



E4S: Extreme-Scale Scientific Software Stack

<https://e4s.io>

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Extreme-Scale Scientific Software Stack (E4S)

<https://e4s.io>

- Spack [<http://spack.io>] is the primary means for software delivery
- SDKs
- Containers for HPC that include ECP ST products.
- Container runtimes supported
 - Docker
 - Dockerhub: [exascaleproject/sdk:AHM19](https://hub.docker.com/r/exascaleproject/sdk/AHM19)
 - Charliecloud
 - Shifter
 - Singularity
- VirtualBox Open Virtualization Appliance (OVA) image that contains these runtimes
- MPI replacement strategies to use native network interconnect

Docker

% docker pull exascaleproject/sdk:AHM19

- Using USB stick or images from <http://e4s.io>:
- % cd /Volumes/ECP_SDK/Docker;
- % gunzip -c ecp.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/ecp/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-lrmti32xdgyckyh5vr5okrxtniv2pb5
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-cdtptdmouswp5a4nvwxylld3u3mcj62
15: magma :          magma@2.4.0 /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-4.8.5/magma-2.4.0-7cc275vlzmhypm5uuubj4krfsqshhmr
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-rze7qodn6y6pbvuv15hw7pyekuqtui
35: umpire :          umpire@master /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/umpire-master-4bditlgpbuznpnshpf3poxthmadefq
36: unifycr :         unifycr@master /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/unifycr-master-kmxew2he475saeh4jc3edhi4nbsywpekl
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-bqeuj73eeiodsoknvtmqakstg3hp3zav
```

Extreme-Scale Scientific Software Stack (E4S)

<http://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 openssl@1.0.2n  py-mako@1.0.4   scr@1.2.2   zlib@1.2.11
font-util@1.3.1 intel-tbb@2018.2  libxdmcp@1.1.2  oftf2@2.1    py-markupsafe@1.0 snappy@1.1.7   zsh@5.4.2
fontconfig@2.12.3 jdk@8u141-b15   libxext@1.3.3  pango@1.41.0  py-matplotlib@2.2.2
```

Extreme-Scale Scientific Software Stack (E4S)

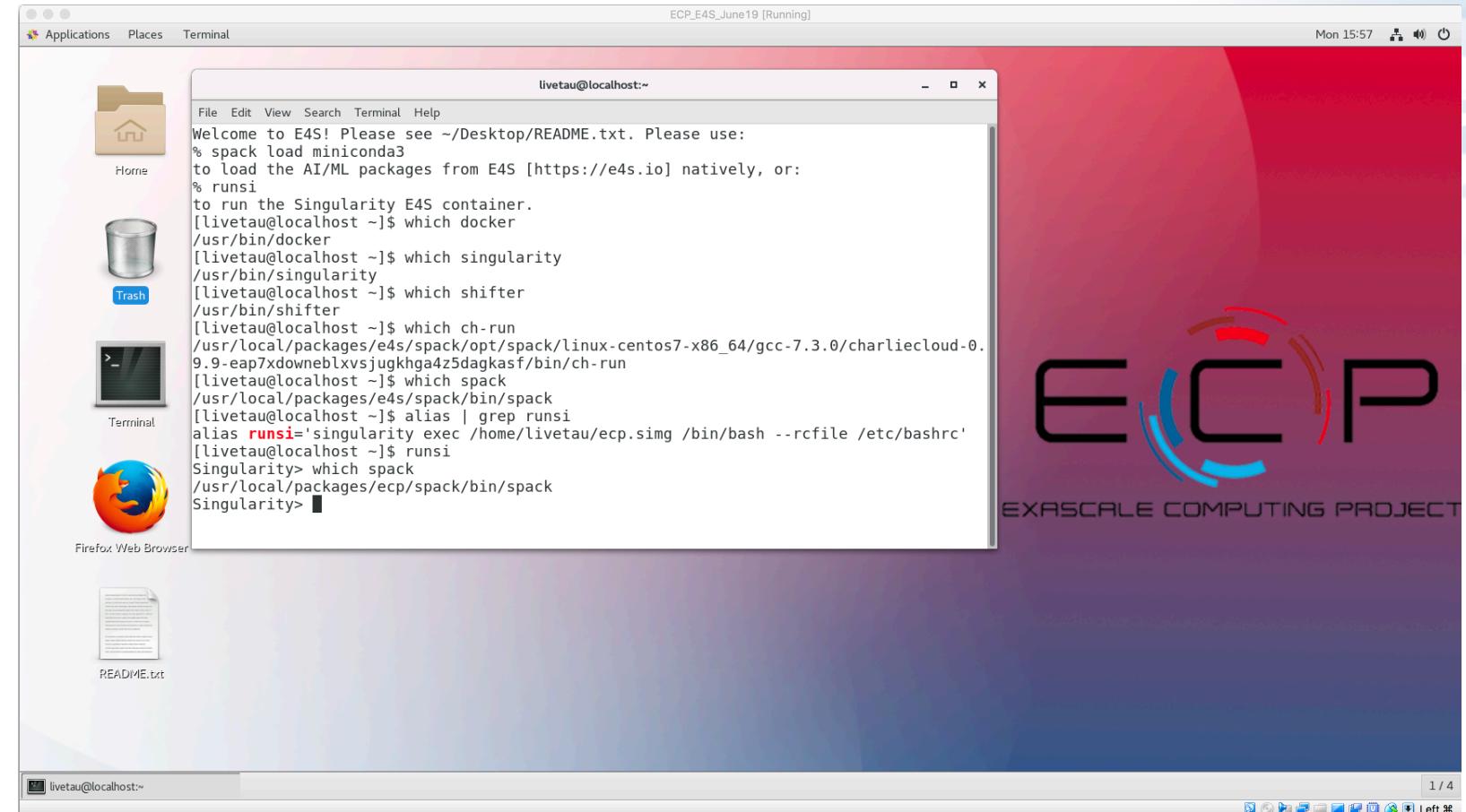
<http://e4s.io>

```
% 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   libModelLaplace.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
libInfo_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
libkokosalgorithms.so.12.12.1   libstokhos_sacado.so.12.12.1
libkokoscontainers.so.12.12.1  libstokhos.so.12.12.1
%
3. ssh
```

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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