



# E4S: Extreme-Scale Scientific Software Stack

<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](https://sc19.supercomputing.org/presentation/?id=tut129&sess=sess206)

# 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)

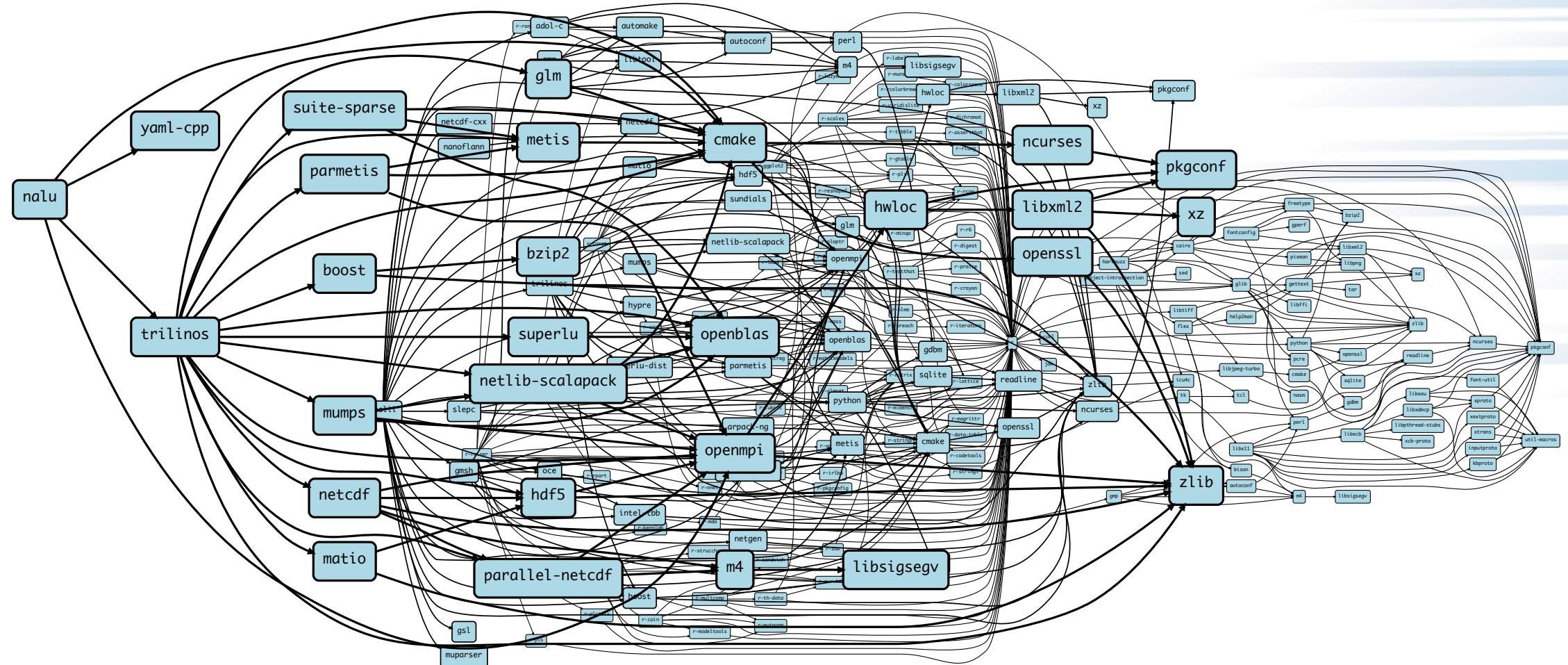
<https://e4s.io>

- 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 practices, 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](https://hub.docker.com/r/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

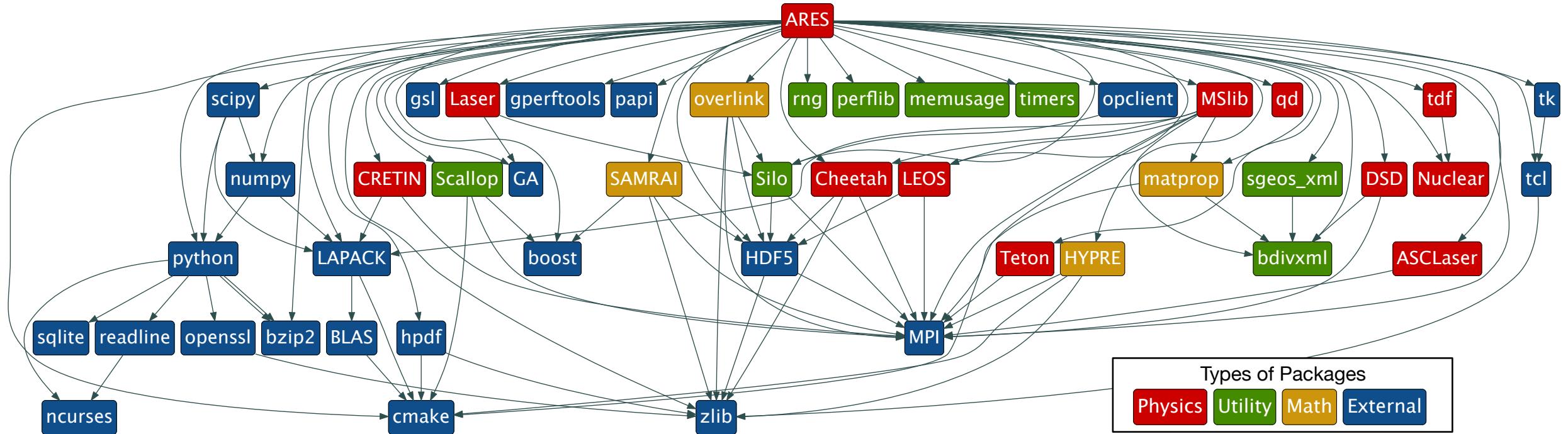
- E4S uses the Spack package manager for software delivery
- Spack provides the ability to specify versions of software packages that are and are not interoperable.
- Spack is a build layer for not only E4S software, but also a large collection of software tools and libraries outside of ECP ST.
- Spack 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**



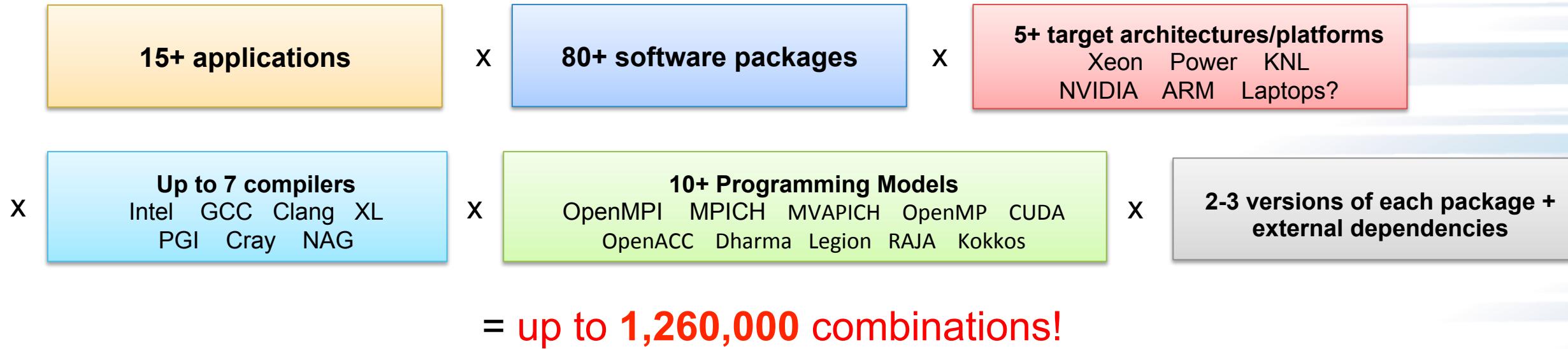
# Nalu: Generalized Unstructured Meshes for Efficient Parallel Mapping and Flow

# Even proprietary codes are based on many open source libraries



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

# The Exascale Computing Project is building an entire ecosystem



- 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

```
(gluon):~$ port install libelf
```

# How to install software on a supercomputer

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

**configure** **make**

```
configure make
```

TIGHE MCILROY : :

make

Tweak configure args...

**configure**   **make**

**make install**    **configure**    **make**

A vertical black and white spectrogram with a dark background. It features numerous horizontal bands of varying intensities, representing different frequencies. The bands are more concentrated at the top and become sparser towards the bottom. A thin vertical line is visible along the right edge of the plot area.

卷之三

**make install**

**cmake**   **make**   **make install**

**make** **make** **make** **install**

**make install**

ake install

Run code  
**Segfault!?**  
Start over.

# Segfault!?

**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 is insufficient**
  - 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



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

# Spack is a flexible package manager for HPC

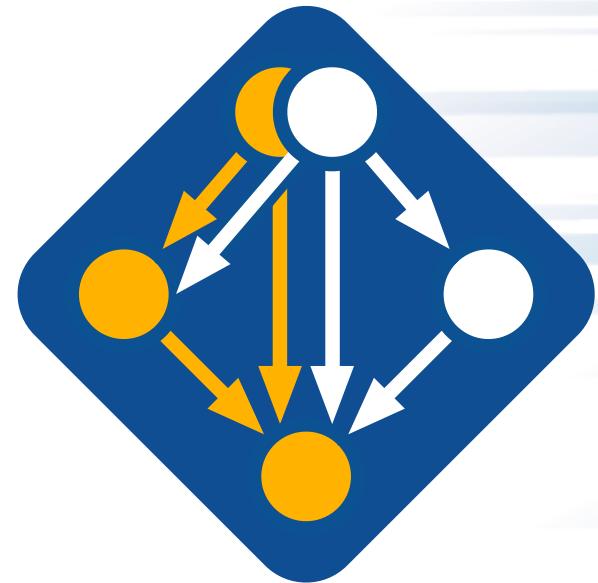
- How to install Spack (works out of the box):

```
$ 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](http://spack.io)



[github.com/spack/spack](https://github.com/spack/spack)



@spackpm

# 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-care            r-webshot
activeharmony   glimmer        nanoflann      py-fiona          r-caret           r-whisker
adept-utils     glm            nanopb         py-fiscalyear     r-catools         r-withr
adios           global          nasm           py-flake8         r-cdcfluvview    r-xde
adios2          globalarrays   nauty          py-flake8-polyfill  r-cellranger     r-xgboost
adlx            globus-toolkit ncbi-magicblast py-flask          r-checkmate      r-xlconnect
adol-c          glog            ncbl-mlblastn  py-flask-compress  r-checkpoint      r-xlconnectjars
aegean          gloo            ncbl-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
amrviz          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       rachel
ant              googletest     netcdf-fortran  py-greenlet       r-corhmm          raja
antlr            gotcha         netgauge        py-griddataformats  r-corpco          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-numumpy@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

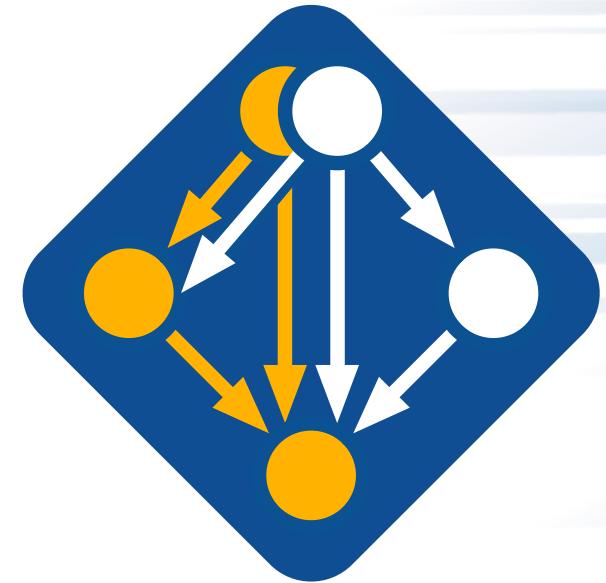
-- linux-rhel7-x86_64 / intel@15.0.0 --
adept-utils@1.0.1      boost@1.55.0    libdwarf@20130729  libelf@0.8.13  mpich@3.0.4

-- 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](http://spack.io)



[github.com/spack/spack](https://github.com/spack/spack)



@spackpm



EXASCALE  
COMPUTING  
PROJECT

# 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.

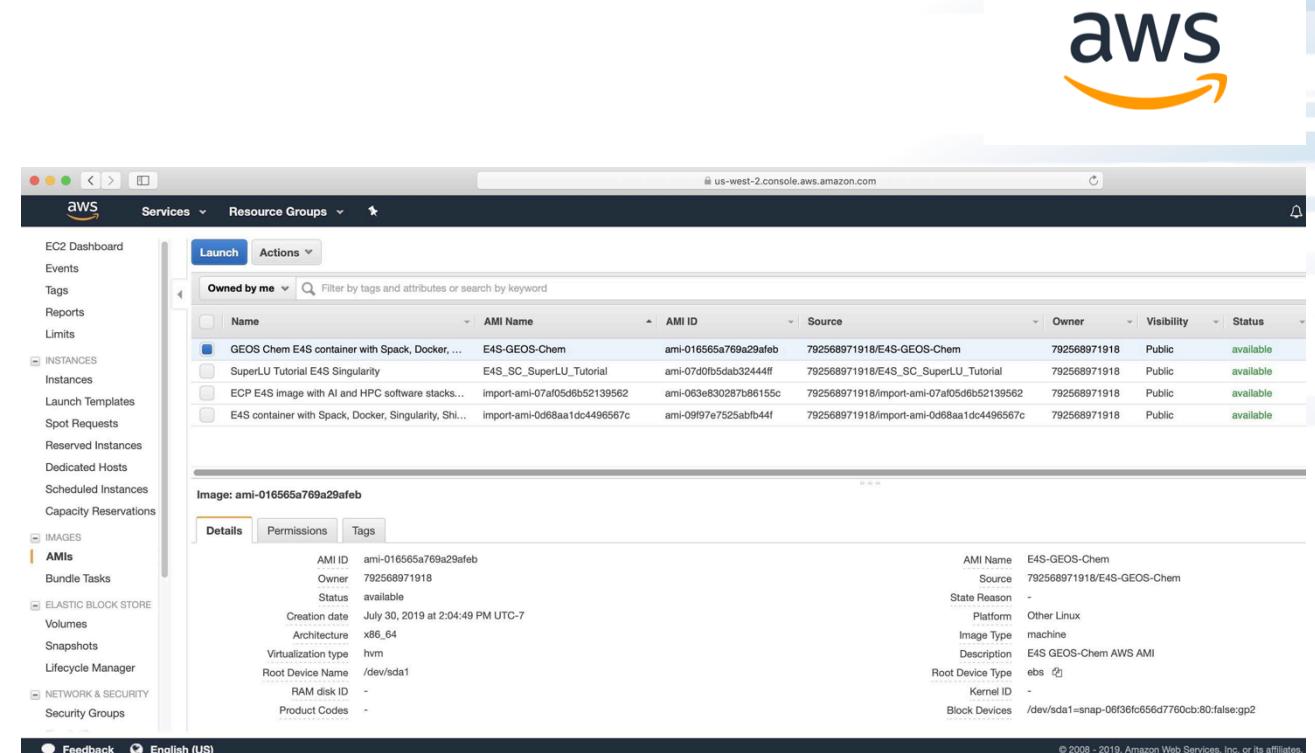


# Integration and Interoperability: E4S

- 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

The screenshot shows a web browser window displaying the Spack E4S Build Cache. The title bar reads "Spack E4S Build Cache". Below it, a message says "Last updated: 13-Oct-2019 07:43 PST". A sub-header indicates "1363 Spack binaries in the build cache". A search bar is present. The main content area lists various software packages and their variants. One package, "dyninst@10.1.0", is highlighted with a yellow background and a callout bubble containing the text "Click on the full spec link to find out more.". A table below this highlights specific builds for "dyninst@10.1.0" across different architectures (x86\_64) and operating systems (centos7, rhel7, ubuntu18.04). The table columns are Link, Arch, OS, Compiler, Created, and Full Hash. The first row of the table is underlined, indicating it is the current selection.

Link	Arch	OS	Compiler	Created	Full Hash
<a href="#">Full Spec</a>	x86_64	centos7	gcc@7.3.0	18-Sep-2019 19:07	m46bcmvfkvly5iz5iygg4mmta7myiers
<a href="#">Full Spec</a>	x86_64	centos7	gcc@7.3.0	18-Sep-2019 19:11	v2wfu3g3n7x4gndevks2vblmgc53qs7o
<a href="#">Full Spec</a>	x86_64	rhel7	gcc@7.3.0	15-Sep-2019 22:08	cwadhszs6dnell5dw2kvhgti5477uxjv
<a href="#">Full Spec</a>	x86_64	rhel7	gcc@7.3.0	15-Sep-2019 22:13	nokyntwy4poce4ips3qlam2sft5s7sk
<a href="#">Full Spec</a>	x86_64	ubuntu18.04	gcc@7.3.0	18-Sep-2019 19:16	lke6kpqlc5tpwxnwltihstek3wpefydy
<a href="#">Full Spec</a>	x86_64	ubuntu18.04	gcc@7.3.0	18-Sep-2019 19:21	e25zc3763g75iaas5wwbsfnuxjybqjfz

dyninst@10.1.0

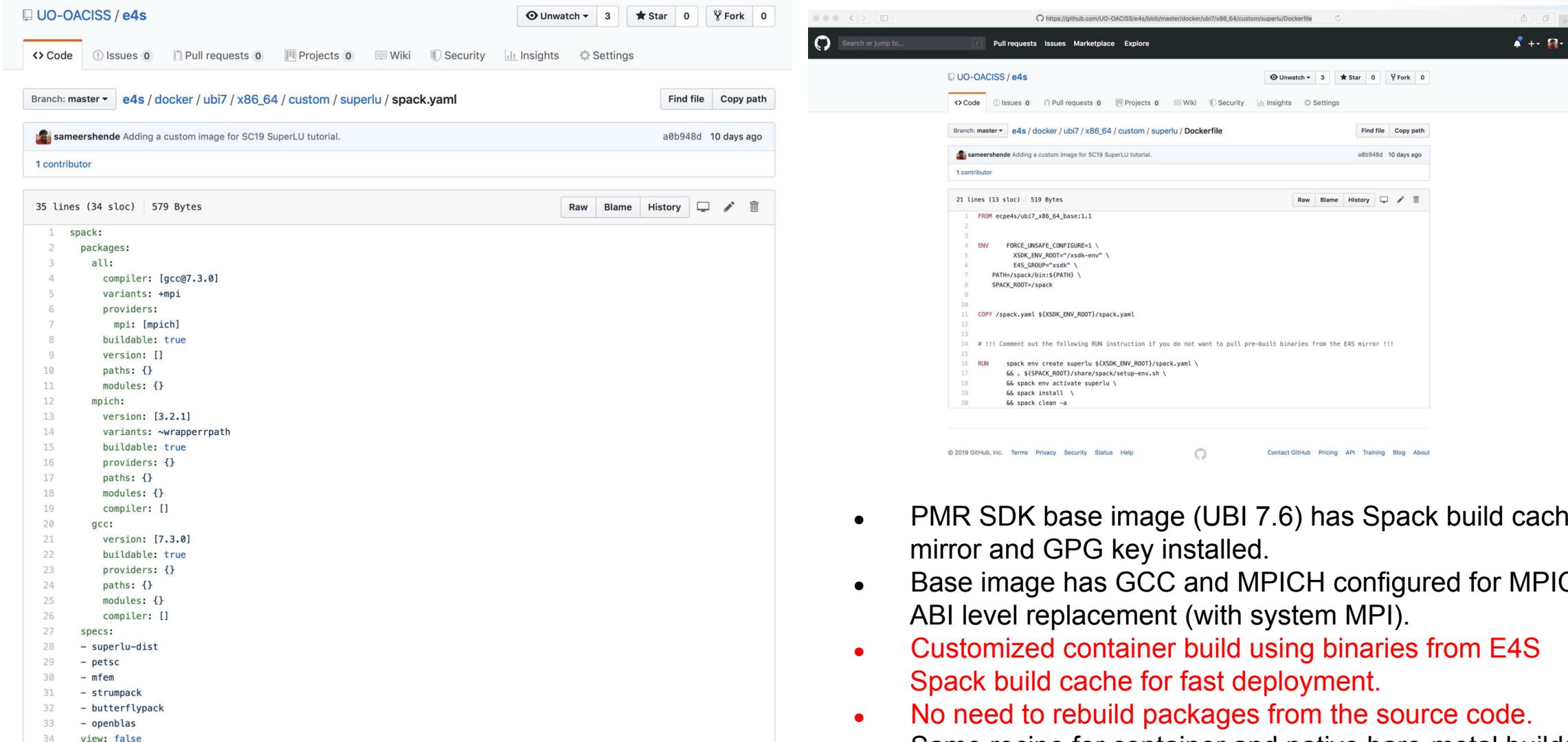
Click on the full spec link to find out more.

Link	Arch	OS	Compiler	Created	Full Hash
<a href="#">Full Spec</a>	x86_64	centos7	gcc@7.3.0	18-Sep-2019 19:07	m46bcmvfkvly5iz5iygg4mmta7myiers
<a href="#">Full Spec</a>	x86_64	centos7	gcc@7.3.0	18-Sep-2019 19:11	v2wfu3g3n7x4gndevks2vblmgc53qs7o
<a href="#">Full Spec</a>	x86_64	rhel7	gcc@7.3.0	15-Sep-2019 22:08	cwadhszs6dnell5dw2kvhgti5477uxjv
<a href="#">Full Spec</a>	x86_64	rhel7	gcc@7.3.0	15-Sep-2019 22:13	nokyntwy4poce4ips3qlam2sft5s7sk
<a href="#">Full Spec</a>	x86_64	ubuntu18.04	gcc@7.3.0	18-Sep-2019 19:16	lke6kpqlc5tpwxnwltihstek3wpefydy
<a href="#">Full Spec</a>	x86_64	ubuntu18.04	gcc@7.3.0	18-Sep-2019 19:21	e25zc3763g75iaas5wwbsfnuxjybqjfz

elfutils@0.176 emacs@26.2 environment-modules@4.3.0 environment-modules@4.3.1 er@0.0.3 exmcutils@0.5.7 expat@2.2.5 faodel@1.1906.1 findutils@4.6.0 flatcc@0.5.3 flecsi@develop flex@2.6.4 font-util@1.3.2 fontconfig@2.12.3 fontsproto@2.1.3 freetype@2.9.1 gasnet@2019.3.0 gawk@4.1.4 gcc@7.3.0 gdbm@1.18.1 geopm@1.0.0-rc2 gettext@0.19.8.1 git@2.21.0 glib@2.56.3 glm@0.9.7.1 globalarrays@5.7 glproto@1.4.17 gmp@6.1.2 googletest@1.8.1

<https://oaciss.uoregon.edu/e4s>

# Reproducible Container Builds using E4S Base Images



The image shows two GitHub repository pages side-by-side. The left page displays the file `spack.yaml` from the `e4s / docker / ubi7 / x86_64 / custom / superlu` directory. The right page displays the `Dockerfile` from the same directory. Both files were last updated 10 days ago by user `sameershende`.

**spack.yaml Content:**

```
1 spack:
2   packages:
3     all:
4       compiler: [gcc@7.3.0]
5       variants: +mpi
6       providers:
7         mpi: [mpich]
8       buildable: true
9       version: []
10      paths: {}
11      modules: {}
12
13      mpich:
14        version: [3.2.1]
15        variants: ~wrapperrpath
16        buildable: true
17        providers: {}
18        paths: {}
19        modules: {}
20        compiler: []
21
22      gcc:
23        version: [7.3.0]
24        buildable: true
25        providers: {}
26        paths: {}
27        modules: {}
28        compiler: []
29
30      specs:
31        - superlu-dist
32        - petsc
33        - mfm
34        - strumpack
35        - butterflypack
36        - openblas
37        view: false
```

**Dockerfile Content:**

```
1 FROM ecp4s/ubi7_x86_64_base:1.1
2
3 ENV FORCE_UNSAFE_CONFIGURE=1 \
4     XSDK_ENV_ROOT=/xdk-env \
5     E4S_GROUP=xdk \
6     PATH=/spack/bin:$PATH \
7     SPACK_ROOT=/spack
8
9 COPY /spack.yaml ${XSDK_ENV_ROOT}/spack.yaml
10
11 # !!! Comment out the following RUN instruction if you do not want to pull pre-built binaries from the E4S mirror !!!
12
13 RUN spack env create superlu ${XSDK_ENV_ROOT}/spack.yaml \
14     && . ${SPACK_ROOT}/share/spack/setup-env.sh \
15     && spack env activate superlu \
16     && spack install \
17     && spack clean -a
```

- 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

The screenshot shows the Dockerhub search interface for the user 'ecpe4s'. The search term 'ecpe4s' is entered in the search bar. The results are filtered by 'Containers'. The results are sorted by 'Most Popular'. There are four search results:

- ecpe4s/ubi7\_x86\_64\_base**: By ecpe4s, Updated a day ago. 37 Downloads. Container, Linux, x86-64.
- ecpe4s/superlu\_sc**: By ecpe4s, Updated 22 days ago. 17 Downloads. Container, Linux, x86-64.
- ecpe4s/e4s\_base**: By ecpe4s, Updated 8 months ago. 15 Downloads. Container, Linux, x86-64. Description: Base E4S container, using spack/centos:7 as the base. This adds gcc 7.4.0 from spack.
- ecpe4s/ubuntu1804\_aarch64\_base**: By ecpe4s, Updated 21 days ago. 13 Downloads. Container, Linux, x86-64.

- **ecpe4s**

- **x86\_64**
- **ppc64le**
- **aarch64**

- **Centos 7.6**
- **Ubuntu 18.04**
- **RHEL/UBI 7.6**

# Docker Recipes on GitHub

The screenshot shows a GitHub repository page for the URL [https://github.com/UO-OACISS/e4s/blob/master/docker-recipes/ubi7/x86\\_64/e4s/spack.yaml](https://github.com/UO-OACISS/e4s/blob/master/docker-recipes/ubi7/x86_64/e4s/spack.yaml). The page displays a YAML configuration file for Spack. The file defines a package named 'spack' with the following specifications:

```
1 spack:
2   packages:
3     all:
4       compiler: [gcc@7.3.0]
5       variants: +mpi
6       providers:
7         mpi: [mpich]
8       buildable: true
9       version: []
10      paths: {}
11      modules: {}
```

- Base images
- SDKs
- E4S

# Spack Build Caches from E4S Base Images

Name	Last modified	Size	Description
Parent Directory		-	
adios2-2.4.0/	19-Sep-2019 06:25	-	
argpack-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	-	
bintools-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	-	
boostedflypack-1.0.1/	12-Sep-2019 17:35	-	
bzip2-1.0.6/	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	-	
dtemp-1.1.0/	19-Sep-2019 06:28	-	
dyninst-10.1.0/	15-Sep-2019 22:13	-	
elfutils-0.176/	15-Sep-2019 17:58	-	
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	-	
faadef1-1.1906.1/	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	-	
gim-0.9.7.1/	29-Aug-2019 12:43	-	
glibproto-1.4.17/	27-Aug-2019 11:43	-	
googletest-1.8.1/	27-Aug-2019 09:09	-	
gotcha-0.0.2/	10-Sep-2019 11:11	-	
hdbs-1.10.5/	19-Sep-2019 06:21	-	
heinzmann-1.47.8/	28-Aug-2019 08:17	-	
httpcookie-2019.08.14/	15-Sep-2019 22:17	-	
hwloc-2.1.11/	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	-	
krbproto-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	-	
libadnl-0.9.1/	17-Sep-2019 17:30	-	
libadnl-0.9.2021029/	16-Sep-2019 12:27	-	
libadnl-1.1-20170329/	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	-	
libpaciaccess-0.13.5/	17-Sep-2019 17:30	-	
libpbfm-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	-	
libsigeev-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

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	-	
argbots-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	-	
dtemp-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	-	
flacc-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	-	
hdfs-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	-	
libsigeev-2.11/	18-Sep-2019 12:31	-	
libsodium-1.0.17/	20-Sep-2019 09:37	-	
libtcool-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 libpcicaccess@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
adlbox@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
adlbox@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 librender@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@41.0.1 tcl@8.6.8
atk@2.30.0 er@0.0.3 harfbuzz@2.3.1 libiberty@2.31.1 libxtst@1.2.2 nettle@1.8.2 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-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-enums@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
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
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
binutils@2.27 fixesproto@5.0 help2man@1.47.4 libpcicaccess@0.13.5 lua-luaposix@33.4.0 openssl@1.0.2n py-jinja2@2.9.6 python@2.7.14
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
binutils@2.32 flecsi@develop hpctoolkit@2017.06 libpng@1.6.34 lwgrp@1.0.2 oftf2@2.1 py-jsonpointer@1.9 python@3.7.4 upcxx@2019.3.2
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
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
bmi@develop font-util@1.3.1 hwloc@1.11.1 libsigsegv@2.11 lzma@4.32.7 papyrus@develop qthreads@1.12
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-lit@0.5.0 r@3.4.3
boost@1.66.0 fontconfig@2.12.3 hypre@2.13.0 libodium@1.0.17 lzo@2.10 paraview@5.6.2 raja@0.5.3
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
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 rankstr@0.0.2
boost@1.70.0 freetype@2.7.1 icu4c@64.1 libtiff@4.0.10 margo@0.4.3 patch@2.7.6 readline@7.0
boost@1.70.0 freetype@2.9.1 inputproto@2.3.2 libtool@2.4 matio@1.5.9 patchelf@0.9 py-markupsafe@1.0 recordproto@1.14.2
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
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
c-blosc@1.12.1 gdb@8.0.1 intltltool@0.51.0 libunwind@1.1 mesa@18.3.6 pcre@8.42 py-natsort@5.2.0
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 rempi@1.1.0
cairo@1.14.12 gdbm@1.18.1 json@0.13.1 libx11@1.6.5 metis@5.1.0 pcre2@10.31 py-numexpr@2.6.1
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
cairo@1.16.0 geomp@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
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
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
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
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
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
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
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
damageproto@1.2.1 glm@0.9.7.1 libarchive@3.3.2 libxfixes@5.0.2 mpifileutils@develop pixman@0.38.0
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-v7jzygyie7n542qppgoz2izthu6xeaj5
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-yb2tk7rst4yc1kluaqixaardes3slhgve
7: dyninst    /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/dyninst-10.1.0-g30gsuc2yztrb2agfgk4ga2ik7w6kg45
8: faodel     /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/faodel-1.1906.1-gpadaotmehed2wejfxyege7bxewtmsclc
9: flecsi     /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/flecsi-develop-2zth7esblvxalqdhnvbxota6jfx2xzis3i
10: gasnet     /home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/gasnet-1.30.0-hp4d5xsbnhg5isbkmopd6pkqmgrczo
11: geopm      /home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/geopm-0.4.0-qhho4nxuyymvurjeuajfm14u42b7a3t6
12: globalarrays /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/globalarrays-5.7-7zsme3slnsmzkuzgq6ac4ggbdnoakal
13: gotcha     /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/gotcha-develop-dcaqsrz3n36z73pqsmd2d745rx5bzvr2hq
14: hdf5       /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/hdf5-1.10.5-qhy2hcx6t7aunew3g7pn4ljdqzw474i
15: hptoolkit   /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/hptoolkit-2017.06-boqjp7bdarhaysswzp6p6w5skt5wa423
16: hypre      /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/hypre-2.13.0-3kjvf17rz3e7f6eojvojyfegcwld6ehb
17: kokkos     /home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/kokkos-2.03.00-a3ksyhg6ffflnlufs5sfanqfwxeheeogey
18: legion     /home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/legion-17.10.0-cjomljrvctxzbhwlnzfc5luw6vviubnyr
19: libnrm     /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/libnrm-0.1.0-ddwgupy5gg4dgyqhcpirzmxgdvcgsrd
20: libquo     /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/libquo-1.3-cdtptdmouswp5x5a4nwxylld3u3mcj62
21: magma      /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-4.8.5/magma-2.4.0-7cc275vlzmhypm5uuubj4krfsqshmr
22: mercury    /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/mercury-1.0.1-rxg3lgg5mratnsokdtqq676pqfs5md37
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-jdotps6duoamzzdzi5udvaohrix5sc
26: ninja      /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/ninja-1.9.0-vwu3smyjyej50lkvhzsyt4t4piilcmql
27: openmpi     /home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/openmpi-3.0.1-hdjeffn2fs3i1dk3whvv6smbrnmzqq3e
28: papi       /home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/papi-5.5.1-abkudkdhua3p4lnn7m6ssj3or45fjri
29: papyrus    /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/papyrus-develop-77kv64iizzvjx222zbrpiexka7fmjsjgr
30: parallel-netcdf /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/parallel-netcdf-1.11.2-bzsg3ky62qc7c3y6h3txvyyouc3h3vdx
31: pdt        /home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/pdt-3.25-fjjddrbx7lx4hrqmfwssq4oz46zvij5p
32: petsc      /home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/petsc-3.8.4-7naeokjkiniftmekcngpcn736bvnrdh1
33: qthreads   /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/qthreads-1.12-npxk43id5zewkrbsv6apr76qisoobzpu
34: raja       /home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/raja-0.5.3-zrjr35xwjrfz6wacs4k361lw45m6qg6
35: rempi      /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/rempi-1.1.0-rpzp7upbe4c3m2auq312we5rjx162xd2
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-q4wvcyff7lzrrbw6np5jxezv6iix7ig
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-5.2.2-2b5bmvyjyjr4b26gz6iekaha6axpu6ujf
40: sz         /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/sz-1.4.12.3-dgykqp27gsnnyc2ktm6rn6bfqgxwq7vq
41: tasmanian  /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/tasmanian-6.0-fv7z3ninw7agbv1w2jhau2hyx5ofyt4k
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-12.1-kobl2zztgzukmx5tktvmyradjt6qym7
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-4bd1tlkgpbuznpnnshpf3poxthmadefq
46: unifyfs    /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/unifyfs-develop-s47fumqvwo7gxjdswnadribvkleppn5
47: upcxx      /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/upcxx-2019.3.2-uezjtlvwssi5ztt6qltejmzr7v6etkh2
48: veloc     /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/veloc-1.0-jmamhwdagwurlxq2ugn7gyuqradj4jz5p
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-kbmhpgxrfimhbhop6upwuj7herhm7pz
```

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           libsplib.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     libstokhos_ifpack2.so.12.12.1 libtpetraclassicclinalg.so.12.12.1
libexodus_for.so.12.12.1       liblocalapack.so.12.12.1     libstokhos_muelu.so.12.12.1  libtpetraclassicnodeapi.so.12.12.1
libexodus.so.12.12.1            libloca.so.12.12.1           libstokhos_amesos2.so.12.12.1 libtpetraclassic.so.12.12.1
libexoIIv2for32.so.12.12.1     liblocathyra.so.12.12.1      libstokhos_sacado.so.12.12.1  libtpetraext.so.12.12.1
libgaleri-epetra.so.12.12.1    libmapvarlib.so.12.12.1     libstokhos_so.12.12.1        libtpetrainout.so.12.12.1
libgaleri-xpetra.so.12.12.1    libml.so.12.12.1             libstokhos_tpetra.so.12.12.1  libtpetra.so.12.12.1
libgtest.so.12.12.1             libModeLaplace.so.12.12.1   libstratimikosamesos.so.12.12.1 libtrilinoscouplings.so.12.12.1
libifpack2-adapters.so.12.12.1 libmuelu-adapters.so.12.12.1  libstratimikosaztecoo.so.12.12.1 libtrilinossso.12.12.1
libifpack2.so.12.12.1           libmuelu-interface.so.12.12.1 libstratimikosbelos.so.12.12.1 libtriutils.so.12.12.1
libifpack.so.12.12.1            libmuelu.so.12.12.1          libstratimikosifpack.so.12.12.1 libxpetra.so.12.12.1
libIoexo_fac.so.12.12.1         libnemesis.so.12.12.1        libstratimikosml.so.12.12.1   libxpetra-sup.so.12.12.1
libIoex.so.12.12.1              libnoxepetra.so.12.12.1      libstratimikos_so.12.12.1    libzoltan2.so.12.12.1
libIofx.so.12.12.1              libnoxlapack.so.12.12.1     libsunes.so.12.12.1          libzoltan.so.12.12.1
libIogn.so.12.12.1              libnox.so.12.12.1           libsplib_cpp.so.12.12.1
libIohb.so.12.12.1              libpamgen_extras.so.12.12.1  libsplib_c.so.12.12.1
libbio_info_lib.so.12.12.1      libpamgen.so.12.12.1
```

# 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 $LD_LIBRARY_PATH ]]
    then
        eval 'export LD_LIBRARY_PATH=/ds1'$realpath
    else
        eval 'export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/ds1'$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)
  Grind time (us/z/c) = 6.1409471 (per dom) (0.095952298 overall)
  FOM                = 10421.845 (z/s)
  Elapsed time      =      16.58 (s)
  Grind 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 LLLNL

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'
```

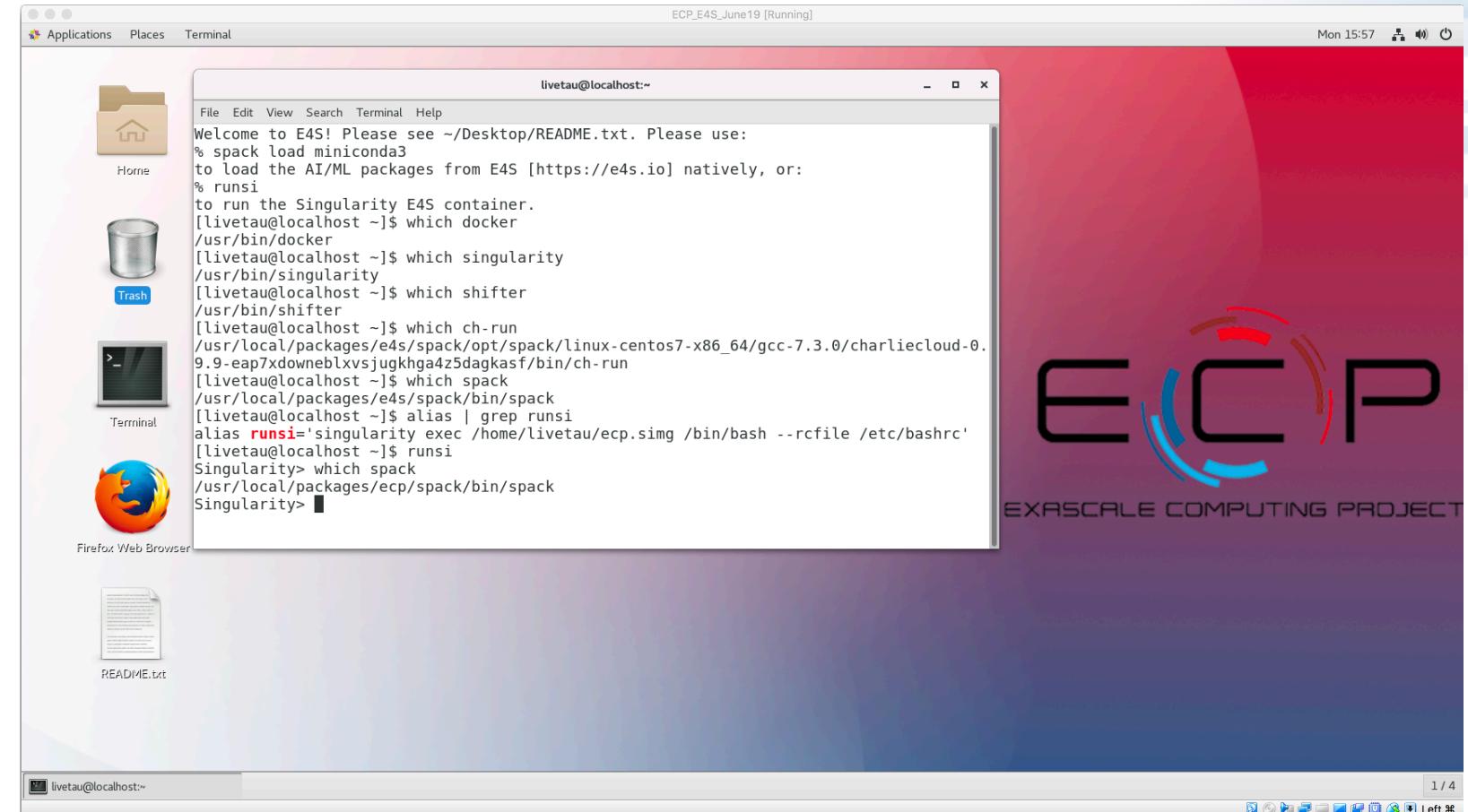
# Replacing MPI with Shifter on Cori.nersc.gov

```
% 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'
```

# 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: livetau
  - 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**
  - **1<sup>st</sup> 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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