



E4S: Extreme-Scale Scientific Software Stack

<https://e4s.io>



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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)

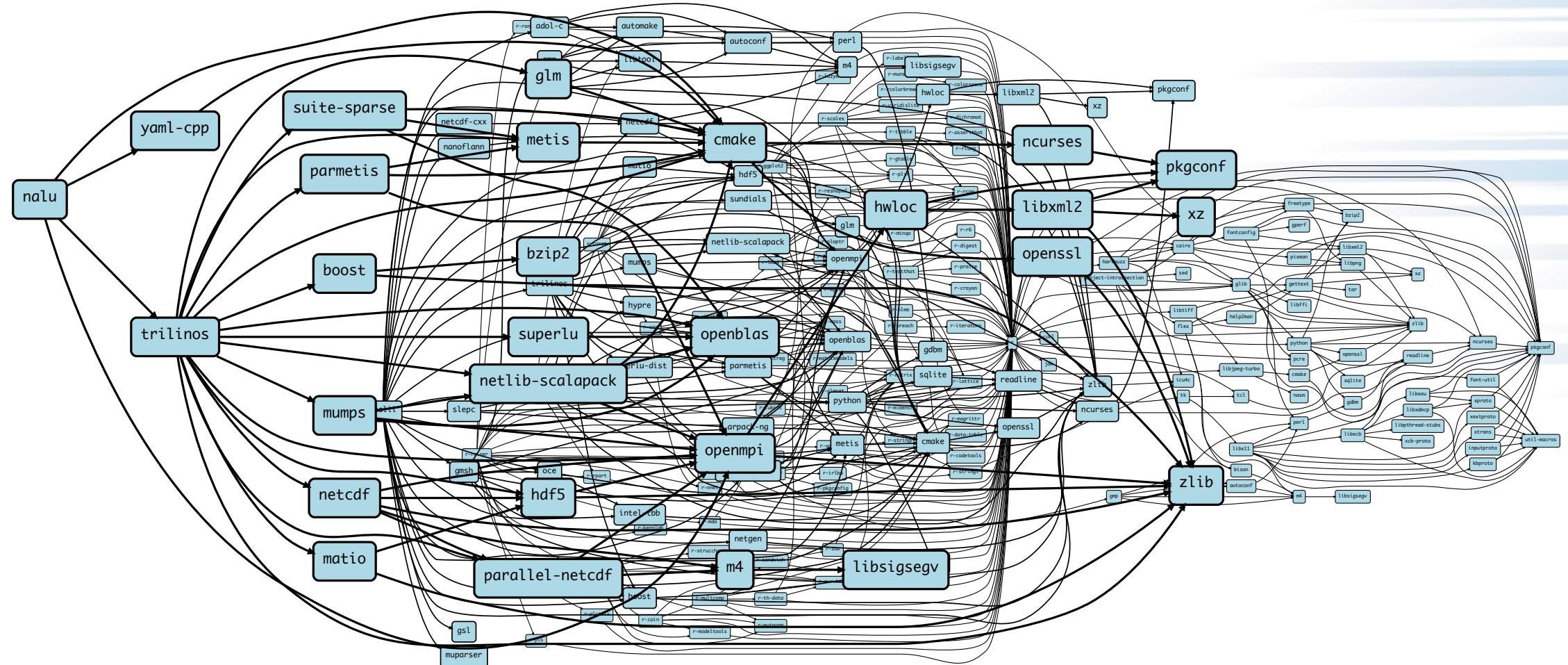
<https://e4s.io>

- 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

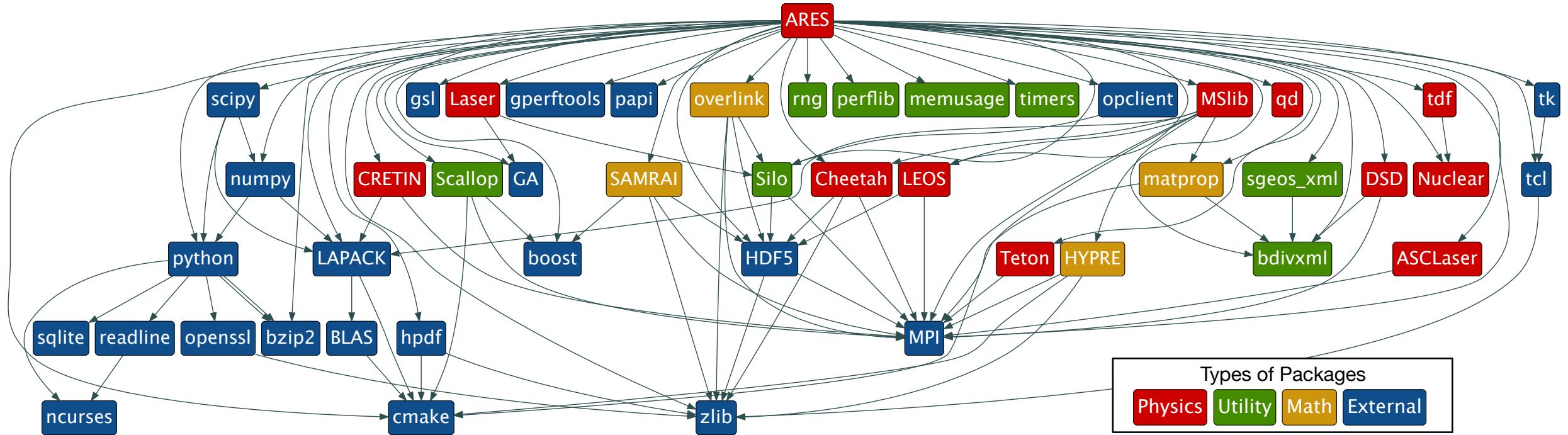
- E4S uses the Spack package manager for software delivery
- Spack provides the ability to specify versions of software packages that are and are not interoperable.
- Spack is a build layer for not only E4S software, but also a large collection of software tools and libraries outside of ECP ST.
- Spack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



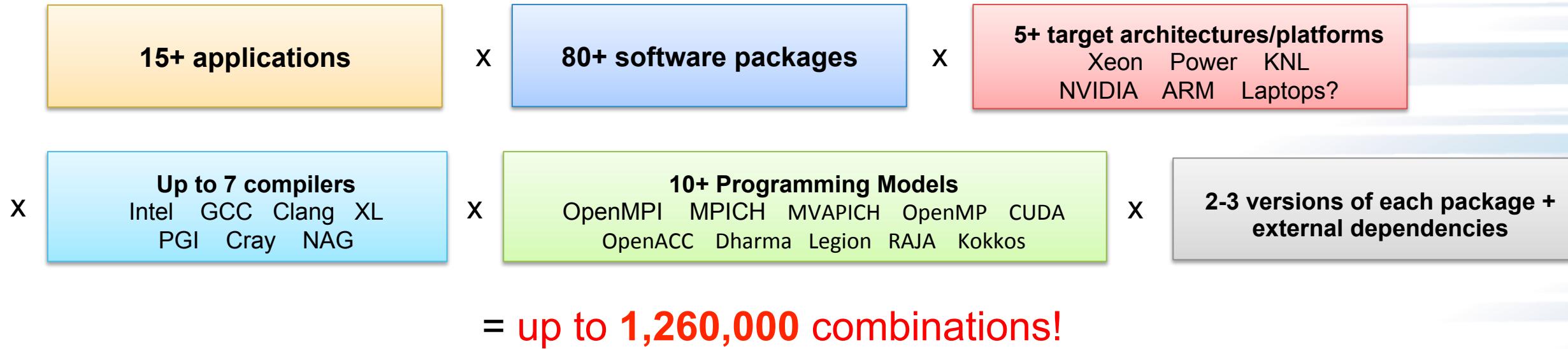
Nalu: Generalized Unstructured Meshes for Efficient Parallel Mapping and Flow

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**

卷之三

make install

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

20

make

install

Run code
Segmentation fault!?
Start over..



EXASCALE
COMPUTING
PROJECT

What about modules?

- Most supercomputers deploy some form of *environment modules*

- TCG modules (date back to 1995) and load (from TACC) are the most common

```
$ 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

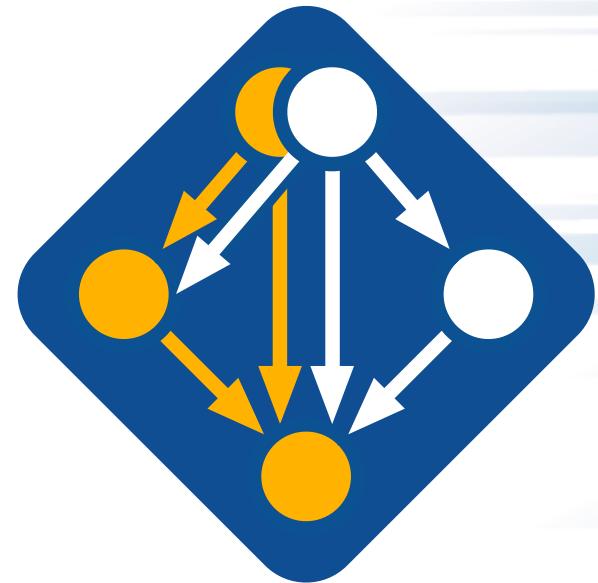
- How to install Spack (works out of the box):

```
$ 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



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-cdcfluview    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



github.com/spack/spack



@spackpm



Docker container of E4S

% docker pull exascaleproject/sdk:AHM19

- Using USB stick or images from <https://e4s.io>:
- % gunzip -c ect.tgz | docker load
% docker images
- Mount home directory:

% docker -i -v \$HOME:\$HOME -t exascaleproject/sdk:AHM19 /bin/bash

% which spack

% cp -r /usr/local/packages/ect/demo . ; cd demo; cat README

E4S Second Release (37+ ST products) exascaleproject/sdk:AHM19 (on Dockerhub)

```
1: adios :           adios@1.13.1 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/adios-1.13.1-v7jyzgyie7n542qppgoz2izthu6xeaj5
2: bolt :           bolt@1.0b1 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/bolt-1.0b1-jenaxkneyprxgq6abwaihlkuuoko4pwv
3: caliper :        caliper@1.8.0 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/caliper-1.8.0-lrmti32xdgycykh5vr5okrxtniv2pb5
4: darshan-runtime : darshan-runtime@3.1.6 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/darshan-runtime-3.1.6-yb2tk7rst4yclkluaixardes3slhgve
5: gasnet :          gasnet@1.30.0 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/gasnet-1.30.0-hp4d5xsbnhg5gisbkmgopd6pkqmgrcz0
6: globalarrays :   globalarrays@5.7 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/globalarrays-5.7-7zbsme3slnsmzkuzgq6ac4ggbndoakal
7: gotcha :          gotcha@develop /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/gotcha-develop-dcqzs3n36z73pqsm2d745rx5bzvr2hq
8: hdf5 :            hdf5@1.10.1 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/hdf5-1.10.1-jizgfu54nfiqzemokjopdyml3tov7md
9: hpctoolkit :    hpctoolkit@2017.06 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/hpctoolkit-2017.06-boqjpb7darhaysswp6p6w5skt5wa423
10: hypre :          hypre@2.13.0 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/hypre-2.13.0-3kjvf17rz3e7f6eoijvojyfegcwdl6ehb
11: geomp :          geomp@0.4.0 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/geomp-0.4.0-qhh04xnuyymvurjeuqjfml4u42b7a3t6
12: Jupyter :        /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/miniconda3-4.3.30-6hmm62lkf5v6n3fulsw3latyjy2phlba/bin/jupyter
12: kokkos :         kokkos@2.03.00 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/kokkos-2.03.00-a3ksyhg6fflnlufs5sfanqfwxeeeohey
13: legion :         legion@17.10.0 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/legion-17.10.0-cjomljrvcxzblznfc5luw6vwiubnyr
14: libquo :         libquo@1.3 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/libquo-1.3-cdtptdmouswpx5a4nvwxylld3u3mcj62
15: magma :          magma@2.4.0 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-4.8.5/magma-2.4.0-7cc275vlzmhypm5uuubj4krfsoqshhmr
16: mfem :           mfem@3.3.2 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0-mfem-3.3.2-sdrntzuhztzqphdl63b3ujmzy5ytb4g
17: mpich :          mpich@3.2.1 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/mpich-3.2.1-5j57f4j36vhcsxgn2pwdouz27qe4ij4
18: netcdf :         netcdf@4.4.1.1 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/netcdf-4.4.1.1-7vei7dnyaskclsuhpyr6wqdp4xjmdadx
19: openmpi :        openmpi@3.0.1 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/openmpi-3.0.1-hdjeffn2fs3iidk3whvv6smbrnmzqq3e
20: papi :           papi@5.5.1 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/papi-5.5.1-abkudkdzhua3p4lnn7m6ssj3or45fjri
21: papyrus :        papyrus@develop /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/papyrus-develop-77k6v4izzvjx222zbrpiexka7fmjsjgr
22: paraview :       paraview@5.4.1 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/paraview-5.4.1-qxvvvn5qs435z25jefz2ijlhoivd3f4
23: petsc :          petsc@3.8.4 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/petsc-3.8.4-7naeokjkinftmkcngpcn736bvnrndl
24: pdt :            pdt@3.25 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/pdt-3.25-fjjddrbx7lx4hrmqfwssq4oz46zvj5p
25: qthreads :       qthreads@1.12 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/qthreads-1.12-npkx43id5wewkrbsv6qpr76qisoozbpu
26: raja :           raja@0.5.3 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/raja-0.5.3-zrjr35xwjrfz6wacs4k36ilwc45m6gq6
27: scr :            scr@1.2.2 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/scr-1.2.2-fdqkevg2nf6yedg4qhwersf6ojwikxqz
28: spack :          /usr/local/packages/ecp/spack/bin/spack
28: strumpack :     strumpack@3.1.1 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/strumpack-3.1.1-q4wwcyff7lzzrbwc6np5jxezv6iix7ig
29: sundials :       sundials@3.1.0 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/sundials-3.1.0-xrqsfvumk2jw7aqidjsj7lya4w5kqm3p
30: sz :             sz@1.4.12.3 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/sz-1.4.12.3-dgykqp27gsnnyc2ktm6rn6bfgxwq7vq
31: tasmanian :     tasmanian@6.0 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/tasmanian-6.0-fv7z3ninw7agbvlw2jhau2hyx5ofyt4k
32: tau :            tau@2.28 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/tau-2.28-2zm23cf4lu74wfp2ufrzo7bu22popu4x
33: trilinos :      trilinos@12.12.1 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/trilinos-12.12.1-kobl2zztgzckmx5tktvmyradjt6qym7
34: vtkm :           vtkm@1.1.0 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/vtkm-1.1.0-rze7qodn6y6pbvuv15hw7pyekuqtuit
35: umpire :         umpire@master /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/umpire-master-4bditlkgpbzunpnnsnshpf3poxthmadefq
36: unifycr :        unifycr@master /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/unifycr-master-kmxew2he475aeh4jc3edhi4nbsywpekl
37: zfp :            zfp@0.5.0 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/zfp-0.5.0-bqeuj3eeiodsoknvtmqakstg3hp3zav
```

Extreme-scale Scientific Software Stack (E4S)

<https://e4s.io>

- Containers for HPC that include ECP ST products.

```
3. ssh
-- linux-centos7-x86_64 / gcc@4.8.5 --
autoconf@2.69    cuda@9.1.85    gmp@6.1.2      kokkos@2.03.00   libxml2@2.9.4    mpich@3.2.1     openssl@1.0.2n  readline@7.0
automake@1.15.1  flex@2.6.4     help2man@1.47.4  libpciaccess@0.13.5 m4@1.4.18       ncurses@6.0     papi@5.5.1      tar@1.29
bison@3.0.4     gcc@7.3.0     hwloc@1.11.9    libsigsegv@2.11  magma@2.4.0     numactl@2.0.11  pdt@3.25       util-macros@1.19.1
bzip2@1.0.6     gdbm@1.14.1   hwloc@2.0.1     libtool@2.4.6    mpc@1.1.0      openblas@0.2.20  perl@5.24.1   xz@5.2.3
cmake@3.11.1    gettext@0.19.8.1  isl@0.19      libunwind@1.1    mpfr@4.0.1     openmpi@3.0.1    pkgconf@1.4.0   zlib@1.2.11

-- linux-centos7-x86_64 / gcc@7.3.0 --
adios@1.13.1    freetype@2.7.1   json@0.13.1    libfixes@5.0.2   papi@5.5.1      py-mccabe@0.6.1  sqlite@3.22.0
adlbx@0.8.0     gasnet@1.30.0   kbproto@1.0.7   libxml2@2.9.4    papyrus@develop  py-mock@2.0.0   stc@0.7.3
adlbx@0.8.0     gasnet@1.30.0   kokkos@2.03.00  libshmfc@1.2    paraview@5.4.1   py-mpi4py@3.0.0  strumpack@3.1.1
ant@1.9.9       gdb@8.0.1     kvtree@1.0.2    libxt@1.1.5     parmetis@4.0.3   py-natsort@5.2.0 suite-sparse@5.2.0
autoconf@2.69   gdbm@1.14.1   lcms@2.8      libxv@1.0.10   patch@2.7.6     py-nose@1.3.7   sundials@3.1.0
automake@1.14   geopm@0.4.0   legion@17.10.0  libxvmc@1.0.9   pcre@8.41      py-numexpr@2.6.1 superlu@5.2.1
automake@1.15.1 gettext@0.19.8.1  leveldb@1.20   libyogrt@1.20-6 pcre@8.41      py-numpy@1.13.3 superlu-dist@5.2.2
axl@0.1.1       git@2.15.1    libarchive@3.3.2  lmod@7.7.13    pdsh@2.31      py-pandas@0.21.1 swig@3.0.12
binutils@2.27   glib@2.56.0   libbsd@0.8.6    lua@5.3.4     pdt@3.25      py-pbr@3.1.1    sz@1.4.12.3
binutils@2.29.1 glm@0.9.7.1   libcircle@0.2.1-rc.1  lua-luafilesystem@1_6.3 perl@5.24.1   py-pillow@3.2.0 tar@1.29
bison@3.0.4     globalarrays@5.7  libedit@3.1-20170329  lua-luaposix@33.4.0 petsc@3.8.4    py-pkgconfig@1.2.2 tasmanian@6.0
bolt@1.0b1      glproto@1.4.17  libffi@3.2.1    lwgrp@1.0.2    pflotran@xsdk-0.3.0 py-py@1.4.33   tau@2.28
boost@1.66.0    gmp@6.1.2     libice@1.0.9    lz4@1.8.1.2   pixman@0.34.0   py-pycodestyle@2.3.1 tcl@8.6.8
boost@1.66.0    gobject-introspection@1.49.2 libiconv@1.15   lzma@4.32.7   pkgconf@1.4.0   py-pyflakes@1.6.0 texinfo@6.5
boost@1.68.0    gotcha@0.0.2   libjpeg-turbo@1.5.3  lzo@2.09    presentproto@1.0  py-pyparsing@2.2.0 tk@8.6.8
bzip2@1.0.6     gotcha@develop  libmng@2.0.3    m4@1.4.18    protobuf@3.5.1.1 py-pytable@3.3.0 trilinos@12.12.1
c-blosc@1.12.1 gperf@3.0.4   libpciaccess@0.13.5  matio@1.5.9   py-argparse@1.4.0 py-pytest@3.6.0 turbine@1.0.0
cairo@1.14.12   harfbuzz@1.4.6   libpfm4@4.8.0   metis@5.1.0   py-babel@2.4.0   py-pytz@2017.2 turbine@1.0.0
caliper@1.8.0   hdf5@1.8.19   libpng@1.6.34   mfem@3.3.2   py-bottleneck@1.0.0 py-scipy@1.0.0  umpire@master
cmake@3.11.1   hdf5@1.8.19   libpthread-stubs@0.4 miniconda2@4.3.30 py-configparser@3.5.0 py-setupools@39.0.1 unifycr@master
conduit@master  hdf5@1.10.1   libquo@1.3     miniconda3@4.3.30 py-cycler@0.10.0 py-six@1.11.0  util-macros@1.19.1
curl@7.59.0    hdf5@1.10.1   libsigsegv@2.11  mpich@3.2.1   py-cython@0.28.1 py-subprocess32@3.2.7 veloc@1.0
damageproto@1.2.1 hdf5@1.10.1   libsm@1.2.2    mumps@5.1.1   py-dateutil@2.5.2 python@2.7.14  videoproto@2.3.3
darshan-runtime@3.1.6 hdf5@1.10.1   libtiff@4.0.6   nasm@2.13.03  py-enum34@1.1.6 qhull@2015.2 vtkm@master
darshan-util@3.1.6 help2man@1.47.4   libtiff@4.0.8   ncurses@6.0   py-flake8@3.5.0 qthreads@1.12 vtkm@1.1.0
doxygen@1.8.12  hpctoolkit@2017.06 libtool@2.4     netcdf@4.4.1.1 py-funcsigs@0.4 r@3.4.3  xcb-proto@1.13
dtcmp@1.1.0     hpctoolkit-externals@2017.06 libtool@2.4.2   netlib-scalapack@2.0.2 py-functools32@3.2.3-2 raja@0.5.3  xextproto@7.3.0
er@0.0.3        hwloc@1.11.9   libtool@2.4.6   nettle@3.3    py-h5py@2.7.1   rankstr@0.0.2  xproto@7.0.31
exmcutils@0.5.3 hwloc@2.0.1     libunwind@1.1   ninja@1.8.2   py-hypothesis@3.7.0 readline@7.0
expat@2.2.2     hypre@2.13.0   libx11@1.6.5   numactl@2.0.11 py-jinja2@2.9.6 redset@0.0.3  xtrans@1.3.5
fftw@3.3.7      hypre@2.13.0   libxau@1.0.8   openblas@0.2.20 py-kiwisolver@1.0.1 ruby@2.2.0  xz@5.2.3
fixesproto@5.0   icu4c@60.1    libxcb@1.13    openmpi@3.0.1   py-lit@0.5.0   ruby-ronn@0.7.3 zfp@0.5.0
flex@2.6.4      inputproto@2.3.2  libxdamage@1.1.4 opensl@1.0.2n  py-mako@1.0.4   scr@1.2.2   zsh@5.4.2
font-util@1.3.1 intel-tbb@2018.2  libxdmcp@1.1.2  oftf2@2.1    py-markupsafe@1.0 shuffle@0.0.3  zstd@1.3.0
fontconfig@2.12.3 jdk@8u141-b15   libxext@1.3.3  pango@1.41.0  py-matplotlib@2.2.2 snappy@1.1.7
```

Extreme-scale Scientific Software Stack (E4S)

<https://e4s.io>

```
3. ssh
% cd `spack location -i trilinos`/lib
% ls *.so*1
libamesos2.so.12.12.1      libkokkoscore.so.12.12.1
libamesos.so.12.12.1        libkokkoskernels.so.12.12.1
libanasaziepetra.so.12.12.1 libkokkostsqr.so.12.12.1
libanasazi.so.12.12.1       liblocaepetra.so.12.12.1
libanasazitpetra.so.12.12.1 liblocalapack.so.12.12.1
libaprepro_lib.so.12.12.1   libloca.so.12.12.1
libaztecoo.so.12.12.1       liblocathra.so.12.12.1
libbelosepetra.so.12.12.1  libmapvarlib.so.12.12.1
libbelos.so.12.12.1         libml.so.12.12.1
libbelostpetra.so.12.12.1  libModeLaplace.so.12.12.1
libchaco.so.12.12.1         libmuelu-adapters.so.12.12.1
libepetraext.so.12.12.1    libmuelu-interface.so.12.12.1
libepetra.so.12.12.1         libmuelu.so.12.12.1
libexodus_for.so.12.12.1   libnemesis.so.12.12.1
libexodus.so.12.12.1        libnoxepetra.so.12.12.1
libexoIIv2for32.so.12.12.1 libnoxlapack.so.12.12.1
libgaleri-epetra.so.12.12.1 libnox.so.12.12.1
libgaleri-xpetra.so.12.12.1 libpamgen_extras.so.12.12.1
libgtest.so.12.12.1         libpamgen.so.12.12.1
libifpack2-adapters.so.12.12.1 librtop.so.12.12.1
libifpack2.so.12.12.1       libsacado.so.12.12.1
libifpack.so.12.12.1        libshyLU.so.12.12.1
libIoexo_fac.so.12.12.1   libstk_expreval.so.12.12.1
libIoex.so.12.12.1          libstk_search.so.12.12.1
libIofx.so.12.12.1          libstk_topology.so.12.12.1
libIogn.so.12.12.1          libstk_transfer_impl.so.12.12.1
libIohb.so.12.12.1          libstk_util_diag.so.12.12.1
lib_info_lib.so.12.12.1    libstk_util_env.so.12.12.1
libIonit.so.12.12.1         libstk_util_parallel.so.12.12.1
libIopg.so.12.12.1          libstk_util_registry.so.12.12.1
libIopx.so.12.12.1          libstk_util_use_cases.so.12.12.1
libIoss.so.12.12.1          libstk_util_util.so.12.12.1
libIotr.so.12.12.1          libstokhos_amesos2.so.12.12.1
libIovs.so.12.12.1          libstokhos_ifpack2.so.12.12.1
libisorropia.so.12.12.1    libstokhos_muelu.so.12.12.1
libkoksalgorithms.so.12.12.1 libstokhos_sacado.so.12.12.1
libkoksalgorithms.so.12.12.1 libstokhos.so.12.12.1
% 
```

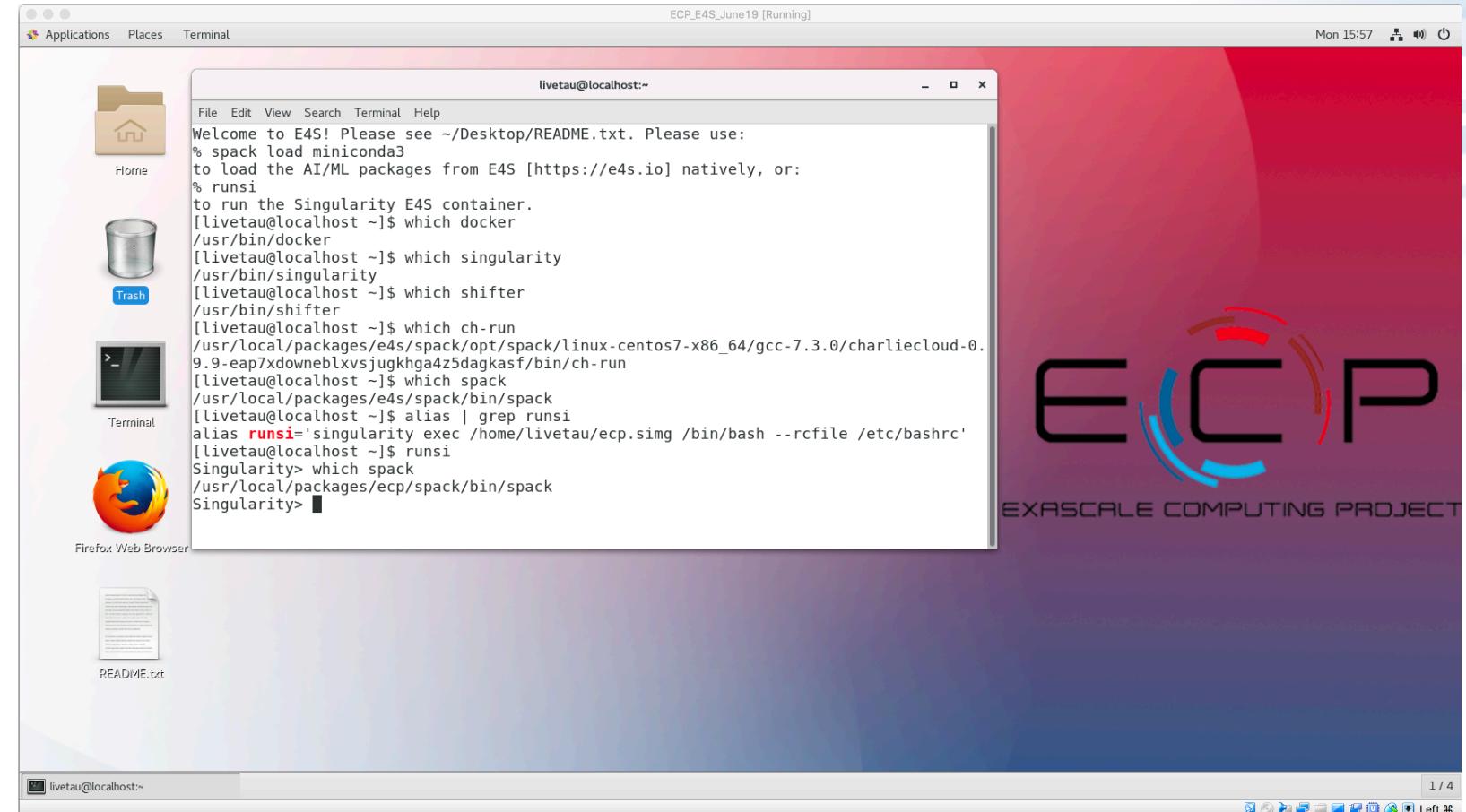
Running MPI applications on other systems

- 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!

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: ****



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'
```

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

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