Running an HPC app on the E4S container

https://e4s.io

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Tutorial, “Container Computing for HPC and Scientific Workloads”

Sunday, Nov. 17, 2019, 3:30 – 4:00 pm, Room # 207, Denver, CO.

https://sc19.supercomputing.org/presentation/?id=tut129&sess=sess206

Outline

- 13:30 – 13:45 Introduction to Containers in HPC (Younge)
- 13:45 – 14:15 How to build your first Docker container (Canon)
- 14:15 – 14:45 How to deploy a container on a supercomputer (Canon)
- 14:45 – 15:00 Best Practices (Canon)
- 15:00 – 15:30 -- Break –
- **15:30 – 16:00 Running an HPC app on the E4S container (Shende)**
- 16:00 - 16:30 How to build a Singularity container image (Arango)
- 16:30 - 16:50 Running Singularity on a supercomputer & adv features (Arango)
- 16:50 - 17:00 Success Stories & Summary (Canon)

Link: https://tinyurl.com/sc19tut

Extreme-scale Scientific Software Stack (E4S) https://e4s.io

- E4S is a community effort to provide open source software packages for developing, deploying, and running scientific applications on HPC platforms.
- E4S provides both source builds and containers of a broad collection of HPC software packages.
- E4S exists to accelerate the development, deployment and use of HPC software, lowering the barriers for HPC users.
- E4S provides containers and turn-key, from-source builds of 80+ popular HPC software packages:
  - MPI: MPICH and OpenMPI
  - Development tools: TAU, HPCToolkit, and PAPI
  - Math libraries: PETSc and Trilinos
  - Data and Viz tools: Adios, HDF5, and Paraview

Extreme-scale Scientific Software Stack (E4S) https://e4s.io

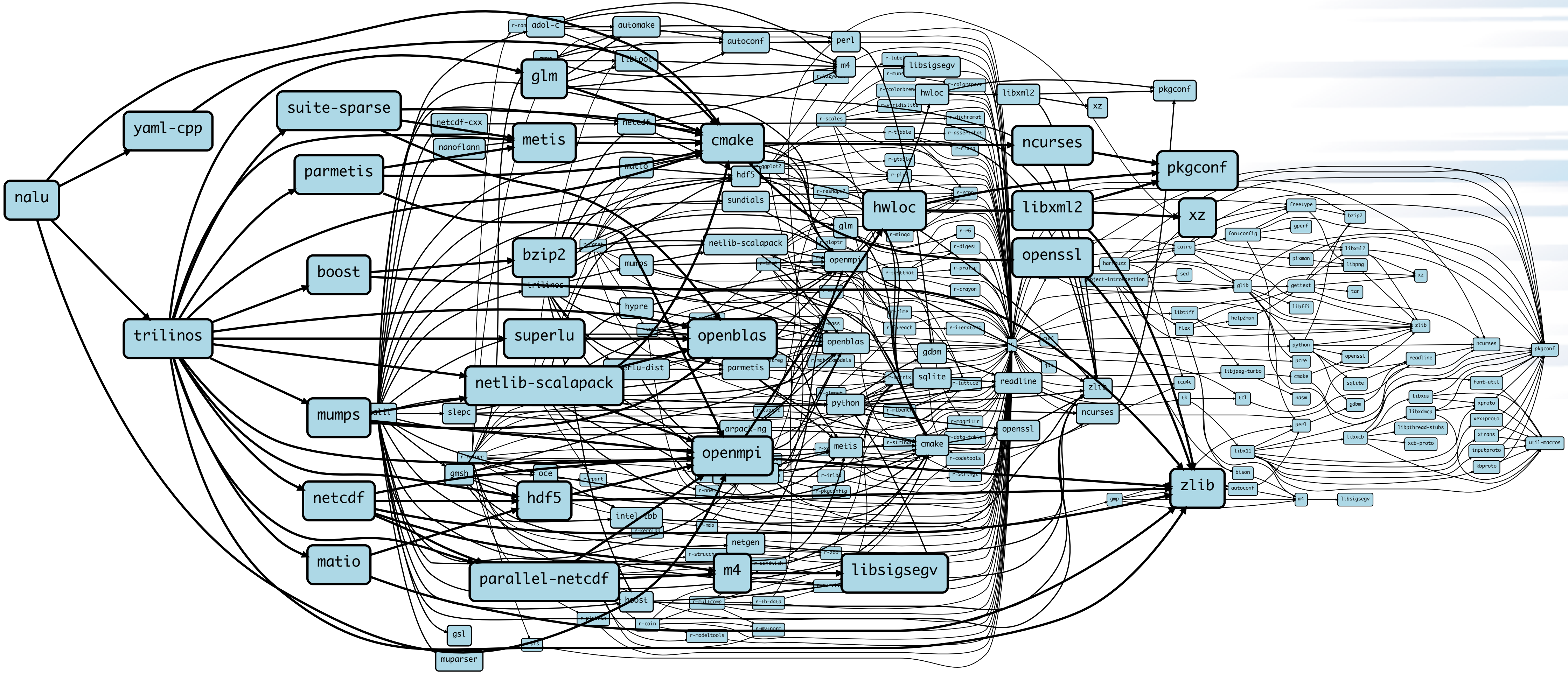
- Spack [http://spack.io] is the primary means for software delivery
- SDKs: collection of related ECP ST products where coordination across package teams will improve usability and practicies, and foster community growth among teams that develop similar and complimentary capabilities. An SDK involves several products.
- Containers of pre-built binaries of ECP ST products.
- Container runtimes supported
  - Docker: Dockerhub: exascaleproject/sdk:AHM19
  - Charliecloud
  - Shifter
  - Singularity
  - Inception at NCAR
- VirtualBox Open Virtualization Appliance (OVA) image that contains these runtimes
- MPI replacement strategies to use native network interconnect

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.
- Acknowledgement: The remaining Spack slides in this presentation are from a talk given by the Spack PI, Todd Gamblin, CASC, LLNL.

- Next: Motivation for Spack!

Scientific software is becoming extremely complex

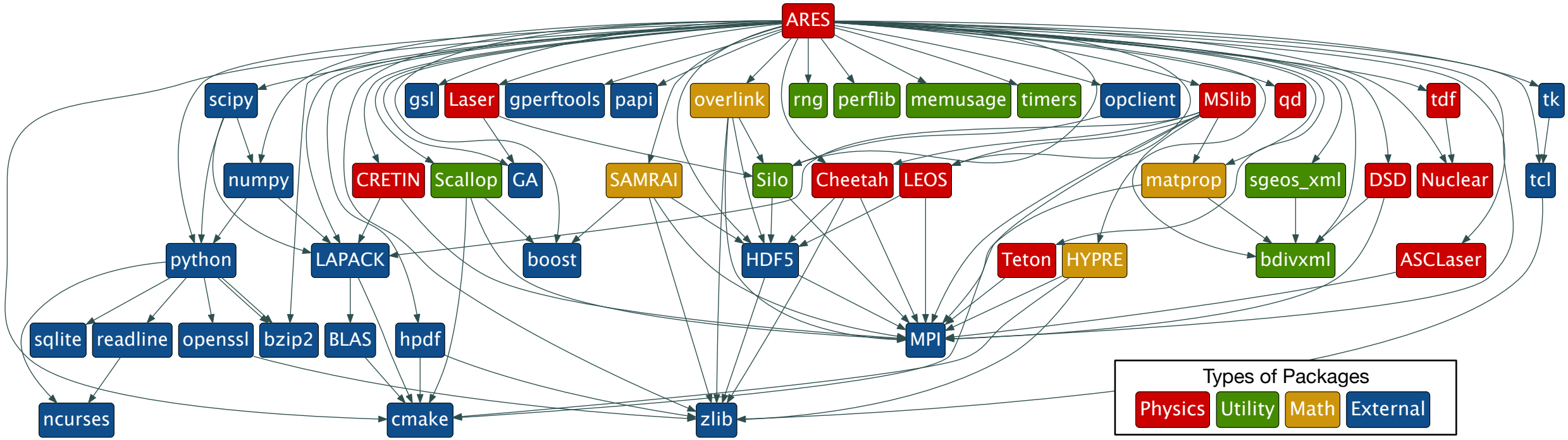


Nalu: Generalized Unstructured Massively Parallel Low Mach Flow

dealii: C++ Finite Element Library

EXASCALE COMPUTING PROJECT

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!

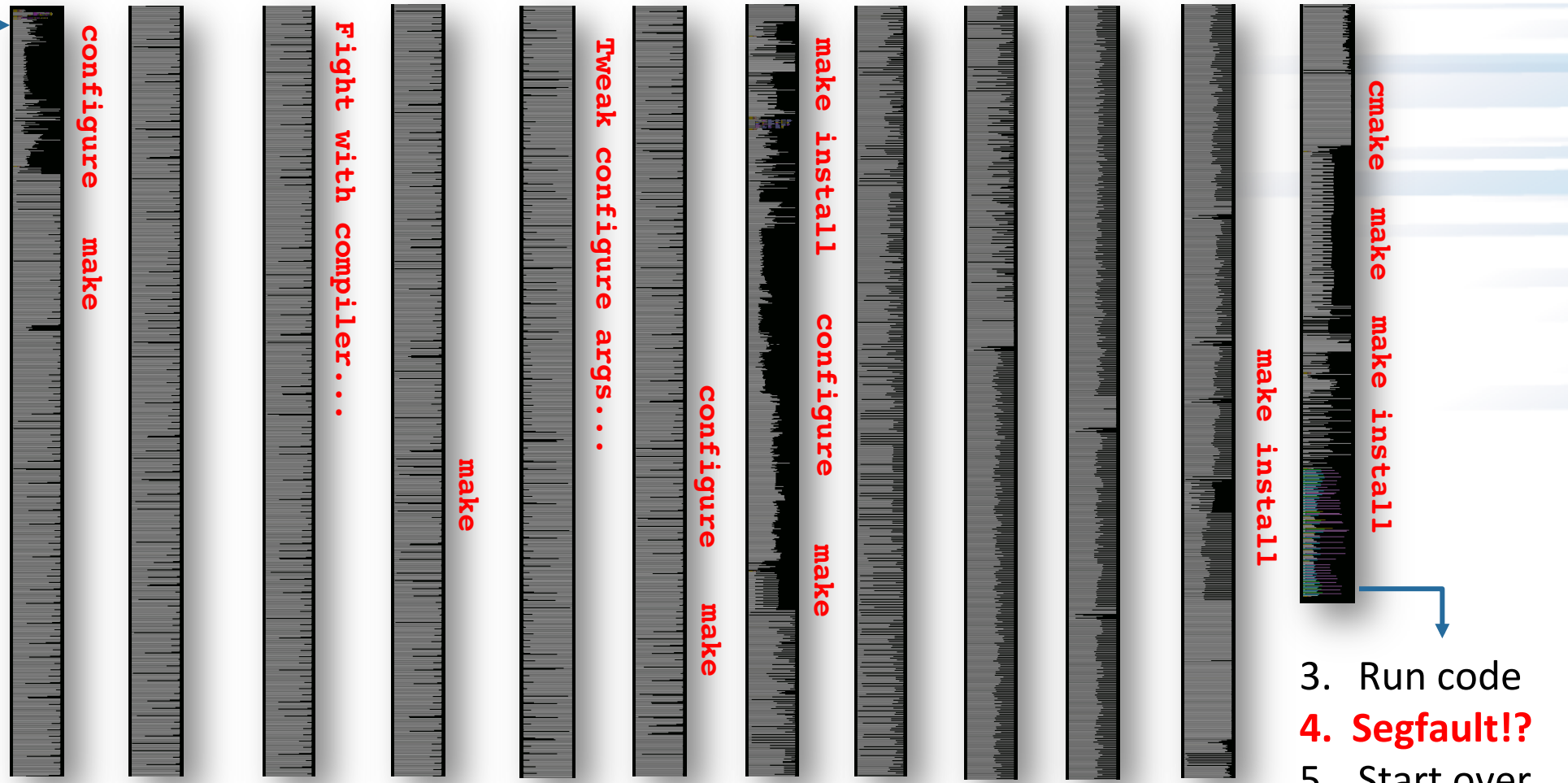
- Every application has its own stack of dependencies.
- Developers, users, and facilities dedicate (many) FTEs to building & porting.
- Often trade reuse and usability for performance.

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

How to install software on a Mac laptop, circa 2013

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

What about containers?

- **Containers provide a great way to reproduce and distribute an already-built software stack**
- **Someone needs to build the container!**
  - This isn't trivial
  - Containerized applications still have hundreds of dependencies
- **Using the OS package manager inside a container may not be enough**
  - Most binaries are built unoptimized
  - Generic binaries, not optimized for specific architectures
- **Developing with an OS software stack can be painful**
  - Little freedom to choose versions
  - Little freedom to choose compiler options, build options, etc. for packages

We need something more flexible to **build** the containers

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 hdf5
```

- HDF5 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

EXASCALE COMPUTING PROJECT

Spack provides the *spec* syntax to describe custom configurations

```
$ spack install mpileaks                          unconstrained
$ spack install mpileaks@3.3                      @ custom version
$ spack install mpileaks@3.3 %gcc@4.7.3           % custom compiler
$ spack install mpileaks@3.3 %gcc@4.7.3 +threads  +/- build option
$ spack install mpileaks@3.3 cxxflags="-O3 -g3"   setting compiler flags
$ spack install mpileaks@3.3 os=cnl10 target=haswell  setting target for X-compile
$ spack install mpileaks@3.3 ^mpich@3.2 %gcc@4.9.3    ^ 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 list` shows what packages are available

```
$ spack list
==> 3041 packages.
abinit                  glew                    nalu                    py-fastaindex           r-cairo                 r-viridislite
abyss                   glfmultiples            nalu-wind               py-fasteners            r-callr                 r-visnetwork
accfft                  glib                    namd                    py-faststructure        r-car                   r-vsn
ack                     glibmm                  nano                    py-filelock             r-caret                 r-webshot
activeharmony           glimmer                 nanoflann               py-fiona                r-category              r-whisker
adept-utils             glm                     nanopb                  py-fiscalyear           r-catools               r-withr
adios                   global                  nasm                    py-flake8               r-cdcfluview            r-xde
adios2                  globalarrays            nauty                   py-flake8-polyfill      r-cellranger            r-xgboost
adlbx                   globus-toolkit          ncbi-magicblast         py-flask                r-checkmate             r-xlconnect
adol-c                  glog                    ncbi-rmblastn           py-flask-compress       r-checkpoint            r-xlconnectjars
aegean                  gloo                    ncbi-toolkit            py-flask-socketio       r-chemometrics          r-xlsx
aida                    glpk                    nccl                    py-flexx                r-chron                 r-xlsxjars
albany                  glproto                 nccmp                   py-fn                   r-circlize              r-xmapbridge
albert                  glvis                   ncdu                    py-fparser              r-class                 r-xml
alglib                  gmake                   ncftp                   py-funcsigs             r-classint              r-xml2
allinea-forge           gmap-gsnap              ncl                     py-functools32          r-cli                   r-xnomial
allinea-reports         gmime                   nco                     py-future               r-clipr                 r-xtable
allpaths-lg             gmodel                  ncurses                 py-futures              r-cluster               r-xts
alquimia                gmp                     ncview                  py-fypp                 r-clustergeneration     r-xvector
alsa-lib                gmsh                    ndiff                   py-gdbgui               r-clusterprofiler       r-yaml
aluminum                gmt                     nek5000                 py-genders              r-cner                  r-yapsa
amg                     gnat                    nekbone                 py-genshi               r-coda                  r-yaqcaffy
amg2013                 gnu-prolog              nekcem                  py-geopandas            r-codetools             r-yarn
amp                     gnupg                   nektar                  py-gevent               r-coin                  r-zlibbioc
ampliconnoise           gnuplot                 neovim                  py-git-review           r-colorspace            r-zoo
amrex                   gnutls                  nest                    py-git2                 r-combinat              r3d
amrvis                  go                      netcdf                  py-gnuplot              r-complexheatmap        racon
andi                    go-bootstrap            netcdf-cxx              py-goatools             r-compositions          raft
angsd                   gobject-introspection   netcdf-cxx4             py-gpaw                 r-convevol              ragel
ant                     googletest              netcdf-fortran          py-greenlet             r-corhmm                raja
antlr                   gotcha                  netgauge                py-griddataformats      r-corpcor               randfold
ants                    gource                  netgen                  py-guidata              r-corrplot              random123
ape                     gperf                   netlib-lapack           py-guiqwt               r-covr                  randrproto
. . .
```

- Spack has over 3,000 builtin package recipes.

`spack find` shows what is installed

```
$ spack find
==> 103 installed packages.
-- linux-rhel7-x86_64 / gcc@4.4.7 ------------------------------
ImageMagick@6.8.9-10  glib@2.42.1        libtiff@4.0.3     pango@1.36.8          qt@4.8.6
SAMRAI@3.9.1          graphlib@2.0.0     libtool@2.4.2     parmetis@4.0.3        qt@5.4.0
adept-utils@1.0       gtkplus@2.24.25    libxcb@1.11       pixman@0.32.6         ravel@1.0.0
atk@2.14.0            harfbuzz@0.9.37    libxml2@2.9.2     py-dateutil@2.4.0     readline@6.3
boost@1.55.0          hdf5@1.8.13        llvm@3.0          py-ipython@2.3.1      scotch@6.0.3
cairo@1.14.0          icu@54.1           metis@5.1.0       py-nose@1.3.4         starpu@1.1.4
callpath@1.0.2        jpeg@9a            mpich@3.0.4       py-numpy@1.9.1        stat@2.1.0
dyninst@8.1.2         libdwarf@20130729  ncurses@5.9       py-pytz@2014.10       xz@5.2.0
dyninst@8.1.2         libelf@0.8.13      ocr@2015-02-16    py-setuptools@11.3.1  zlib@1.2.8
fontconfig@2.11.1     libffi@3.1         openssl@1.0.1h    py-six@1.9.0
freetype@2.5.3        libmng@2.0.2       otf@1.12.5salmon  python@2.7.8
gdk-pixbuf@2.31.2     libpng@1.6.16      otf2@1.4          qhull@1.0

-- linux-rhel7-x86_64 / gcc@4.8.2 ------------------------------
adept-utils@1.0.1  boost@1.55.0  cmake@5.6-special  libdwarf@20130729  mpich@3.0.4
adept-utils@1.0.1  cmake@5.6     dyninst@8.1.2      libelf@0.8.13      openmpi@1.8.2

-- linux-rhel7-x86_64 / intel@14.0.2 ---------------------------
hwloc@1.9  mpich@3.0.4  starpu@1.1.4

-- linux-rhel7-x86_64 / intel@15.0.0 ---------------------------
adept-utils@1.0.1  boost@1.55.0  libdwarf@20130729  libelf@0.8.13  mpich@3.0.4

-- linux-rhel7-x86_64 / intel@15.0.1 ---------------------------
adept-utils@1.0.1  callpath@1.0.2  libdwarf@20130729  mpich@3.0.4
boost@1.55.0       hwloc@1.9       libelf@0.8.13      starpu@1.1.4
```

- 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

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Exascale Platform Preparation

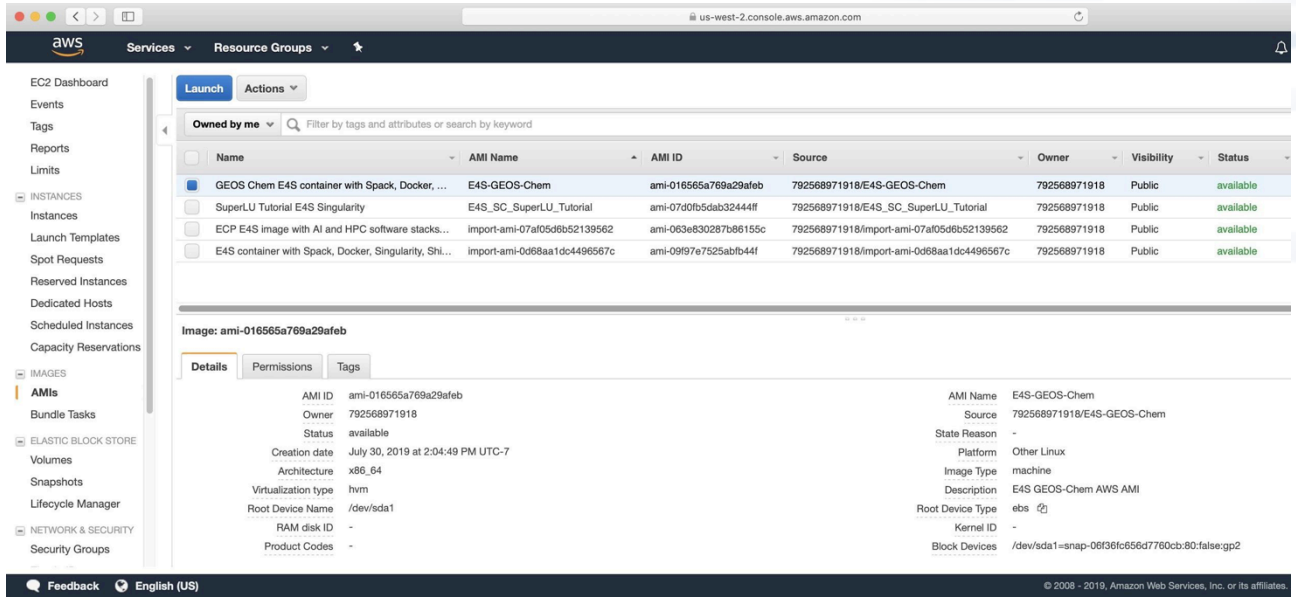
- SDK Exascale platform preparation is focused on interoperable delivery.
- ST products from SDKs are released in the Extreme-scale Scientific Software Stack (E4S) [https://e4s.io].
  - E4S: a community effort to provide open source software packages for developing, deploying, and running scientific applications on HPC platforms
- E4S containers and Spack based builds currently support the following pre-exascale systems:
  - Theta at ALCF (Cray XC).
  - Cori at NERSC (Cray XC).
  - Summit, Sierra, Butte, RZAnsel (IBM Power 9 AC922).
  - Linux x86_64 systems at LANL (Grizzly), Sandia (Voltrino), LLNL (Quartz).
  - Other NSF platforms including Frontera (TACC).
- E4S preparation for future Exascale systems includes testing on AMD and Intel systems.

Integration and Interoperability: E4S

- E4S is released twice a year. Two versions have been released to date and we are planning for a release at SC19. The E4S 0.2 release supports:
  - Containers and turn-key, from-source builds of 80+ popular HPC software packages
  - 37 full release ECP ST products including:
    - MPI: MPICH and OpenMPI
    - Development tools: TAU, HPCToolkit, and PAPI
    - Math libraries: PETSc and Trilinos
    - Data and Viztools: Adios, HDF5, and Paraview
  - Limited access to 10 additional ECP ST products
  - Docker
  - Singularity
  - Shifter
  - Charliecloud
  - Inception
  - Open Virtualization Appliance (OVA) for VirtualBox features Spack, E4S containers, and support for container environments

Integration and Interoperability: E4S on AWS

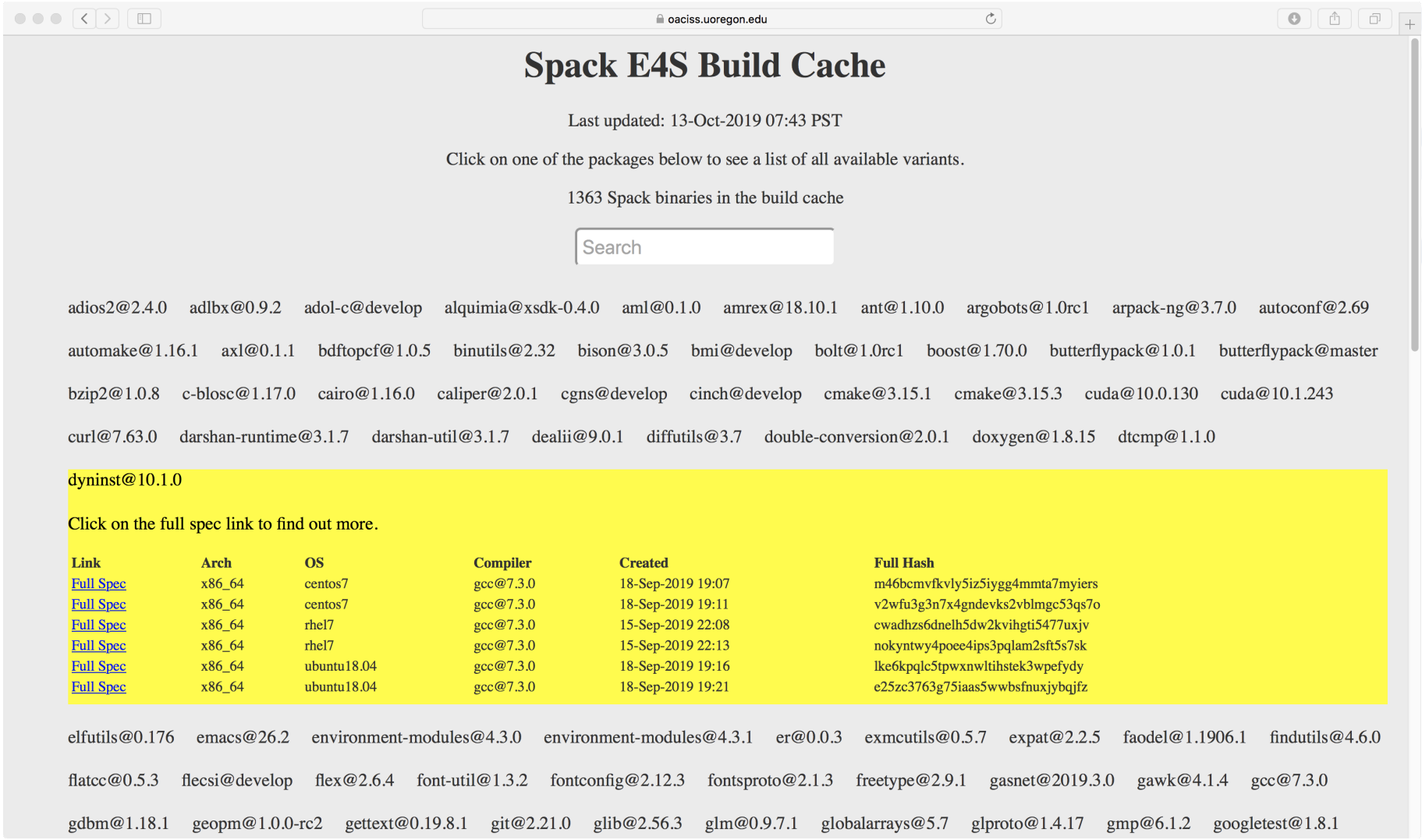
- E4S AWS public image ami-063e830287b86155c (US-West-2 Oregon) has following container runtimes:
  - Docker
  - Shifter
  - Singularity
  - Charliecloud
- Spack with base PMR components
- E4S full featured Singularity image
  - (exascaleproject/sdk:AHM19)
- Used in ISC-HPC 2019 tutorials
- Used as base image for NASA GEOS-Chem E4S public image
- Resources provided by AWS AI/ML team



Reproducible, Customizable Container Builds & Spack Mirrors

- E4S provides base images and recipes for building Docker containers based on SDKs
  - Git: https://github.com/UO-OACISS/e4s
  - Base images released (September 2019):
    - UBI 7.6 (RHEL Universal Binary Image for container builds) for x86_64
    - Centos 7.6 for x86_64
    - Ubuntu 18.04 for x86_64
    - UBI 7.6 (RHEL) for ppc64le
- E4S provides build caches for Spack for native bare-metal as well as container builds based installation of ST products
  - Build caches: https://oaciss.uoregon.edu/e4s
    - The build cache model can be extended to target platforms, and can be managed by facilities staff when appropriate.

E4S Build Cache Binaries



https://oaciss.uoregon.edu/e4s

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

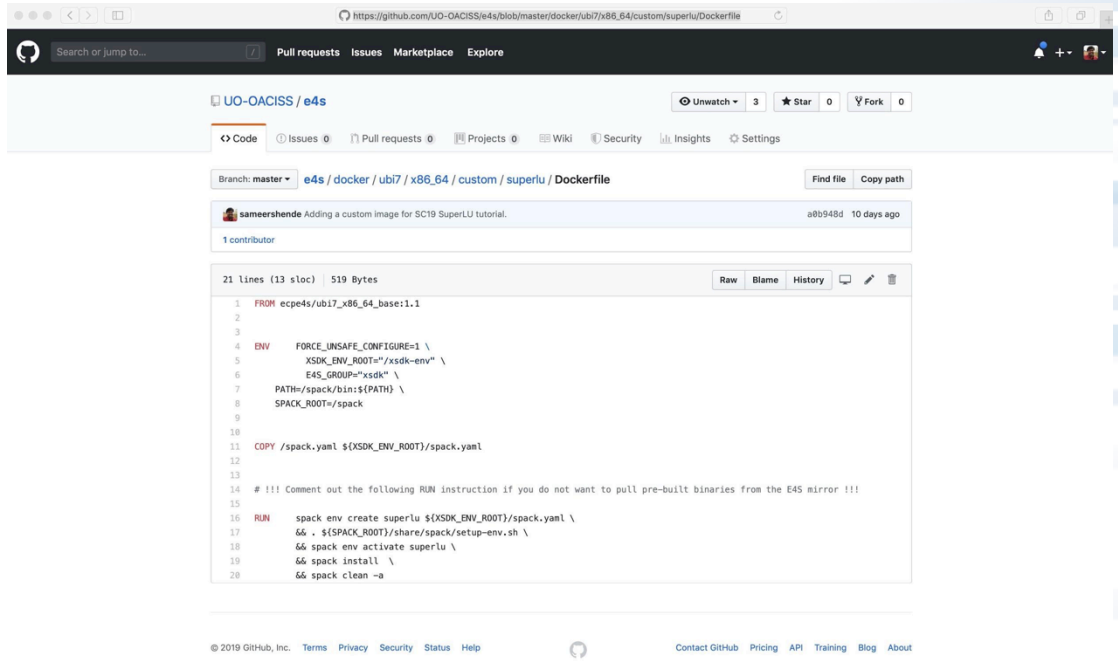
Branch: master — e4s / docker / ubi7 / x86_64 / custom / superlu / spack.yaml — Find file | Copy path

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

1 contributor

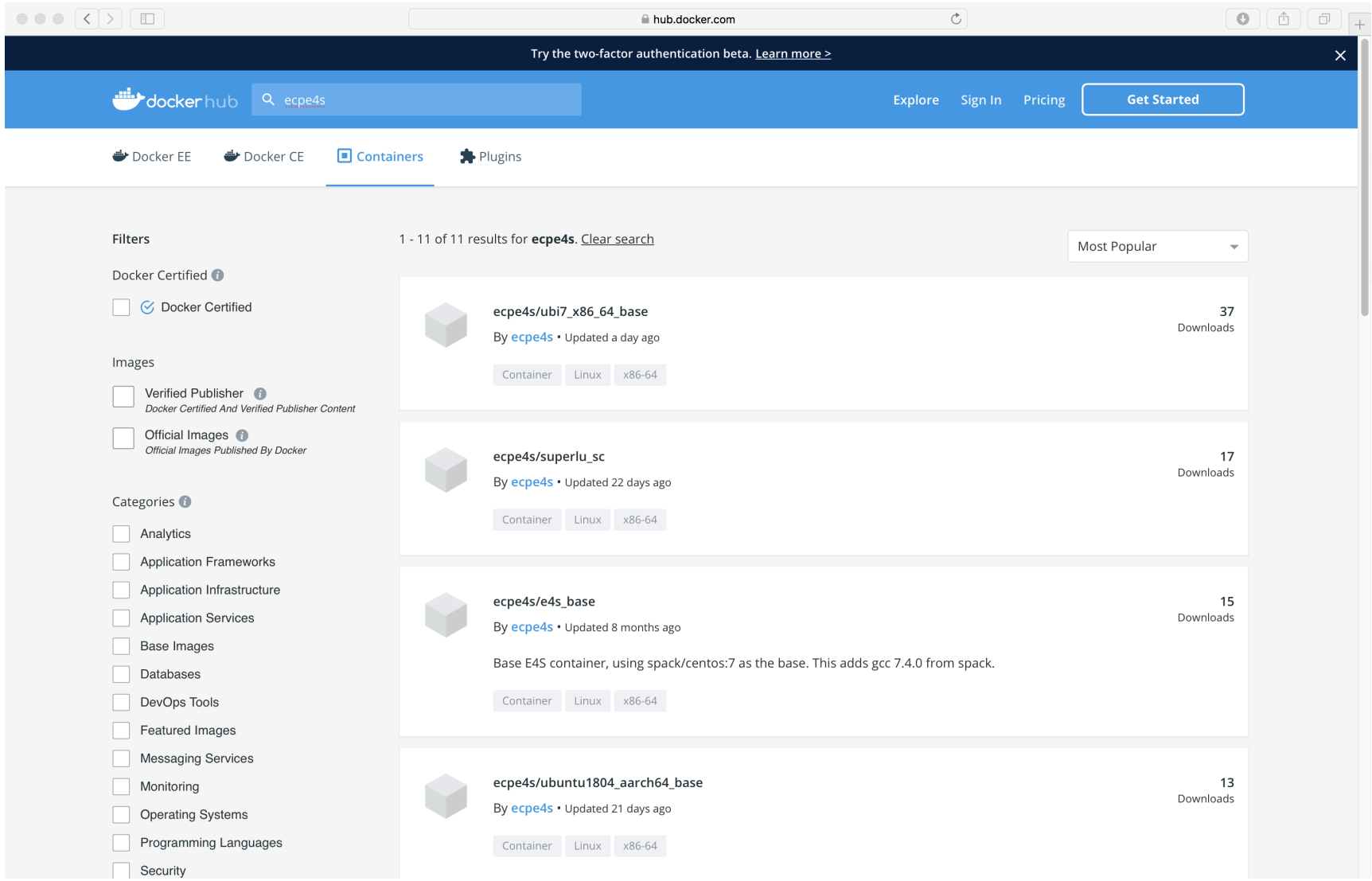
35 lines (34 sloc) | 579 Bytes — Raw | Blame | History

```
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
```



- PMR SDK base image (UBI 7.6) 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!

Reproducible Base Images on Dockerhub

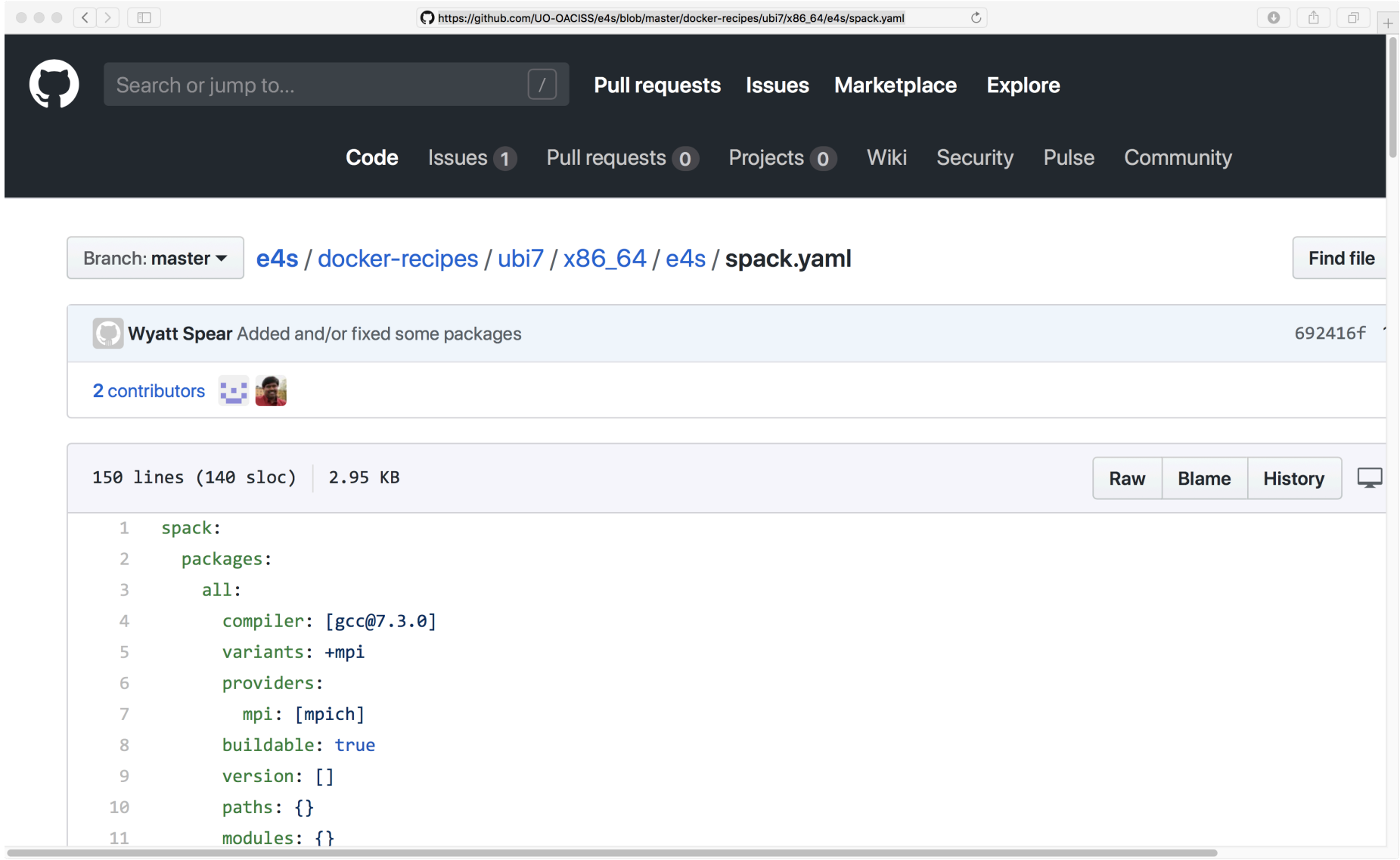


- ecpe4s

- x86_64
- ppc64le
- aarch64

- Centos 7.6
- Ubuntu 18.04
- RHEL/UBI 7.6

Docker Recipes on GitHub



- Base images
- SDKs
- E4S

https://github.com/UO-OACISS/e4s

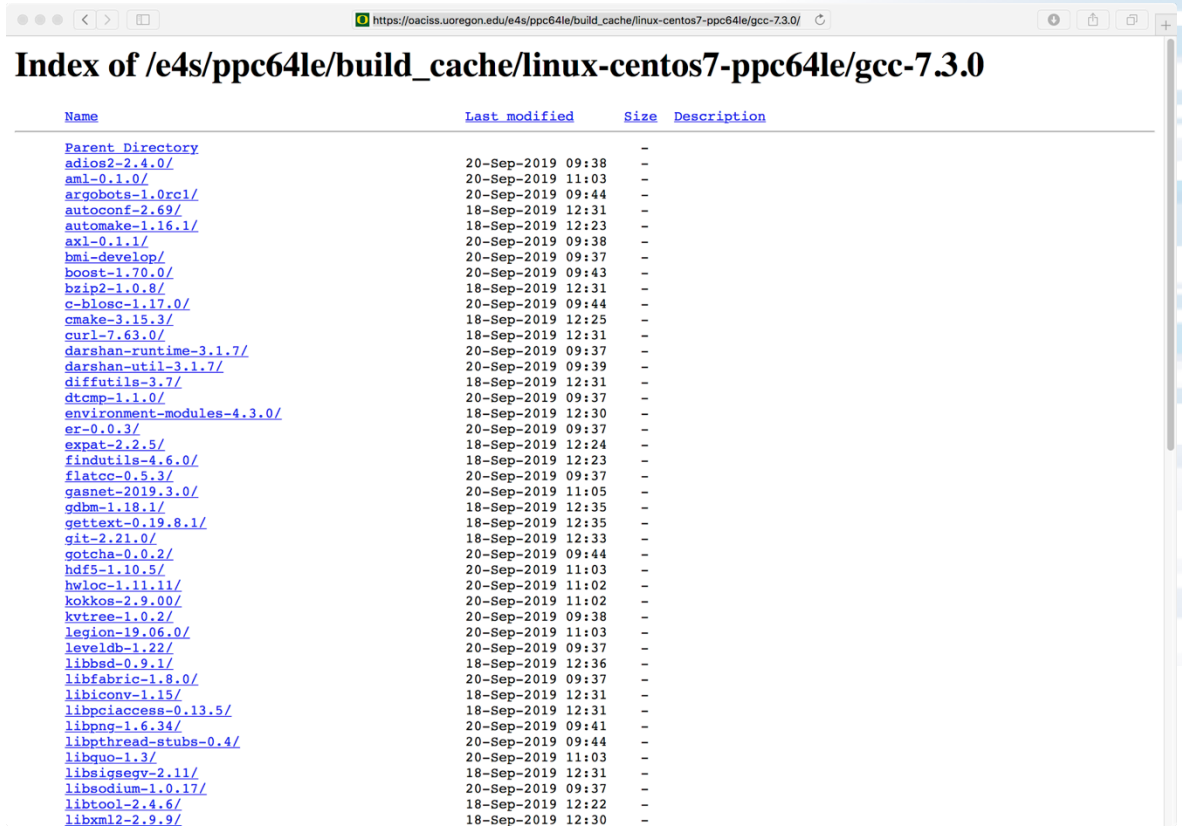
Spack Build Caches from E4S Base Images

https://oaciss.uoregon.edu/e4s/x86_64/build_cache/linux-rhel7-x86_64/gcc-7.3.0/

Index of /e4s/x86_64/build_cache/linux-rhel7-x86_64/gcc-7.3.0

Name	Last modified	Size	Description
Parent Directory		-	
adios2-2.4.0/	19-Sep-2019 06:25	-	
arpack-ng-3.7.0/	12-Sep-2019 12:35	-	
autoconf-2.69/	17-Sep-2019 17:24	-	
automake-1.16.1/	17-Sep-2019 17:31	-	
axl-0.1.1/	19-Sep-2019 06:28	-	
binutils-2.32/	15-Sep-2019 21:57	-	
bison-3.0.5/	28-Aug-2019 08:17	-	
boost-1.70.0/	19-Sep-2019 06:16	-	
butterflypack-1.0.1/	12-Sep-2019 12:35	-	
bzip2-1.0.8/	17-Sep-2019 17:47	-	
c-blosc-1.17.0/	27-Aug-2019 09:04	-	
caliper-2.0.1/	06-Sep-2019 08:41	-	
cinch-develop/	28-Aug-2019 18:57	-	
cmake-3.15.1/	17-Sep-2019 17:57	-	
cmake-3.15.3/	18-Sep-2019 13:17	-	
cuda-10.0.130/	05-Sep-2019 12:59	-	
cuda-10.1.243/	11-Sep-2019 13:42	-	
curl-7.63.0/	17-Sep-2019 18:03	-	
darshan-runtime-3.1.7/	19-Sep-2019 06:22	-	
darshan-util-3.1.7/	27-Aug-2019 09:02	-	
diffutils-3.7/	18-Sep-2019 14:23	-	
dtcmp-1.1.0/	19-Sep-2019 06:28	-	
dyninst-10.1.0/	15-Sep-2019 22:13	-	
elfutils-0.176/	15-Sep-2019 21:58	-	
environment-modules-4.3.0/	17-Sep-2019 17:59	-	
er-0.0.3/	19-Sep-2019 06:29	-	
expat-2.2.5/	17-Sep-2019 17:24	-	
faodel-1.1906.1/	19-Sep-2019 06:27	-	
findutils-4.6.0/	17-Sep-2019 17:24	-	
flecsi-develop/	18-Sep-2019 14:44	-	
flex-2.6.4/	28-Aug-2019 08:17	-	
freetype-2.9.1/	27-Aug-2019 11:48	-	
gasnet-2019.3.0/	27-Aug-2019 10:18	-	
gdbm-1.18.1/	17-Sep-2019 17:47	-	
gettext-0.19.8.1/	17-Sep-2019 17:26	-	
git-2.21.0/	17-Sep-2019 18:03	-	
glm-0.9.7.1/	29-Aug-2019 12:43	-	
glproto-1.4.17/	27-Aug-2019 11:43	-	
googletest-1.8.1/	27-Aug-2019 09:09	-	
gotcha-1.0.2/	10-Sep-2019 13:01	-	
hdf5-1.10.5/	19-Sep-2019 06:21	-	
help2man-1.47.8/	28-Aug-2019 08:17	-	
hpctoolkit-2019.08.14/	15-Sep-2019 22:17	-	
hwloc-1.11.11/	15-Sep-2019 18:27	-	
hypre-2.16.0/	17-Aug-2019 09:08	-	
hypre-2.17.0/	29-Aug-2019 12:55	-	
inputproto-2.3.2/	27-Aug-2019 11:48	-	
intel-mkl-2019.3.199/	05-Sep-2019 13:09	-	
intel-tbb-2019.4/	10-Sep-2019 12:49	-	
intel-xed-2019.03.01/	10-Sep-2019 12:57	-	
kbproto-1.0.7/	28-Aug-2019 08:27	-	
kokkos-2.8.00/	10-Aug-2019 07:35	-	
kokkos-2.9.00/	27-Aug-2019 10:16	-	
kvtree-1.0.2/	19-Sep-2019 06:25	-	
legion-19.06.0/	27-Aug-2019 10:19	-	
libbsd-0.9.1/	17-Sep-2019 17:30	-	
libdwarf-20180129/	10-Sep-2019 12:57	-	
libedit-3.1-20170329/	27-Aug-2019 11:48	-	
libelf-0.8.13/	10-Sep-2019 12:48	-	
libfabric-1.8.0/	27-Aug-2019 09:04	-	
libffi-3.2.1/	05-Sep-2019 13:15	-	
libiberty-2.31.1/	10-Sep-2019 12:52	-	
libice-1.0.9/	27-Aug-2019 11:48	-	
libiconv-1.15/	17-Sep-2019 17:59	-	
libjpeg-turbo-2.0.2/	28-Aug-2019 08:28	-	
libmonitor-2018.07.18/	10-Sep-2019 12:48	-	
libpciaccess-0.13.5/	17-Sep-2019 17:30	-	
libpfm4-4.10.1/	10-Sep-2019 13:02	-	
libpng-1.6.34/	27-Aug-2019 09:03	-	
libpthread-stubs-0.4/	27-Aug-2019 09:03	-	
libquo-1.3/	27-Aug-2019 10:16	-	
libsigsegv-2.11/	17-Sep-2019 17:54	-	
libsm-1.2.2/	27-Aug-2019 11:43	-	
libsodium-1.0.17/	27-Aug-2019 09:02	-	

- x86_64 build cache
  - 40 GB on disk



https://oaciss.uoregon.edu/e4s/ppc64le/build_cache/linux-centos7-ppc64le/gcc-7.3.0/

Index of /e4s/ppc64le/build_cache/linux-centos7-ppc64le/gcc-7.3.0

Name	Last modified	Size	Description
Parent Directory		-	
adios2-2.4.0/	20-Sep-2019 09:38	-	
aml-0.1.0/	20-Sep-2019 11:03	-	
argobots-1.0rc1/	20-Sep-2019 09:44	-	
autoconf-2.69/	18-Sep-2019 12:31	-	
automake-1.16.1/	18-Sep-2019 12:23	-	
axl-0.1.1/	20-Sep-2019 09:38	-	
bmi-develop/	20-Sep-2019 09:37	-	
boost-1.70.0/	20-Sep-2019 09:43	-	
bzip2-1.0.8/	18-Sep-2019 12:31	-	
c-blosc-1.17.0/	20-Sep-2019 09:44	-	
cmake-3.15.3/	18-Sep-2019 12:25	-	
curl-7.63.0/	18-Sep-2019 12:31	-	
darshan-runtime-3.1.7/	20-Sep-2019 09:37	-	
darshan-util-3.1.7/	20-Sep-2019 09:39	-	
diffutils-3.7/	18-Sep-2019 12:31	-	
dtcmp-1.1.0/	20-Sep-2019 09:37	-	
environment-modules-4.3.0/	18-Sep-2019 12:30	-	
er-0.0.3/	20-Sep-2019 09:37	-	
expat-2.2.5/	18-Sep-2019 12:24	-	
findutils-4.6.0/	18-Sep-2019 12:23	-	
flatcc-0.5.3/	20-Sep-2019 09:37	-	
gasnet-2019.3.0/	20-Sep-2019 11:05	-	
gdbm-1.18.1/	18-Sep-2019 12:35	-	
gettext-0.19.8.1/	18-Sep-2019 12:35	-	
git-2.21.0/	18-Sep-2019 12:33	-	
gotcha-0.0.2/	20-Sep-2019 09:44	-	
hdf5-1.10.5/	20-Sep-2019 11:03	-	
hwloc-1.11.11/	20-Sep-2019 11:02	-	
kokkos-2.9.00/	20-Sep-2019 11:02	-	
kvtree-1.0.2/	20-Sep-2019 09:38	-	
legion-19.06.0/	20-Sep-2019 11:03	-	
leveldb-1.22/	20-Sep-2019 09:37	-	
libbsd-0.9.1/	18-Sep-2019 12:36	-	
libfabric-1.8.0/	20-Sep-2019 09:37	-	
libiconv-1.15/	18-Sep-2019 12:31	-	
libpciaccess-0.13.5/	18-Sep-2019 12:31	-	
libpng-1.6.34/	20-Sep-2019 09:41	-	
libpthread-stubs-0.4/	20-Sep-2019 09:44	-	
libquo-1.3/	20-Sep-2019 11:03	-	
libsigsegv-2.11/	18-Sep-2019 12:31	-	
libsodium-1.0.17/	20-Sep-2019 09:37	-	
libtool-2.4.6/	18-Sep-2019 12:22	-	
libxml2-2.9.9/	18-Sep-2019 12:30	-	

- IBM Power 9 (ppc64le) build cache
  - 2.6 GB on disk
  - early stages of effort
  - Initial ARM 64 build cache is underway

Docker container of E4S

% docker pull exascaleproject/e4s_x86_64:1.0

- Using USB stick or images from https://e4s.io:
- % unxz −c e4s_x86_64.xz | docker load
  % docker images
- Mount home directory:

% docker −i −v $HOME:$HOME −t exascaleproject/e4s_x86_64:1.0 /bin/bash

% which spack

% cp −r /usr/local/packages/ecp/demo . ; cd demo; cat README

Using Shifter at NCSA BlueWaters

Load shifter module and E4S image on the compute node

- Allocate a node
  - % qsub -I -l nodes=1:ppn=32 -l walltime=01:15:00 -l gres=shifter16
- Load the shifter module
  - % module load shifter
- Pull the image (once)
  - % shifterimg pull exascaleproject/sdk:AHM19
- Launch the image
  - % shifter --image=exascaleproject/sdk:AHM19 -- /bin/bash
  - % unset CRAYPE_VERSION; . /etc/bashrc
  - % spack find

Extreme-scale Scientific Software Stack (E4S) https://e4s.io

```
-- linux-centos7-x86_64 / gcc@4.8.5 -----------------------------
autoconf@2.69    bzip2@1.0.6   flex@2.6.4   gettext@0.19.8.1  hwloc@1.11.9  kokkos@2.03.00      libtool@2.4.6  m4@1.4.18    mpfr@4.0.1   numactl@2.0.11  openssl@1.0.2n  pkgconf@1.4.0  util-macros@1.19.1
automake@1.15.1  cmake@3.11.1  gcc@7.3.0    gmp@6.1.2         hwloc@2.0.1   libpciaccess@0.13.5 libunwind@1.1  magma@2.4.0  mpich@3.2.1  openblas@0.2.20 papi@5.5.1      readline@7.0   xz@5.2.3
bison@3.0.4      cuda@9.1.85   gdbm@1.14.1  help2man@1.47.4   isl@0.19      libsigsegv@2.11     libxml2@2.9.4  mpc@1.1.0    ncurses@6.0  openmpi@3.0.1   perl@5.24.1     tar@1.29       zlib@1.2.11

-- linux-centos7-x86_64 / gcc@7.3.0 -----------------------------
adios@1.13.1           dbus@1.12.8                 gmp@6.1.2                   libbsd@0.9.1          libxi@1.7.6           nasm@2.13.03          presentproto@1.0      py-pytables@3.3.0      superlu-dist@5.2.2
adios2@2.4.0           diffutils@3.7               gobject-introspection@1.49.2 libcircle@0.2.1-rc.1 libxkbcommon@0.8.2   nasm@2.14.02          protobuf@3.5.1.1      py-pytest@3.6.0        swig@3.0.12
adlbx@0.8.0            docbook-xml@4.5             gobject-introspection@1.56.1 libcircle@0.2.1-rc.1 libxkbfile@1.0.9     ncurses@6.0           py-argparse@1.4.0     py-pytz@2017.2         swig@4.0.0
adlbx@0.8.0            docbook-xsl@1.79.2          googletest@1.8.1            libedit@3.1-20170329  libxml2@2.9.4         ncurses@6.1           py-argparse@1.4.0     py-pyyaml@3.13         swig@4.0.0
aml@0.1.0              double-conversion@2.0.1     gotcha@0.0.2                libedit@3.1-20170329  libxml2@2.9.9         netcdf@4.4.1.1        py-babel@2.4.0        py-scipy@1.0.0         sz@1.4.12.3
ant@1.9.9              doxygen@1.8.12              gotcha@develop              libfabric@1.8.0       libxrender@0.9.10     netcdf@4.7.0          py-bottleneck@1.0.0   py-scipy@1.3.1         tar@1.29
argobots@1.0rc1        dtcmp@1.1.0                 gperf@3.0.4                 libffi@3.2.1          libxshmfence@1.2      netlib-lapack@3.8.0   py-cffi@1.12.2        py-setuptools@39.0.1   tar@1.31
arpack-ng@3.7.0        dtcmp@1.1.0                 graphlib@3.0.0              libfontenc@1.1.3      libxslt@1.1.33        netlib-scalapack@2.0.2 py-configparser@3.5.0 py-setuptools@41.0.1   tasmanian@6.0
at-spi2-atk@2.26.2     dyninst@10.1.0              graphviz@2.40.1             libgcrypt@1.8.4       libxt@1.1.5           nettle@3.3            py-cycler@0.10.0      py-setuptools@41.0.1   tau@2.28
at-spi2-core@2.28.0    elfutils@0.176              harfbuzz@1.4.6              libgpg-error@1.36     libxt@1.1.5           nettle@3.4.1          py-cython@0.28.1      py-setuptools-scm@3.1.0 tcl@8.6.8
atk@2.30.0             er@0.0.3                    harfbuzz@2.3.1              libiberty@2.31.1      libxtst@1.2.2         ninja@1.8.2           py-cython@0.29.7      py-six@1.11.0          texinfo@6.5
autoconf@2.69          exmcutils@0.5.3             hdf5@1.8.19                 libice@1.0.9          libxv@1.0.10          ninja@1.9.0           py-dateutil@2.5.2     py-six@1.12.0          texinfo@6.5
autoconf@2.69          expat@2.2.2                 hdf5@1.8.19                 libiconv@1.15         libxvmc@1.0.9         nrm@0.1.0             py-enum34@1.1.6       py-subprocess32@3.2.7  tk@8.6.8
automake@1.14          expat@2.2.5                 hdf5@1.10.1                 libjpeg-turbo@1.5.3   libyogrt@1.20-6       numactl@2.0.11        py-flake8@3.5.0       py-tornado@5.1.1       trilinos@12.12.1
automake@1.15.1        faodel@1.1906.1             hdf5@1.10.1                 libjpeg-turbo@2.0.2   llvm@8.0.0            numactl@2.0.12        py-funcsigs@0.4       py-vcversioner@2.16.0.0 turbine@1.0.0
automake@1.16.1        fast-global-file-status@1.1 hdf5@1.10.1                 libmng@2.0.3          lmod@7.7.13           openblas@0.2.20       py-functools32@3.2.3-2 py-warlock@1.3.3      turbine@1.0.0
axl@0.1.1              fftw@3.3.7                  hdf5@1.10.1                 libmng@2.0.3          lua@5.3.4             openblas@0.3.7        py-h5py@2.7.1         py-zmq@17.1.2          umpire@master
bdftopcf@1.0.5         findutils@4.6.0             hdf5@1.10.5                 libnrm@0.1.0          lua-luafilesystem@1_6_3 openmpi@3.0.1       py-hypothesis@3.7.0   python@2.7.14          unifycr@master
binutils@2.27          fixesproto@5.0              help2man@1.47.4             libpciaccess@0.13.5   lua-luaposix@33.4.0   openssl@1.0.2n        py-jinja2@2.9.6       python@2.7.14          unifyfs@develop
binutils@2.29.1        flatcc@0.5.3                help2man@1.47.8             libpfm4@4.8.0         lwgrp@1.0.2           openssl@1.1.1c        py-jsonpatch@1.23     python@2.7.16          upcxx@2019.3.2
binutils@2.32          flecsi@develop              hpctoolkit@2017.06          libpng@1.6.34         lwgrp@1.0.2           otf2@2.1              py-jsonpointer@1.9    python@3.7.4           util-macros@1.19.1
bison@3.0.4            flex@2.6.4                  hpctoolkit-externals@2017.06 libpthread-stubs@0.4 lz4@1.8.1.2       pango@1.41.0          py-jsonschema@2.6.0   qhull@2015.2           veloc@1.0
bison@3.0.5            flex@2.6.4                  hwloc@1.11.9                libquo@1.3            lz4@1.9.0             papi@5.5.1            py-kiwisolver@1.0.1   qt@5.10.0              videoproto@2.3.3
bmi@develop            font-util@1.3.1             hwloc@1.11.11               libsigsegv@2.11       lzma@4.32.7           papyrus@develop       py-lit@0.5.0          qthreads@1.12          vtkm@1.1.0
bolt@1.0b1             font-util@1.3.2             hwloc@2.0.1                 libsm@1.2.2           lzo@2.09              parallel-netcdf@1.11.2 py-mako@1.0.4        r@3.4.3                vtkm@master
boost@1.66.0           fontconfig@2.12.3           hypre@2.13.0                libsodium@1.0.17      lzo@2.10              paraview@5.6.2        py-mako@1.0.4         raja@0.5.3             xcb-proto@1.13
boost@1.66.0           fontconfig@2.12.3           hypre@2.13.0                libtiff@4.0.6         m4@1.4.18             parmetis@4.0.3        py-markupsafe@1.0     rankstr@0.0.2          xcb-util@0.4.0
boost@1.68.0           fontsproto@2.1.3            icu4c@60.1                  libtiff@4.0.8         m4@1.4.18             parmetis@4.0.3        py-markupsafe@1.0     readline@7.0           xcb-util-image@0.4.0
boost@1.70.0           freetype@2.7.1              icu4c@64.1                  libtiff@4.0.10        margo@0.4.3           patch@2.7.6           py-matplotlib@2.2.2   readline@7.0           xcb-util-keysyms@0.4.0
boost@1.70.0           freetype@2.9.1              inputproto@2.3.2            libtool@2.4           matio@1.5.9           patchelf@0.9          py-mccabe@0.6.1       recordproto@1.14.2     xcb-util-renderutil@0.3.9
bzip2@1.0.6            gasnet@1.30.0               intel-tbb@2018.2            libtool@2.4.2         mercury@1.0.1         pcre@8.41             py-mock@2.0.0         redset@0.0.3           xcb-util-wm@0.4.1
bzip2@1.0.8            gasnet@1.30.0               intel-tbb@2019.4            libtool@2.4.6         mercury@1.0.1         pcre@8.41             py-mpi4py@3.0.0       rempi@1.1.0            xextproto@7.3.0
c-blosc@1.12.1         gdb@8.0.1                   intltool@0.51.0             libunwind@1.1         mesa@18.3.6           pcre@8.42             py-natsort@5.2.0      renderproto@0.11.1     xkbcomp@1.3.1
c-blosc@1.17.0         gdbm@1.14.1                 jdk@8u141-b15               libuuid@1.0.3         meson@0.49.1          pcre@8.42             py-nose@1.3.7         ruby@2.2.0             xkbdata@1.0.1
cairo@1.14.12          gdbm@1.18.1                 json-c@0.13.1               libx11@1.6.5          metis@5.1.0           pcre2@10.31           py-numexpr@2.6.1      ruby-ronn@0.7.3        xproto@7.0.31
cairo@1.16.0           gdk-pixbuf@2.38.0           kbproto@1.0.7               libx11@1.6.7          metis@5.1.0           pdsh@2.31             py-numpy@1.13.3       scr@1.2.2              xtrans@1.3.5
cairo@1.16.0           geopm@0.4.0                 kokkos@2.03.00              libxau@1.0.8          mfem@3.3.2            pdt@3.25              py-numpy@1.17.2       shared-mime-info@1.9   xz@5.2.3
caliper@1.8.0          gettext@0.19.8.1            kvtree@1.0.2                libxcb@1.13           miniconda2@4.3.30     perl@5.24.1           py-pandas@0.21.1      shuffile@0.0.3         xz@5.2.4
cinch@develop          gettext@0.19.8.1            launchmon@1.0.2             libxcb@1.13           miniconda3@4.3.30     perl@5.26.2           py-pbr@3.1.1          snappy@1.1.7           zeromq@4.3.2
cmake@3.11.1           git@2.15.1                  lcms@2.8                    libxdamage@1.1.4      mkfontdir@1.0.7       perl-data-dumper@2.173 py-pillow@3.2.0      snappy@1.1.7           zfp@0.5.0
cmake@3.15.3           git@2.21.0                  lcms@2.9                    libxdmcp@1.1.2        mkfontscale@1.1.2     perl-xml-parser@2.44  py-pkgconfig@1.2.2    sqlite@3.22.0          zfp@0.5.4
conduit@master         glib@2.56.0                 legion@17.10.0              libxdmcp@1.1.2        mount-point-attributes@1.1 petsc@3.8.4      py-py@1.4.33          sqlite@3.29.0          zlib@1.2.11
curl@7.59.0            glib@2.56.3                 leveldb@1.20                libxext@1.3.3         mpich@3.2.1           pflotran@xsdk-0.3.0   py-py@1.5.4           stc@0.7.3              zsh@5.4.2
curl@7.63.0            glib@2.56.3                 leveldb@1.22                libxext@1.3.3         mpich@3.2.1           pixman@0.34.0         py-pycodestyle@2.3.1  strumpack@3.1.1        zstd@1.3.0
damageproto@1.2.1      glm@0.9.7.1                 libarchive@3.3.2            libxfixes@5.0.2       mpifileutils@develop  pixman@0.38.0         py-pycparser@2.18     suite-sparse@5.2.0     zstd@1.4.2
darshan-runtime@3.1.6  globalarrays@5.7            libarchive@3.3.2            libxfixes@5.0.2       mrnet@5.0.1-3         pkgconf@1.4.0         py-pyflakes@1.6.0     sundials@3.1.0
darshan-util@3.1.6     glproto@1.4.17              libbsd@0.8.6                libxfont@1.5.2        mumps@5.1.1           pkgconf@1.6.1         py-pyparsing@2.2.0    superlu@5.2.1
```

E4S v1.0 Release (50 Products):

45. tutorial@ip-172-31-1-143:~ (ssh)

```
1: adios        /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/adios-1.13.1-v7jyzgyie7n542qppgoz2izthu6xeaj5
2: aml  /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/aml-0.1.0-ao2r76pzk5k6mdfvx3cixvqlyg7hzppt
3: argobots     /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/argobots-1.0rc1-4kbgyfusscwopqzl76oaxpiglf6itptm
4: bolt         /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/bolt-1.0b1-jenaxkneyprxgq6abwaihlkuuoko4pwv
5: caliper      /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/caliper-1.8.0-lrmti32xdgyckyhk5vr5okrxtniv2pb5
6: darshan-runtime      /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/darshan-runtime-3.1.6-yb2tk7rst4yclkluqaixardes3slhgve
7: dyninst      /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/dyninst-10.1.0-g3ogsuc2yztrb2agfgk4ga2ik7w6kg45
8: faodel       /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/faodel-1.1906.1-gpadaotmehed2wejfxyeg7bxewtmsclc
9: flecsi       /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/flecsi-develop-2zth7esblvxalqdnvbxota6jfx2xzi3i
10: gasnet      /home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/gasnet-1.30.0-hp4d5xsbnhg5gisbkmgopd6pkqmgrczo
11: geopm       /home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/geopm-0.4.0-qhho4xnuyymvurjeuqjfml4u42b7a3t6
12: globalarrays        /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/globalarrays-5.7-7zbsme3slnsmzkuzgq6ac4ggbdnoakal
13: gotcha      /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/gotcha-develop-dcqszr3n36z73pqsm2d745rx5bzvr2hq
14: hdf5        /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/hdf5-1.10.5-qhy2hcxb6t7aunew3g7pn4ljdqzw474i
15: hpctoolkit  /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/hpctoolkit-2017.06-boqjp7bdarhaysswzp6p6w5skt5wa423
16: hypre       /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/hypre-2.13.0-3kjvfl7rz3e7f6eojvojyfegcwdl6ehb
17: kokkos      /home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/kokkos-2.03.00-a3ksyhg6fflnlufs5sfanqfwxeeeogey
18: legion      /home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/legion-17.10.0-cjomljrvcxzbhwlznfc5luw6vwiubnyr
19: libnrm      /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/libnrm-0.1.0-ddwgupy5gg4dgyqhcpirzmxdgvcdgsrd
20: libquo      /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/libquo-1.3-cdtptdmouswpx5a4nvwxfyld3u3mcj62
21: magma       /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-4.8.5/magma-2.4.0-7cc275vlzmhypm5uuubj4krfsoqshhmr
22: mercury     /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/mercury-1.0.1-rxg3lgg5mratnsokdtqg676pqfs5md37
23: mfem        /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/mfem-3.3.2-sdrntzuthtzqophdl63b3ujmzy5ytb4g
24: mpich       /home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/mpich-3.2.1-5j57f4j36vhcsxgn2pwndouz27qe4ij4
25: mpifileutils        /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/mpifileutils-develop-jdotps6duoaumzzdzi5udvaohrix5scc
26: ninja       /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/ninja-1.9.0-vwu3smyjyej5olkvhzsy4t4piilcgmql
27: openmpi     /home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/openmpi-3.0.1-hdjeffn2fs3iidk3whvv6smbrnmzqq3e
28: papi        /home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/papi-5.5.1-abkudkdhzua3p4lnn7m6ssj3or45fjri
29: papyrus     /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/papyrus-develop-77k6v4izzvjx222zbrpiexka7fmjsjgr
30: parallel-netcdf     /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/parallel-netcdf-1.11.2-bzsg3ky62qc7c3y6h3txvvyouc3h3vdx
31: pdt         /home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/pdt-3.25-fjjddrbx7lx4hrqmqfwssq4oz46zvj5p
32: petsc       /home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/petsc-3.8.4-7naeokjkiniftmkecngpcn736bvnrdhl
33: qthreads    /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/qthreads-1.12-npkx43id5wewkrbsv6qpr76qisoozbpu
34: raja        /home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/raja-0.5.3-zrjr35xwjrfz6wacs4k36ilwc45m6gq6
35: rempi       /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/rempi-1.1.0-rpzp7upbe4c3m2auq3l2we5rjxl62xd2
36: scr         /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/scr-1.2.2-fdqkevg2nf6yedg4qhwersf6ojwikxqz
37: strumpack   /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/strumpack-3.1.1-q4wwcyff7lzrrbwc6np5jxezv6iix7ig
38: sundials    /home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/sundials-3.1.0-xrqsfvumk2jw7aqidjsj7lya4w5kqm3p
39: superlu-dist        /home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/superlu-dist-5.2.2-2b5bmvyyjr4b26gz6iekaha6axpu6ujf
40: sz  /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/sz-1.4.12.3-dgykqp27gsnnyc2ktm6rnb6bfgxwq7vq
41: tasmanian   /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/tasmanian-6.0-fv7z3ninw7agbvlw2jhau2hyx5ofyt4k
42: tau         /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/tau-2.28-2zm23cf4lu74wfp2ufrzo7bu22popu4x
43: trilinos    /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/trilinos-12.12.1-kobl2zztgzcukmx5tktvmyradjt6qym7
44: turbine     /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/turbine-1.0.0-6ct6q2xwav5n22xvf2exbmgpjwknkgho
45: umpire      /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/umpire-master-4bditlkgpbuznpnnshpf3poxthmadefq
46: unifyfs     /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/unifyfs-develop-s47fumvqwo7gxjdspwnadribvrkeppn5
47: upcxx       /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/upcxx-2019.3.2-uezjtlwvssi5ztt6qltejmxzrv6etkh2
48: veloc       /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/veloc-1.0-jmamhwdqgwurlxq2ugn7gyuqrdj4jz5p
49: vtkm        /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/vtkm-master-g6zjyz5ja7olj7fbj2iga7ohfy4hx3f5
50: zfp         /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/zfp-0.5.4-kbmhpghxrfimhbhop6upwuj7herhm7pz
```

exascaleproject/e4s_x86_64:1.0
on Dockerhub

Extreme-scale Scientific Software Stack (E4S)
https://e4s.io

```
Singularity> cd `spack location -i trilinos`/lib
Singularity> ls *.so*1
libamesos2.so.12.12.1           libIonit.so.12.12.1             librtop.so.12.12.1              libsuplib.so.12.12.1
libamesos.so.12.12.1            libIopg.so.12.12.1              libsacado.so.12.12.1            libteuchoscomm.so.12.12.1
libanasaziepetra.so.12.12.1     libIopx.so.12.12.1              libshylu.so.12.12.1             libteuchoscore.so.12.12.1
libanasazi.so.12.12.1           libIoss.so.12.12.1              libstk_expreval.so.12.12.1      libteuchoskokkoscomm.so.12.12.1
libanasazitpetra.so.12.12.1     libIotr.so.12.12.1              libstk_search.so.12.12.1        libteuchoskokkoscompat.so.12.12.1
libaprepro_lib.so.12.12.1       libIovs.so.12.12.1              libstk_topology.so.12.12.1      libteuchosnumerics.so.12.12.1
libaztecoo.so.12.12.1           libisorropia.so.12.12.1         libstk_transfer_impl.so.12.12.1 libteuchosparameterlist.so.12.12.1
libbelosepetra.so.12.12.1       libkokkosalgorithms.so.12.12.1  libstk_util_diag.so.12.12.1     libteuchosremainder.so.12.12.1
libbelos.so.12.12.1             libkokkoscontainers.so.12.12.1  libstk_util_env.so.12.12.1      libthyracore.so.12.12.1
libbelostpetra.so.12.12.1       libkokkoscore.so.12.12.1        libstk_util_parallel.so.12.12.1 libthyraepetraext.so.12.12.1
libchaco.so.12.12.1             libkokkoskernels.so.12.12.1     libstk_util_registry.so.12.12.1 libthyraepetra.so.12.12.1
libepetraext.so.12.12.1         libkokkostsqr.so.12.12.1        libstk_util_use_cases.so.12.12.1 libthyratpetra.so.12.12.1
libepetra.so.12.12.1            liblocaepetra.so.12.12.1        libstk_util_util.so.12.12.1     libtpetraclassiclinalg.so.12.12.1
libexodus_for.so.12.12.1        liblocalapack.so.12.12.1        libstokhos_amesos2.so.12.12.1   libtpetraclassicnodeapi.so.12.12.1
libexodus.so.12.12.1            libloca.so.12.12.1              libstokhos_ifpack2.so.12.12.1   libtpetraclassic.so.12.12.1
libexoIIv2for32.so.12.12.1      liblocathyra.so.12.12.1         libstokhos_muelu.so.12.12.1     libtpetraext.so.12.12.1
libgaleri-epetra.so.12.12.1     libmapvarlib.so.12.12.1         libstokhos_sacado.so.12.12.1    libtpetrainout.so.12.12.1
libgaleri-xpetra.so.12.12.1     libml.so.12.12.1                libstokhos.so.12.12.1           libtpetra.so.12.12.1
libgtest.so.12.12.1             libModeLaplace.so.12.12.1       libstokhos_tpetra.so.12.12.1    libtpi.so.12.12.1
libifpack2-adapters.so.12.12.1  libmuelu-adapters.so.12.12.1    libstratimikosamesos.so.12.12.1 libtrilinoscouplings.so.12.12.1
libifpack2.so.12.12.1           libmuelu-interface.so.12.12.1   libstratimikosaztecoo.so.12.12.1 libtrilinosss.so.12.12.1
libifpack.so.12.12.1            libmuelu.so.12.12.1             libstratimikosbelos.so.12.12.1  libtriutils.so.12.12.1
libIoexo_fac.so.12.12.1         libnemesis.so.12.12.1           libstratimikosifpack.so.12.12.1 libxpetra.so.12.12.1
libIoex.so.12.12.1              libnoxepetra.so.12.12.1         libstratimikosml.so.12.12.1     libxpetra-sup.so.12.12.1
libIofx.so.12.12.1              libnoxlapack.so.12.12.1         libstratimikos.so.12.12.1       libzoltan2.so.12.12.1
libIogn.so.12.12.1              libnox.so.12.12.1               libsupes.so.12.12.1             libzoltan.so.12.12.1
libIohb.so.12.12.1              libpamgen_extras.so.12.12.1     libsuplib_cpp.so.12.12.1
libio_info_lib.so.12.12.1       libpamgen.so.12.12.1            libsuplib_c.so.12.12.1
Singularity>
```

Running MPI applications on other systems

- Applications built with MPI in the E4S container can be replaced by the system MPI!
- This allows fast inter-node communication using the native interconnect.
- Application and data are external to the E4S container.
- Programming models, compilers, runtime libraries, and tools are inside the container.
- We can replace MPI using the MPICH ABI compatibility layer.
- Goal: Build an MPI binary once and run it un-modified on all HPC Linux x86_64 clusters!

Using E4S on NCSA BlueWaters and replacing MPI

Step 1: Allocate a node with the E4S image

- qsub -I -l nodes=2:ppn=32 -l walltime=01:15:00 -l gres=shifter16 -v UDI=exascaleproject/sdk:AHM19
- This allocates a single node for 1:15h
- Specifies the use of Shifter as the container environment
- The image is exascaleproject/sdk:AHM19
- This image was pulled on a compute node previously using:
  - %module load shifter; shifterimg pull exascaleproject/sdk:AHM19
- After this qsub step, we can now launch the job using aprun

Using E4S on NCSA BlueWaters Replacing MPI

Step 2: Create a file called ~/shifter_mpi.sh

```
% cat ~/shifter_mpi.sh
#!/bin/bash
# set up LD_LIBRARY_PATH
for dir in $(echo $CRAY_LD_LIBRARY_PATH:/opt/cray/wlm_detect/default/lib64 | tr
':' ' ')
do
    realpath=$(readlink -f "$dir")
    if [[ -z $LD_LIBRARY_PATH ]]
    then
        eval 'export LD_LIBRARY_PATH=/dsl'$realpath
    else
        eval 'export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/dsl'$realpath
    fi
done
```

Replacing MPI using cray-mpich-abi package

Step 3: Source this ~/shifter_mpi and setup LD_LIBRARY_PATH

```
% cat run.sh
#!/bin/bash
export CRAY_ROOTFS=SHIFTER
module load shifter
module unload PrgEnv-cray # or any other PrgEnv module currently loaded
module load PrgEnv-gnu # or PrgEnv-intel
module unload cce
module unload cray-mpich
module load cray-mpich-abi
export LD_LIBRARY_PATH=$CRAY_MPICH_DIR/lib:$LD_LIBRARY_PATH
source ~/shifter_mpi.sh
export LD_LIBRARY_PATH=/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/
gcc-7.3.0/hwloc-1.11.9-7xxgxbg65an7zmrztfcuu3hs73puj6v3/lib:$LD_LIBRARY_PATH
export OMP_NUM_THREADS=2
aprun -b -n 64 -- ./lulesh.host  -i 100
```

Replacing MPI using cray-mpich-abi package

Step 4: run the example

```
% ./run.sh
Running problem size 30^3 per domain until completion
Num processors: 64
Num threads: 2
Total number of elements: 1728000
…
Run completed:
   Problem size        =  30
   MPI tasks           =  64
   Iteration count     =  100
   Final Origin Energy = 8.465100e+07
   Testing Plane 0 of Energy Array on rank 0:
        MaxAbsDiff   = 7.916242e-09
        TotalAbsDiff = 3.030168e-08
        MaxRelDiff   = 1.224484e-13

Elapsed time         =      16.58 (s)
Grid time (us/z/c)   =  6.1409471 (per dom)  (0.095952298 overall)
FOM                  =  10421.845 (z/s)
Elapsed time         =      16.58 (s)
Grid time (us/z/c)   =  6.0131382 (per dom)  (0.22270882 overall)
FOM                  =  4490.1679 (z/s)

Application 81575093 resources: utime ~442s, stime ~20s, Rss ~45404, inblocks ~9110
```

Singularity on Theta at ALCF

```
% qsub -A ECP_SDK -t 30 -n 2  -q debug-cache-quad  -I
% /projects/ECP_SDK/tutorial/run_job.sh
```

```
module swap PrgEnv-intel PrgEnv-gnu

module swap cray-mpich cray-mpich-abi

export SINGULARITYENV_LIBWLM_DETECT=/opt/cray/wlm_detect/
1.3.2-6.0.6.0_3.8__g388ccd5.ari/lib64

aprun -n 16 -N 8 singularity exec -H $HOME    -B /projects/ECP_SDK:/projects/ECP_SDK:ro
-B /opt:/opt:ro -B /var/opt:/var/opt:ro /projects/ECP_SDK/containers/singularity/ecp.simg bash
-c 'unset CRAYPE_VERSION; source /usr/local/packages/ecp/misc/bashrc; spack load
trilinos hypre parmetis hdf5 metis openblas superlu zlib netcdf matio boost@1.66.0 scalapack
suite-sparse tau ;spack unload openmpi mpich ;  export
LD_LIBRARY_PATH=$LIBWLM_DETECT:$CRAY_LD_LIBRARY_PATH:
$CRAYPAT_LD_LIBRARY_PATH:$LD_LIBRARY_PATH   ; /projects/ECP_SDK/tutorial/demo/
trilinos/Zoltan/Zoltan; '
```

Singularity on Quartz at LLNL

MVAPICH2 needs /lib. Mount it as /hostlib64 and add it to LD_LIBRARY_PATH

```
% salloc -N 2
% srun -n 4 -c 2 singularity exec -B /lib64:/hostlib64 -B
$SLURM_SUBMIT_DIR:$SLURM_SUBMIT_DIR -B /usr/tce:/usr/tce ./ecp.simg /
bin/bash -c ' . /etc/bashrc ; spack load trilinos hypre parmetis hdf5 metis
openblas superlu zlib netcdf matio boost@1.66.0 scalapack suite-sparse tau;
spack unload openmpi mpich; export LD_LIBRARY_PATH=/usr/tce/packages/
mvapich2/mvapich2-2.2-intel-18.0.1/lib:$LD_LIBRARY_PATH:/hostlib64; ./Zoltan'
```

Replacing MPI with Shifter on Cori.nersc.gov

% shifterimg images

exascaleproject/sdk:AHM19 …

% To replace MPI with system MPI:

salloc -N 2 -q interactive -t 00:30:00 --image=exascaleproject/sdk:AHM19 -C haswell -L SCRATCH

~sameer/run_shifter.sh

cat ~/run_shifter.sh

srun −n 32 shifter -- /bin/bash -c 'unset CRAYPE_VERSION; . /etc/bashrc ; spack load trilinos hypre parmetis hdf5 metis openblas superlu zlib netcdf matio boost@1.66.0 scalapack suite-sparse tau; spack unload openmpi mpich; ./Zoltan'

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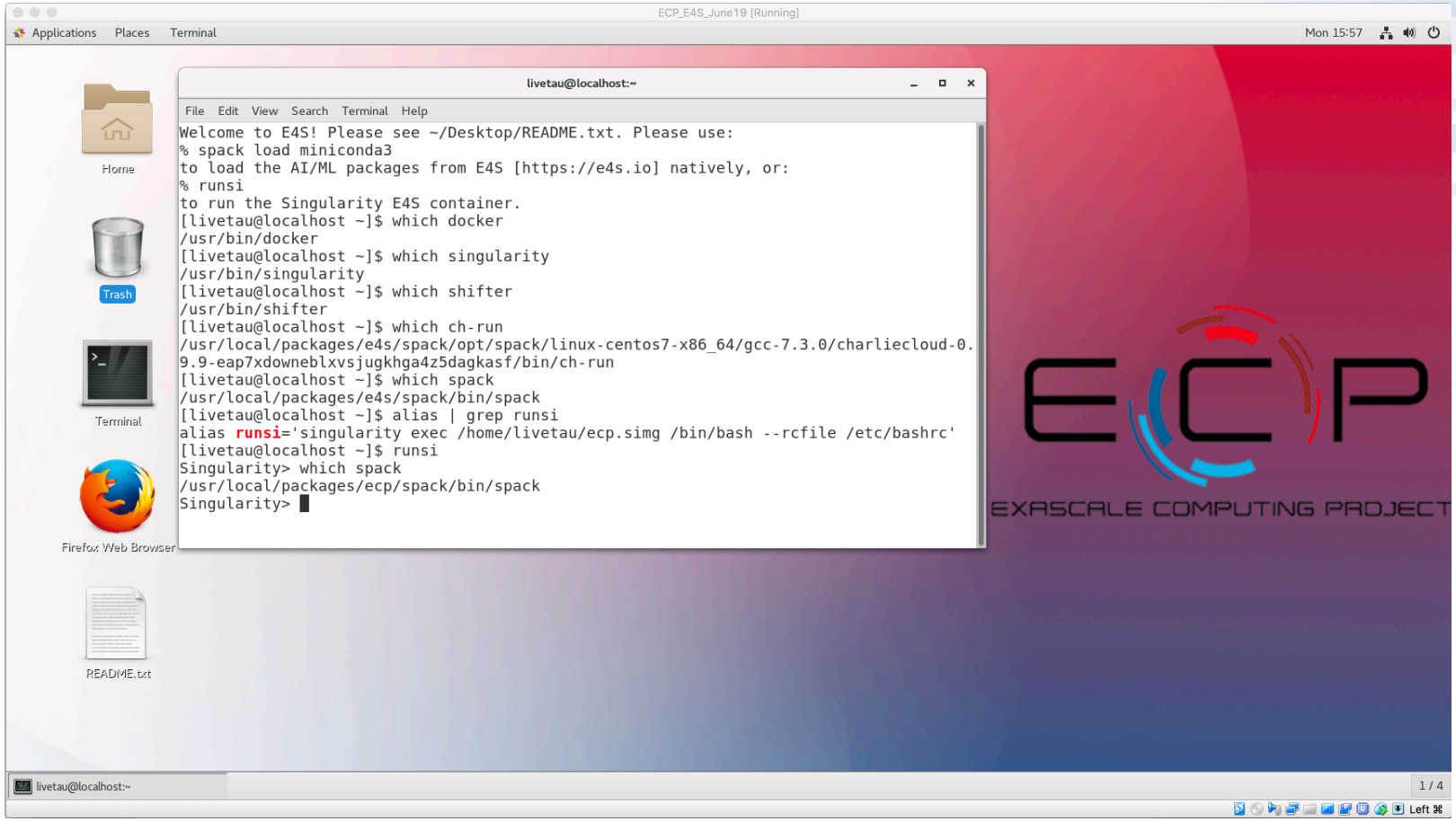
E4S VirtualBox OVA image

Contains all four container runtimes and the E4S Singularity image!

- Docker
- Singularity
- Shifter
- Charliecloud



E4S image on Amazon AWS

Contains all four container runtimes and the E4S Singularity image!

- AWS AMI ID (Oregon, us-west-2 region):
  - ami-063e830287b86155c
- Royalty free, public image with HPC, AI, and 4 container runtimes
- Launch EC2 instance with this AMI
  - Login: tutorial
  - Password: ****

Future work, issues…

- Increasing the number of ST packages in E4S
- Porting to IBM and ARM platforms
- Support for GPUs and visualization tools
- Addition of CI testing
- Facility deployment
- Scalable startup with full-featured “Supercontainers”
- Improving the launch of MPI applications

E4S: How to get involved

- **E4S BoF at SC19**
  - **Tuesday, Nov. 19, 12:15pm – 1:15pm, Room 405-406-407**
- **CANOPIE-HPC Workshop at SC19**
  - **1st Workshop on Containers and New Orchestration Paradigms for Isolated Environments in HPC**
  - **Monday, Nov. 18, 2019, 2pm – 5:30pm, Room 704-706**
  - https://canopie-hpc.nersc.gov/

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