E4S at DOE Facilities with Deep Dive at NERSC

Sameer Shende, University of Oregon
E4S Technical Lead

Monday, Oct. 4, 2021, 9am – noon PT

Zoom: https://exascaleproject.zoomgov.com/j/1612548862

Slides: https://e4s.io/talks/E4S_NERSC21.pdf

EXASCALE COMPUTING PROJECT

National Nuclear Security Administration

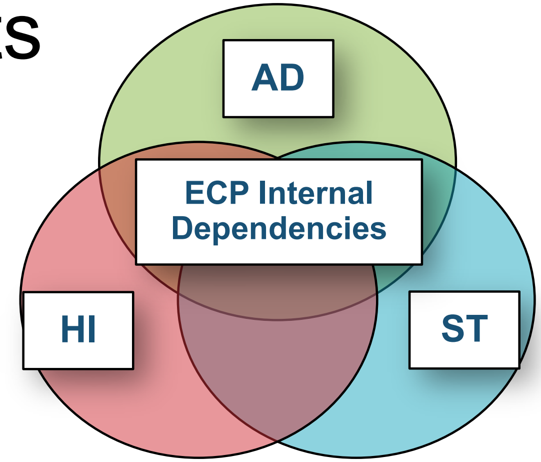
U.S. DEPARTMENT OF ENERGY | Office of Science

The Growing Complexity of Scientific Application Software Stacks

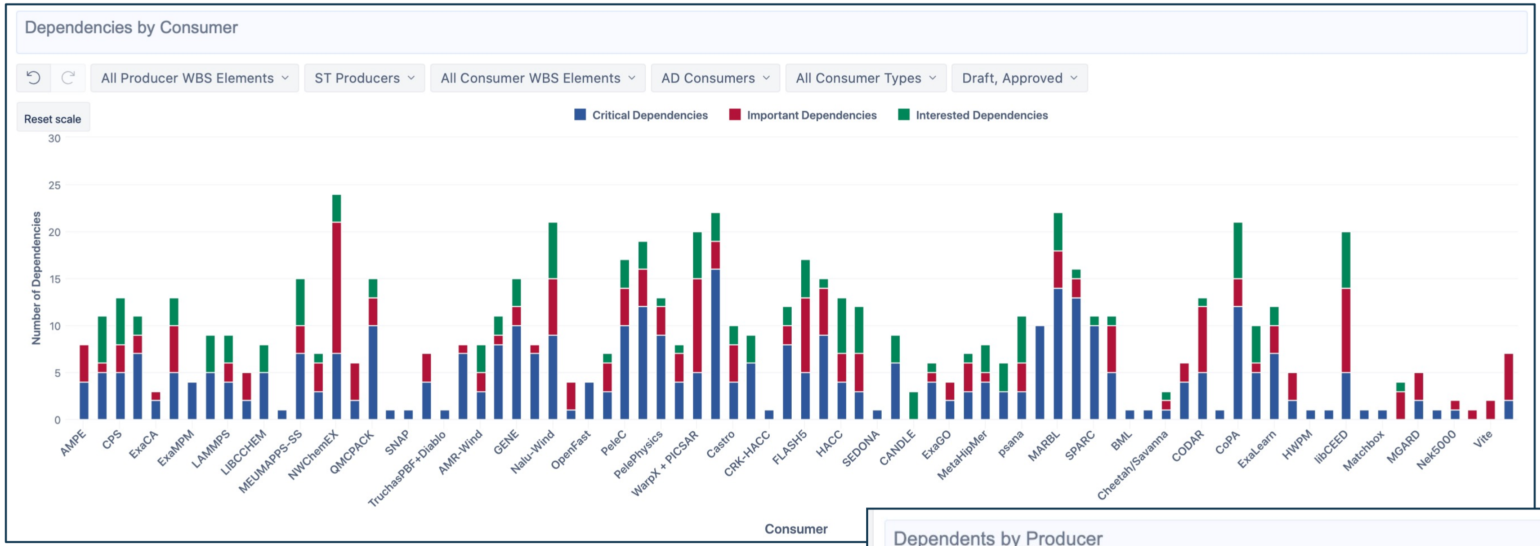
Challenges

- As our software gets more complex, it is getting harder to install tools and libraries correctly in an integrated and interoperable software stack.

ECP apps (AD) are primary consumers of ST products

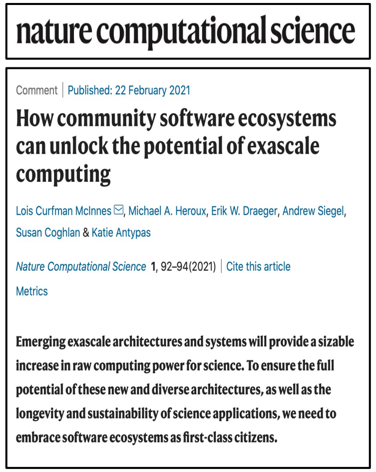


Dependency Database



View by AD consumers

https://dx.doi.org/10.1038/s43588-021-00033-y


nature computational science

Comment | Published: 22 February 2021

How community software ecosystems can unlock the potential of exascale computing

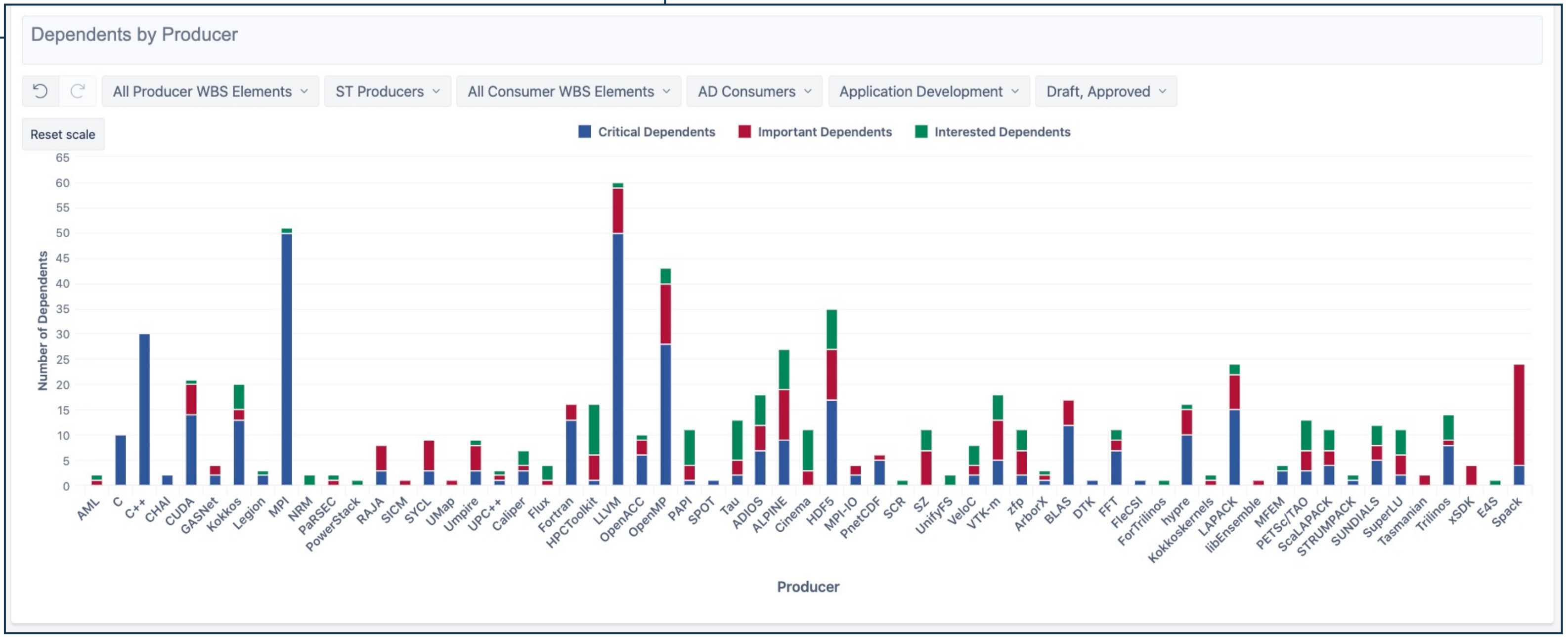
Lois Curfman McInnes, Michael A. Heroux, Erik W. Draeger, Andrew Siegel, Susan Coghlan & Katie Antypas

Nature Computational Science 1, 92–94(2021) | Cite this article

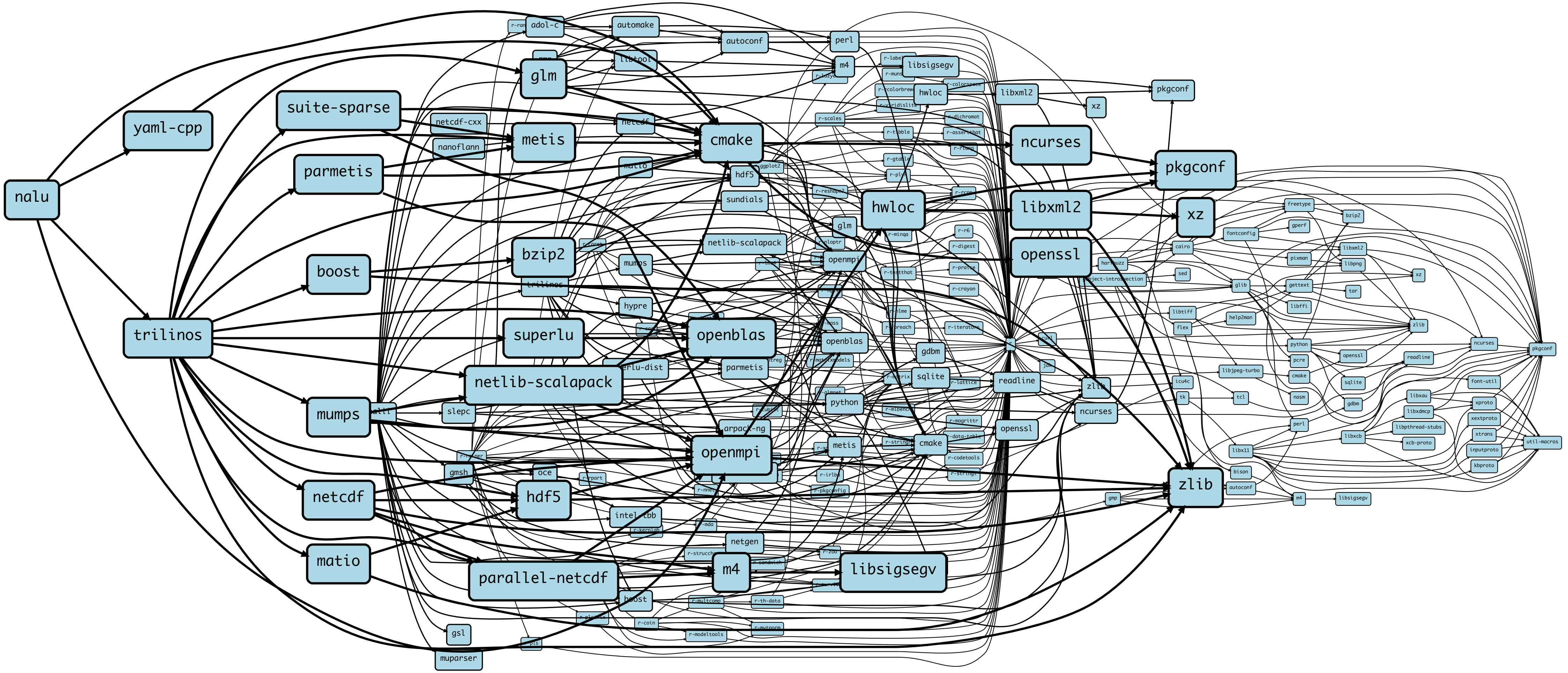
Metrics

Emerging exascale architectures and systems will provide a sizable increase in raw computing power for science. To ensure the full potential of these new and diverse architectures, as well as the longevity and sustainability of science applications, we need to embrace software ecosystems as first-class citizens.

View by ST producers



Scientific software is becoming extremely complex



Nalu: Generalized Unstructured Massively Parallel Low Mach Flow

dealii: C++ Finite Element Library

R Miner: R Data Mining Library

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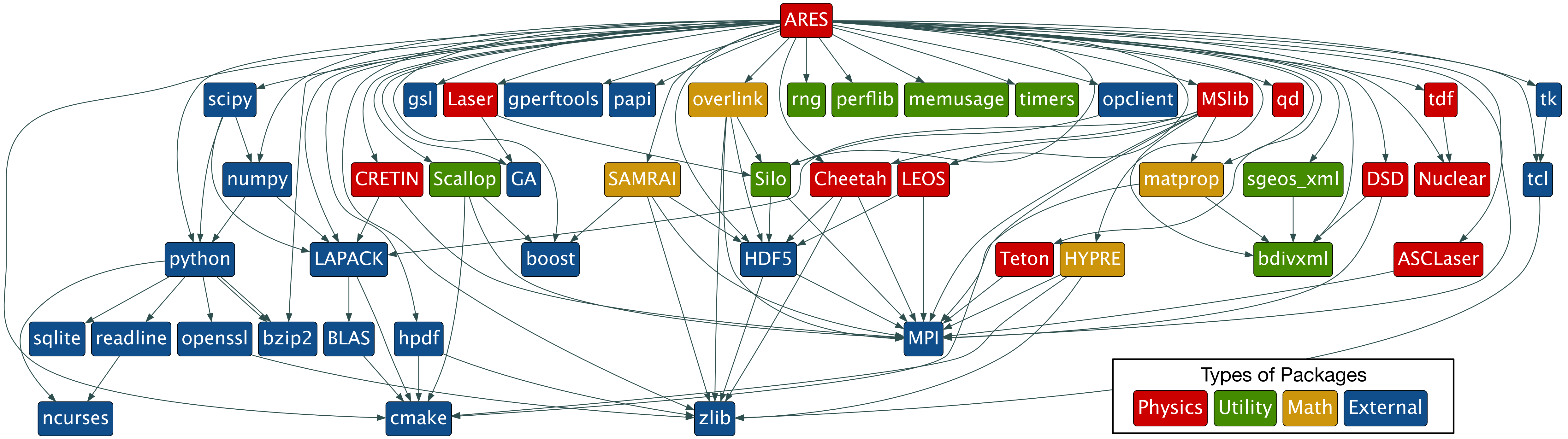
Even proprietary codes are based on many open source libraries



- 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**

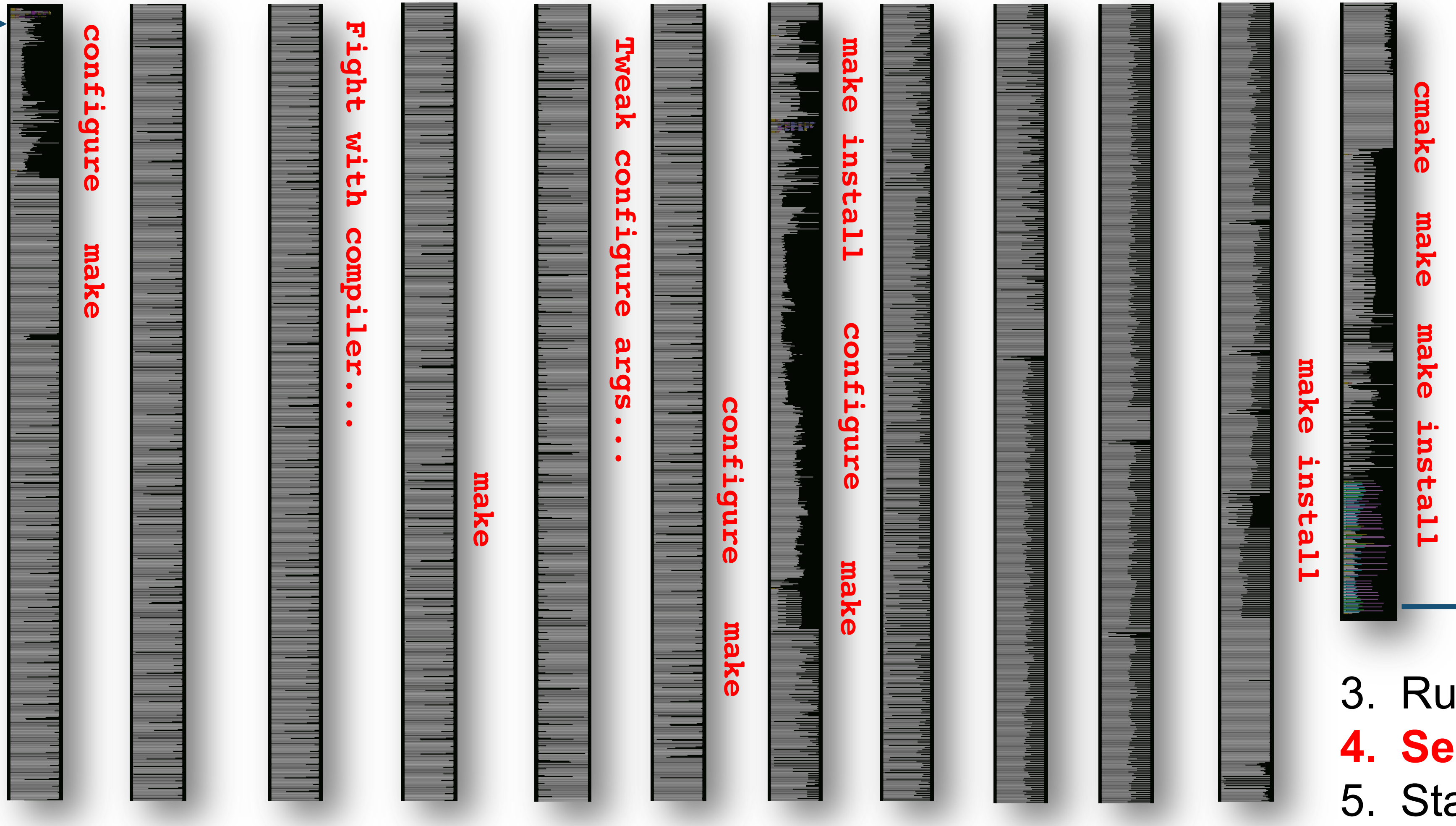
= up to **1,260,000** combinations!

- 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 Overview

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

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

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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@2.30.1                                    @ custom version
$ spack install tau@2.30.1 %gcc@9.3.0                         % custom compiler
$ spack install tau@2.30.1 %gcc@9.3.0 +level_zero +openmpi    +/- build option
$ spack install tau@2.30.1 %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

```
Singularity> spack find
==> 319 installed packages
-- linux-ubuntu18.04-power9le / gcc@7.3.0 -----------------------
autoconf@2.69     diffutils@3.7     libiconv@1.16      m4@1.4.18     ncurses@6.2               openssl@1.1.1g      texinfo@6.5
automake@1.16.2   findutils@4.6.0   libpciaccess@0.16  matio@1.5.17  netcdf-c@4.7.4            parmetis@4.0.3      trilinos@13.0.0
boost@1.74.0      glm@0.9.7.1       libsigsegv@2.12    metis@5.1.0   netlib-scalapack@2.1.0    perl@5.26.1         util-macros@1.19.1
bzip2@1.0.8       hdf5@1.10.7       libtool@2.4.6      mpich@3.2.1   omega-h@9.29.0            pkgconf@1.7.3       xz@5.2.5
cmake@3.18.4      hypre@2.20.0      libxml2@2.9.10     mumps@5.3.3   openblas@0.3.10           suite-sparse@5.7.2  zlib@1.2.11

-- linux-ubuntu18.04-ppc64le / gcc@7.3.0 ------------------------
adiak@0.1.1             flit@2.1.0              libpfm4@4.11.0              papyrus@develop              py-more-itertools@7.2.0     qthreads@1.14
adios@1.13.1            gasnet@2020.3.0         libpng@1.6.37               parallel-netcdf@1.12.1       py-mpi4py@3.0.3             raja@0.12.1
adios2@2.6.0            gasnet@2020.3.0         libpthread-stubs@0.4        parmetis@4.0.3               py-nbclient@0.5.0           rankstr@0.0.2
adlbx@0.9.2             gdbm@1.18.1             libquo@1.3.1                pcre@8.44                    py-nbconvert@6.0.1          readline@8.0
aml@0.1.0               gettext@0.20.2          libsigsegv@2.12             pcre2@10.35                  py-nbformat@5.0.7           redset@0.0.3
amrex@20.10             gettext@0.21            libsodium@1.0.18            pdsh@2.31                    py-nest-asyncio@1.4.0       rempi@1.1.0
arborx@0.9-beta         ginkgo@1.3.0            libtool@2.4.6               pdt@3.25.1                   py-notebook@6.1.4           scr@2.0.0
argobots@1.0            git@2.28.0              libunistring@0.9.10         perl@5.26.1                  py-numpy@1.19.2             shuffile@0.0.3
arpack-ng@3.7.0         git@2.28.0              libunwind@1.4.0             petsc@3.13.6                 py-oauthlib@3.1.0           slate@develop
ascent@develop          glm@0.9.7.1             libunwind@1.4.0             petsc@3.14.0                 py-pamela@1.0.0             slepc@3.14.0
autoconf@2.69           globalarrays@5.7        libuuid@1.0.3               pkgconf@1.7.3                py-pandocfilters@1.4.2      snappy@1.1.8
automake@1.16.2         gmake@4.2.1             libxml2@2.9.10              plasma@20.9.20               py-parso@0.6.1              sqlite@3.31.1
axl@0.3.0               gmp@6.1.2               libyogrt@1.24               precice@2.1.1                py-petsc4py@3.13.0          strumpack@5.0.0
axom@0.3.3              googletest@1.10.0       libzmq@4.3.2                pumi@2.2.2                   py-pexpect@4.7.0            suite-sparse@5.7.2
bash@5.0                gotcha@0.0.2            lmod@8.3                    py-alembic@1.0.7             py-pickleshare@0.7.5        sundials@5.4.0
binutils@2.33.1         gotcha@1.0.3            lua@5.3.5                   py-argon2-cffi@20.1.0        py-prometheus-client@0.7.1  superlu@5.2.1
bmi@develop             gperftools@2.7          lua-luafilesystem@1_7_0_2   py-asn1crypto@0.24.0         py-prompt-toolkit@2.0.9     superlu-dist@6.3.0
bolt@1.0                hdf5@1.8.21             lua-luaposix@33.4.0         py-async-generator@1.10      py-psutil@5.7.2             superlu-dist@6.3.1
boost@1.73.0            hdf5@1.8.21             lwgrp@1.0.3                 py-attrs@19.3.0              py-ptyprocess@0.6.0         swig@4.0.2
boost@1.73.0            hdf5@1.10.6             lz4@1.9.2                   py-babel@2.7.0               py-py@1.8.0                 sz@1.4.12.3
boost@1.73.0            hdf5@1.10.6             lzo@2.10                    py-backcall@0.1.0            py-pycparser@2.20           sz@2.0.2.0
boost@1.73.0            hpctoolkit@2020.08.03   m4@1.4.18                   py-bleach@3.1.0              py-pyelftools@0.26          sz@2.1.10
butterflypack@1.2.0     hpx@1.5.1               magma@2.5.4                 py-blinker@1.4               py-pygments@2.6.1           tar@1.32
bzip2@1.0.8             hwloc@1.11.11           margo@0.4.3                 py-certifi@2020.6.20         py-pyjwt@1.7.1              tasmanian@7.3
c-blosc@1.17.0          hwloc@2.2.0             matio@1.5.17                py-certipy@0.1.3             py-pyopenssl@19.0.0         tau@2.29
caliper@2.4.0           hypre@2.18.2            mbedtls@2.16.7              py-cffi@1.14.3               py-pyrsistent@0.15.7        tcl@8.6.10
cinch@master            hypre@2.20.0            mercury@1.0.1               py-chardet@3.0.4             py-pytest-runner@5.1        texinfo@6.5
cmake@3.17.3            intel-tbb@2020.3        mercury@1.0.1               py-cryptography@2.7          py-python-dateutil@2.8.0    turbine@1.2.3
conduit@master          kokkos@3.2.00           metis@5.1.0                 py-cython@0.29.21            py-python-editor@1.0.4      umap@2.1.0
conduit@master          kokkos-kernels@3.2.00   mfem@4.1.0                  py-decorator@4.4.2           py-python-oauth2@1.1.1      umpire@4.0.1
cuda@10.2.89            kvtree@1.0.2            mpark-variant@1.4.0         py-defusedxml@0.6.0          py-pytz@2020.1              umpire@4.0.1
curl@7.72.0             legion@20.03.0          mpich@3.2.1                 py-entrypoints@0.3           py-pyzmq@18.1.0             unifyfs@0.9.0
darshan-runtime@3.2.1   leveldb@1.22            mpifileutils@develop        py-idna@2.8                  py-requests@2.24.0          unzip@6.0
da Snapz Pro X 3.2.1    libarchive@3.4.1        mumps@5.3.3                 py-importlib-metadata@2.0.0  py-send2trash@1.5.0         upcxx@2020.3.0
di[illegible]s@3.7      libbsd@0.10.0           ncurses@6.2                 py-ipykernel@5.3.4           py-setuptools@50.1.0        util-macros@1.19.1
```

- 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.

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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

The Extreme-Scale Scientific Software Stack (E4S) Components

E4S: Extreme-scale Scientific Software Stack Components

- 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
- 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
- August 2021: E4S 21.08 - 88 full release products

https://e4s.io

Lead: Sameer Shende (U Oregon)

Also include other products .e.g.,
AI: PyTorch, TensorFlow, Horovod
Co-Design: AMReX, Cabana, MFEM

Using E4S with containers

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

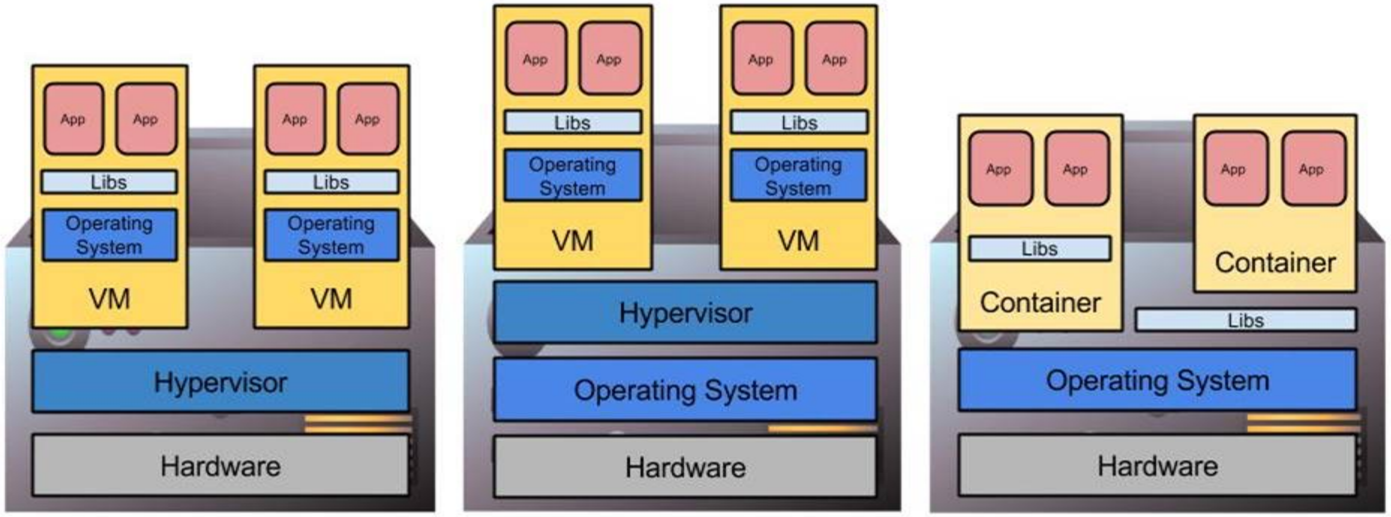
Creates a portable* software ecosystem

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**

E4S Docker and Singularity Containers

https://e4s-project.github.io/download.html

Using E4S Containers

The current E4S container offerings include Docker images for Red Hat Enterprise Linux 7, Red Hat Enterprise Linux 8, Ubuntu 18.04 (Bionic), and Ubuntu 20.04 (Focal Fossa). Our images can run on X86_64, PPC64LE, and AARCH64 depending on the particular image. In addition to offering a full E4S image containing a comprehensive selection of E4S software released on a quarterly cycle, we also offer a set of minimal base images suitable for use in Continuous Integration (CI) pipelines.

Docker images are available on the E4S Docker Hub.

Recipes for building images from scratch are available on the E4S GitHub repository.

Our recipes make use of Spack packages available as pre-built binaries in the E4S Build Cache.

Container Releases

- Docker Downloads
- Singularity x86_64 Download
- Singularity ppc64le Download
- OVA Download

From source with Spack

Visit the Spack Project

Spack contains packages for all of the products listed in the E4S 2021.08 Full Release category (see above 2021.02 Release Notes). General instructions for building software with Spack can be found at the Spack website. For more information, see /usr/local/packages/ecp in the container referenced here. Questions concerning building those packages are deferred to the associated package development team.

AWS EC2 Image

The E4S 21.05 release is also available on AWS as an EC2 AMI with ID ami-057d49e585d0c6c7d in the US-West-2 (Oregon) region.

Note on Container Images

Container images contain binary versions of the Full Release packages listed above. A clone of Spack is also available in the container which can be used to compile the Full Release and Partial Release packages. Example Spack "recipes" (lists of configuration commands) are available in the container. See the README.txt file for more details. This release also includes an OVA file that has Docker, Charliecloud, Shifter, and Singularity preinstalled in it. The Docker container image is also available from Dockerhub:

```
# docker pull ecpe4s/ubuntu18.04-e4s-gpu
```

E4S base images for custom container deployment and CI images

https://e4s-project.github.io/download.html

E4S GPU Images

Multi-Arch Image (X86_64 and PPC64LE)

This is a multi-arch image, meaning that the same image name can be used to pull the appropriate image for your architecture.

ecpe4s/ubuntu18.04-e4s-gpu docker GitHub

Continuous Integration Images

X86_64

ecpe4s/rhel7-runner-x86_64 docker GitHub

ecpe4s/rhel8-runner-x86_64 docker GitHub

ecpe4s/ubuntu18.04-runner-x86_64 docker GitHub

ecpe4s/ubuntu20.04-runner-x86_64 docker GitHub

PPC64LE

ecpe4s/rhel7-runner-ppc64le docker GitHub

ecpe4s/rhel8-runner-ppc64le docker GitHub

ecpe4s/ubuntu18.04-runner-ppc64le docker GitHub

ecpe4s/ubuntu20.04-runner-ppc64le docker GitHub

Custom Images

ecpe4s/ubuntu1804_aarch64_waggle docker GitHub

ecpe4s/superlu_sc docker GitHub

E4S Facility Deployment

NERSC

OLCF

21.08 Release: 88 Official Products + dependencies (x86_64 gcc)

```
1: adios2       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/adios2-2.7.1-27vgcpqdhek4p6twmy7afio2tgmxiy5e
2: aml  /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/aml-0.1.0-rkblv6wpaf6wts534fffwav7u2d66df6
3: amrex        /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/amrex-21.08-d7y3vig7gdvjqcrrxdmoirvg43cubymi
4: arborx       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/arborx-1.0-fivuanyy3gcizpuu77ibic2x4hrczpfb
5: archer       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/archer-2.0.0-bg45ysged6t757qet5iyoxkfqxaca7di
6: argobots     /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/argobots-1.1-2ohkpy7o25d3f37gk6f5hnu3zvxru3eo
7: ascent       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/ascent-0.7.1-yzfv4m5fpp5i7t4i4224r4ris73so5i4
8: axom         /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/axom-0.5.0-7sbph4rnb2mtynfqizhgatof4pzaxqr7
9: bolt         /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/bolt-2.0-sux27szhh5drrqcm33ar3pbpqgzxdszc
10: cabana      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/cabana-0.3.0-w5gtkjavtkjpa37vdlnr4mwtj7azwzxo
11: caliper     /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/caliper-2.6.0-5swnlis5idlmyhk4yvsehyq7dhkbvctn
12: chai        /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/chai-2.3.0-uscxbayu7u57awdvshkwfcsehckgr7q7
13: charliecloud        /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/charliecloud-0.24-2rmscb2hg3a7grngz4ocfqjbi77vc7yq
14: conduit     /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/conduit-0.7.2-qzfdcvrojq3hxnshglaud3vaglyb2xni
15: darshan-runtime     /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/darshan-runtime-3.3.1-zk5hlc5o4noyp6ucm2f3ykrt4ycyyv2x
16: datatransferkit     /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/datatransferkit-3.1-rc2-4mwojqjufucbz67wurdpnql4cnyrokhd
17: dyninst     /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/dyninst-11.0.1-tgx3yorce4aknwzwsgym2ii5a5mat6qf
18: faodel      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/faodel-1.1906.1-zw3imhpuewnrszis3fxg7q4tk7petcmg
19: flecsi      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/flecsi-1.4.2-pef3qn2qy72w4gkiqjpt3qjv5xizlssa
20: flit        /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/flit-2.1.0-fxbnhrqdsyfyh4bnqatpxq724hna67ak
21: flux-core   /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/flux-core-0.28.0-afwbrgcp64iqzvtafgstoyw3l7o3rfdb
22: fortrilinos         /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/fortrilinos-2.0.0-e2wcf2okviq3mb7dfa4lqyvo6bu4riab
23: gasnet      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/gasnet-2021.3.0-k6ghuyl57vd2lrveo4kkjp7mn4dugm3i
24: geopm       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/geopm-1.1.0-nozivxl4pqdw5hjpt6cahrppv7c5fiuf
25: ginkgo      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/ginkgo-1.3.0-wfanvywkbnfnko6elyeuk2s76nx3cvzp
26: globalarrays        /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/globalarrays-5.8-qsupbbxerp5pzm5ztvik6er7l4n5gtub
27: gotcha      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/gotcha-1.0.3-zd4bbdeflybaltl7d6z3qsqoonfzcy2n
28: hdf5        /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/hdf5-1.12.0-gu7ywoxzerehevp6w4rftkf4fmcyqapa
29: heffte      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/heffte-2.1.0-paam77fhaqkaorcum4zmujqfbrgafzzt
30: hpctoolkit  /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/hpctoolkit-2021.05.15-vg2l6c45hvaqafzqpcl6kg4eavw63qkv
31: hpx         /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/hpx-1.7.1-e5tyu2igpw5rxgipugzwhi7trum6xjqd
32: hypre       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/hypre-2.22.0-5hio4z4qrg24lgcwcabjbt4gjcg7lyp4
33: kokkos      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/kokkos-3.4.00-upyjzufpcuk2pwmke27lpiavhvdwfmjx
34: kokkos-kernels      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/kokkos-kernels-3.2.00-m2c6w6kjavdf3qbyddorda7oqcqv2n32
35: legion      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/legion-21.03.0-44i7yagoviqomn5r654ywrry4dxmioyj
36: libnrm      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/libnrm-0.1.0-7b4a3z4gisn44m3xscyz3yrh4bbviosr
37: libquo      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/libquo-1.3.1-fhkkhwbgwneq2tgojzveu5z2pq3eiyqg
38: llvm-doe    /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/llvm-doe-uo-jtjbxu4fmcomsktujfwo4byicpu6xtnb
39: loki        /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/loki-0.1.7-ak2py6nz74lhsxwb3wnfvjw6zt6npbve
40: magma       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/magma-2.6.1-xmw3vx34flufaarkuqhivrqsjjj6dkz3
41: mercury     /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/mercury-2.0.1-c6ffa2yzrptsk5rv56watttknatafste
42: metall      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/metall-0.15-tpem27xlmealt2kkznrsshkns5krpf5m
43: mfem        /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/mfem-4.3.0-xyj4x5zn5sst43oxtpr5nviagyctkyg5
44: mpich       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/mpich-3.4.2-nolyq2e5hpk6732d3bqgxbg5y2gbaxy3
```

Support for GPUs

- nvhpc 21.7
- cuda 11.4
- oneAPI 2021.1.1
- ROCm 3.8

21.08 Release: 88 Official Products + dependencies (x86_64 gcc)

```
45: mpark-variant      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/mpark-variant-1.4.0-gkduikmh7z3bgja2cpbeyru4q2ztsf7c
46: mpifileutils       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/mpifileutils-0.11-zjma6o6gyrpcn2hnwqnmeqkeavetvpwt
47: ninja       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/ninja-1.10.2-yve7omxowuaybwm2wsxouxnl2b5ryfb5
48: nrm         /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/nrm-0.1.0-vovfl5qv5qjfxocympruezpncpfafhed
49: omega-h     /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/omega-h-9.32.5-joavfvt5ab3ve5oasydgcijzqrtxbq5r
50: openpmd-api        /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/openpmd-api-0.13.4-ars3ve5sm4afg5qjh4oeilxwpceyyu3c
51: openmpi     /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/openmpi-4.1.1-hjdyfjwrv4qujcrp5p7dsiib5hjbkibe
52: papi        /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/papi-6.0.0.1-lbnepjda4cajdibucrhe2nwk55ukfxzk
53: papyrus     /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/papyrus-1.0.1-x3dqutritvg3h4lmg76cl3b5jplxmwv2
54: parallel-netcdf    /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/parallel-netcdf-1.12.2-uqd2rsergw7sjbnu2nqhjhnhfhbhkhes
55: paraview    /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/paraview-5.9.1-uaheirmp3awdb7w37yvgezbyarw3r4ai
56: parsec      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/parsec-3.0.2012-5ctbj5apqu237unoim47ws7ah4o3huvh
57: pdt         /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/pdt-3.25.1-kvi5wuu5y72fypijti3nxqvdn7zpj6ni
58: petsc       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/petsc-3.15.3-d2rafhfv46h2zzses5ik7w4vemu3azvn
59: phist       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/phist-1.9.4-zmytghdqb6xdrhbubfo7dctlxzlzijct
60: plasma      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/plasma-20.9.20-zrtx37x4g2cfxrj24wswomin6lh5e4z6
61: precice     /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/precice-2.2.1-metv4fwpilqrcgu7da4qqjvfre7ake6u
62: pumi        /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/pumi-2.2.6-rnffroq76i74svtkxdi7a6nfofnm4xnv
63: py-jupyterhub      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/py-jupyterhub-1.0.0-zmy7ykvaklbucevdy7enygo6nedlqdxd
64: py-libensemble     /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/py-libensemble-0.7.2-q5woewa4j6pm3rqpnklzqlozzk7f5fzl
65: qthreads    /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/qthreads-1.16-56f6xq6wjalrnyuive6vpml4wfblmz75
66: raja        /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/raja-0.13.0-vzuvvb5ga6qyhjoawb53yrjsd7jksouj
67: rempi       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/rempi-1.1.0-jojz6u5u7xoieurju5gmtqt5dmmkcgow
68: scr         /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/scr-3.0rc1-jdifh5evccpmfb5yjthfllnec247bhij
69: slate       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/slate-2021.05.02-3ccegp7i4sjnmuliixdug7cswztzecz4
70: slepc       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/slepc-3.15.1-exod3rsgxmr472evjoduslqlzufpzcwf
71: stc         /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/stc-0.9.0-wtqpqgjdnx6ec35vgfosfyupqv3f45dz
72: strumpack   /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/strumpack-5.1.1-yj5fhgmqlk3gs7gdd3cmfnayrrkjyni2
73: sundials    /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/sundials-5.7.0-ddgmhlcdzhpjmkpyl7m54rolssuzkjzg
74: superlu-dist       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/superlu-dist-6.4.0-jal2ts3mruwwwz7wlybwtbn5brgwim73
75: swig        /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/swig-4.0.2-fortran-nhtva752i5uwrxddcmcrtz7xypzmg6bn
76: sz  /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/sz-2.1.12-jbq7prb4khprrmnysjxviegxmelu64fi
77: tasmanian   /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/tasmanian-7.5-spsudttdsxyetjuysuzqodapugbn4nwv
78: tau         /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/tau-2.30.1-xc5ipw5pdangiif52753ijrex4gululv
79: trilinos    /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/trilinos-13.0.1-bpq5bmu6ifdurm7sfdtmq3rr7iwy2sec
80: turbine     /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/turbine-1.3.0-rytfvqxv7eqcowra6ydwrjcpjsccjzzm
81: umap        /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/umap-2.1.0-r2kjvkblf2muxddcekd3mnrioeibekyz
82: umpire      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/umpire-4.1.2-rnaubxwefw7m5f2isnnp64q75yno2o6g
83: unifyfs     /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/unifyfs-0.9.1-px4skkbhgyxkngyrms7q5ojmqv2sdhaq
84: upcxx       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/upcxx-2021.3.0-xwqhvlonec356hk6cy2yfwkv5uckqf3x
85: veloc       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/veloc-1.4-hqgau6iv5ofvyfmjaf5nxbqibn4fz6wu
86: vtk-m       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/vtk-m-1.6.0-nuq45xqbwmspxzr2tus6qausszeyual2
87: warpx       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/warpx-21.08-dmzohb67o7xmqupswcpollmjk6a5viyc
88: zfp         /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/zfp-0.5.5-wgf57w7huzhw4f2ksgpqa4ardvcsqpz4
```

- GCC
- DOE fork of LLVM

AI/ML frameworks
- PyTorch
- Tensorflow

21.08 Release: x86_64 clang (DOE fork of LLVM)

```
1: adios2       /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/adios2-2.7.1-yxtyyzqd6g7ind3y5cztga53khnoj75e
2: aml  /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/aml-0.1.0-ivmjn5vwzm5n2kvzmpbailjm5zwwtrct
3: amrex        /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/amrex-21.08-4j66rudlgccjaf7q2weucnwjjdbbnx22
4: arborx       /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/arborx-1.0-qrxyddgckb6rlkphgghnztpspm4zrqa7
5: argobots     /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/argobots-1.1-sbcw2q7jswchkeils5shcpjx5cxnwkqn
6: axom         /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/axom-0.5.0-qaqmuswnnre2bzmpp244tfq5i2n6kssz
7: bolt         /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/bolt-2.0-ixposfomlcop4tjqrbcy3646xuowtbc2
8: cabana       /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/cabana-0.3.0-w3g2d566mlhrtrph7rpdljpbl3as4kxx
9: chai         /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/chai-2.3.0-xpr2bqk2gzxlvsu64crvdhcbjit4ih3o
10: conduit     /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/conduit-0.7.2-igt54l25gukjexgqnwwr2t74jglhj6ka
11: darshan-runtime     /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/darshan-runtime-3.3.1-k5f5yweveeuwtzdvpvac6f372u5ptrwu
12: datatransferkit     /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/datatransferkit-3.1-rc2-mjahapr7lz2txjtadspin4pbb7exos3z
13: faodel      /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/faodel-1.1906.1-g6ywaor7dafiz5dpywj72s42ywparoel
14: flit        /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/flit-2.1.0-p5fbffuymo2mmy4sxaolyp76u4uupgop
15: flux-core   /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/flux-core-0.28.0-lzfiz67owgoxzt4bymt33iwykcvsvgrr
16: fortrilinos         /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/fortrilinos-2.0.0-dysp5ba76qlujisp2dwxk57ldvptk3tv
17: gasnet      /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/gasnet-2021.3.0-3vh4oyk7xfcujsujzod2tjhbkxkng7nd
18: ginkgo      /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/ginkgo-1.3.0-x3i7rqviv47kzagu7pvvbbvn4qsm7uxp
19: globalarrays        /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/globalarrays-5.8-54crw4v3u5yqvpe7xd23t6fox6ttvkyo
20: gotcha      /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/gotcha-1.0.3-wjrccm7hkkqfl7qzz6l35yndktv46v35
21: hdf5        /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/hdf5-1.12.0-dh6tu6soyt5egqkkjk7azcqyh3u4gk2w
22: heffte      /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/heffte-2.1.0-ufviwwrhmityfbgfhovyf63jf6l43rwm
23: hpx         /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/hpx-1.7.1-jndohnv3doqragtq6eguzamak7s6kbfl
24: hypre       /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/hypre-2.22.0-gknkkcoz5yt7onukotflkv7a3rtotgtq
25: kokkos      /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/kokkos-3.4.00-kv3r5fujhuvjlh3jycqzabbvl5bxxans
26: kokkos-kernels      /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/kokkos-kernels-3.2.00-4e4tynmks77av2cdsfoas3rut7b4p5h6
27: legion      /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/legion-21.03.0-6kkayvju7r6rq5dtqj3tycygh6alqjj7
28: libnrm      /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/libnrm-0.1.0-yv66qlntuoflclak6aykdn3q6g7ki2sd
29: libquo      /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/libquo-1.3.1-mnqscmfqlzeip2jb6ecshvcfywkuitpx
30: loki        /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/loki-0.1.7-i4kkqcj5w5tmxb5ztfx5goykttqzmmeg
31: mercury     /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/mercury-2.0.1-rix6tbnldtrt77zm6mymv4jczzigjpdx
32: metall      /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/metall-0.15-adxx4qyolz26p53xd7olz4d7e2hggywm
33: mfem        /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/mfem-4.3.0-f24a6fvjnvary5zcrkrasarju45upmyv
34: mpich       /usr/local/mpich
```

21.08 Release: x86_64 clang (DOE fork of LLVM)

```
35: mpark-variant       /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/mpark-variant-1.4.0-2ttpmydvy2xvgqrdhcjmhttmx66skioa
36: mpifileutils        /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/mpifileutils-0.11-a5345yd3v52qzwlvkko7hdfsjfogmqvs
37: ninja       /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/ninja-1.10.2-wwed7qfgm4jhtfel7sqvibcthjp4b2al
38: nrm         /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/nrm-0.1.0-7cj5wc66nwqzl7esyt2lyepct2hgd4xj
39: openpmd-api         /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/openpmd-api-0.13.4-jik2lrmryedetymolopqf4zvoe5336zp
40: openmpi     /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/openmpi-4.1.1-mi5bkj3ztbr5pwyrms3gwg66n4sqr4mv
41: papi        /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/papi-6.0.0.1-fmjwmas7zbbtauekt3f5w5j6rns36sfc
42: papyrus     /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/papyrus-1.0.1-k62ikiw57max2z4nz2x5zyan47v2c4sb
43: parallel-netcdf     /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/parallel-netcdf-1.12.2-ifxcaprlsbg6yici5thrauenrrsni6rf
44: parsec      /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/parsec-3.0.2012-skubbhmuerh2girwaaxzjvbrhh32y7vc
45: pdt         /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/pdt-3.25.1-26xpd4lciazzhyty5e4a3m7mg2j4pw7s
46: petsc       /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/petsc-3.15.3-k47bmlzv45mt5bvseit4jvc2dyguirtq
47: precice     /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/precice-2.2.1-srjr2zgocc3ytbkmd3f6s2qmdnvr6zsz
48: pumi        /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/pumi-2.2.6-jcuodiq4bszr7lrg5bkrdwpeke7k42a5
49: py-libensemble      /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/py-libensemble-0.7.2-2x2kmeoh3ap2rzhuudvzwolzctascl3z
50: qthreads    /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/qthreads-1.16-wfk6b3rpmkoknbsqzzrh5ntyvyrv2aar
51: raja        /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/raja-0.13.0-gy2js2b5mgwcojgnx346qd3zwcmm2acb
52: slate       /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/slate-2021.05.02-osr65v4fm4b4lqo2e6gl7gc25nuvcftv
53: slepc       /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/slepc-3.15.1-wpl3du3po6mw5hwywut3ima45lf3xyop
54: stc         /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/stc-0.9.0-rtxsbh2curyo677tad2es6errx4ks4ak
55: strumpack   /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/strumpack-5.1.1-kg7z3vorexd5qkbgjxnq3mmxhj45nhu7
56: sundials    /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/sundials-5.7.0-2g3b7x2qcrtj5lnb6rkpeimkalphzqqk
57: superlu-dist        /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/superlu-dist-6.4.0-celyerjnxknvlo7knbxshos66hjyjjnj
58: swig        /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/swig-4.0.2-fortran-5abclen45xtkqz2zlracludgl64hyyma
59: sz  /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/sz-2.1.12-rol3fpnarlcal47esdajmdhw6v53dhrx
60: tasmanian   /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/tasmanian-7.5-txw2jfti7onplz7ivgxwdhochi2jy2jl
61: trilinos    /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/trilinos-13.0.1-j56hfmk5th6gtygy2p65cf4mkv3wba3g
62: turbine     /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/turbine-1.3.0-6pujosdllzqwk4vyd7nf6xdn2bbzwyle
63: umpire      /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/umpire-4.1.2-ihxehibuvy6jgz5eaylcsii2dtxgq4iz
64: upcxx       /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/upcxx-2021.3.0-4642kludhepbxiviirgpbcacd35nfgmc
65: veloc       /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/veloc-1.4-j6fbijfh65qgnr32vzfppr6pswjojvtz
66: vtk-m       /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/vtk-m-1.6.0-54pffiakg4osgntzc4bcp6qjw44d3gdh
67: warpx       /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/warpx-21.08-h5z7l7d7to7e2lnqfauo7ld3wg7fmmet
68: zfp         /spack/opt/spack/linux-ubuntu18.04-x86_64/clang-13.0.0/zfp-0.5.5-hjkdysnxx5nlj46apm467t2ahg54mteb
```

EXASCALE COMPUTING PROJECT

21.08 Release: 88 Official Products + dependencies (ppc64le gcc)

```
1: adios2       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/adios2-2.7.1-5ypq4cpy5saarjfhorbxsv5neybf2ssn
2: aml  /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/aml-0.1.0-756lbduqno2kffsx6hzv6zjhv2bgh7vc
3: amrex        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/amrex-21.08-pi6s5ebemynnxaos34vcr4kiheacdw7a
4: arborx       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/arborx-1.0-znhysvf6mscyvqhpd7ooteslnv4upszk
5: archer       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/archer-2.0.0-qwvexfzn5qcxy3syo6fzc3ygz7r6ruly
6: argobots     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/argobots-1.1-zr2jx6dqcu3yvqhtinwcvewkpt46m4if
7: ascent       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/ascent-0.7.1-v6zgmtzcr6v5wbshjndiq2c4vub7zqms
8: axom         /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/axom-0.5.0-mzarurrq3pm6sdgg6tuv5mmuncqievyw
9: bolt         /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/bolt-2.0-eqxc7tio6l5idbxocc67lyrendkxldvv
10: cabana      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/cabana-0.3.0-v5enrdkttmz2dagtswfro7fco6ky5zc4
11: caliper     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/caliper-2.6.0-72lypcuy6sunwumc5uodzxeggwlwkyel
12: chai        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/chai-2.3.0-jnjmiios3dnrlsgew2l4gmkjhey4mb5i
13: charliecloud        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/charliecloud-0.24-nw4mwua6qy3hxfhqfzvhlrwcwr3k5awk
14: conduit     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/conduit-0.7.2-yn76rqhb556flxddh7ywvc6m6iu6ff5h
15: darshan-runtime     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/darshan-runtime-3.3.1-5yubw26b2r2naliejw35jw2rils7odd2
16: datatransferkit     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/datatransferkit-3.1-rc2-dkcpm6zd4xqakw5pwosgbit773ew7u7p
17: dyninst     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/dyninst-11.0.1-7ajspbfdrsrvsntcs6lg2ubwwoo5xpxs
18: faodel      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/faodel-1.1906.1-o7lz62bpelvkb4jzldsxs4dnavsnpdoe
19: flecsi      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/flecsi-1.4.2-vdjk5wq4xg5iks2hk7ast3jlq6qwhi2m
20: flit        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/flit-2.1.0-7444nergpy2artrg2is73o3btwurldnm
21: flux-core   /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/flux-core-0.28.0-lkzlgwxw4lsnueb6o6cflkvsuceepbph
22: fortrilinos         /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/fortrilinos-2.0.0-4ebbyxzs2l4cna74apwkbnfyyfzgq7au
23: gasnet      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/gasnet-2021.3.0-3dcjcmjoezerqszd6erumbompcsb5lgx
24: ginkgo      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/ginkgo-1.3.0-eehwgpl74hjha7asdxmr62vmwgrlv6hi
25: globalarrays        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/globalarrays-5.8-i56xnbjkepmyyef2jfxp27wecpsp74nd
26: gotcha      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/gotcha-1.0.3-lx2grawxujh2zcrsgg72zq6jgcbgodvk
27: hdf5        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/hdf5-1.12.0-kragbxub77idtxrazuuckq66v7ojjpri
28: heffte      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/heffte-2.1.0-vqmohwnqhyryfgkc43pomzilk6wjqoap
29: hpctoolkit  /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/hpctoolkit-2021.05.15-av4ie6mgrw2ukxpcsf7tk2ch5p2facov
30: hpx         /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/hpx-1.7.1-7272vqgygknfk5rlb4gxjzmdugvxjc2b
31: hypre       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/hypre-2.22.0-z4v2y4syakr4xxhpiifkddzvkhiup43t
32: kokkos      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/kokkos-3.4.00-dpda6rfkntqkdmtbzuwzkiy2nfhfvzsk
33: kokkos-kernels      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/kokkos-kernels-3.2.00-etrpvii2orcpwldtcer5p63iik4l4yzt
34: legion      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/legion-21.03.0-ikxkqp6m3r4etdjlnwywiyqytrfkms5p
35: libnrm      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/libnrm-0.1.0-qfikafns6vepq7cxu5ajocjqrwqdchwo
36: libquo      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/libquo-1.3.1-tjuqmxav3vsudgs3oqeq7pvwo66q3wjp
37: llvm-doe    /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/llvm-doe-uo-nplo7xkc5mewsdi36egeevlt4dzxzgo4
38: loki        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/loki-0.1.7-75yfeguryaey75ifjz34myucsxkntlbn
39: magma       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/magma-2.6.1-wuq4swyyegmvfn7ovxiq3kby45aepoyw
40: mercury     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mercury-2.0.1-top7xbsvpbuoehcycbl6flkwgqvvdhck
41: metall      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/metall-0.15-l6zegrxqr4js7ntap7qrbniwkylnetej
42: mfem        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mfem-4.3.0-6b67y2spjmr3xwhkievytkml2ib52sxq
43: mpich       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mpich-3.4.2-zotxlduewt5l6xfz72zor4xjt6qmoq7m
44: mpark-variant       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mpark-variant-1.4.0-uglub2prq64a3grjxebvalgzf5fyyjeh
```

Support for GPUs

- nvhpc 21.7
- cuda 11.4.0

EXASCALE COMPUTING PROJECT

21.08 Release: 88 Official Products + dependencies (ppc64le gcc)

```
45: mpifileutils      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mpifileutils-0.11-4r2yyylqgcn4hxuzgihryikmggqinw2i
46: netlib-scalapack  /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/netlib-scalapack-2.1.0-3ocusnxqwmpd2lzn7gdtuzwzdcvzjvls
47: ninja       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/ninja-1.10.2-nyszbmxf6pwatvxzmtbk33ws3g4h7z6e
48: nrm         /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/nrm-0.1.0-lfcz5mxq47tq6g3h7zvf6pjcx5rtsejt
49: omega-h     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/omega-h-9.32.5-k3dbv6fzmy24wrnnimz3ou6343wdve3m
50: openmpi     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/openmpi-4.1.1-6radczo4upfnv3flhbhj4bafq532dpvf
51: openpmd-api       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/openpmd-api-0.13.4-xghlpjwaomjdtqjdfpnwlslwym7nbze2
52: papi        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/papi-6.0.0.1-jdzpki5fslvwcjs6xikughssbyin3y7q
53: papyrus     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/papyrus-1.0.1-ei7kgyj6pfxx4lg3lwreynsaimo752vi
54: parallel-netcdf   /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/parallel-netcdf-1.12.2-elfqmjesbu7ypq3vw5kv27cvsjksiror
55: paraview    /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/paraview-5.9.1-y5kaqeeu4cxc2vlapraga35dlv6iabsn
56: parsec      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/parsec-3.0.2012-ts42udsitpsvkz4vrgr2y7japkbpbmqq
57: pdt         /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/pdt-3.25.1-ilht5xwcligeas4yrobr7ttod2lhkvfx
58: petsc       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/petsc-3.15.3-xpinmm5a5xdwkdyd2t3bpe5cufax6b7w
59: plasma      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/plasma-20.9.20-m5jru2byq5a3nn7aaibfixhaot3ix5rp
60: precice     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/precice-2.2.1-xoakvlsmedn6ccqx44arxzshpw2zvund
61: pumi        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/pumi-2.2.6-vfese5drtybcelsrmqcdylgpa5rpuqzm
62: py-jupyterhub     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-jupyterhub-1.0.0-iput7vbst5vfkr3ee2rvarktxn5co7hn
63: py-libensemble    /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-libensemble-0.7.2-cmvpizlxbfr3ebhzobs43wb7pgq4tifj
64: py-warpx    /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-warpx-21.08-w43bz3xvl4xaz2ak3yy5ih7pxobuym5p
65: qthreads    /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/qthreads-1.16-7cckh2xagt6wxvog7et3qov2oh4cruyn
66: raja        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/raja-0.13.0-t2gfqkglc452raitdisocv7lsyu2qio7
67: rempi       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/rempi-1.1.0-tk23cayw6akduy2p4worwdm4dqfwo4qd
68: scr         /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/scr-3.0rc1-j5re3dcmt3oly67fx3fwqymgd7tfvgup
69: slate       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/slate-2021.05.02-ydt6cjyewdms65yi3skccyhwrbr33fgz
70: slepc       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/slepc-3.15.1-ezj2y3a5257ftdszsem7pzctxqm4q22w
71: stc         /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/stc-0.9.0-fyrfwpaxwlusgwewwnzmyi3uofx6dql4
72: strumpack   /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/strumpack-5.1.1-ifm6u3c7xp7z3vmrw5jnj5jojms6gxvp
73: sundials    /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/sundials-5.7.0-a3xt4ve7rtuvokvcczginthrp656iwyt
74: superlu-dist      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/superlu-dist-6.4.0-f5dky6ukrhde3uhdgoljn47sabtzbl45
75: swig        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/swig-4.0.2-fortran-ymkhsbcjuruoqfddhua5o2o4ni4hqh7o
76: sz  /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/sz-2.1.12-f4stpek6xecauyz3td27xdv7nvnvmd3r
77: tasmanian   /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/tasmanian-7.5-z24lhbk6cqvlgtkxbq57oxnicu5rwjsu
78: tau         /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/tau-2.30.1-npsshipn6qypsycpyhhq2k22ki2zu3fd
79: trilinos    /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/trilinos-13.0.1-xhjaaxy5jzlu22laevkitkngtibahnym
80: turbine     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/turbine-1.3.0-xhczvdoaofhwtj54msko4h6ies3fa5k5
81: umap        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/umap-2.1.0-pfpnanzkevlsv7s7jvymtnof7su7gg4k
82: umpire      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/umpire-4.1.2-fmg5gdiea7b6pi5f6mkcbbyi33gcw4ej
83: unifyfs     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/unifyfs-0.9.1-pgwglf2tuiahnw4iwb2qkdf2fjzrfb4t
84: upcxx       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/upcxx-2021.3.0-guxznj2jbl7l7v5v6nu5jiaz5wgvvkyg
85: veloc       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/veloc-1.4-3jyuj6wyb44cgd3pcbv3bklic2okqlrm
86: vtk-m       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/vtk-m-1.6.0-tuzuw57aed54t4d447gy2skcgfxioa4c
87: warpx       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/warpx-21.08-qvqrlvxxr6wvn5uykpvpufzaldopt2jh
88: zfp         /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/zfp-0.5.5-2tiii5lc66cfhfajvs57fyq2lgdmp4wc
```

EXASCALE COMPUTING PROJECT

21.08 Release: 88 Official Products + dependencies (ppc64le llvm)

```
1: adios2        /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/adios2-2.7.1-43ls77z7pfxbnwu3dqo345zwcaqa6w7c
2: aml  /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/aml-0.1.0-ganh5ug63lak6rieiidorqh7qm2zqvmy
3: amrex         /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/amrex-21.08-ndffpysecvrvoxlc2k4eskrdb4b2bzca
4: arborx        /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/arborx-1.0-y4fwqwigysw7dy32gttky6ibuvqsohh5
5: argobots      /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/argobots-1.1-j5jbf7tvgz2nlmxnkyqp7ax3xmexxizj
6: axom          /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/axom-0.5.0-5wy37is6crmquyyls3mli2pr7b6h2xw4
7: bolt          /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/bolt-2.0-pgyj3k3ozbaxy7l7sao2ddec5aallbcz
8: cabana        /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/cabana-0.3.0-vtd2oatmkbkvmxrxlhiav2nneywuttnw
9: chai          /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/chai-2.3.0-4jeoitrfnrhjhkimp7k4fiwmwwmy6xxi
10: conduit      /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/conduit-0.7.2-tqwrg7mmo3ncypjmobvuqnaqv7b5r3pv
11: darshan-runtime      /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/darshan-runtime-3.3.1-ktykjyehwslgciuy364jojimjdki5okr
12: faodel       /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/faodel-1.1906.1-glwjunqrsffr2di2yuccr4gtumwhznsd
13: flit         /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/flit-2.1.0-2prfvul7hywta5fuqotwcd2xjabfkdin
14: flux-core    /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/flux-core-0.28.0-dndcnrfym66vdrfjuk7wapxkeo7fe5lw
15: gasnet       /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/gasnet-2021.3.0-7ddmgdkmblog5ytdfdtarsjj42c77oac
16: ginkgo       /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/ginkgo-1.3.0-xfaibi6kt6is4xfklpdmr2ngs3aiptjj
17: gotcha       /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/gotcha-1.0.3-2zklpafyyz3s42t6i5ld5lzonvgeiogd
18: hdf5         /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/hdf5-1.12.0-rgeyyx36ww4vh46lw3uupecokm2ng5on
19: heffte       /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/heffte-2.1.0-t6p3aa7xtiqgqku75itbotlkmj5pv3pu
20: hpx          /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/hpx-1.7.1-rayqo5aeoicbubk3u7ttdxpaqg6pvjay
21: kokkos       /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/kokkos-3.4.00-mrywpj45t2suizxmrkrosuxd7ak6ylmx
22: kokkos-kernels       /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/kokkos-kernels-3.2.00-zag6wptuazibeglxobd7odsi5wihrlvf
23: legion       /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/legion-21.03.0-mxpfgriqu3omjsggsgjscnvcjz5fwm3v
24: libquo       /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/libquo-1.3.1-eaa4ko2v5abilqai4wbtl27kgnwi6khn
25: loki         /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/loki-0.1.7-avcj4mvkofozfqdmzxewvrvmz6vcaltd
26: mercury      /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/mercury-2.0.1-7izboj2r5hjjqsguk22lip3i7inizonw
```

21.08 Release: 88 Official Products + dependencies (ppc64le llvm)

```
27: metall      /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/metall-0.15-3hddyrdj37qhzuirxllaufmxl6h73ts3
28: mpich       /usr/local/mpich
29: mpark-variant       /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/mpark-variant-1.4.0-y3cdl4uwjbg7vukhr6nphmvjrd6okb2i
30: mpifileutils        /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/mpifileutils-0.11-5j7x4oazncd5ayqq5hbgfbbtreutbxk2
31: ninja       /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/ninja-1.10.2-gfx5xvn52iopbxtjuid4bbkq37gbzcht
32: openpmd-api         /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/openpmd-api-0.13.4-kdnxdlnpiwgizngh6iiwpupyncuycrym
33: openmpi     /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/openmpi-4.1.1-mxaoo5uz6rvzvvlwax2grnuxifwibz65
34: papi        /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/papi-6.0.0.1-izlyfej6re2uhh7cipdbizqsyafyw6mk
35: papyrus     /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/papyrus-1.0.1-tpavqisuz3dlhzqeizlchkehc2b7j6ji
36: parallel-netcdf     /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/parallel-netcdf-1.12.2-m3oqli7hzito72tizhimyhvnheodklrq
37: parsec      /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/parsec-3.0.2012-l2j623hjgucv4w7p7i6s6cmxektb7hxf
38: pdt         /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/pdt-3.25.1-g5zoacjhk7d2juffmpybsjo7ccvyop7n
39: pumi        /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/pumi-2.2.6-el5rrb2e4bjnagdnub4dcbdcbrj44xxe
40: qthreads    /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/qthreads-1.16-532w6nlsalov23famjbmbud3pliokbi7
41: raja        /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/raja-0.13.0-2u3642wb7anactofwbxglft47plizoha
42: stc         /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/stc-0.9.0-agqqshmxw3i536f6og26luw4lnpfm6h4
43: sundials    /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/sundials-5.7.0-qmvw42l6vqyghtwyfg7guwhaibjmjday
44: swig        /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/swig-4.0.2-fortran-4q36y7ilx4qqrwiyxue6u6f5d3xlbc3p
45: sz  /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/sz-2.1.12-5a53cw7wls3ybrvh6d74p4bhaxzt3dz2
46: tasmanian   /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/tasmanian-7.5-zt6sj4dsxjhoocsdisnsvh2kyoinvl5e
47: turbine     /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/turbine-1.3.0-srocuaodmb3uu3q4sqcw22g4rwppy3x7
48: umpire      /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/umpire-4.1.2-2lwdxnbczlq2fwylpopqgldfembbc7i3
49: upcxx       /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/upcxx-2021.3.0-7r6unth4batyuwvrpk2m6zpfd2g3yjdn
50: vtk-m       /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/vtk-m-1.6.0-zy6r5uunhmujtiulgsxq6lyqk4zj3l3u
51: warpx       /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/warpx-21.08-l4ukqhs6exsuvtvy56jkdkue5k7rjcsi
52: zfp         /spack/opt/spack/linux-ubuntu18.04-ppc64le/clang-13.0.0/zfp-0.5.5-5h72cs57h6tump4skthbponh2xcjtm7f
```

Using E4S with Shifter on Cori

```
% shifterimg images | grep e4s
% cd; cp -r /global/homes/s/sameer/demo/testsuite/ .;ln -s ~/testsuite/trilinos/Zoltan ~/
% shifter -E --image=ecpe4s/ubuntu18.04-e4s-gpu:21.08 -- /bin/bash --rcfile /etc/bashrc
% spack find; cd ~/Zoltan; ./compile.sh
% which mpicc
% exit
% cat /etc/os-release
% cat run.job
#!/bin/bash
#SBATCH -N 4 -t 5
#SBATCH --image=ecpe4s/ubuntu18.04-e4s-gpu:21.08
#SBATCH -C haswell
srun -n 4 shifter -- /bin/bash -c 'unset CRAYPE_VERSION; unset MODULEPATH; .
  /spack/share/spack/setup-env.sh; spack load --first trilinos%gcc ; spack unload mpich;
  ./Zoltan'

% sbatch run.job
% cat *.out
```

EXASCALE COMPUTING PROJECT

Using E4S with Shifter on Perlmutter

```
% cd; cp -r ~sameer/demo/NPB3.1 .
% shifter -E --image=ecpe4s/ubuntu18.04-e4s-gpu:latest -- /bin/bash --rcfile /etc/bashrc
% spack find
% spack load --first trilinos % gcc
% which mpicc
% cd ~/NPB3.1; make clean; make ; cd bin; mpirun -np 4 ./lu.W.4
```

EXASCALE COMPUTING PROJECT

E4S Download from https://e4s.io


https://e4s-project.github.io/download.html

E4S

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Extreme-Scale Scientific Software Stack (E4S) version 21.08

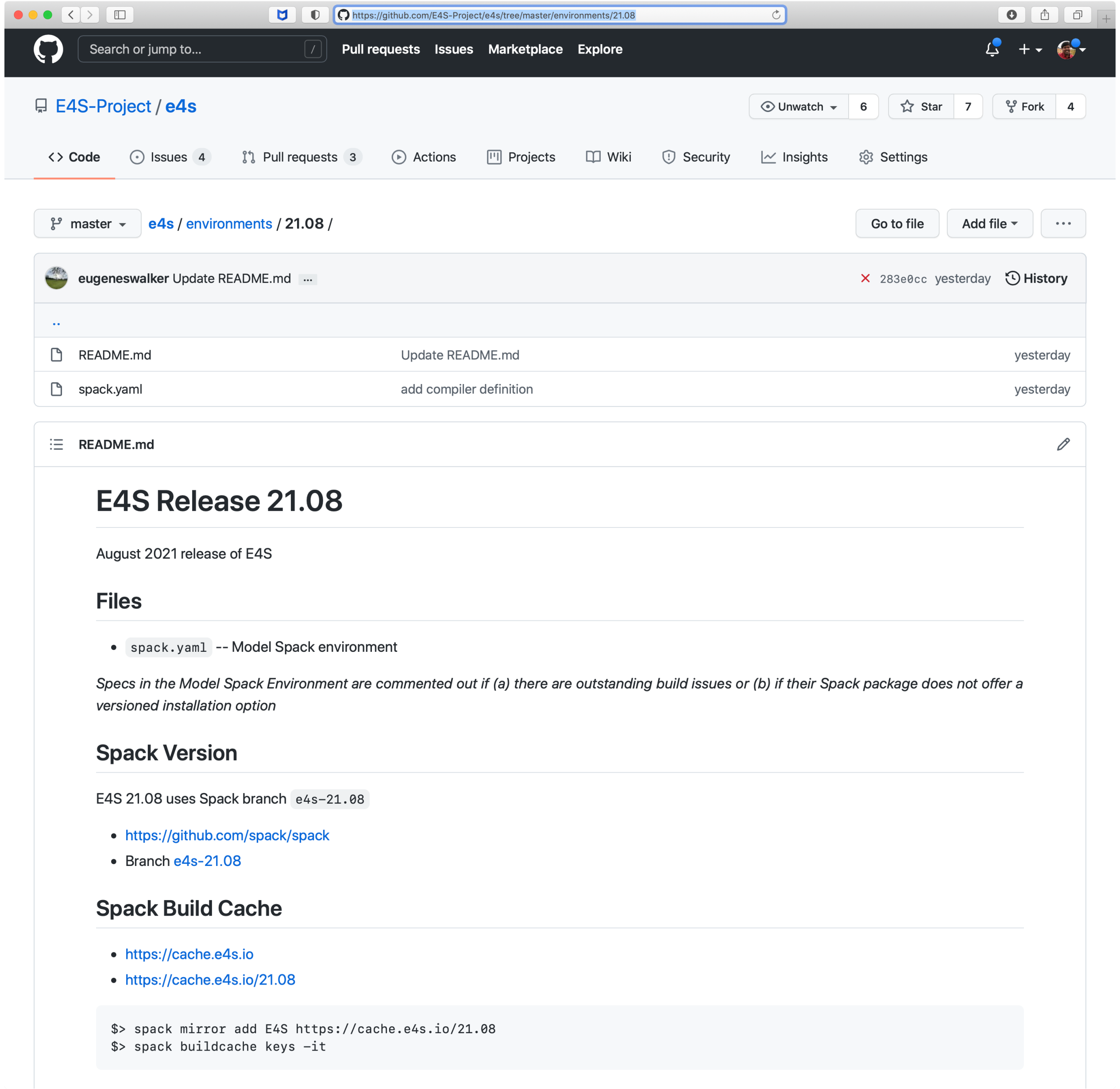
Exascale Computing Project (ECP) Software Technologies (ST) software, Extreme-Scale Scientific Software Stack (E4S) v21.08, includes a subset of ECP ST software products, and demonstrates the target approach for future delivery of the full ECP ST software stack. Also available are a number of ECP ST software products that support a Spack package, but are not yet fully interoperable. As the primary purpose of the v21.08 is demonstrating the ST software stack release approach, not all ECP ST software products were targeted for this release. Software products were targeted primarily based on existing Spack package maturity, location within the scientific software stack, and ECP SDK developer experience with the software. Each release will include additional software products, with the ultimate goal of including all ECP ST software products.

E4S v21.08 Notes.

E4S Container Installation Instructions.

ECP EXASCALE COMPUTING PROJECT

E4S for bare-metal installation



E4S Release 21.08

August 2021 release of E4S

Files

- `spack.yaml` -- Model Spack environment

Specs in the Model Spack Environment are commented out if (a) there are outstanding build issues or (b) if their Spack package does not offer a versioned installation option

Spack Version

E4S 21.08 uses Spack branch `e4s-21.08`

- https://github.com/spack/spack
- Branch e4s-21.08

Spack Build Cache

- https://cache.e4s.io
- https://cache.e4s.io/21.08

```
$> spack mirror add E4S https://cache.e4s.io/21.08
$> spack buildcache keys -it
```

EXASCALE COMPUTING PROJECT

E4S: Spack Build Cache at U. Oregon and AWS

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

E4S Build Cache for Spack 0.16.2

To use this build cache, just add it to your Spack

spack mirror add E4S https://cache.e4s.io

spack buildcache keys -it

Click on one of the packages below to see a list of all available variants.

All Architectures   PPC64LE   X86_64

All Operating Systems   Centos 7   Centos 8   RHEL 7   RHEL 8   Ubuntu 18.04   Ubuntu 20.04   Amazon Linux 2

Last updated: 05-22-2021 23:03 PDT

53991 Spack packages

Search

adiak@0.1.1 adiak@0.2.1 adios2@2.5.0 adios2@2.6.0 adios2@2.7.0 adios2@2.7.1 adios@1.13.1 adlbx@0.9.2 adlbx@1.0.0 adol-c@2.7.2 amg@1.2 aml@0.1.0

amr-wind@ascent amr-wind@main amrex@20.07 amrex@20.09 amrex@20.10 amrex@20.11 amrex@20.12 amrex@21.01 amrex@21.02 amrex@21.03 amrex@21.04

amrex@21.05 ant@1.10.0 ant@1.10.7 arborx@0.9-beta arborx@1.0 argobots@1.0 argobots@1.0rc1 argobots@1.0rc2 argobots@1.1 arpack-ng@3.7.0

arpack-ng@3.8.0 ascent@0.6.0 ascent@0.7.0 ascent@0.7.1 ascent@develop ascent@pantheon_ver assimp@4.0.1 assimp@5.0.1 autoconf-archive@2019.01.06

autoconf@2.69 autoconf@2.70 automake@1.16.1 automake@1.16.2 automake@1.16.3 axl@0.1.1 axl@0.3.0 axl@0.4.0 axom@0.3.3 axom@0.4.0

axom@0.5.0

Click on the full spec link to find out more.

Link	Arch	OS	Compiler	Created	Full Hash
Full Spec	ppc64le	rhel7	gcc@9.3.0	05-19-2021 23:33 PDT	7m3n6ldvbv26h2xlbflxzqposyeqrhwm
Full Spec	ppc64le	rhel8	gcc@8.3.1	05-19-2021 23:39 PDT	3sussuga5t3f24xiyw6skvtmdhmdk7wd
Full Spec	ppc64le	ubuntu18.04	gcc@7.5.0	05-19-2021 22:16 PDT	d66vwasmnnz3mgagzoqnbei6vctddwhq
Full Spec	ppc64le	ubuntu20.04	gcc@9.3.0	05-19-2021 22:17 PDT	naokmt4c776tdajlb6wlkppns5jll4s2
Full Spec	x86_64	rhel7	gcc@9.3.0	05-19-2021 21:30 PDT	wfmbfgibmf2cxkdrzxkigu5arb3xvzxp
Full Spec	x86_64	rhel7	gcc@9.3.0	05-22-2021 20:26 PDT	aaj2zlurf7wdvusngcvgj2l6l4xc7d72
Full Spec	x86_64	rhel8	gcc@8.3.1	05-19-2021 21:30 PDT	mpqhhargaocfpbspnnlzmygjntqogiuc
Full Spec	x86_64	rhel8	gcc@8.3.1	05-22-2021 20:21 PDT	co6kkiurfbbaudif5lsapfebgofx3pr5
Full Spec	x86_64	ubuntu18.04	gcc@7.5.0	05-19-2021 21:28 PDT	rxslnbkn6p6svy5gfwvon5y3vlcktm5u
Full Spec	x86_64	ubuntu18.04	gcc@7.5.0	05-22-2021 20:24 PDT	7fsv5m7i6w6o4vgs6ljpcqiyjph3pifa
Full Spec	x86_64	ubuntu20.04	gcc@9.3.0	05-19-2021 21:33 PDT	jwr5ek7brob3d3tknpupxdsmom5zsl43
Full Spec	x86_64	ubuntu20.04	gcc@9.3.0	05-22-2021 20:27 PDT	fvnwh3mq4k3ghoccwmlyvm7z74pyfxqh

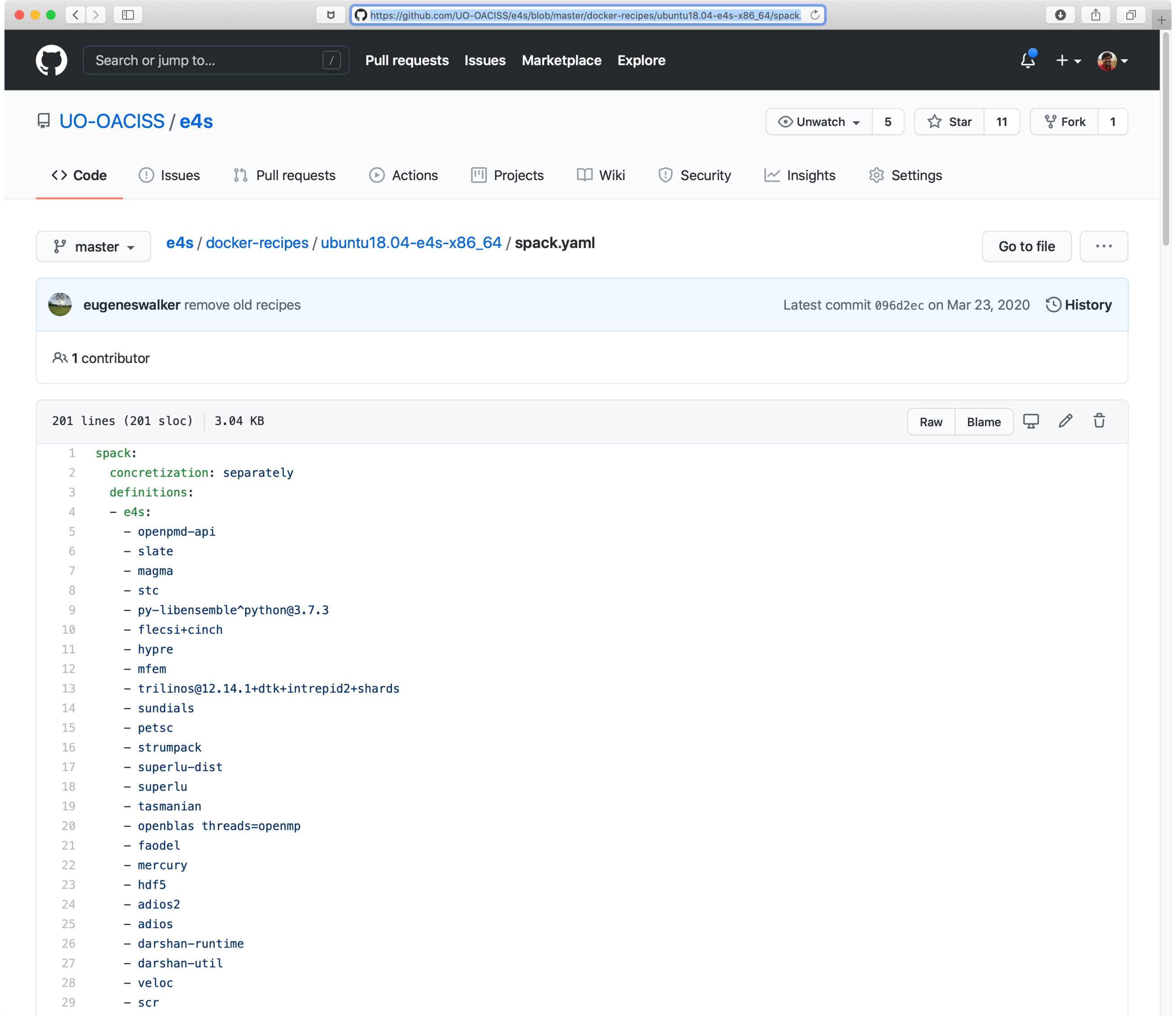
- 50,000+ binaries
- S3 mirror
- No need to build from source code!

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

EXASCALE COMPUTING PROJECT

Using E4S: From source using Spack and build caches

E4S Spack environment spack.yaml




```yaml
spack:
  concretization: separately
  definitions:
  - e4s:
    - openpmd-api
    - slate
    - magma
    - stc
    - py-libensemble^python@3.7.3
    - flecsi+cinch
    - hypre
    - mfem
    - trilinos@12.14.1+dtk+intrepid2+shards
    - sundials
    - petsc
    - strumpack
    - superlu-dist
    - superlu
    - tasmanian
    - openblas threads=openmp
    - faodel
    - mercury
    - hdf5
    - adios2
    - adios
    - darshan-runtime
    - darshan-util
    - veloc
    - scr
```

- Bare-metal install
  % cat spack.yaml
  % spack -e . install

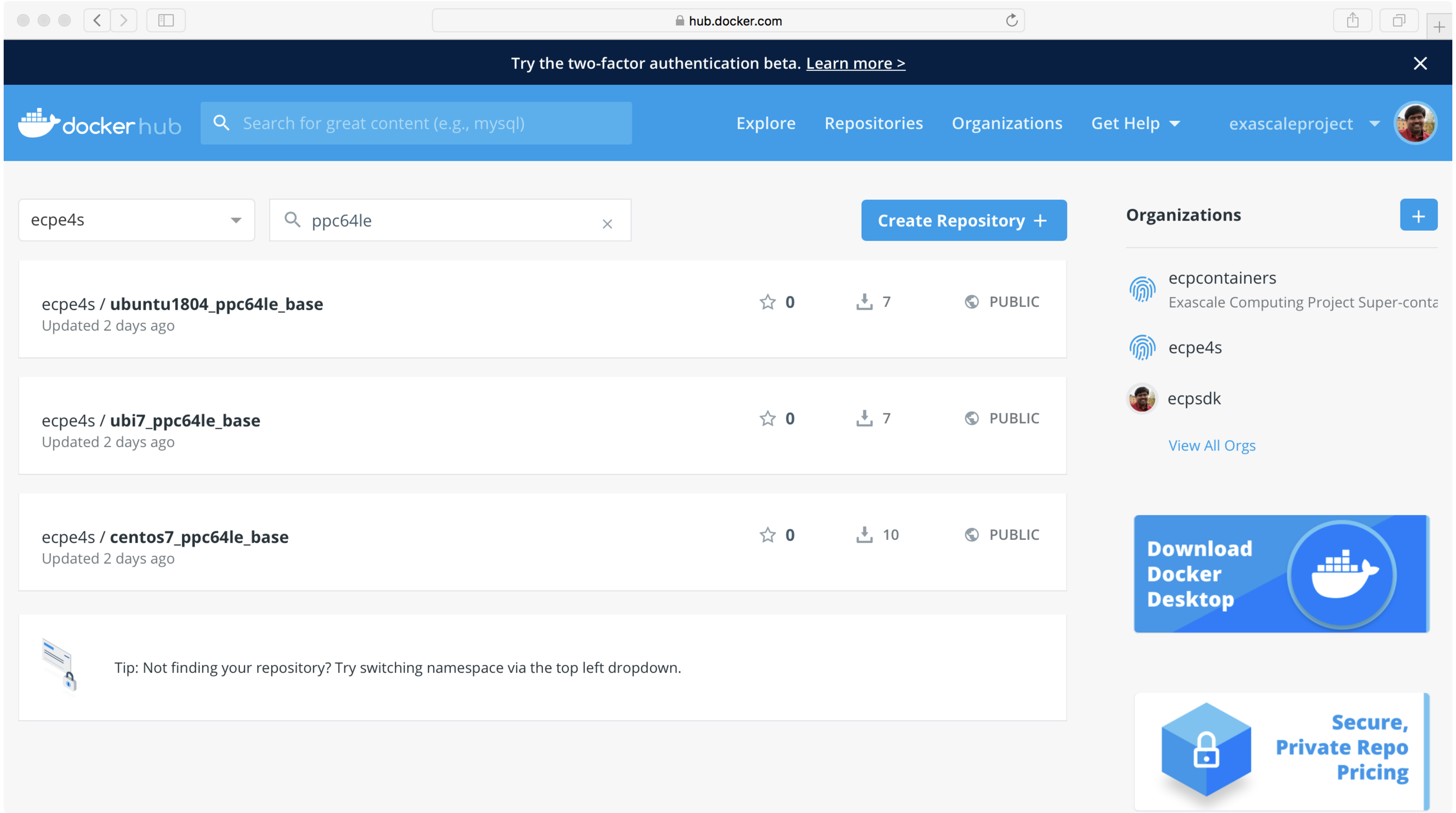
- Docker build:

Executable File | 2 lines (2 sloc) | 78 Bytes

```bash
#!/bin/bash -x
docker build --no-cache -t ecpe4s/ubuntu18.04-e4s-x86_64:1.2 .
```

EXASCALE COMPUTING PROJECT

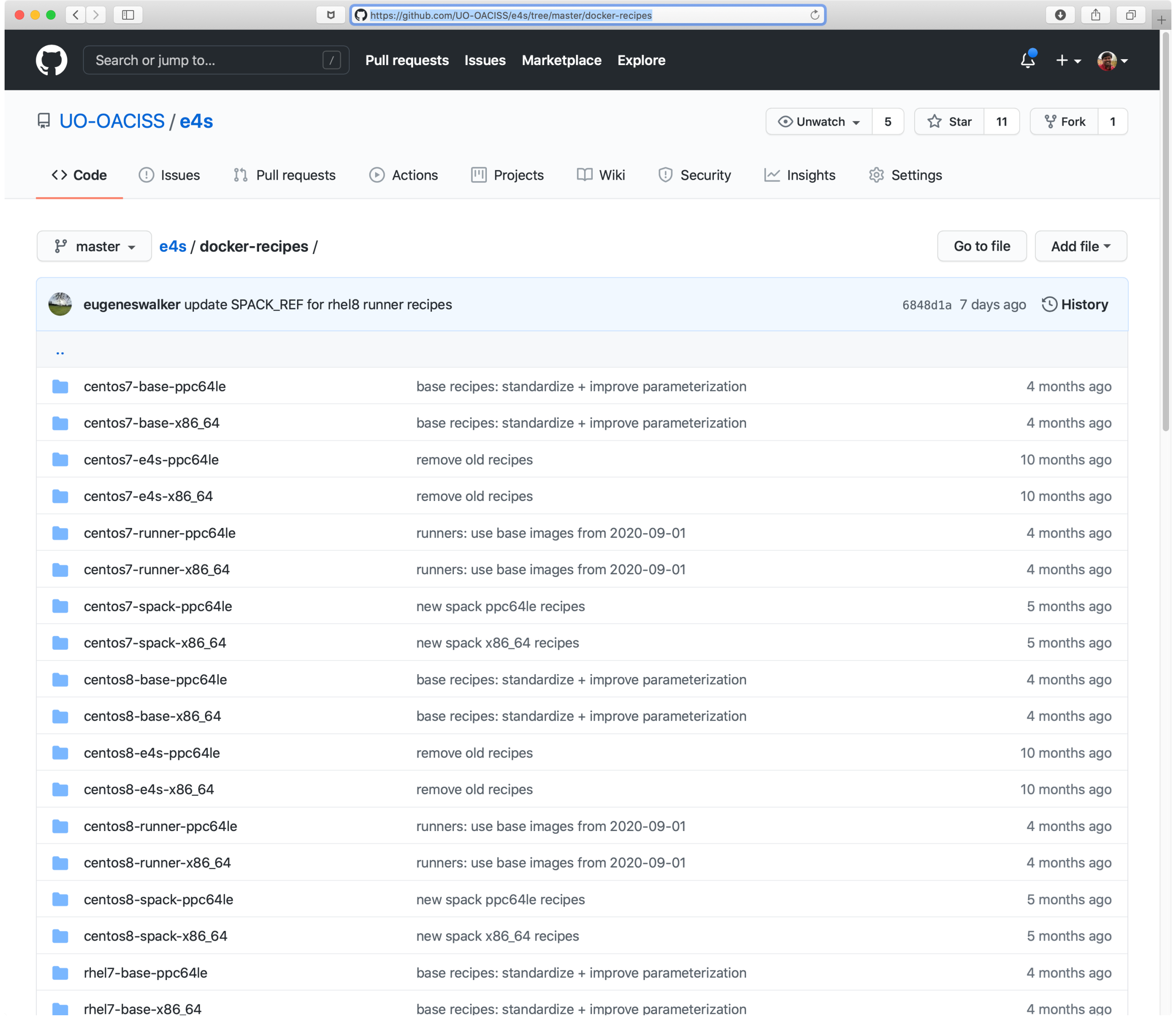
E4S: ppc64le Base Container Images



- Hub.docker.com
- ecpe4s

- Ubuntu 18.04
- RHEL/UBI 7.6
- Centos 7.6

Multi-platform E4S Docker Recipes

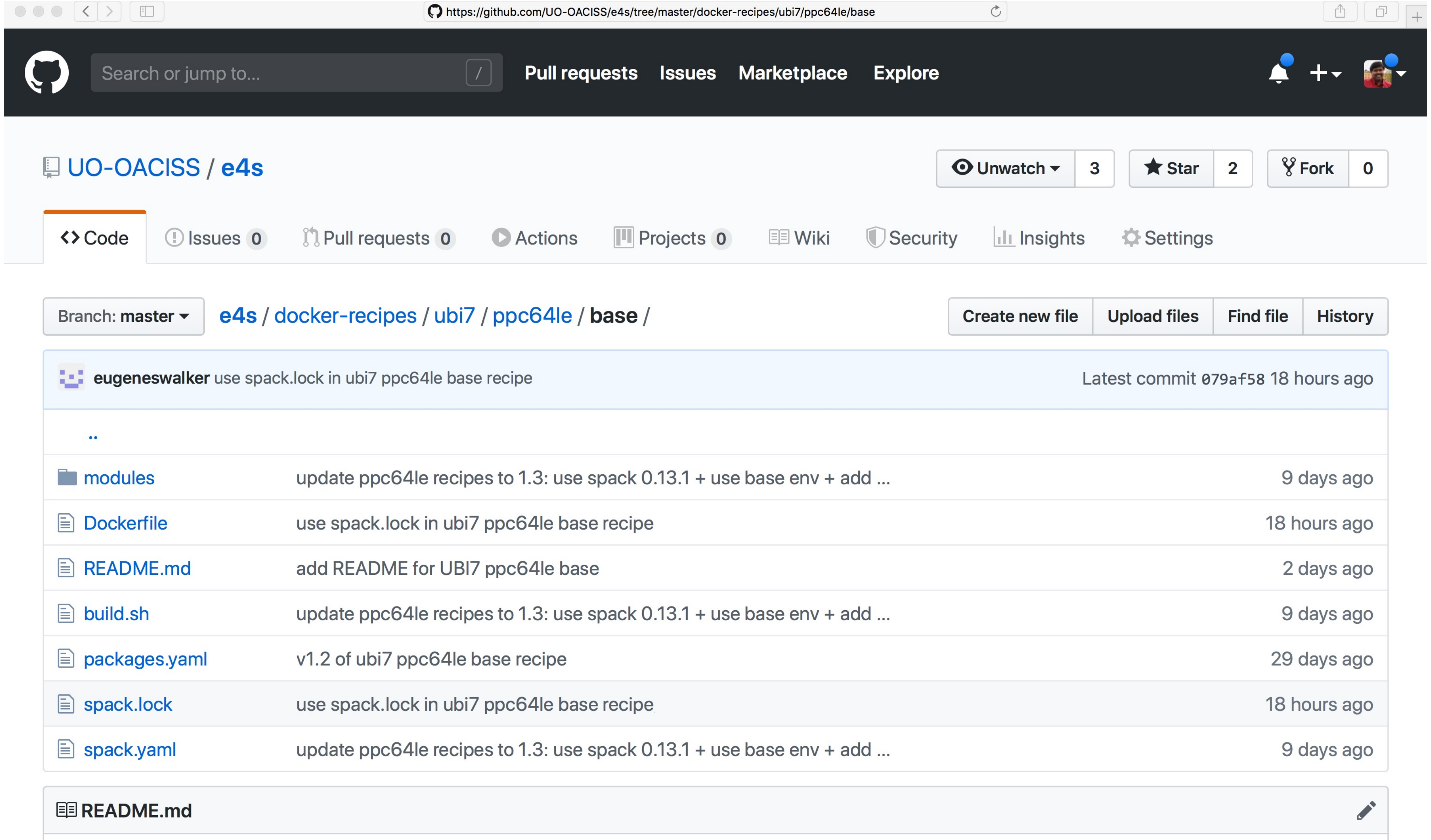


10 lines (6 sloc) | 178 Bytes

```
FROM ecpe4s/ubuntu18.04-spack-x86_64:0.14.1

WORKDIR /e4s-env

COPY /spack.yaml .

RUN spack install --cache-only \
 && spack clean -a && rm -rf /tmp/root/spack-stage

WORKDIR /
```

EXASCALE COMPUTING PROJECT

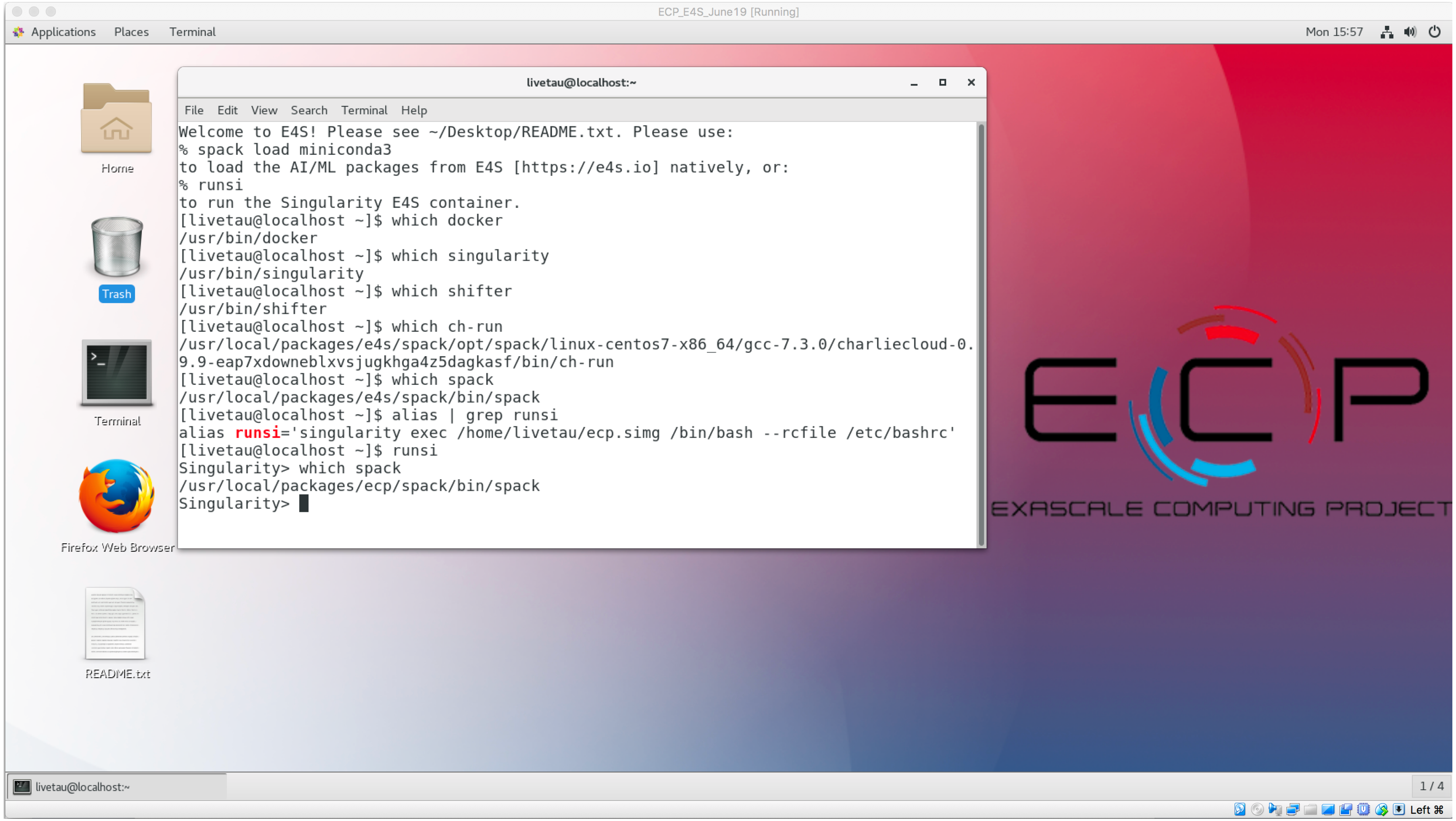
E4S: Multi-platform Reproducible Docker Recipes



E4S
- x86_64
- ppc64le
- aarch64

https://e4s.io

E4S VirtualBox Image



Container Runtimes

- Docker
- Shifter
- Singularity
- Charliecloud

https://e4s.io

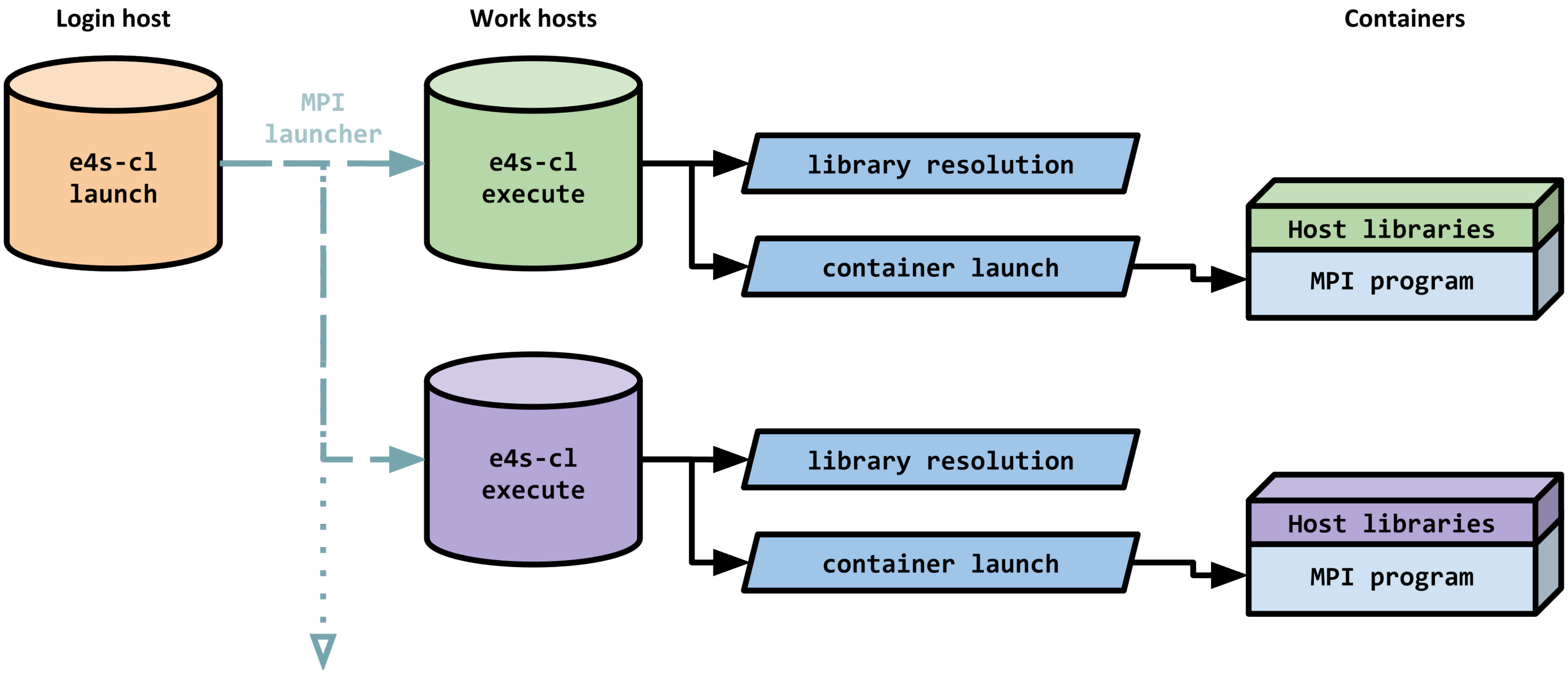
e4s-cl: A tool to simplify the launch of MPI jobs in E4S containers

- E4S containers support replacement of MPI libraries using MPICH ABI compatibility layer.
- 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:
    1. e4s-cl init --backend singularity --image ~/ecp.simg --soure ~/source.sh
    2. e4s-cl mpirun -np <N> -hosts <> <command>

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

EXASCALE COMPUTING PROJECT

e4s-cl Container Launcher



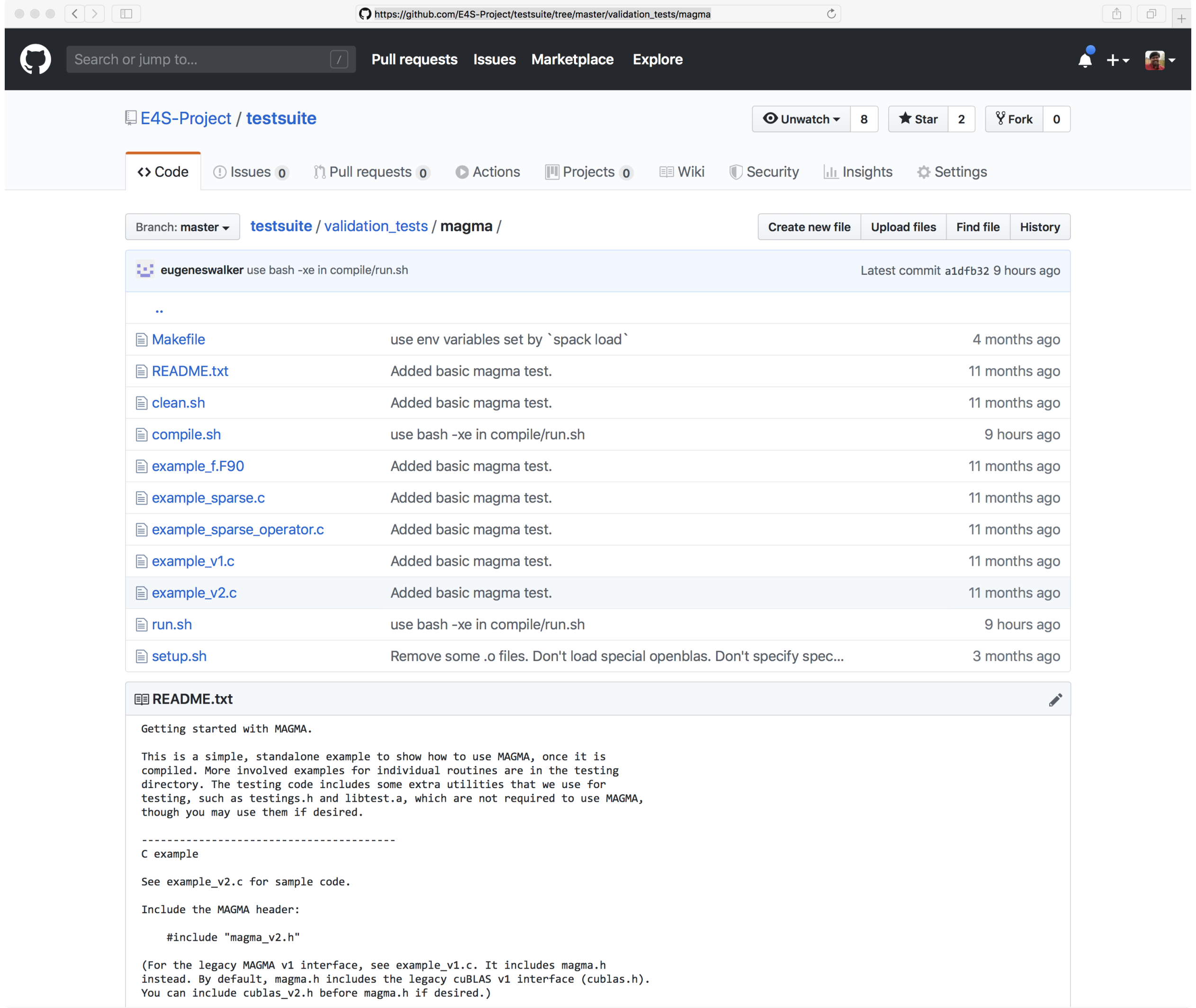
EXASCALE COMPUTING PROJECT

https://e4s.io

E4S Continuous Integration Testing

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

Reproducible Container Builds using E4S Base Images

UO-OACISS / e4s

Unwatch 3 | Star 0 | Fork 0

Code | Issues 0 | Pull requests 0 | Projects 0 | Wiki | Security | Insights | Settings

Branch: master | e4s / docker / ubi7 / x86_64 / custom / superlu / spack.yaml | Find file | Copy path

sameershende Adding a custom image for SC19 SuperLU tutorial. a0b948d 10 days ago

1 contributor

35 lines (34 sloc) | 579 Bytes | Raw | Blame | History

```yaml
spack:
  packages:
    all:
      compiler: [gcc@7.3.0]
      variants: +mpi
      providers:
        mpi: [mpich]
      buildable: true
      version: []
      paths: {}
      modules: {}
    mpich:
      version: [3.2.1]
      variants: ~wrapperrpath
      buildable: true
      providers: {}
      paths: {}
      modules: {}
      compiler: []
    gcc:
      version: [7.3.0]
      buildable: true
      providers: {}
      paths: {}
      modules: {}
      compiler: []
  specs:
  - superlu-dist
  - petsc
  - mfem
  - strumpack
  - butterflypack
  - openblas
  view: false
```

https://github.com/UO-OACISS/e4s/blob/master/docker/ubi7/x86_64/custom/superlu/Dockerfile

Search or jump to... | Pull requests | Issues | Marketplace | Explore

UO-OACISS / e4s

Unwatch 3 | Star 0 | Fork 0

Code | Issues 0 | Pull requests 0 | Projects 0 | Wiki | Security | Insights | Settings

Branch: master | e4s / docker / ubi7 / x86_64 / custom / superlu / Dockerfile | Find file | Copy path

sameershende Adding a custom image for SC19 SuperLU tutorial. a0b948d 10 days ago

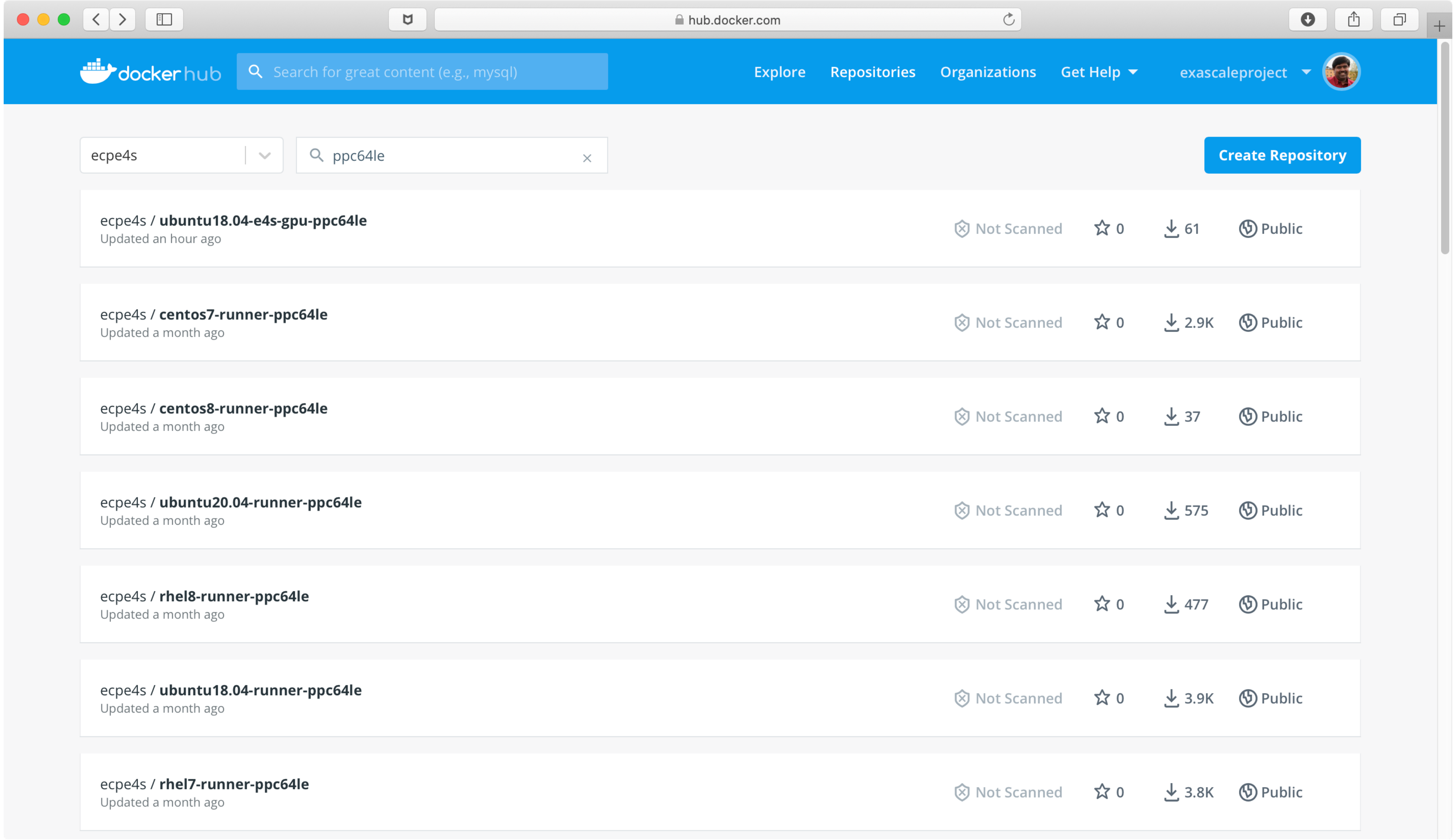
1 contributor

21 lines (13 sloc) | 519 Bytes | Raw | Blame | History

```dockerfile
FROM ecpe4s/ubi7_x86_64_base:1.1


ENV     FORCE_UNSAFE_CONFIGURE=1 \
          XSDK_ENV_ROOT="/xsdk-env" \
          E4S_GROUP="xsdk" \
    PATH=/spack/bin:${PATH} \
    SPACK_ROOT=/spack


COPY /spack.yaml ${XSDK_ENV_ROOT}/spack.yaml


# !!! Comment out the following RUN instruction if you do not want to pull pre-built binaries from the E4S mirror !!!

RUN     spack env create superlu ${XSDK_ENV_ROOT}/spack.yaml \
        && . ${SPACK_ROOT}/share/spack/setup-env.sh \
        && spack env activate superlu \
        && spack install  \
        && spack clean -a
```


- PMR SDK base image has Spack build cache mirror and GPG key installed.
- Base image has GCC and MPICH configured for MPICH ABI level replacement (with system MPI).
- Customized container build using binaries from E4S Spack build cache for fast deployment.
- No need to rebuild packages from the source code.
- Same recipe for container and native bare-metal builds with Spack!

E4S: GitLab Runner Images



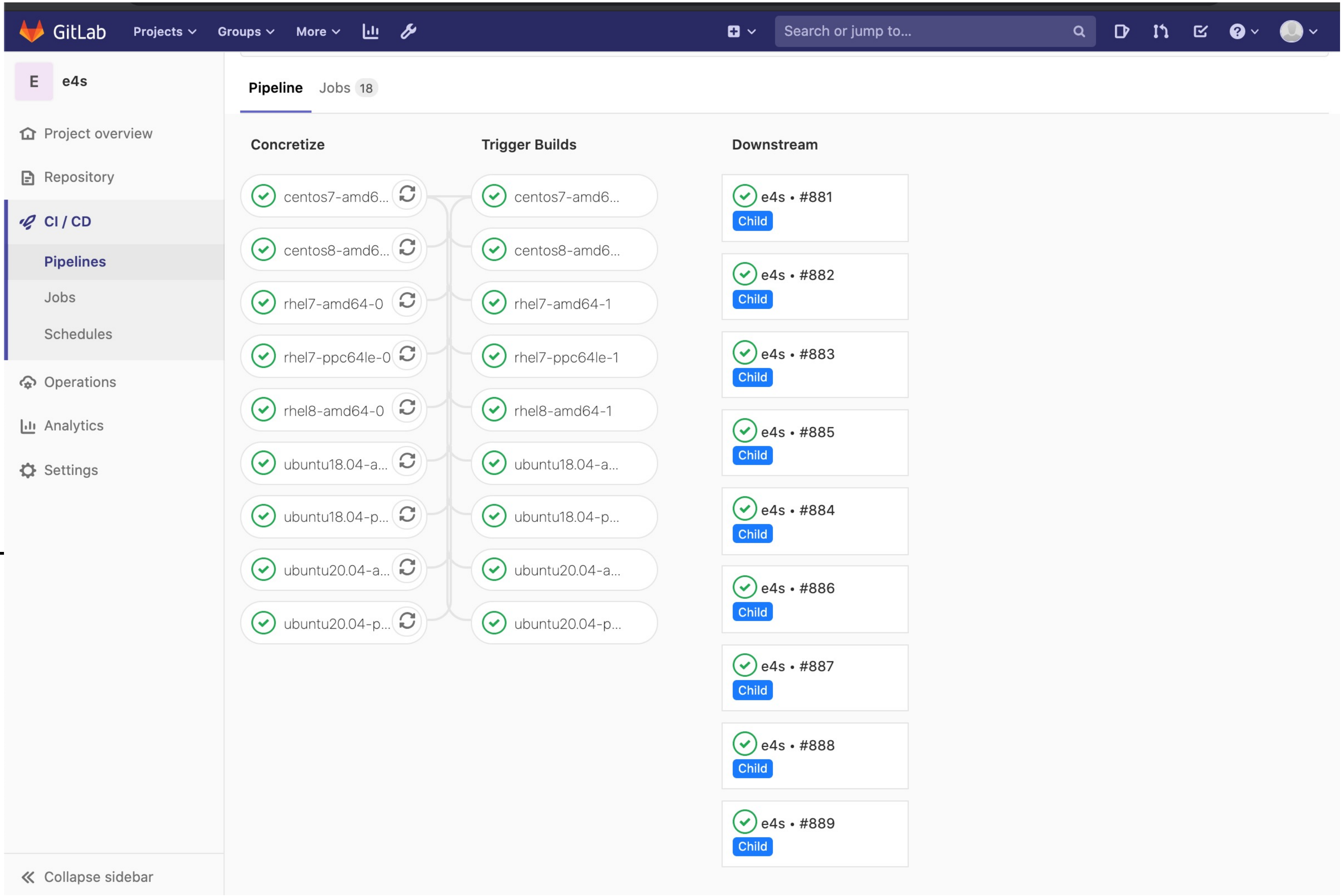
- Dockerhub
- Bare-bones
- Multi-platfrom
- Build E4S

EXASCALE COMPUTING PROJECT

University of Oregon GitLab CI

E4S Builds:
•Ubuntu 18.04
•Ubuntu 20.04
•RHEL 7.6
•RHEL 8
•CentOS 7
•CentOS 8

Architectures:
ppc64le and x86_



• https://gitlab.e4s.io

EXASCALE COMPUTING PROJECT

GitLab GPU Runners on Frank, U. Oregon

Recent searches | uo-illyad | Created date — Runners currently online: 11

Type/State	Runner token	Description	Version	IP Address	Projects	Jobs	Tags	Last contact
shared locked paused	9yUY6sjq	uo-illyad	13.9.0	192.168.165.1...	n/a	0	a100 avx avx2 huge large medium nvidia-gpu public small spack uo x86_64 xlarge	3 minutes ago

A100 NVIDIA GPU

Recent searches | uo-jupiter | Created date — Runners currently online: 11

Type/State	Runner token	Description	Version	IP Address	Projects	Jobs	Tags	Last contact
specific locked paused	E_zdx2ry	uo-jupiter	13.9.0	192.168.165.1...	2	105	avx avx2 avx512 cooper-lake dg1 huge intel-gpu large medium public small spack uo x86_64 xlarge	4 minutes ago

DG1 Intel GPU

Recent searches | uo-instinct | Created date — Runners currently online: 11

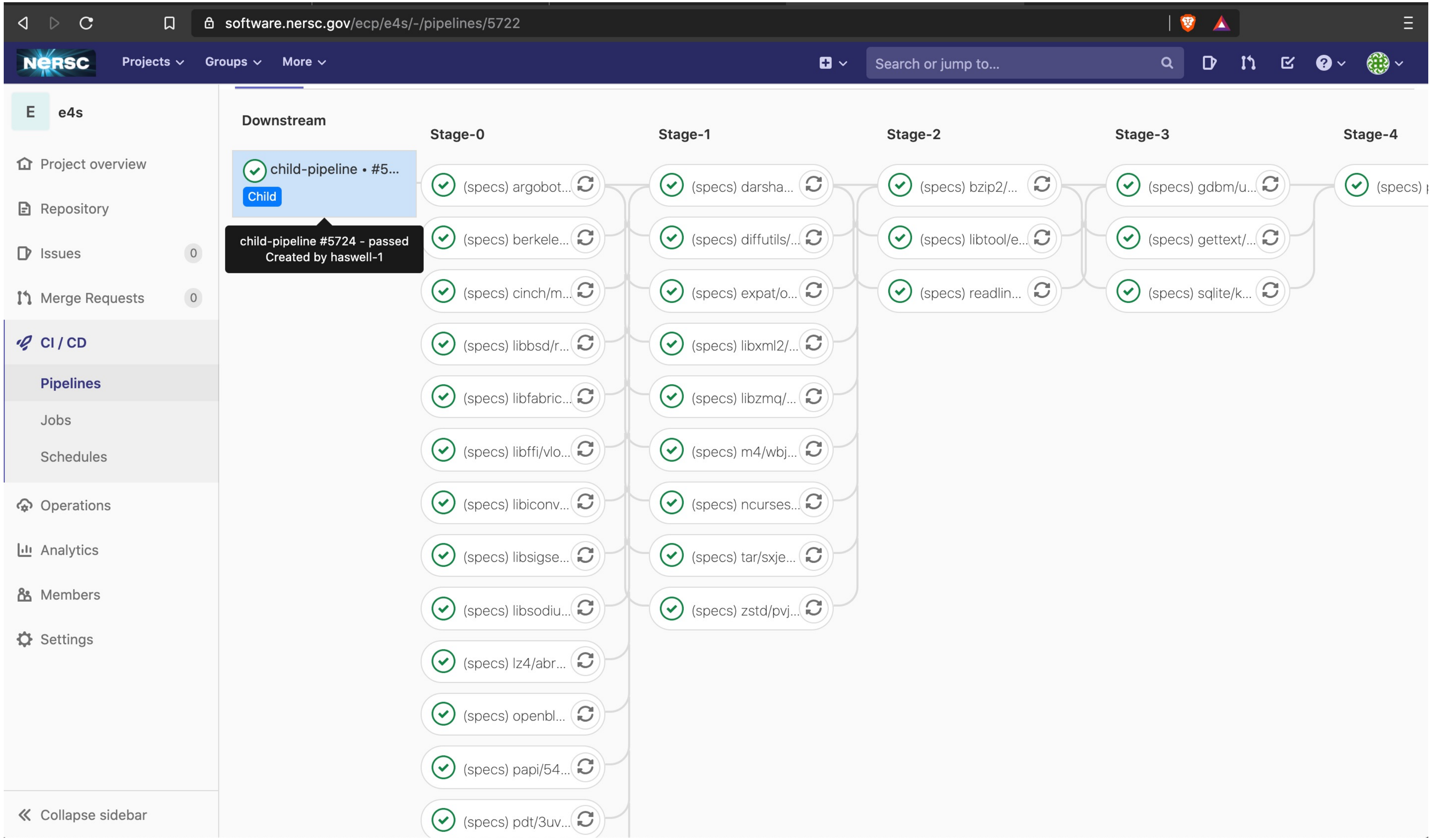
Type/State	Runner token	Description	Version	IP Address	Projects	Jobs	Tags	Last contact
shared locked paused	xPVjy9oY	uo-instinct	13.9.0	192.168.165.1...	n/a	0	amd-gpu avx avx2 huge large medium mi50 public small spack uo x86_64 xlarge	5 minutes ago

MI50 AMD GPU

Frank @ UO: https://oaciss.uoregon.edu/frank

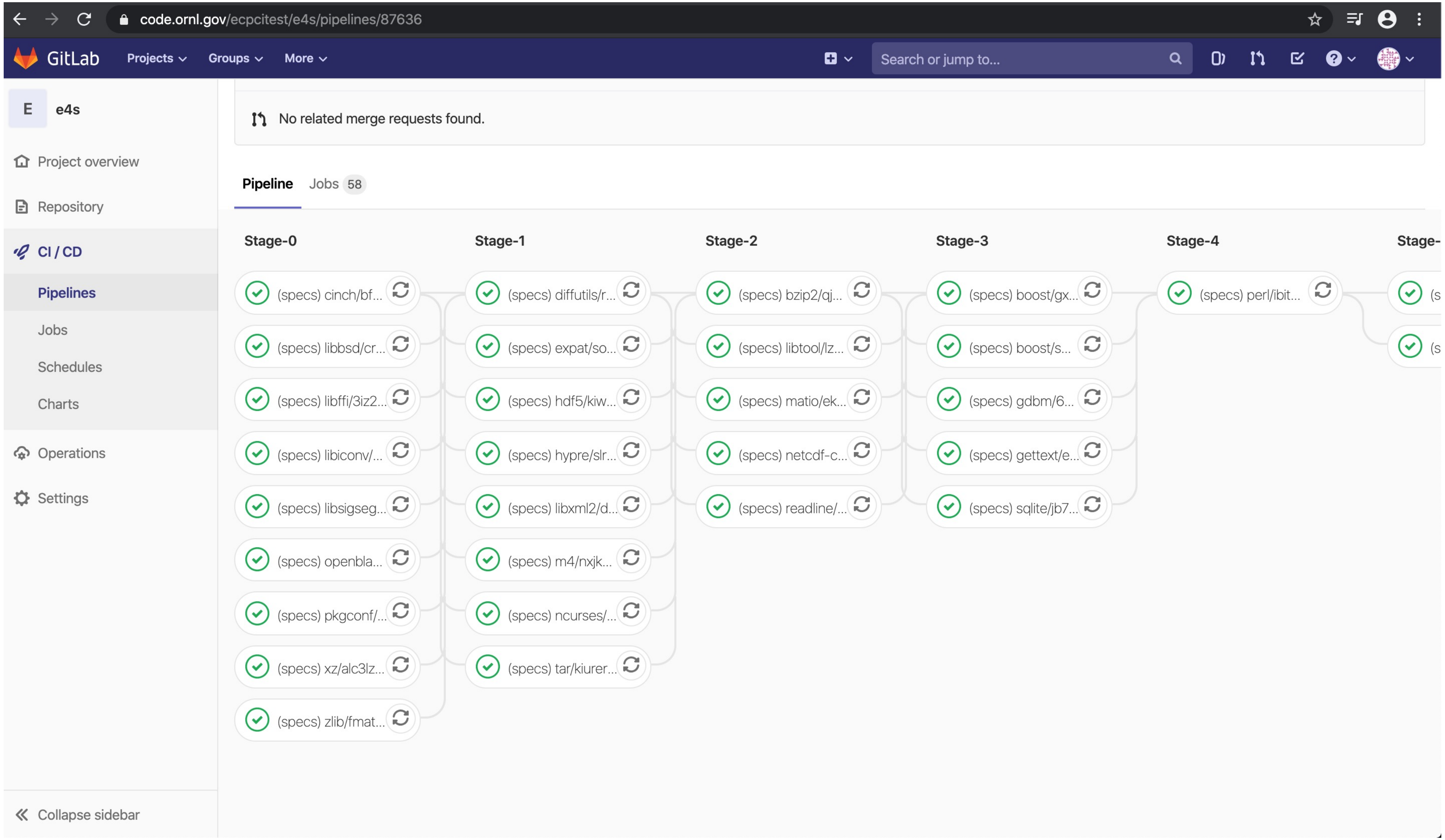
EXASCALE COMPUTING PROJECT

Multi-stage E4S CI Build Pipeline on Cori, NERSC



EXASCALE COMPUTING PROJECT

ORNL GitLab Build Pipeline for E4S Spack Build Cache



- ppc64le (Ascent @ ORNL)
- Reproducible container builds

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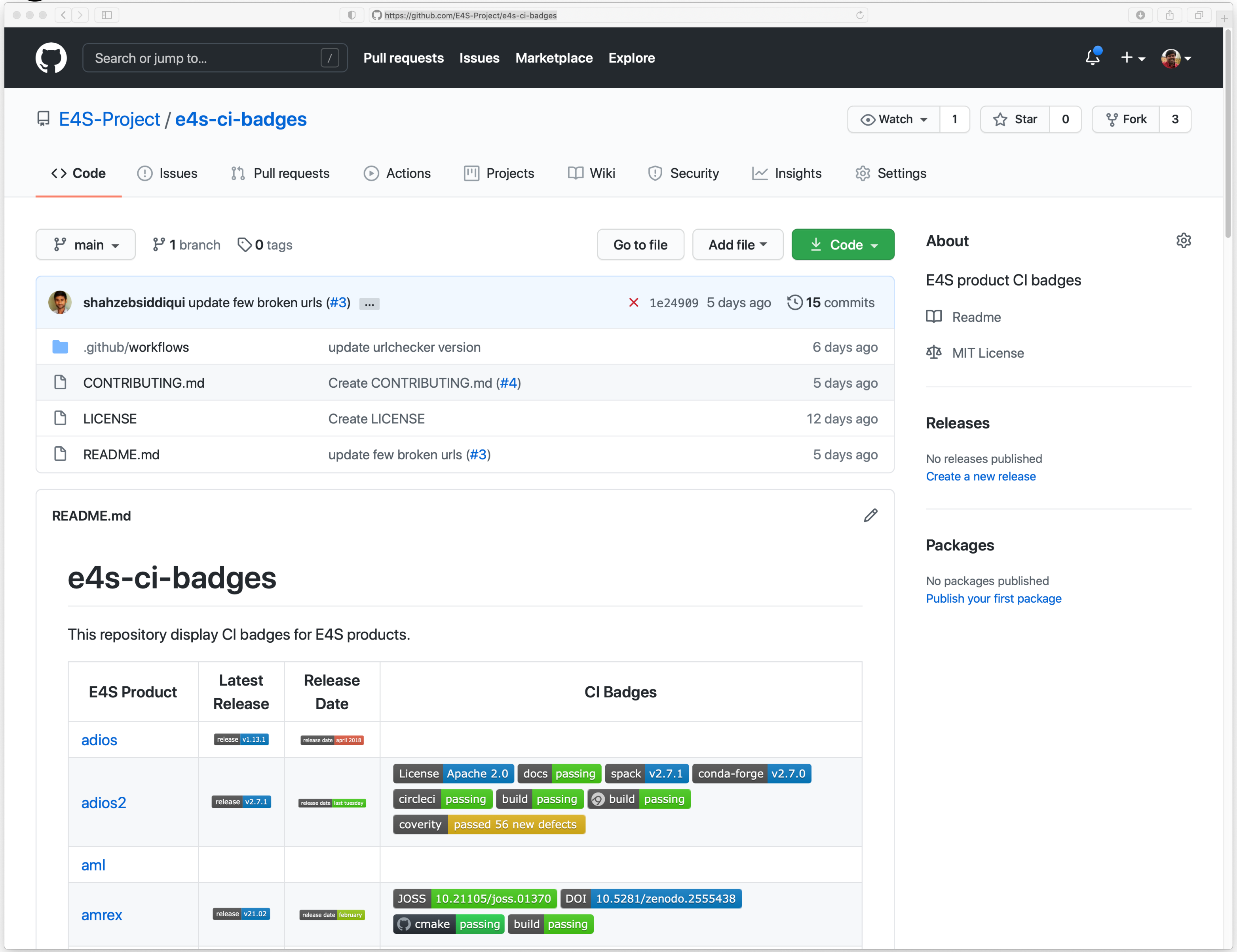
E4S CI Badges



E4S Community Engagement

Opportunities via E4S

- E4S enables portfolio strategy for ASCR R&D software delivery:
  - Facilities: Robust planning, delivery, integration and testing at Facilities
  - Community: MPI Forum, C++, OpenMP, LLVM
  - Vendor: Coordinated integration into vendor software stacks
  - Users: Turnkey delivery of capabilities to DOE program offices, US agencies, industry, international partners
- E4S provides incentives and support for high-quality research software products
  - Community policies: Drives quality by explicit expectations and clear view of gaps
  - SDKs for community interaction: Build awareness and collaboration across independent teams
  - Transparency: E4S DocPortal, build, test, integration shows quality (good or poor) of a product
- E4S provides direct path for software teams to reach users and other stakeholders
  - Example: ArborX is brand new geometric search library
    - Part of E4S, available at DocPortal, tested regularly on many platforms
    - Installed anywhere E4S is installed, users can count on it being there
    - Without E4S: ArborX would take years to become visible and available
  - Availability and adoption timeline reduced from years (or never) to months

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 for ECP & beyond, including AI and Quantum.
• A monolithic, take-it-or-leave-it software behemoth.	• Full collection if compatible software capabilities **and** • Manifest of a la carte selectable software capabilities.
• A commercial product.	• Vehicle for delivering high-quality reusable software products in collaboration with others. • New entity in the HPC ecosystem enabling first-of-a-kind relationships with Facilities, vendors, other DOE program offices, other agencies, industry & international partners.
• A simple packaging of existing software.	• Hierarchical software framework to enhance (via SDKs) software interoperability and quality expectations. • Conduit for future leading edge HPC software targeting scalable computing platforms.

Looking Forward

Lessons learned from E4S/ECP ST to carry forward

- Deliver DOE reusable software as a portfolio
  - E4S value is already more than the sum of its parts
  - Community policies drive quality, membership
  - DocPortal, testing, containerization, cloud, build caches, modules, etc., greatly improve access & usability
  - Poor performing products are ID’ed, then improved or removed
- E4S is ready to extend to next-generation software and hardware needs
  - AI/ML products already in portfolio, ready for any new products
  - Quantum, FPGA, neuromorphic devices likely to be accelerators
    - From a macro software architecture, similar to GPUs
    - Software for these devices can and should be part of the same stack for holistic HPC environment
- DOE software as a portfolio is a first-class entity in the ecosystem
  - E4S planning, executing, tracking, assessing is peer collaboration with Facilities, program offices, vendors, etc
  - E4S can become a perennial asset for DOE/ASCR as part of its mission impact within and beyond DOE

Final points

- E4S is a curated software stack with quality improvement incentives, moving toward turnkey use
- With DOE program managers ECP is starting
  - Software ecosystem sustainability planning
  - E4S strategic plan (will include monthly townhalls)
- We believe
  - E4S has reduced important gaps that limit usefulness of DOE software for industry
  - But some gaps remain
- Next steps:
  - Better characterize these gaps
  - Explore models to further reduce and close gaps
  - Plan and execute toward sustainability

Thank you

https://www.exascaleproject.org

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

EXASCALE COMPUTING PROJECT

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