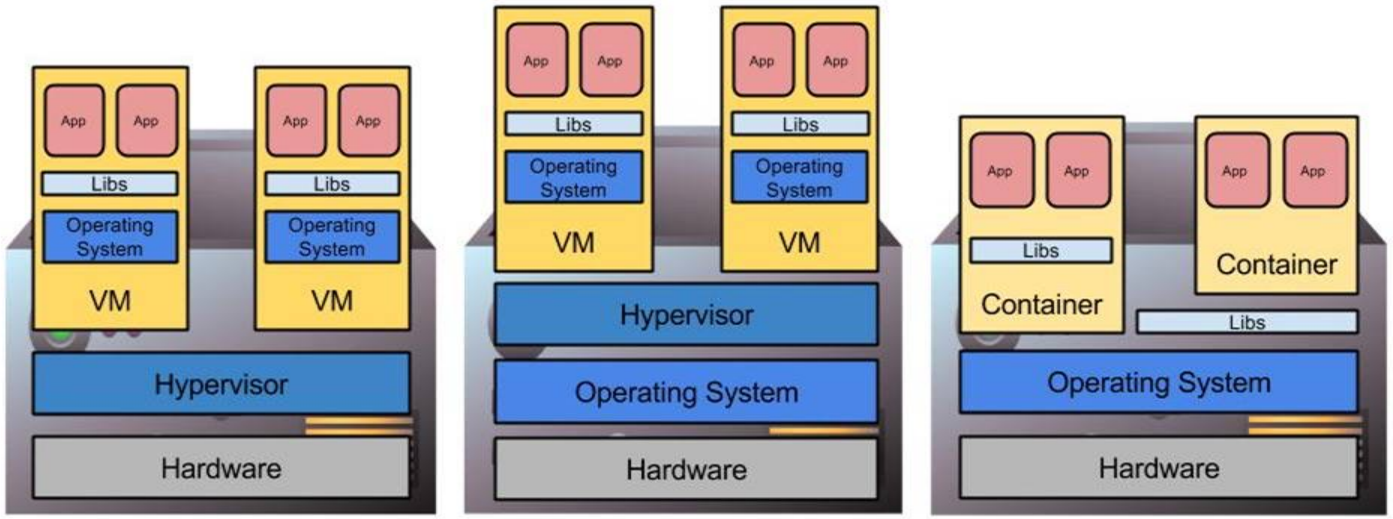
What are containers

- A lightweight collection of executable software that encapsulates everything needed to run a single specific task
  - Minus the OS kernel
  - Based on Linux only
- Processes and all user-level software is isolated
- Creates a portable* software ecosystem
- Think `chroot` on steroids
- Docker most common tool today
  - Available on all major platforms
  - Widely used in industry
  - Integrated container registry via Dockerhub



Hypervisors and Containers

- Type 1 hypervisors insert layer below host OS
- Type 2 hypervisors work as or within the host OS
- Containers do not abstract hardware, instead provide “enhanced chroot” to create isolated environment
- Location of abstraction can have impact on performance
- All enable custom software stacks on existing hardware



Type 1 Hypervisor Type 2 Hypervisor Containers

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:22.05
```

```
# docker pull ecpe4s/e4s-rocm:22.05
```

```
# docker pull ecpe4s/e4s-oneapi:22.05
```

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:22.05 docker

e4s-rocm-22.05.sif mirror 1

NVIDIA CUDA (x86_64, ppc64le)

ecpe4s/e4s-cuda:22.05 docker

e4s-cuda-x86_64-22.05.sif mirror 1

e4s-cuda-ppc64le-22.05.sif mirror 1

Intel OneAPI (x86_64)

ecpe4s/e4s-oneapi:22.05 docker

e4s-oneapi-22.05.sif mirror 1

https://e4s.io

Download E4S 22.05 Base GPU Container Images

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:22.05 docker

e4s-base-cuda-x86_64-22.05.sif mirror 1

e4s-base-cuda-aarch64-22.05.sif mirror 1

e4s-base-cuda-ppc64le-22.05.sif mirror 1

ROCM X86_64

ecpe4s/e4s-base-rocm:22.05 docker

e4s-base-rocm-22.05.sif mirror 1

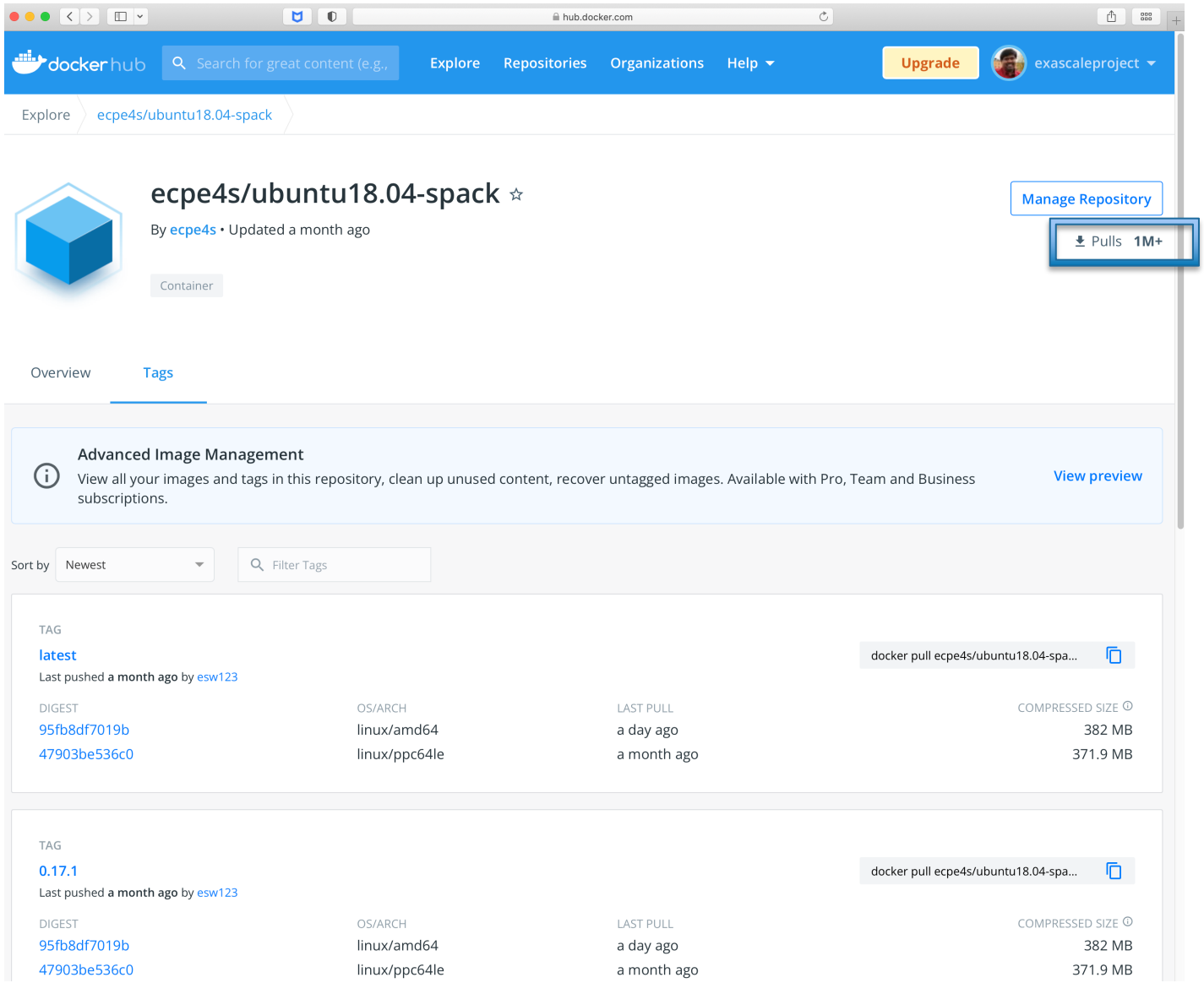
Intel OneAPI X86_64

ecpe4s/e4s-base-oneapi:22.05 docker

e4s-base-oneapi-22.05.sif mirror 1

https://e4s.io

Minimal Spack base image on Dockerhub



- Create custom container images
- 1M+ downloads!

22.05 Release: 101 Official Products + dependencies (gcc, x86_64)

```
 1: adios2          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/adios2-2.8.0-5fxpauervqbotprybms3mwkgh7t6jc6v
 2: alquimia        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/alquimia-1.0.9-mkugz7joihpf4umcyidflg3dwik2nvlr
 3: aml             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/aml-0.1.0-ogtiuh4diyg4tq47tfjdpw7nue7sa5ka
 4: amrex           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/amrex-22.05-7tgphdtmt3fmoijkfrfsnwbqzpikxqfs
 5: arborx          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/arborx-1.2-a5j5wjdwqatoqsvs6xjckootv76g5h32
 6: archer          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/archer-2.0.0-zurunmhys3lwxhqn3ffapnelmezog2gl
 7: argobots        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/argobots-1.1-prj5il35vpp7sgcclenbh2thzqvrylwf
 8: ascent          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/ascent-0.8.0-qgivng4ownyfzct535vkvzle6irkjaq2
 9: axom            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/axom-0.6.1-ammuobdcyxxfsoyl7pyvbgyvw3kysoaj
10: bolt            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/bolt-2.0-mb62bsxs7cvgisgkww4m46qffxvfknfz
11: bricks          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/bricks-r0.1-5qkeva7iiqimec7zwsgvd33tz4mddslz
12: butterflypack   /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/butterflypack-2.1.1-fhncpxhwa4agoogz7magi6flubctqdp6
13: cabana          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/cabana-0.4.0-obd2epyboqn4pifoqwfiojyszqi6npoc
14: caliper         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/caliper-2.7.0-5scpuxjsztlwgbpclgpw3kafmfvbp3ub
15: chai            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/chai-2.4.0-l6nclfuapgjlbctkriikyeo3mhdatl5l
16: charliecloud    /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/charliecloud-0.26-wgnmvl3rceimjvrcstuogmhlzhelz466
17: conduit         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/conduit-0.8.3-hm2j65mka5alpsg4uc4dswqvp7fusqvz
18: darshan-runtime /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/darshan-runtime-3.3.1-ausjp6wozamwgyhgxiv22qcsarxvoixy
19: datatransferkit /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/datatransferkit-3.1-rc3-xd57qoqxv4ikmz7ypfowrmnboqtohwq4
20: dyninst         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/dyninst-12.1.0-du56qu4uijap4synulxijiwury3dni5h
21: faodel          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/faodel-1.2108.1-kvw27w57ny2achbuhpiu3cweudqnin7h
22: flecsi          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/flecsi-1.4.2-fzhunvoffnf7l4sssl6l5ufukbrftc5u
23: flit            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/flit-2.1.0-j4naqyymm6h4mofj5id6sfit5ngr4xh6
24: flux-sched      /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/flux-sched-0.22.0-nfljuuoxqlk4r7zx3yoepyzjjjfxsqkz
25: fortrilinos     /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/fortrilinos-2.0.0-uobhjnniqweeclzx7awlhcmvxitktwo5
26: gasnet          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/gasnet-2022.3.0-ep4xyqocdziblie475bojotd6qgpfpse
27: geopm           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/geopm-1.1.0-3bxmokjvkuh4gmymmu6b4iqhss5zq352
28: ginkgo          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/ginkgo-1.4.0-l6ahxdmshvwqrl6rmke7w4p3i5d5ehyd
29: globalarrays    /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/globalarrays-5.8-y42lqtmfsq6nddv7vu5z3bjxbqjz6yww
30: gotcha          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/gotcha-1.0.3-cidwbtn2h7xjqzvajljks3idskhr3dcv
31: gptune          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/gptune-3.0.0-bjtlsqmghh24awymzp5g3fxt6wiequ3n
32: h5bench         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/h5bench-1.2-x5gqhbii26t7f4e3bpscw5wbhfg5qlhb
33: hdf5            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/hdf5-1.12.2-75qn37lp7leuvlsrbizprz5o5yr3ekjo
```

22.05 Release: 101 Official Products + dependencies (gcc, x86_64)

```
34: heffte                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/heffte-2.2.0-hqigomw3nlexreke2rgquwvdazenvhb2
35: hpctoolkit            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/hpctoolkit-2022.04.15-cqz4vlmjclq6qmxp4sonlrqiz4twl2sh
36: hpx                   /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/hpx-1.7.1-o7y77tofbg4jg2vcvfhjgdsqtckzhw3v
37: hypre                 /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/hypre-2.24.0-c7vk7oprzxpfs6njr42xn632tksu64ax
38: kokkos                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/kokkos-3.6.00-fy3onzyijziq2x2laoxu7rttrwhaqufj
39: kokkos-kernels        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/kokkos-kernels-3.6.00-gn7fvng67ekhwt324xo45lizuxea327n
40: lammps                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/lammps-20220107-pmr5l5hzxruzhpzkucukg7qqr6os5iir
41: legion                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/legion-21.03.0-g3tu5cdevxuzsrvcqinaxrgduik3ea54
42: libnrm                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/libnrm-0.1.0-gjllhvje7in4rp3kvvaywywr7uyjprxj
43: libquo                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/libquo-1.3.1-2o7zqn3e2f7je3o3z4hcwsqgkn6bjmme
44: loki                  /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/loki-0.1.7-66nzpehhmoidzifzm6khyxhnbfgmppoa
45: magma                 /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/magma-2.6.2-mmx2xmmz7cbcjbc2j3vn6eoxrwgivu24
46: mercury               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mercury-2.1.0-yzp4mkdsnmcf5dgsein4ek2co7eag763
47: metall                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/metall-0.20-6o2ewhyu2ilxbco74j5qqdeunqjkmgta
48: mfem                  /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mfem-4.4.0-cra7q4353kgqdow7futlc5vik5hf4bu6
49: mpich                 /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mpich-4.0.2-ssbmd2ccbxzkbxk7fzrlekupe23rokw2
50: mpifileutils          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mpifileutils-0.11.1-zvlai7bnjegicp5dzelxnvwmvu6sye5j
51: netlib-scalapack      /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/netlib-scalapack-2.2.0-l2chii6rgvnp6rswldzqxza7trgpdkib
52: nccmp                 /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/nccmp-1.9.0.1-ef6vn4ls3rj7wieuygnpf5c2i4trzpvo
53: nco                   /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/nco-5.0.1-xlix5wvr6bprihee7rryknegskv4sjho
54: nrm                   /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/nrm-0.1.0-cyiqhjsurt3q4bkn37u2ylvzhgdtmuuu
55: omega-h               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/omega-h-9.34.1-3d4zvshz6tj7twd3nqcnebls4zwryrvm
56: openpmd-api           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/openpmd-api-0.14.4-6ktbupm7eqmq73vflxkjiapn3kanomm4
57: openmpi               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/openmpi-4.1.3-p5q2yggpo7lhcn2n26deo25ymx3thdwt
58: papi                  /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/papi-6.0.0.1-fxfxybh2varhxhnu6jcrqsg5ixrrcxp2
59: papyrus               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/papyrus-1.0.2-r2wef2ldj24dluqgd43hjn23fxowxet2
60: parallel-netcdf       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/parallel-netcdf-1.12.2-7ruhgcy35hofq4goi6c3d42tteuhqlwl
61: paraview              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/paraview-5.10.1-ohruf5tnfp2yeywlslszty5jfbq6pjw7
62: parsec                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/parsec-3.0.2012-dcaz2iwq6nrz7l6kcwpwsbeftpb3urv6
63: pdt                   /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/pdt-3.25.1-d5jyjfrocerrcl5cxqwsfrbv5l776d7r
64: petsc                 /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/petsc-3.17.1-vffv6b2ykiy3a4lxuoe7dzi4zggbrdqb
65: phist                 /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/phist-1.9.5-vxmwjbns3kywtogpldhhmouoehgi7d2m
66: plasma                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/plasma-21.8.29-hwpchnbrscxsmzgyioeepsjwddgnunxm
```

22.05 Release: 101 Official Products + dependencies (gcc, x86_64)

```
 67: plumed          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/plumed-2.6.3-g6dn67baochvycvcicgeltwjnvotgjk2
 68: precice         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/precice-2.4.0-orye5yx46n4mm2zey7xeg5k5i222twiw
 69: pruners-ninja   /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/pruners-ninja-1.0.1-hn6y2kevr5hgmlykfverjadgbgxkppcn
 70: pumi            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/pumi-2.2.7-zkipah7wz3a4eksedht2syqpx3tcg6ki
 71: py-cinemasci    /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/py-cinemasci-1.7.0-77yj2xigharoeq6lciw4mzngexnegxmc
 72: py-jupyterhub   /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/py-jupyterhub-1.4.1-3cebk5prfze6najqsdabftwxgqkccmwm
 73: py-libensemble  /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/py-libensemble-0.9.1-noalxjfvyidhsvps4zn7mhu4j5hf2wo6
 74: py-parsl        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/py-parsl-1.1.0-ul2cthsh524npmv6zrseklzodp6ej4en
 75: py-radical-saga /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/py-radical-saga-1.11.1-naxx4rp2e6wr7oo24jw3catzys26loya
 76: qthreads        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/qthreads-1.16-v7vcyz7vakzdyzpa3mjdbnov4s55a6vw
 77: raja            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/raja-0.14.0-edjvff74mwcz7fngfj4qlatpplxs5vzl
 78: rempi           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/rempi-1.1.0-yoa3gfri6iafv2l2avkhg25pzpgiftwg
 79: scr             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/scr-3.0rc2-mibyx3jm6nkm4gq7ovpbwe4kpwxnwou6
 80: slate           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/slate-2021.05.02-6krdeny5oeki4o2slafxstn7wa6vgmlq
 81: slepc           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/slepc-3.17.1-fzx6e3h2jqmsvhgbeclbwuirqrax7hkl
 82: stc             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/stc-0.9.0-vd4xaiuv4ryo4tzqzqvnsr4qwtndyyxq
 83: strumpack       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/strumpack-6.3.1-du3qimqp3yrjcso22pw2zsbbswgrtsay
 84: sundials        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/sundials-6.2.0-5iz6lim5mabrkkukic63lipmz5r6lmvb
 85: superlu-dist    /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/superlu-dist-7.2.0-2jp6torp4rjf44hhffm56glemlegfoyb
 86: swig            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/swig-4.0.2-fortran-fjva3hpwop4b3dmrmguisinqdrt2ixyk
 87: sz              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/sz-2.1.12-kzqvvvdo5fvv2s6sgheei7ikwgsbsd7m
 88: tasmanian       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/tasmanian-7.7-5q6657fcerfpwshuhdmrowzvxpoo25tt
 89: tau             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/tau-2.31.1-ikx2r2pk34hej3rmjqoam5ma6rvzbuqm
 90: trilinos        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/trilinos-13.2.0-hmpjtr4o7fnpffcg6m6b4pl73ipr422e
 91: turbine         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/turbine-1.3.0-aztpwwbbjeogl5bwiznmpx2lcyos64cz
 92: umap            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/umap-2.1.0-blwc2edy5e3lkrylgbrwfd55slyuuy4s
 93: umpire          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/umpire-6.0.0-gwbap637zehqkvjwmetuqcgjtkwhzzlo
 94: unifyfs         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/unifyfs-0.9.2-hcid7bugnj4vzetl4oh4zfnah2gzsctb
 95: upcxx           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/upcxx-2022.3.0-fpv2zorgjpac5iuqibffz57h6x3xhrjr
 96: variorum        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/variorum-0.4.1-fcfi26hd2dfvnwe5gehtv4iqx36hafj7
 97: veloc           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/veloc-1.5-avca7jodby7efy3be63siav4mqao2big
 98: vtk-m           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/vtk-m-1.7.1-hbilfvhsgkelno7jrvr6fffyn6guusxf
 99: wannier90       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/wannier90-3.1.0-vzfixrlicq5jrtzj2wpd6bg7nbkqdit6
100: warpx           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/warpx-22.05-gtg2e5dwy3lzr53t7fsyzscbj25gzu2m
101: zfp             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/zfp-0.5.5-3cc5y5ffuvxtdsiurtrt4blcbodbxj2p
```

GPU runtimes

- Intel (oneAPI)
  - 2022.1.0
- AMD (ROCm)
  - 5.1.1
- NVIDIA (CUDA)
  - 11.4
- NVHPC
  - 22.3

E4S 22.05 container deployment on Perlmutter using Shifter

- E4S containers
- Accessing A100 GPUs
- CUDA 11.5

```
sameer@perlmutter:login19:~> shifter --image=ecpe4s/e4s-base-cuda:22.05 /bin/bash --rcfile /etc/bashrc

Inactive Modules:
  1) PrgEnv-gnu     3) cray-libsci     5) craype                7) craype-x86-milan     9) libfabric         11) xpmem
  2) cray-dsmml     4) cray-mpich      6) craype-network-ofi    8) gcc                 10) perftools-base

Lmod is automatically replacing "cray-mpich/8.1.15" with "mpich/4.0.2".

(base) sameer@login19:~$ cat /etc/os-release
NAME="Ubuntu"
VERSION="20.04.4 LTS (Focal Fossa)"
ID=ubuntu
ID_LIKE=debian
PRETTY_NAME="Ubuntu 20.04.4 LTS"
VERSION_ID="20.04"
HOME_URL="https://www.ubuntu.com/"
SUPPORT_URL="https://help.ubuntu.com/"
BUG_REPORT_URL="https://bugs.launchpad.net/ubuntu/"
PRIVACY_POLICY_URL="https://www.ubuntu.com/legal/terms-and-policies/privacy-policy"
VERSION_CODENAME=focal
UBUNTU_CODENAME=focal
(base) sameer@login19:~$ nvidia-smi
Tue Jun 14 07:23:04 2022
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 470.103.01   Driver Version: 470.103.01   CUDA Version: 11.5     |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|                               |                      |               MIG M. |
|===============================+======================+======================|
|   0  NVIDIA A100-PCI...  Off  | 00000000:C3:00.0 Off |                    0 |
| N/A   39C    P0    38W / 250W |      0MiB / 40536MiB |      0%      Default |
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                                  |
|  GPU   GI   CI        PID   Type   Process name                  GPU Memory |
|        ID   ID                                                   Usage      |
|=============================================================================|
|  No running processes found                                                 |
+-----------------------------------------------------------------------------+
(base) sameer@login19:~$ spack find
==> 21 installed packages
-- linux-ubuntu20.04-x86_64 / gcc@9.4.0 --------------------------
cmake@3.23.1  libfabric@1.14.1  libxml2@2.9.13  lua-luafilesystem@1_8_0  ncurses@6.2     readline@8.1  xz@5.2.5
curl@7.83.0   libiconv@1.16     lmod@8.7.2      lua-luaposix@35.0        nvhpc@22.3      tcl@8.6.12    yaksa@0.2
hwloc@2.7.1   libpciaccess@0.16 lua@5.3.5       mpich@4.0.2              openssl@1.1.1o  unzip@6.0     zlib@1.2.12
(base) sameer@login19:~$ which mpicc
/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mpich-4.0.2-ssbmd2ccbxzkbxk7fzrlekupe23rokw2/bin/mpicc
```

E4S 22.05 packages built with support for A100 GPUs in a container

- AI/ML
- HPC

```
sameer@perlmutter:login19:~> shifterimg images | grep e4s | grep :22.05
perlmutter docker     READY    cd20a7d2c5   2022-06-14T06:59:30 ecpe4s/e4s-base-cuda:22.05
perlmutter docker     READY    7832c93f11   2022-06-14T07:53:07 ecpe4s/e4s-cuda:22.05
sameer@perlmutter:login19:~> shifter --image=ecpe4s/e4s-cuda:22.05 /bin/bash --rcfile /etc/bashrc

Inactive Modules:
  1) PrgEnv-gnu     3) cray-libsci     5) craype                7) craype-x86-milan     9) libfabric         11) xpmem
  2) cray-dsmml     4) cray-mpich      6) craype-network-ofi    8) gcc                 10) perftools-base


Lmod is automatically replacing "cray-mpich/8.1.15" with "mpich/4.0.2".

(base) sameer@login19:~$ grep Ubuntu /etc/os-release
NAME="Ubuntu"
PRETTY_NAME="Ubuntu 20.04.4 LTS"
(base) sameer@login19:~$ nvidia-smi
Tue Jun 14 08:39:09 2022
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 470.103.01   Driver Version: 470.103.01   CUDA Version: 11.5     |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|                               |                      |               MIG M. |
|===============================+======================+======================|
|   0  NVIDIA A100-PCI...  Off  | 00000000:C3:00.0 Off |                    0 |
| N/A   41C    P0    38W / 250W |      0MiB / 40536MiB |      0%      Default |
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                                  |
|  GPU   GI   CI        PID   Type   Process name                  GPU Memory |
|        ID   ID                                                   Usage      |
|=============================================================================|
|  No running processes found                                                 |
+-----------------------------------------------------------------------------+
(base) sameer@login19:~$ which mpicc
/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mpich-4.0.2-ssbmd2ccbxzkbxk7fzrlekupe23rokw2/bin/mpicc
(base) sameer@login19:~$ spack find +cuda cuda_arch=80
==> 27 installed packages
-- linux-ubuntu20.04-x86_64 / gcc@9.4.0 --------------------------
adios2@2.8.0   camp@0.2.2    heffte@2.2.0  kokkos@3.6.00          magma@2.6.2      petsc@3.17.1     slepc@3.17.1     superlu-dist@7.2.0  umpire@6.0.0
arborx@1.2     chai@2.4.0    hpx@1.7.1     kokkos@3.6.00          mfem@4.4.0       raja@0.14.0      strumpack@6.3.1  tasmanian@7.7       vtk-m@1.7.1
caliper@2.7.0  ginkgo@1.4.0  hypre@2.24.0  kokkos-kernels@3.6.00  parsec@3.0.2012  slate@2021.05.02 sundials@6.2.0   trilinos@13.2.0     zfp@0.5.5
(base) sameer@login19:~$ python
Python 3.9.7 (default, Sep 16 2021, 13:09:58)
[GCC 7.5.0] :: Anaconda, Inc. on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import tensorflow
>>> tensorflow.config.list_physical_devices('GPU')
[PhysicalDevice(name='/physical_device:GPU:0', device_type='GPU')]
>>>
(base) sameer@login19:~$
```

E4S 22.05 Release: Support for NVIDIA GPUs

```
Singularity> python
Python 3.9.7 (default, Sep 16 2021, 13:09:58)
[GCC 7.5.0] :: Anaconda, Inc. on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import tensorflow as tf
>>> tf.__version__
'2.9.1'
>>> tf.config.list_physical_devices('GPU')
[PhysicalDevice(name='/physical_device:GPU:0', device_type='GPU'), PhysicalDevice(name='/physical_device:GPU:1', device_type='GPU')]
>>> import torch
>>> torch.__version__
'1.11.0+cu113'
>>> torch.cuda.get_device_name(torch.cuda.current_device())
'NVIDIA A100-PCIE-40GB'
>>>
Singularity> spack find -l +cuda cuda_arch=80
==> 27 installed packages
-- linux-ubuntu20.04-x86_64 / gcc@9.4.0 --------------------------
5fxpaue adios2@2.8.0   hqigomw heffte@2.2.0          mmx2xmm magma@2.6.2       fzx6e3h slepc@3.17.1        gwbap63 umpire@6.0.0
a5j5wjd arborx@1.2     o7y77to hpx@1.7.1             cra7q43 mfem@4.4.0        du3qimq strumpack@6.3.1     hbilfvh vtk-m@1.7.1
5scpuxj caliper@2.7.0  c7vk7op hypre@2.24.0          dcaz2iw parsec@3.0.2012   5iz6lim sundials@6.2.0      3cc5y5f zfp@0.5.5
5nftkwe camp@0.2.2     kn4ult3 kokkos@3.6.00         mvt3juo petsc@3.17.1      2jp6tor superlu-dist@7.2.0
l6nclfu chai@2.4.0     fy3onzy kokkos@3.6.00         edjvff7 raja@0.14.0       5q6657f tasmanian@7.7
l6ahxdm ginkgo@1.4.0   gn7fvng kokkos-kernels@3.6.00 6krdeny slate@2021.05.02  hmpjtr4 trilinos@13.2.0
Singularity> spack find -l +cuda cuda_arch=70
==> 27 installed packages
-- linux-ubuntu20.04-x86_64 / gcc@9.4.0 --------------------------
mvzqvxg adios2@2.8.0   zz33g5c heffte@2.2.0          7ddf6kl magma@2.6.2       td7e334 slepc@3.17.1        hjgbyxh umpire@6.0.0
2wllnpi arborx@1.2     zrpfbiq hpx@1.7.1             hyuvayy mfem@4.4.0        66zzxrb strumpack@6.3.1     stzpxgb vtk-m@1.7.1
xb3ix2x caliper@2.7.0  m735zlc hypre@2.24.0          37dtmme parsec@3.0.2012   ykvyvrc sundials@6.2.0      ldaf46p zfp@0.5.5
etalgqv camp@0.2.2     dmru53c kokkos@3.6.00         2lsmpfg petsc@3.17.1      7bbqseb superlu-dist@7.2.0
rjky53t chai@2.4.0     xwt7ck4 kokkos@3.6.00         ttunttv raja@0.14.0       r7artq7 tasmanian@7.7
36fsm5m ginkgo@1.4.0   k47b42d kokkos-kernels@3.6.00 yeairhs slate@2021.05.02  qpycht6 trilinos@13.2.0
Singularity>
```

E4S 22.05 Release: GUI Tools

```
Singularity> module load paraview
Singularity> which paraview
/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/paraview-5.10.1-ohruf5tnfp2yeywlslszty5jfbq6pjw7/bin/paraview
Singularity> module load visit
Singularity> which visit
/usr/local/visit/bin/visit
Singularity> which paraprof
/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/tau-2.31.1-ikx2r2pk34hej3rmjqoam5ma6rvzbuqm/bin/paraprof
Singularity> module load julia
Singularity> julia
               _
   _       _ _(_)_     |  Documentation: https://docs.julialang.org
  (_)     | (_) (_)    |
   _ _   _| |_  __ _   |  Type "?" for help, "]?" for Pkg help.
  | | | | | | |/ _` |  |
  | | |_| | | | (_| |  |  Version 1.7.3 (2022-05-06)
 _/ |\__'_|_|_|\__'_|  |  Official https://julialang.org/ release
|__/                   |

julia>
Singularity> nvidia-smi
Tue May 31 23:33:39 2022
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 470.57.02    Driver Version: 470.57.02    CUDA Version: 11.4     |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|                               |                      |               MIG M. |
|===============================+======================+======================|
|   0  NVIDIA A100-PCI...  Off  | 00000000:25:00.0 Off |                    0 |
| N/A   42C    P0    37W / 250W |      0MiB / 40536MiB |      0%      Default |
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+
|   1  NVIDIA A100-PCI...  Off  | 00000000:E1:00.0 Off |                    0 |
| N/A   38C    P0    37W / 250W |      0MiB / 40536MiB |     32%      Default |
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+
```

E4S 22.02 bare-metal Spack installation environments on GitHub

https://github.com/E4S-Project/e4s/blob/master/environments/22.02/spack-x86_64.yaml

```yaml
packages:
  all:
    compiler:
    - gcc@9.3.0
    providers:
      blas:
      - openblas
      mpi:
      - mpich
    target:
    - x86_64
    variants: +mpi
  binutils:
    variants: +ld +gold +headers +libiberty ~nls
    version:
    - 2.36.1
  cuda:
    version:
    - 11.4.2
  doxygen:
    version:
    - 1.8.20
  elfutils:
    variants: +bzip2 ~nls +xz
  hdf5:
    variants: +fortran +hl +shared
    version:
    - 1.10.7
  libfabric:
    variants: fabrics=sockets,tcp,udp,rxm
  libunwind:
    variants: +pic +xz
  mesa:
    variants: ~llvm
  mesa18:
    variants: ~llvm
  mpich:
    variants: ~wrapperrpath
  ncurses:
    variants: +termlib
  openblas:
    variants: threads=openmp
  python:
    version:
    - 3.8.12
  trilinos:
    variants: +amesos +amesos2 +anasazi +aztec +belos +boost +epetra +epetraext
      +ifpack +ifpack2 +intrepid +intrepid2 +isorropia +kokkos +ml +minitensor +muelu
      +nox +piro +phalanx +rol +rythmos +sacado +stk +shards +shylu +stokhos +stratimikos
      +teko +tempus +tpetra +trilinoscouplings +zoltan +zoltan2 +superlu-dist gotype=long_long
```

spack.yaml

E4S 22.02 bare-metal installation spack.yaml recipe

https://github.com/E4S-Project/e4s/blob/master/environments/22.02/spack-x86_64.yaml

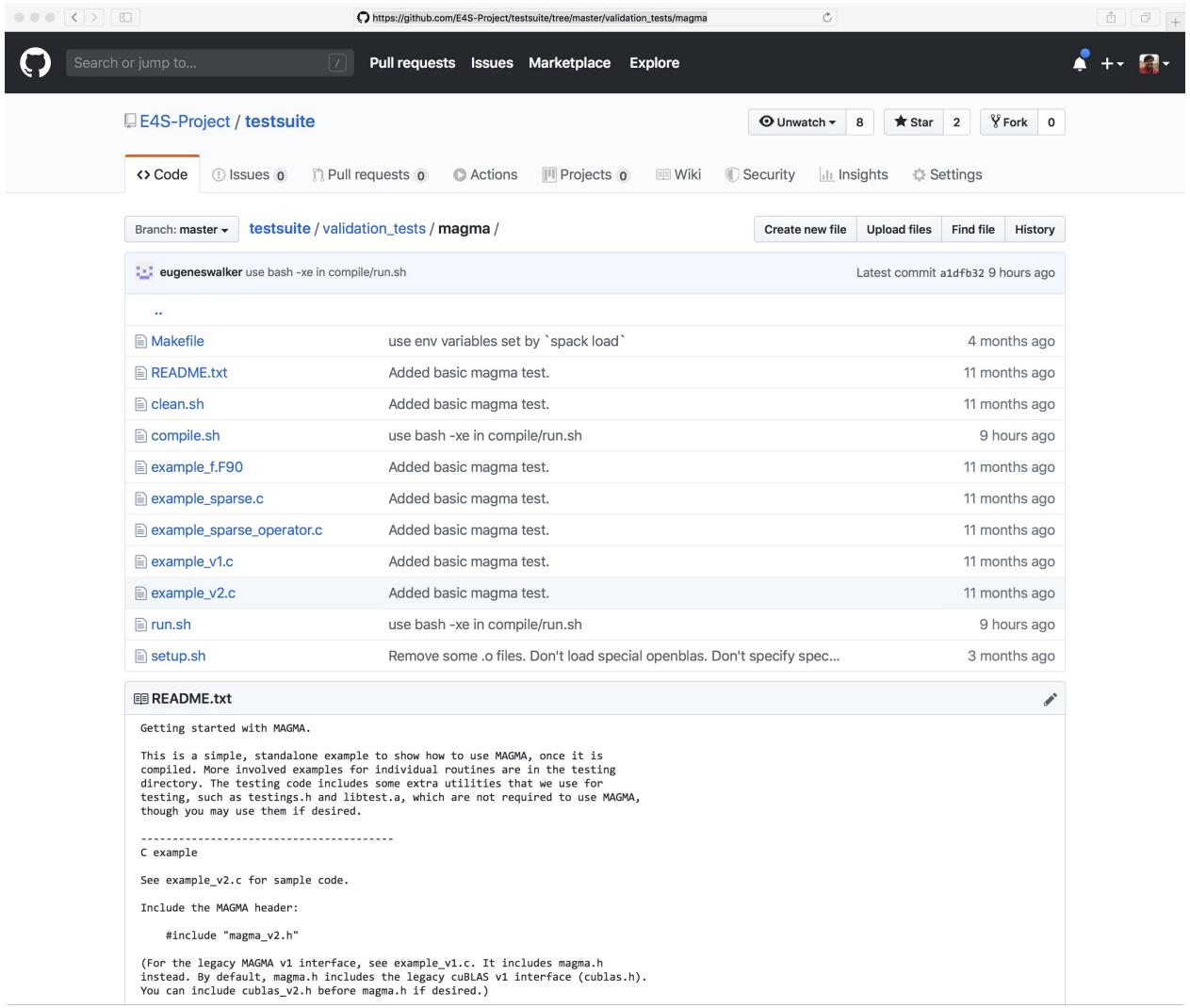
```
  - cuda_specs:
    - amrex@22.02 +cuda cuda_arch=80
    - caliper@2.7.0 +cuda cuda_arch=80
    - chai@2.4.0 ~benchmarks ~tests +cuda cuda_arch=80 ^umpire@6.0.0 ~shared
    - flecsi@2.1.0 +cuda cuda_arch=80
    - flux-core@0.35.0 +cuda # not CudaPackage
    - ginkgo@1.4.0 +cuda cuda_arch=80
    - heffte@2.2.0 +cuda cuda_arch=80
    - hpctoolkit@2022.01.15 +cuda # not CudaPackage
    - hpx@1.7.1 +cuda cuda_arch=80
    - hypre@2.24.0 +cuda cuda_arch=80
    - kokkos-kernels@3.5.00 +cuda cuda_arch=80 ^kokkos@3.5.00 +wrapper +cuda cuda_arch=80
    - kokkos@3.5.00 +wrapper +cuda cuda_arch=80
    - magma@2.6.1 +cuda cuda_arch=80
    - mfem@4.3.0 +cuda cuda_arch=80
    - openmpi@4.1.2 +cuda # not CudaPackage
    - papi@6.0.0.1 +cuda # not CudaPackage
    - parsec@3.0.2012 +cuda cuda_arch=80
    - petsc@3.16.4 +cuda cuda_arch=80
    - raja@0.14.0 +cuda cuda_arch=80
    - slate@2021.05.02 +cuda cuda_arch=80
    - slepc@3.16.2 +cuda cuda_arch=80
    - strumpack@6.3.0 ~slate +cuda cuda_arch=80
    - sundials@6.1.1 +cuda cuda_arch=80
    - superlu-dist@7.2.0 +cuda cuda_arch=80
    - tasmanian@7.7 +cuda cuda_arch=80
    - trilinos@13.2.0 +cuda cuda_arch=80
    - umpire@6.0.0 ~shared +cuda cuda_arch=80
    - vtk-m@1.7.1 +cuda cuda_arch=80
    - zfp@0.5.5 +cuda cuda_arch=80
    #- arborx@1.1 +cuda # not CudaPackage
    #- ascent@0.7.1 ~shared +cuda cuda_arch=80
    #- axom@0.6.1 +cuda cuda_arch=80 ^umpire ~shared
    #- cabana@0.4.0 +cuda # not CudaPackage
    #- dealii@9.3.2 +cuda cuda_arch=80 # gmsh
    #- legion@21.03.0 +cuda cuda_arch=80
    #- llvm@13.0.0 +cuda cuda_arch=80
    #- paraview@5.10.0 +cuda cuda_arch=80
    #- upcxx@2021.9.0 +cuda # not CudaPackage, needs driver

  - rocm_specs:
    - amrex@22.02 +rocm amdgpu_target=gfx908
    - chai@2.4.0 ~benchmarks +rocm amdgpu_target=gfx908
    - ginkgo@1.4.0 +rocm amdgpu_target=gfx908
    - heffte@2.2.0 +rocm amdgpu_target=gfx908
    - hpx@1.7.1 +rocm amdgpu_target=gfx908
    - kokkos@3.5.00 +rocm amdgpu_target=gfx908
    - magma@2.6.1 ~cuda +rocm amdgpu_target=gfx908
    - mfem@4.3.0 +rocm amdgpu_target=gfx908
    - petsc@3.16.4 +rocm amdgpu_target=gfx908
    - raja@0.14.0 ~openmp +rocm amdgpu_target=gfx908
    - slate@2021.05.02 +rocm amdgpu_target=gfx908
    - slepc@3.16.2 +rocm amdgpu_target=gfx908 ^petsc +rocm amdgpu_target=gfx908
    - strumpack@6.3.0 ~slate +rocm amdgpu_target=gfx908
```

- E4S products built with CUDA for A100
- Built with ROCm for MI100 and MI250X
- Built with oneAPI

E4S Validation Test Suite

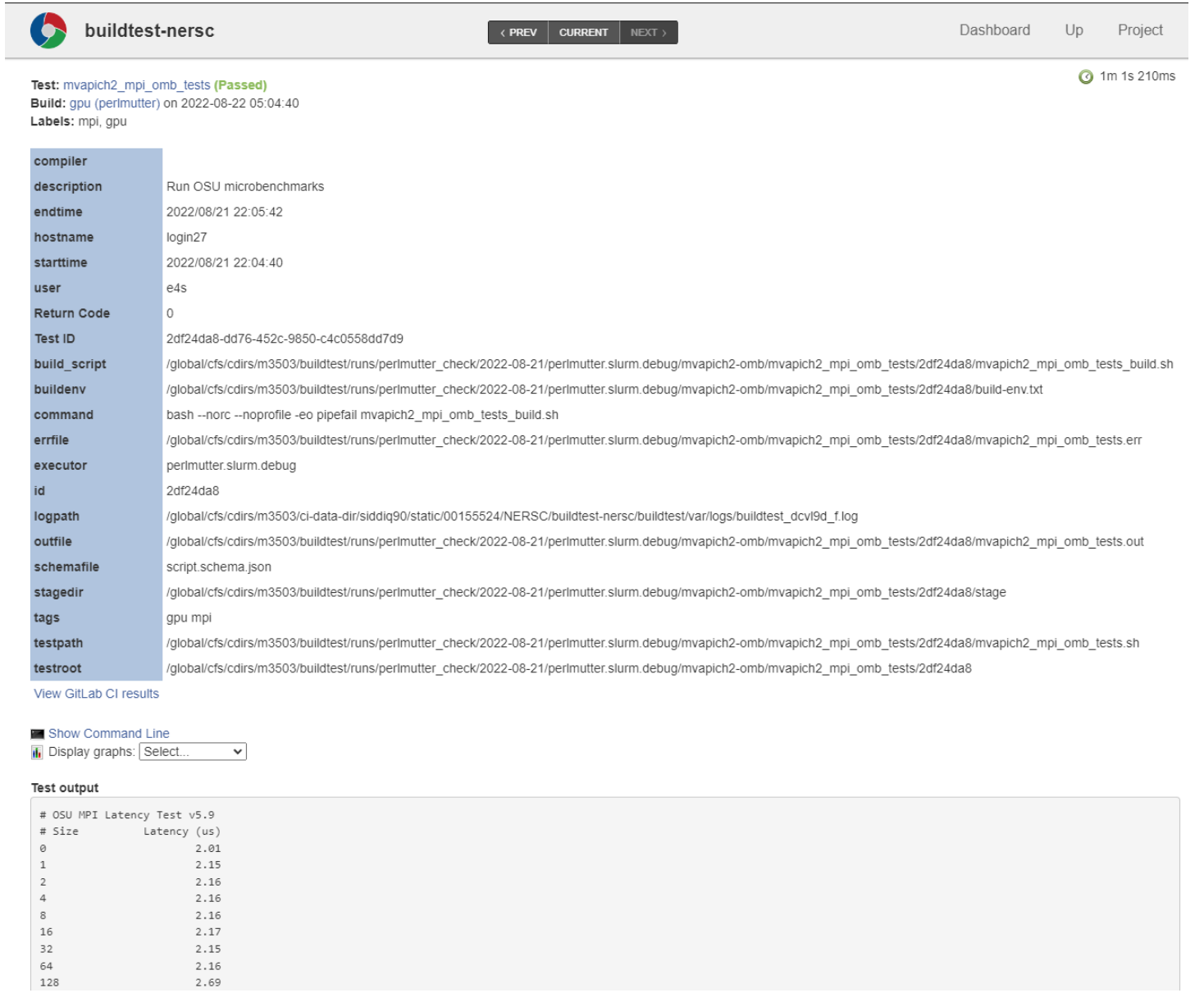
- Provides automated build and run tests
- Validate container environments and products
- New LLVM validation test suite for DOE LLVM



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

E4S MPI Tests (OMB) using Buildtest @ NERSC

- CI/CD using GitLab
- Buildtest integration



buildtest-nersc

‹ PREV | CURRENT | NEXT ›

Dashboard Up Project

1m 1s 210ms

Test: mvapich2_mpi_omb_tests **(Passed)**
Build: gpu (perlmutter) on 2022-08-22 05:04:40
Labels: mpi, gpu

compiler	
description	Run OSU microbenchmarks
endtime	2022/08/21 22:05:42
hostname	login27
starttime	2022/08/21 22:04:40
user	e4s
Return Code	0
Test ID	2df24da8-dd76-452c-9850-c4c0558dd7d9
build_script	/global/cfs/cdirs/m3503/buildtest/runs/perlmutter_check/2022-08-21/perlmutter.slurm.debug/mvapich2-omb/mvapich2_mpi_omb_tests/2df24da8/mvapich2_mpi_omb_tests_build.sh
buildenv	/global/cfs/cdirs/m3503/buildtest/runs/perlmutter_check/2022-08-21/perlmutter.slurm.debug/mvapich2-omb/mvapich2_mpi_omb_tests/2df24da8/build-env.txt
command	bash --norc --noprofile -eo pipefail mvapich2_mpi_omb_tests_build.sh
errfile	/global/cfs/cdirs/m3503/buildtest/runs/perlmutter_check/2022-08-21/perlmutter.slurm.debug/mvapich2-omb/mvapich2_mpi_omb_tests/2df24da8/mvapich2_mpi_omb_tests.err
executor	perlmutter.slurm.debug
id	2df24da8
logpath	/global/cfs/cdirs/m3503/ci-data-dir/siddiq90/static/00155524/NERSC/buildtest-nersc/buildtest/var/logs/buildtest_dcvl9d_f.log
outfile	/global/cfs/cdirs/m3503/buildtest/runs/perlmutter_check/2022-08-21/perlmutter.slurm.debug/mvapich2-omb/mvapich2_mpi_omb_tests/2df24da8/mvapich2_mpi_omb_tests.out
schemafile	script.schema.json
stagedir	/global/cfs/cdirs/m3503/buildtest/runs/perlmutter_check/2022-08-21/perlmutter.slurm.debug/mvapich2-omb/mvapich2_mpi_omb_tests/2df24da8/stage
tags	gpu mpi
testpath	/global/cfs/cdirs/m3503/buildtest/runs/perlmutter_check/2022-08-21/perlmutter.slurm.debug/mvapich2-omb/mvapich2_mpi_omb_tests/2df24da8/mvapich2_mpi_omb_tests.sh
testroot	/global/cfs/cdirs/m3503/buildtest/runs/perlmutter_check/2022-08-21/perlmutter.slurm.debug/mvapich2-omb/mvapich2_mpi_omb_tests/2df24da8

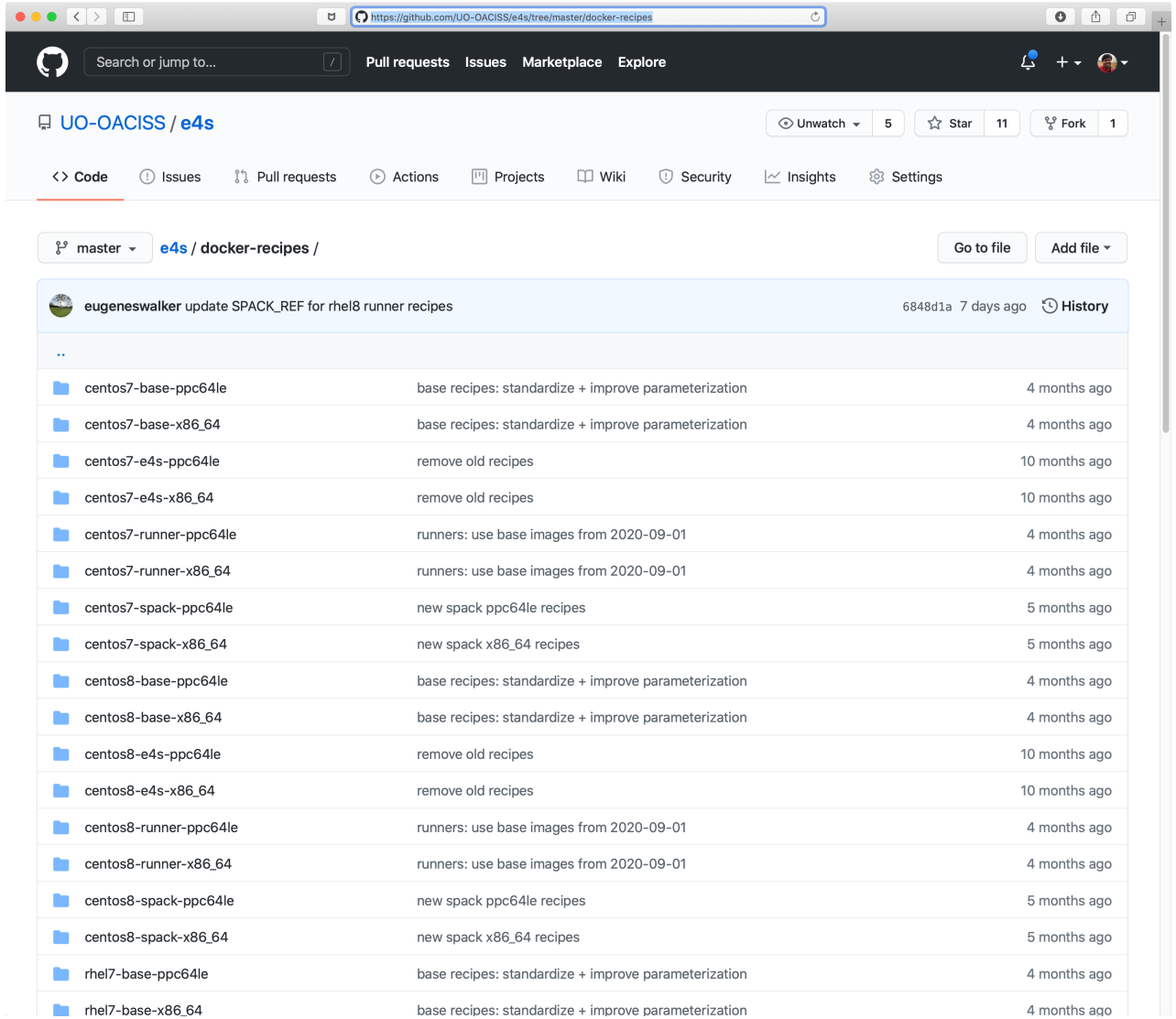
View GitLab CI results

Show Command Line
Display graphs: Select...

Test output

```
# OSU MPI Latency Test v5.9
# Size          Latency (us)
0                       2.01
1                       2.15
2                       2.16
4                       2.16
8                       2.16
16                      2.17
32                      2.15
64                      2.16
128                     2.69
```

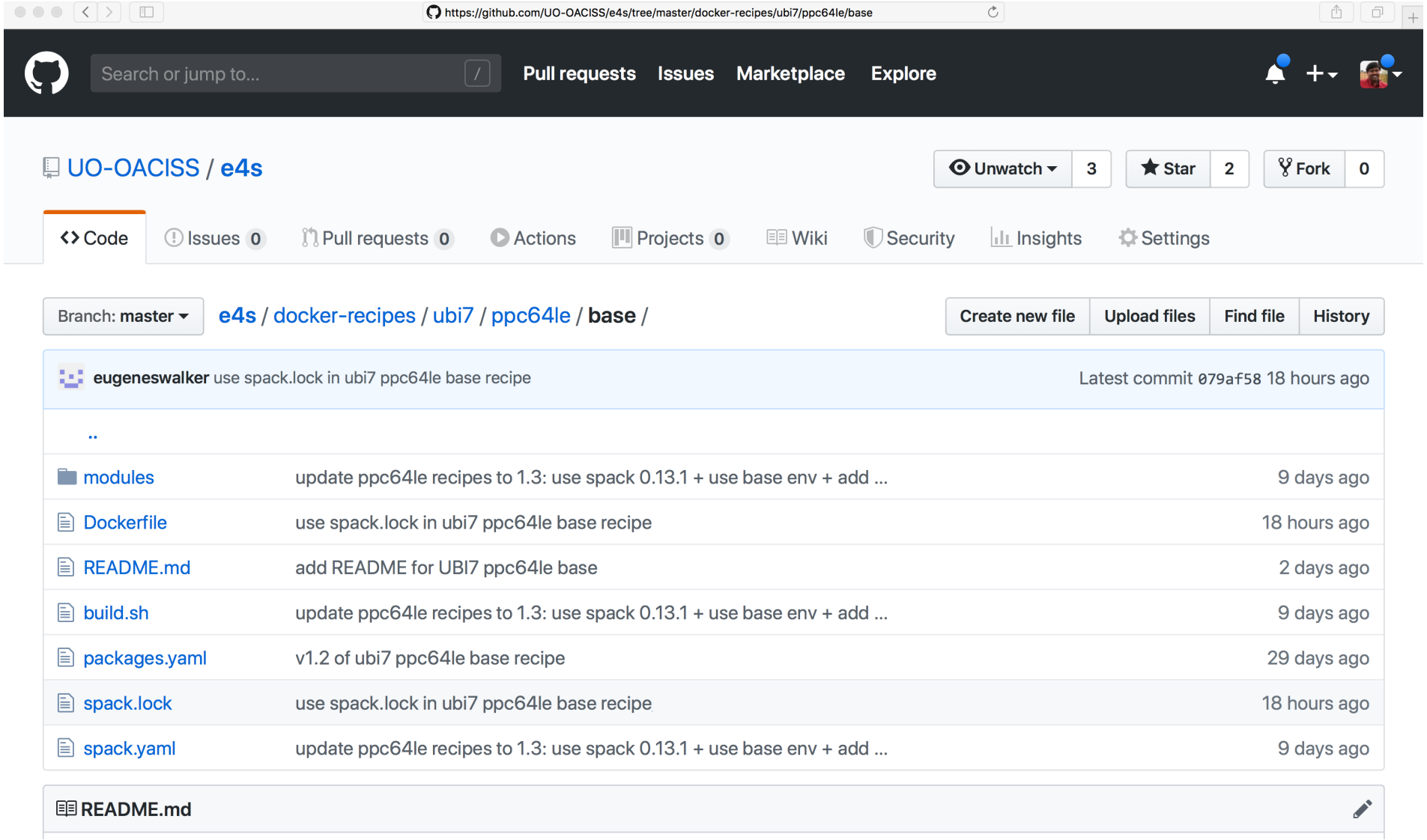
Multi-platform E4S Docker Recipes



10 lines (6 sloc) | 178 Bytes

```
1  FROM ecpe4s/ubuntu18.04-spack-x86_64:0.14.1
2
3  WORKDIR /e4s-env
4
5  COPY /spack.yaml .
6
7  RUN spack install --cache-only \
8   && spack clean -a && rm -rf /tmp/root/spack-stage
9
10 WORKDIR /
```

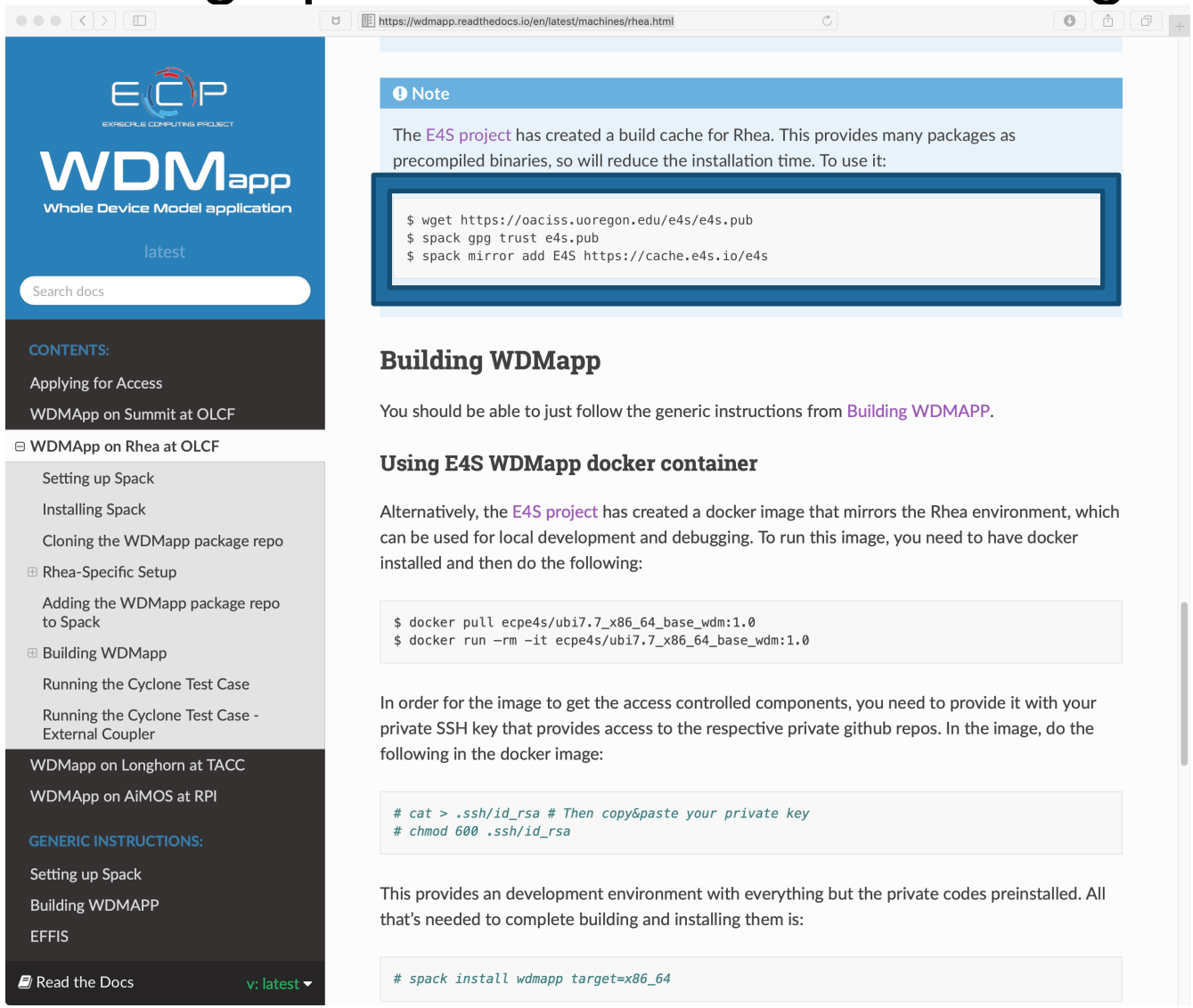
E4S: Multi-platform Reproducible Docker Recipes



E4S
- x86_64
- ppc64le
- aarch64

https://e4s.io

WDMApp: Speeding up bare-metal installs using E4S build cache



- E4S Spack build cache
- Adding E4S mirror
- WDMApp install speeds up!

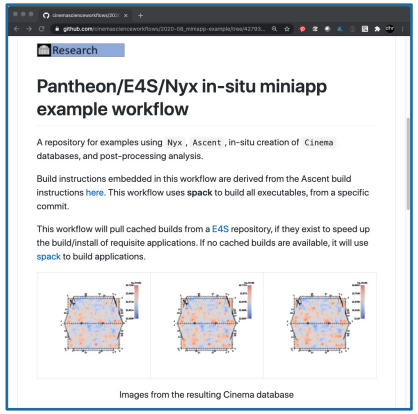
Pantheon and E4S build cache support end-to-end ECP examples

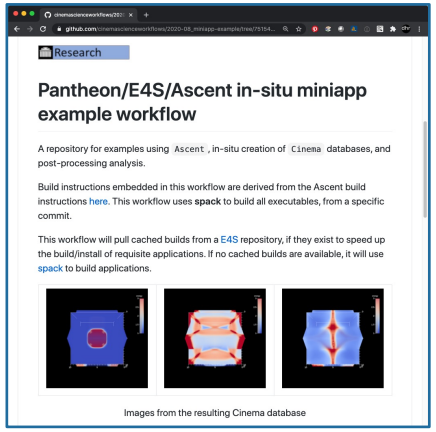
Overview: The Exascale Computing Project (ECP) is a complex undertaking, involving a myriad of technologies working together. An outstanding need is a way to capture, curate, communicate and validate workflows that cross all of these boundaries.

The **Pantheon** and **E4S** projects are collaborating to advance the integration and testing of capabilities, and to promote understanding of the complex workflows required by the ECP project. Utilizing a host of ECP technologies (spack, Ascent, Cinema, among others), this collaboration brings curated workflows to the fingertips of ECP researchers.

Contributions

- Curated end-to-end application/in-situ analysis examples can be run quickly by anyone on Summit. (https://github.com/pantheonscience/ECP-E4S-Examples)
- Pantheon/E4S integration speeds up build/setup times over source builds due to cached binaries (approx.10x speed up).





Instructions page for (top) Nyx, Ascent and Cinema workflow repository, and (bottom) Cloverleaf3d, Ascent, Cinema workflow. These curated workflows use Pantheon, E4S and spack to provide curated workflows for ECP.

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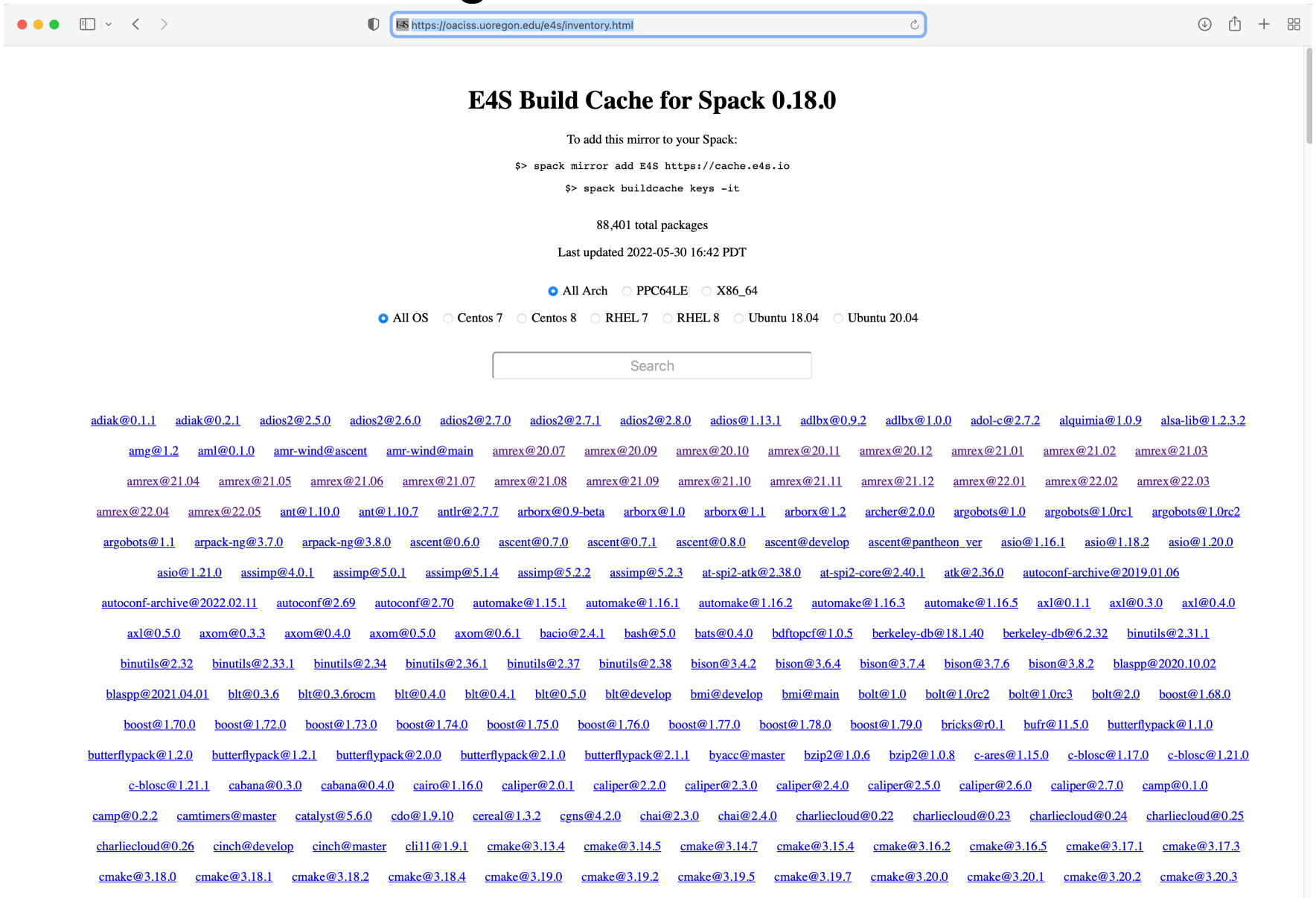
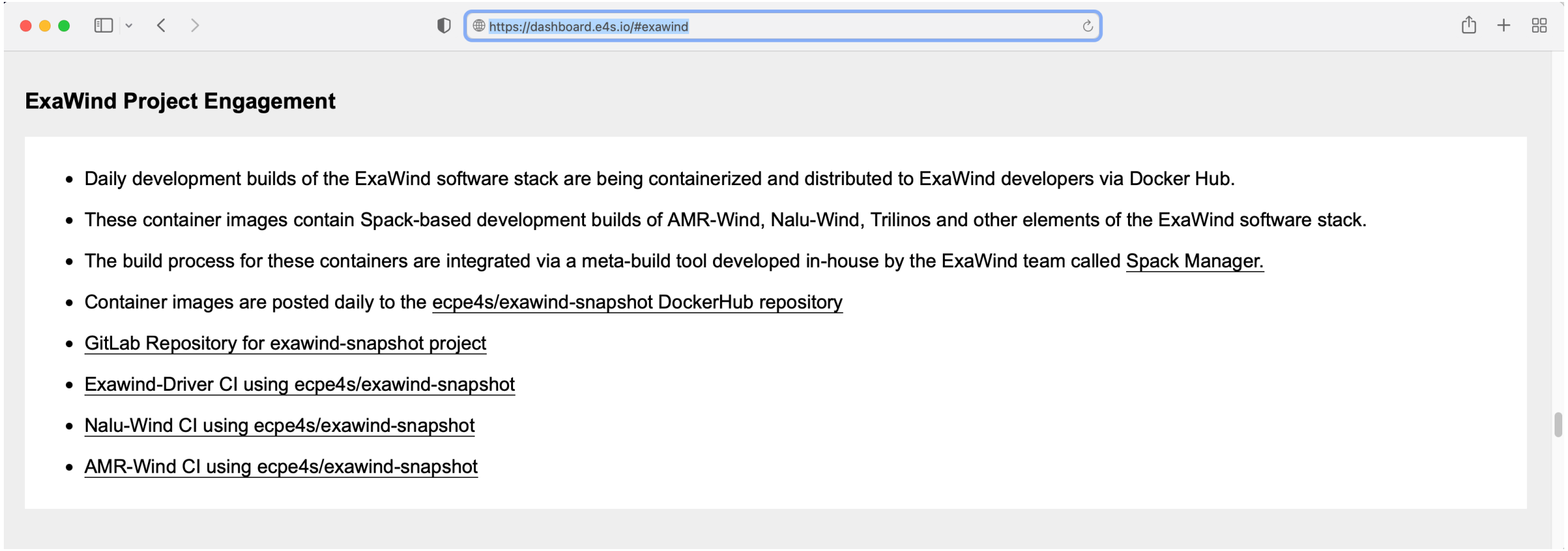
E4S Build Cache at U. Oregon

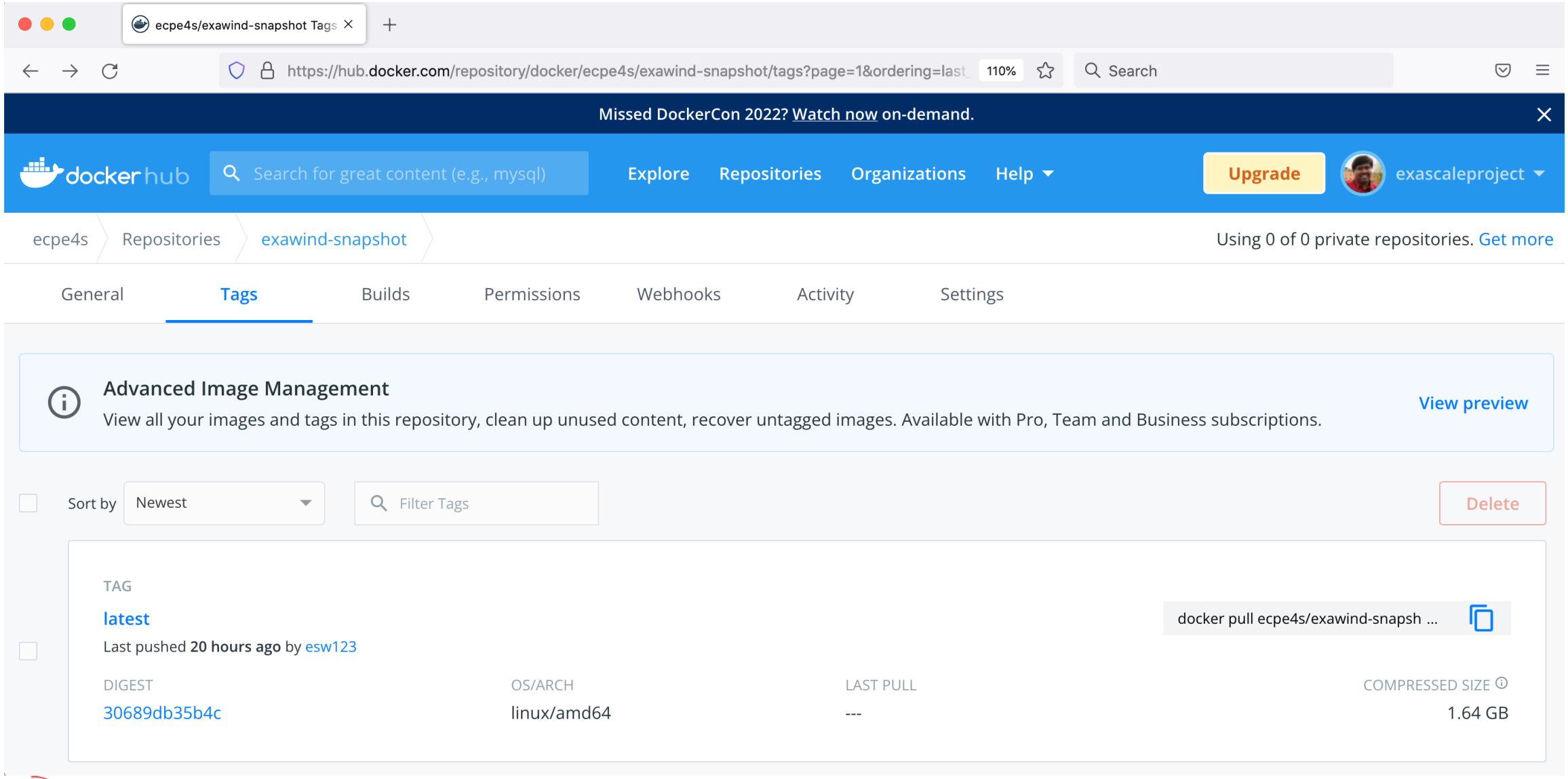


Over 88,000 binaries!

E4S Support for AD teams: ExaWind



E4S Custom Docker Images using E4S Build Cache: ExaWind



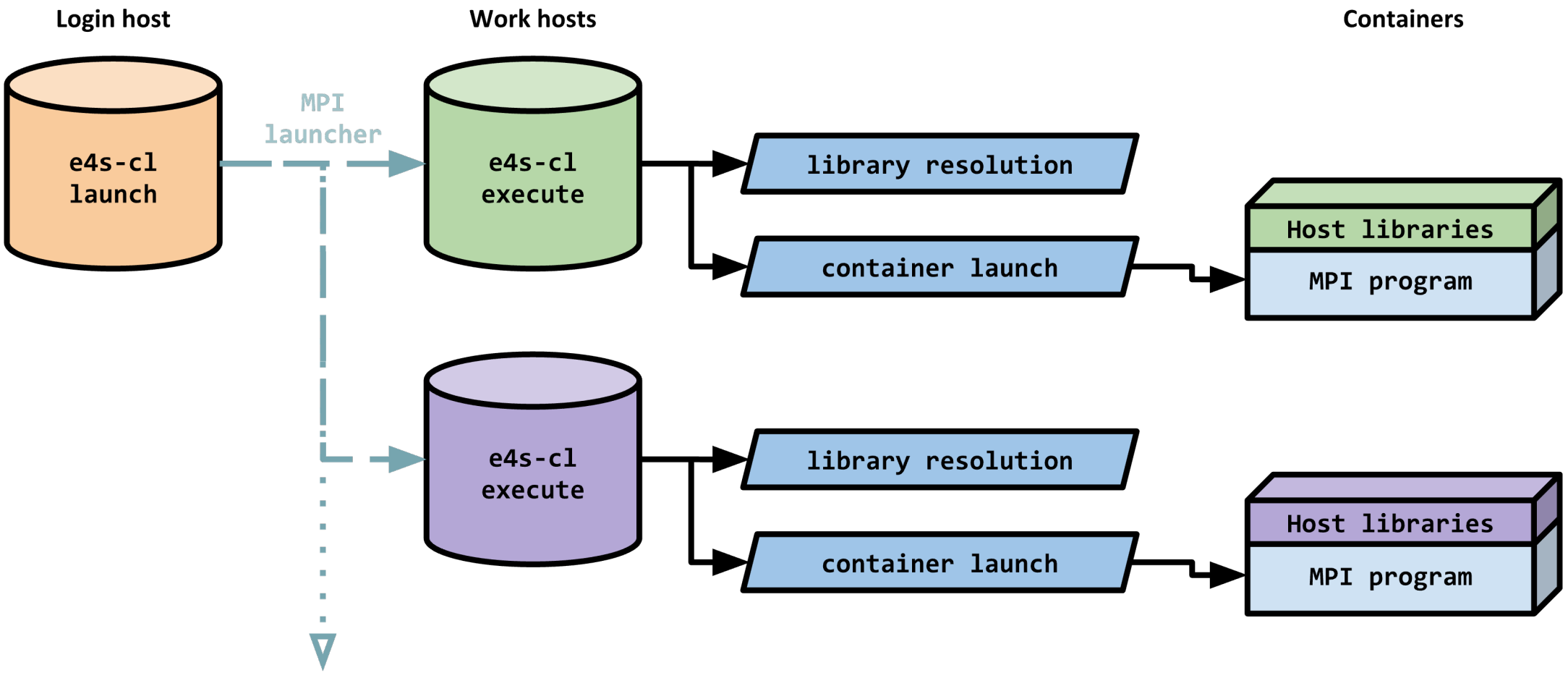
e4s-cl: A tool to simplify the launch of MPI jobs in E4S containers

- E4S containers support replacement of MPI libraries using MPICH ABI compatibility layer and Wi4MPI [CEA] for OpenMPI and MPICH variants.
- 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.
- Usage:

```
. /opt/intel/oneapi/setvars.sh

e4s-cl init --backend singularity --image /home/tutorial/ecp.simg --source /home/tutorial/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
```

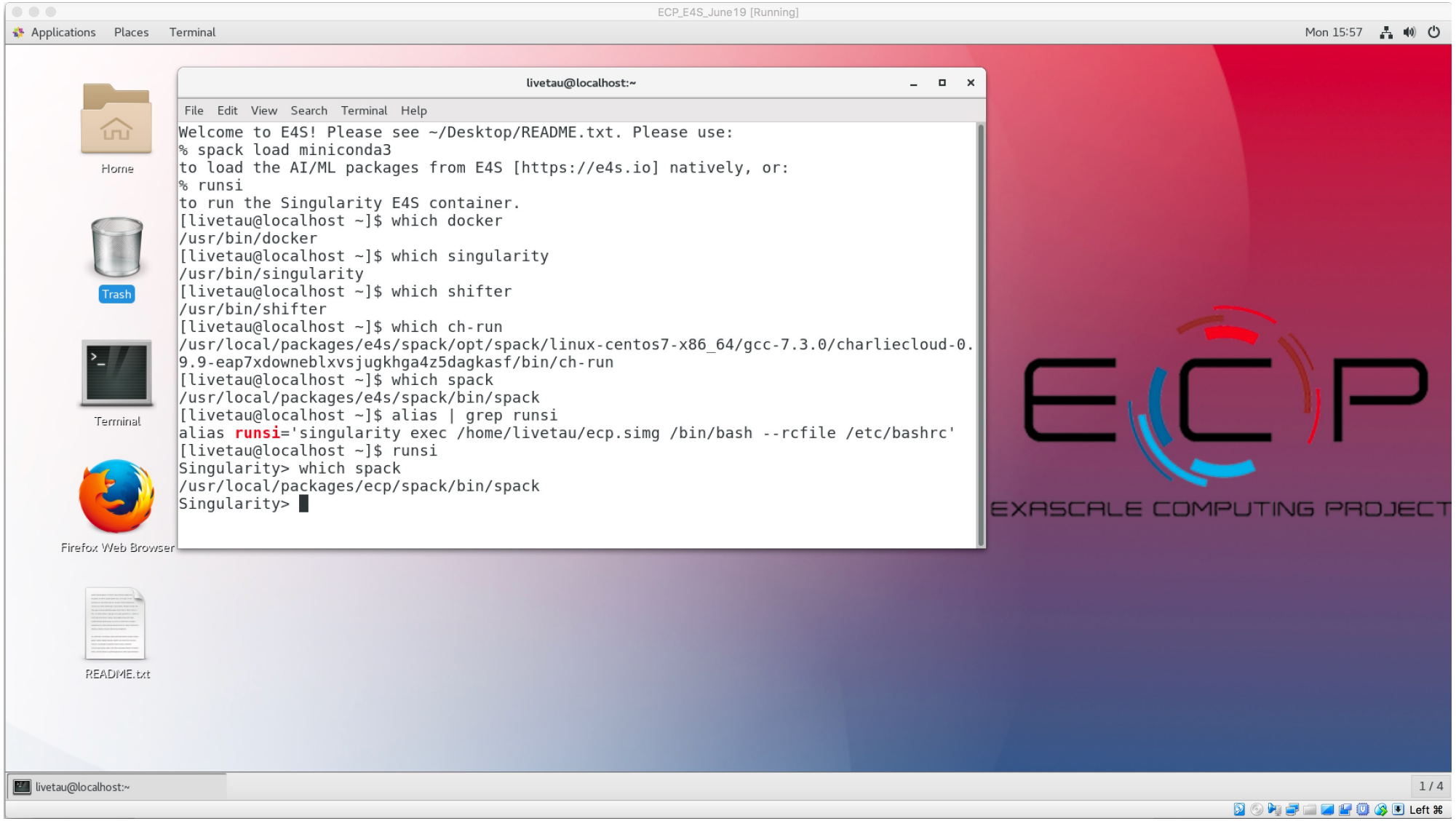
https://github.com/E4S-Project/e4s-cl

e4s-cl Container Launcher



https://e4s.io

E4S VirtualBox Image

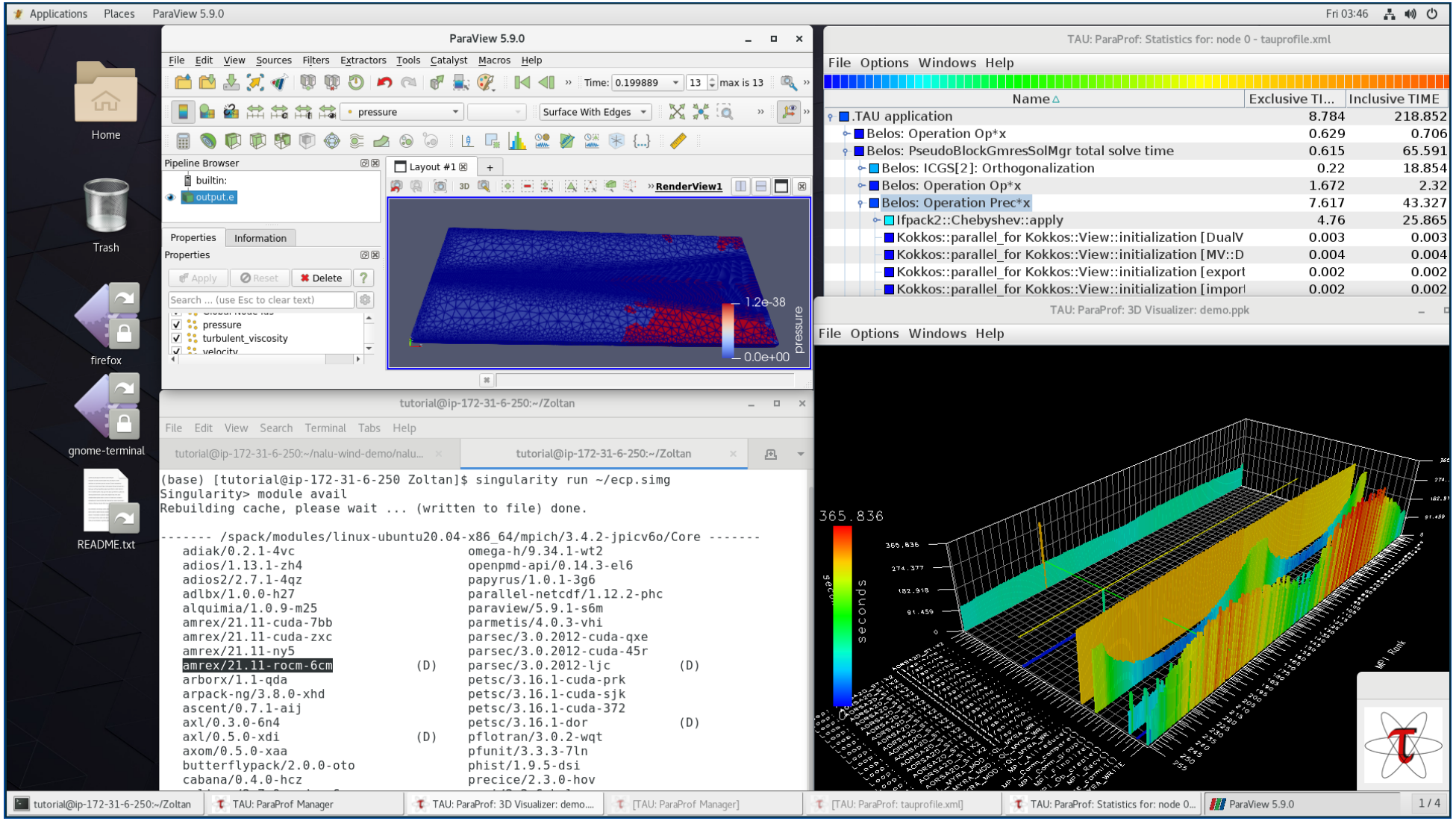


Container Runtimes

- Docker
- Shifter
- Singularity
- Charliecloud

https://e4s.io

E4S 22.05 AWS image: US-West2 (OR) ami-0d7295416d1c63e3a



Private E4S 22.05 image

- Build cache
- Nalu-X demonstration
- Singularity and Docker runtimes
- Discussing a compelling demo in E4S iteration 42
- Was demonstrated at ISC22 and ATPESC.

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.

Acknowledgment

“This research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of two U.S. Department of Energy organizations (Office of Science and the National Nuclear Security Administration) responsible for the planning and preparation of a capable exascale ecosystem, including software, applications, hardware, advanced system engineering, and early testbed platforms, in support of the nation’s exascale computing imperative.”