

HPC-BP Webinar: Extreme-scale Scientific Software Stack (E4S)

Wednesday, January 13th, 2021, 10am – 10:30am PT

ECP HPC-BP Webinar

<https://exascaleproject.zoomgov.com/j/1616523770>

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<https://e4s.io>



Challenges

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

E4S: Extreme-scale Scientific Software Stack

- Curated, Spack based software distribution
- Spack binary build caches for bare-metal installs
 - x86_64, ppc64le (IBM Power 9), and aarch64 (ARM64)
- Container images on DockerHub and E4S website of pre-built binaries of ECP ST products
- Base images and full featured containers (with GPU support)
- GitHub recipes for creating custom images from base images
- GitLab integration for building E4S images
- E4S validation test suite on GitHub
- E4S VirtualBox image with support for container runtimes
 - Docker
 - Singularity
 - Shifter
 - Charliecloud
- AWS and GCP images to deploy E4S

<https://e4s.io>

Extreme-scale Scientific Software Stack (E4S)

- E4S: A Spack-based distribution of ECP ST and related and dependent software tested for interoperability and portability to multiple architectures
 - Provides distinction between SDK usability / general quality / community and deployment / testing goals
 - Will leverage and enhance SDK interoperability thrust
-
- Oct 2018: E4S 0.1 - 24 full, 24 partial release products
 - Jan 2019: E4S 0.2 - 37 full, 10 partial release products
 - Nov 2019: E4S 1.0 - 50 full, 5 partial release products
 - Jan 2020: E4S 1.1 – ppc64le and x86_64 release with 50 full (x86_64), 46 full (ppc64le) release products.
 - Nov. 2020: E4S 1.2 – ppc64le and x86_64 release each with 67 full release products.



<https://e4s.io>

Spack is a flexible package manager for HPC

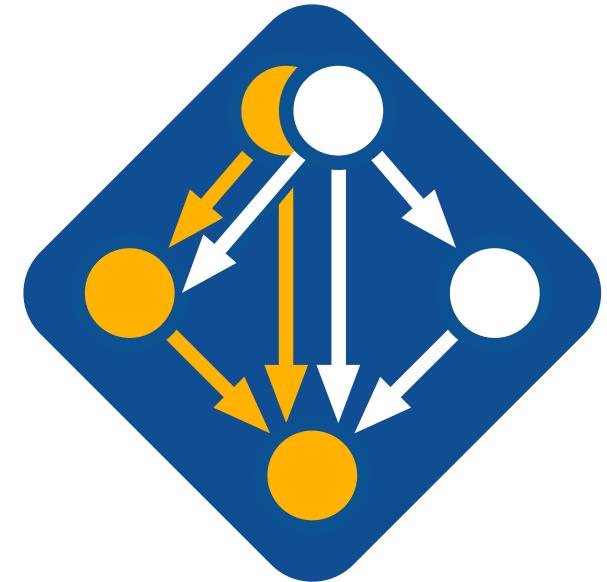
- How to install Spack (works out of the box):

```
$ git clone https://github.com/spack/spack
$ . spack/share/spack/setup-env.sh
```

- How to install a package:

```
$ spack install tau
```

- TAU and its dependencies are installed within the Spack directory.
- Unlike typical package managers, Spack can also install many variants of the same build.
 - Different compilers
 - Different MPI implementations
 - Different build options



Visit spack.io



github.com/spack/spack



@spackpm

Spack provides the *spec* syntax to describe custom configurations

```
$ spack install tau                                unconstrained  
$ spack install tau@2.29                            @ custom version  
$ spack install tau@2.29 %gcc@7.3.0               % custom compiler  
$ spack install tau@2.29 %gcc@7.3.0 +mpi+python+pthreads +/- build option  
$ spack install tau@2.29 %gcc@7.3.0 +mpi ^mvapich2@2.3~wrapperrpath ^ dependency information
```

- Each expression is a ***spec*** for a particular configuration
 - Each clause adds a constraint to the spec
 - Constraints are optional – specify only what you need.
 - Customize install on the command line!
- Spec syntax is recursive
 - Full control over the combinatorial build space

`spack find` shows what is installed

```
Singularity> spack find
==> 319 installed packages
-- linux-ubuntu18.04-power9le / gcc@7.3.0 -----
autoconf@2.69  diffutils@3.7  libiconv@1.16  m4@1.4.18
automake@1.16.2  findutils@4.6.0  libpciaccess@0.16  matio@1.5.17
boost@1.74.0  glm@0.9.7.1  libsigsegv@2.12  metis@5.1.0
bzip2@1.0.8  hdf5@1.10.7  libtool@2.4.6  mpich@3.2.1
cmake@3.18.4  hypre@2.20.0  libxml2@2.9.10  mumps@5.3.3
cups@2.3.0  libcurl@7.68.0  libedit@3.1.20  ncurses@6.2
curl@7.72.0  libgcc@10.2.0  libiconv@1.16  netcdf-c@4.7.4
curlpp@0.12.0  libgccxml@0.9.9  libltdl@2.4.0  netlib-scalapack@2.1.0
curlxx@0.12.0  libgfortran@8.1.0  libmpc@3.1.0  openssl@1.1.1g
curlxx@0.12.0  libgccxml@0.9.9  libmpc++@3.1.0  parmetis@4.0.3
curlxx@0.12.0  libgfortran@8.1.0  libmpfr@4.0.2  perl@5.26.1
curlxx@0.12.0  libgccxml@0.9.9  libquadmath@3.1.0  pkgconf@1.7.3
curlxx@0.12.0  libgfortran@8.1.0  libstdc++@9.3.0  suite-sparse@5.7.2
curlxx@0.12.0  libgccxml@0.9.9  libunwind@1.4.0  openblas@0.3.10
curlxx@0.12.0  libgfortran@8.1.0  libxml2@2.9.10  texinfo@6.5
curlxx@0.12.0  libgccxml@0.9.9  libxmlsec@1.8.10  trilinos@13.0.0
curlxx@0.12.0  libgfortran@8.1.0  libxerces-c@3.2.3  util-macros@1.19.1
curlxx@0.12.0  libgccxml@0.9.9  libxmlsec@1.8.10  xz@5.2.5
curlxx@0.12.0  libgfortran@8.1.0  libxmlsec@1.8.10  zlib@1.2.11
-- linux-ubuntu18.04-ppc64le / gcc@7.3.0 -----
adiak@0.1.1  flit@2.1.0  libpfm4@4.11.0
adios@1.13.1  gasnet@2020.3.0  libpng@1.6.37
adios2@2.6.0  gasnet@2020.3.0  libpthread-stubs@0.4
adlbox@0.9.2  gdbm@1.18.1  libquo@1.3.1
aml@0.1.0  gettext@0.20.2  libsigsegv@2.12
amrex@20.10  gettext@0.21  libsodium@1.0.18
arborx@0.9-beta  ginkgo@1.3.0  libtool@2.4.6
argobots@1.0  git@2.28.0  libunistring@0.9.10
arpack-ng@3.7.0  git@2.28.0  libunwind@1.4.0
ascent@develop  glm@0.9.7.1  libunwind@1.4.0
autoconf@2.69  globalarrays@5.7
automake@1.16.2  gmake@4.2.1  libxml2@2.9.10
axl@0.3.0  gmp@6.1.2  libyogrt@1.24
axom@0.3.3  googletest@1.10.0  libzmq@4.3.2
bash@5.0  gotcha@0.0.2  lmod@8.3
binutils@2.33.1  gotcha@1.0.3  lua@5.3.5
bmi@develop  gperftools@2.7  lua-luafsystem@1_7_0_2
bolt@1.0  hdf5@1.8.21  lua-luaposix@33.4.0
boost@1.73.0  hdf5@1.8.21  lwgrp@1.0.3
boost@1.73.0  hdf5@1.10.6  lz4@1.9.2
boost@1.73.0  hdf5@1.10.6  lzo@2.10
boost@1.73.0  hptoolkit@2020.08.03  m4@1.4.18
butterflypack@1.2.0  hpx@1.5.1  magma@2.5.4
bzip2@1.0.8  hwloc@1.11.11  margo@0.4.3
c-blosc@1.17.0  hwloc@2.2.0  matio@1.5.17
caliper@2.4.0  hypre@2.18.2  mbedtls@2.16.7
cinch@master  hypre@2.20.0  mercury@1.0.1
cmake@3.17.3  intel-tbb@2020.3  mercury@1.0.1
conduit@master  kokkos@3.2.00  metis@5.1.0
conduit@master  kokkos-kernels@3.2.00  mfem@4.1.0
cuda@10.2.89  kvtree@1.0.2  mpark-variant@1.4.0
curl@7.72.0  legion@20.03.0  mpich@3.2.1
darshan-runtime@3.2.1  leveldb@1.22  mpifileutils@develop
da... Snapz Pro X 3.2.1  libarchive@3.4.1  mumps@5.3.3
di... ...  libbsd@0.10.0  ncurses@6.2
papyrus@develop  py-more-itertools@7.2.0
parallel-netcdf@1.12.1  py-mpi4py@3.0.3
parmetis@4.0.3  py-nbclient@0.5.0
pcre@8.44  py-nbconvert@6.0.1
pcre2@10.35  py-nbformat@5.0.7
pdsh@2.31  py-nest-asyncio@1.4.0
pdt@3.25.1  py-notebook@6.1.4
perl@5.26.1  py-numumpy@1.19.2
petsc@3.13.6  py-oauthlib@3.1.0
petsc@3.14.0  py-pamela@1.0.0
pkgconf@1.7.3  py-pandocfilters@1.4.2
plasma@20.9.20  py-parso@0.6.1
precice@2.1.1  py-petsc4py@3.13.0
pumi@2.2.2  py-pexpect@4.7.0
py-alembic@1.0.7  py-pickleshare@0.7.5
py-argon2-cffi@20.1.0  py-prometheus-client@0.7.1
py-asn1crypto@0.24.0  py-prompt-toolkit@2.0.9
py-async-generator@1.10  py-psutil@5.7.2
py-attrs@19.3.0  py-ptyprocess@0.6.0
py-babel@2.7.0  py-py@1.8.0
py-backcall@0.1.0  py-pycparser@2.20
py-bleach@3.1.0  py-pyelftools@0.26
py-blinker@1.4  py-pygments@2.6.1
py-certifier@2020.6.20  py-pyjwt@1.7.1
py-certipy@0.1.3  py-pyopenssl@19.0.0
py-cffi@1.14.3  py-pyrsistent@0.15.7
py-chardet@3.0.4  py-pytest-runner@5.1
py-cryptography@2.7  py-python-dateutil@2.8.0
py-cython@0.29.21  py-python-editor@1.0.4
py-decorator@4.4.2  py-python-oauth2@1.1.1
py-defusedxml@0.6.0  py-pytz@2020.1
py-entrypoints@0.3  py-pyzmq@18.1.0
py-idna@2.8  py-requests@2.24.0
py-importlib-metadata@2.0.0  py-send2trash@1.5.0
py-ipypkg@5.3.4  py-setuptools@50.1.0
py-ipypkg@5.3.4  util-macros@1.19.1
```

All the versions coexist!

- Multiple versions of same package are ok.

Packages are installed to automatically find correct dependencies.

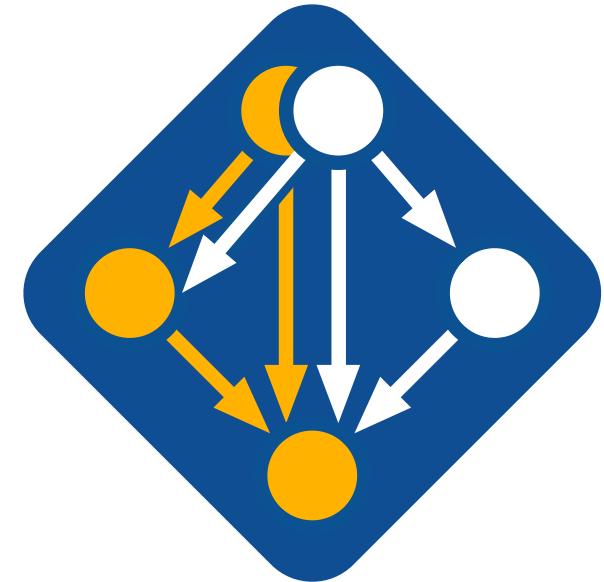
Binaries work *regardless of user's environment*.

Spack also generates module files.

- Don't have to use them.

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

Download E4S v1.2 GPU Container Image

The screenshot shows a web browser window with the URL <https://e4s-project.github.io/download.html>. The page displays a list of Docker container images for E4S v1.2, categorized by host system (RHEL 7, Ubuntu 18.04, CentOS 7) and spack configuration (SPACK MINIMAL, E4S COMPREHENSIVE, CUSTOM). The Ubuntu 18.04 section includes a note about x86_64 and ppc64le versions. A blue box highlights the x86_64 version entry.

Host System	Spack Configuration	Docker Image	Notes
RHEL 7	SPACK MINIMAL	ecpe4s/rhel7-spack	
	E4S COMPREHENSIVE	ecpe4s/rhel7-e4s	
	CUSTOM	ecpe4s/superlu_sc	
Ubuntu 18.04	SPACK MINIMAL	ecpe4s/ubuntu18.04-spack	
	E4S GPU IMAGE	ecpe4s/ubuntu18.04-e4s-gpu	x86_64 version: CUDA and ROCM ppc64le version: CUDA
	E4S COMPREHENSIVE	ecpe4s/ubuntu18.04-e4s	
	SPACK MINIMAL	ecpe4s/ubuntu18.04-spack	
CentOS 7	SPACK MINIMAL	ecpe4s/centos7-spack	
	E4S COMPREHENSIVE	ecpe4s/centos7-e4s	
CUSTOM	SPACK MINIMAL	ecpe4s/centos7-spack	

E4S v1.2 GPU Release for x86_64

```
1: adios2      /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/adios2-2.6.0-nkp24j7enorn3dt7626chuqm3pbkrvfe
2: aml        /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/aml-0.1.0-3mwyb6cf6ervfnruqb5u33v46buyqth
3: arborx     /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/arborx-0.9-beta-qjzxllkgcplto6pnjpwejoh5xpoik3adr
4: argobots   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/argobots-1.0-yoafg2slps7kp4dkmb6pzu5z2a37sgs4
5: ascent     /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/ascent-develop-ciwgq6lh6unw3hjsnu47wr7cpqptqgy
6: axom       /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/axom-0.3.3-tzyejxpy3p3ekaev35k2bhpk74cnuhh
7: bolt        /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/bolt-1.0-uxku5w5qdfnpa4atgzcbraq7wop7lunc
8: caliper    /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/caliper-2.4.0-lfdx3gc6qodg2abbpovib3thdsmsamnn
9: darshan-runtime /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/darshan-runtime-3.2.1-jquggxx2uunyaduo3owhd2snves6mlr
10: dyninst   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/dyninst-10.2.1-xad3v6rvosm6qfa5fc7d4nn3svtzf
11: faodel     /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/faodel-1.1906.1-ijilel2vjionmj56mscckw2hpecfsuy
12: flecsi     /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/flecsi-1-c7sevln2ak4pf2jgq6wh3mwictch5l2
13: flit        /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/flit-2.1.0-yvvog7kmax22ei2yyrwdxj3heinmz5am
14: gasnet     /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/gasnet-2020.3.0-ufrq5hym67eq3jsg4jtttjjqgo4i6hnq
15: ginkgo     /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/ginkgo-1.2.0-r6lorgchpr5qrcwyqqxtewdhtpi4rmt
16: globalarrays /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/globalarrays-5.7-bow6d32j63j6gusotzjuityznwqv64b
17: gotcha     /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/gotcha-1.0.3-7n7bjnzsfn5w5tnihok3otbaedhjmu
18: hdf5        /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/hdf5-1.10.6-k74avubedd5knvnlc73dr3ib5oyw6bcwn
19: hpctoolkit  /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/hpctoolkit-2020.08.03-wck4g3h3jhfvzxorelxqunbe3xesry
20: hpx         /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/hpx-1.5.0-pynmocntkmuwkowy05jxtycvg34w6kue
21: hypre       /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/hypre-2.19.0-vqo72wn6ei7ruitpg7drkje2rdbdfguo
22: kokkos     /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/kokkos-3.2.00-pqv3uugd6cv3qftyur3rx6dm2gao2tg3
23: kokkos-kernels /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/kokkos-kernels-3.1.00-y4veufyptworlbehxusg4yzh6n7anhp
24: legion      /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/legion-20.03.0-zkbz7h2wuze4dgbwcbc04w5fvqltugmog
25: libnrm      /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/libnrm-0.1.0-kp5jb7o4kow25rnggiditwtmdbeebojs
26: libquo      /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/libquo-1.3.1-w45wcw6dqbiajeeaj3ryaeskk7bzx6
27: magma        /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/magma-2.5.3-yksxthffslhjrhzwgcx7smz2tca6ojfn
28: mercury     /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/mercury-1.0.1-ppledtsr3drk2upciytfusuawfxrtjp73q
29: mfem         /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/mfem-4.1.0-kivaike2qintplgufwp5yf2mj3n36ay3
30: mpich        /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/mpich-3.2.1-kgwtpelzbokrvg24ct6padfbhw7nene
31: mpifileutils /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/mpifileutils-develop-djje5g7ts55g3yic3bms426c2zi7gqsj
32: ninja        /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/ninja-1.10.1-7zbbtuslw25nmqo4ur6abyyf3tchnqv
33: omega-h     /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/omega-h-9.29.0-eln73w7ytpvgqtkmkqyjm4gsabsu2w4p
```

- 67 ECP ST products
- Ubuntu v18.04 x86_64
- AI/ML package support
 - TensorFlow 2.3.5
 - PyTorch 1.8
 - Horovod
- Support for GPUs
 - AMD ROCm 3.8
 - NVIDIA CUDA 10.2, 11
- Kokkos with support for AMD GPUs!

E4S v1.2 GPU Release for x86_64

```
34: openpmd-api      /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/openpmd-api-0.12.0-4myph6pbjnupgupxdlvbxvqqeqx6atyp
35: openmpi         /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/openmpi-3.1.6-6yqtoym56as6xso2pdgkmn4bcsoyufku
36: papi            /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/papi-6.0.0.1-gorrfrvrik575lldzgq46qmmu63kxl7x
37: papyrus         /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/papyrus-develop-iu3dgpwwyykgv5mpw2dwcr0l4wbwbai
38: parallel-netcdf   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/parallel-netcdf-1.12.1-tmmkzibn43xr7su76msxxusyzrphdt5
39: pdt              /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/pdt-3.25.1-kvi5wuu5y72fypijti3nxqvdn7zpj6ni
40: petsc            /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/petsc-3.13.4-llg3u4rrt5axrqlim75tt73epewxu4fb
41: plasma           /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/plasma-19.8.1-tji7bojb5ne5hqj2mwn5bqq2tfkm23ke
42: precice          /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/precice-2.1.0-ozdmbat2hlivccha3nklbeahikgynewu
43: pumi             /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/pumi-2.2.2-52czdbxeg7pmjkd55nub5jgxzodcprh
44: py-jupyterhub     /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/py-jupyterhub-1.0.0-tr3wcolaij3kbzb6xm4mbbvakcstwsw3
45: py-libensemble    /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/py-libensemble-0.7.0-mxvqxhiiblqnmlfepbxboyiskqyvbej
46: qthreads          /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/qthreads-1.14-neshsclplh7ttkebm34grztaijqohnxt
47: raja              /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/raja-0.11.0-w25bj2dys6cjqn7isgcjfyvte3tuulev
48: rempi             /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/rempi-1.1.0-sideqdbiik2yseshs3loh4sictbis3t6
49: scr               /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/scr-2.0.0-yh3chyq5gayuk6r4juejjiye6zg3rh3u
50: slate             /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/slate-develop-jnysy2rh5vxhwua5ubtvq4bsfd3py7d5
51: slepc             /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/slepc-3.13.4-q3lalpbqoshiyvjgrnhb2iqiisvnfrp
52: strumpack         /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/strumpack-4.0.0-rlbti5eqc5rjhfisxv2uxevj6m3fn5gg
53: sundials          /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/sundials-5.3.0-3g52gh4a6h4ohucqart5i4m6pi66woj6
54: superlu-dist     /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/superlu-dist-6.3.1-o2hkund66coxn2rrbtlalda2vq35uu7j
55: stc               /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/stc-0.8.3-oxfik7nsmgufoqyy7xilzsRCT7it63ej
56: swig              /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/swig-4.0.1-htxmzjd5sed5yfibw6j7jn5cx6p7g72x
57: sz   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/sz-2.1.9-tcatyiuzh6quctrqd2g3dcli7xa7gvtj
58: tasmanian         /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/tasmanian-7.1-quo3grs5kb2xrvjufpi7vn66cpjfnav
59: tau               /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/tau-2.29-ijw2nbphmlfkt42ubwz7g5a5yru22ikn
60: trilinos          /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/trilinos-13.0.0-6xfnp44g5xm7gpn2en6gkwzfceykdir3x
61: turbine            /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/turbine-1.2.3-q4qjvgxjl3cbuyquo6zrurb4mwf6wkp
62: umap              /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/umap-2.0.0-5tob3exzrmwoitudu5pstbb2dms3xnto
63: umpire            /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/umpire-3.0.0-6woo2uvazcucxikc6xad6g3zksu2ygi
64: unifyfs           /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/unifyfs-0.9.0-be7mqbng7kdeewdlgvldhm4jkxnquiil
65: upcxx              /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/upcxx-2020.3.0-pshe62qyvmnrvesqa4pkj6bdq3fxucf
66: veloc              /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/veloc-1.4-gk3iwfjhmgkwlawp7rmxf2eh37rqpqm2
67: zfp               /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/zfp-0.5.5-6r6yaco7gga5w4gbuvid3zt2iohrnepj
```

E4S Support for Singularity Container Runtime [Sylabs.io]

Docker images are available on the [E4S Docker Hub](#) and in compressed XZ format on E4S servers.

Recipes for building images from scratch are available on the [E4S GitHub repository](#).

Our recipes make use of Spack packages available as pre-built binaries in the [E4S build cache](#).

Container Releases

- [Docker Download](#)
- [Singularity x86_64 Download](#)
- [Singularity ppc64le Download](#)
- [CharlieCloud Download](#)
- [OVA Download](#)

From source with Spack

[Visit the Spack Project](#)

Spack contains packages for all of the products listed in the E4S 1.0 Full Release category (see above 1.0 Release Notes). General instructions for building software with Spack can be found at the Spack website. For more information, see `/usr/local/packages/ecp` in the



- `wget http://tau.uoregon.edu/ecp.simg`
- `singularity exec ecp.simg /bin/bash --rcfile /etc/bashrc`
- `spack find`

E4S v1.2 Release: GPU, ppc64le for Docker Containers

The screenshot shows the Docker Hub interface for the repository `ecpe4s/ubuntu18.04-e4s-gpu-ppc64le`. The top navigation bar includes links for Explore, Repositories, Organizations, Get Help, and the user account `exascaleproject`. The repository page displays basic information like the repository name, a brief description of E4S, and the last push time (2 minutes ago). It also features sections for Docker commands (with a "Public View" button) and recent builds. A sidebar on the left lists tags and scans.

Docker commands

```
docker push ecpe4s/ubuntu18.04-e4s-gpu-ppc64le:tagname
```

Tags and Scans

This repository contains 7 tag(s).

TAG	OS	PUSHED
latest		2 minutes ago
2020-11-04		a day ago
2020-11-01		4 days ago
2020-10-27		9 days ago

VULNERABILITY SCANNING - DISABLED

[Enable](#)

Recent builds

Link a source provider and run a build to see build results here.

- 67 ECP Products
- Support for GPUs
 - NVIDIA (CUDA 10.2)
 - ppc64le and x86_64

% docker pull ecpe4s/ubuntu18.04-e4s-gpu

E4S v1.2 GPU Release: 67 E4S Products (ppc64le)

```
1: adios2      /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/adios2-2.6.0-veoqi5iqkx4kbeddhxoroggvxqqbtvos
2: aml         /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/aml-0.1.0-ftizegmvpbweuyzg75g3ndzhdyjx37op
3: amrex       /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/amrex-20.10-4z5quvlqt3fbzv5n6rrjv5byq7472emy
4: arborx      /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/arborx-0.9-beta-p7lw7eobsrdpqwhb7ispxpathng2tn4nt
5: ascent       /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/ascent-develop-7ktzsmvluqvfd4xoop7hjwddyjetn2ai
6: axom         /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/axom-0.3.3-zfgqs6qa6vxlodjnaojeffmyl26czmp5
7: argobots    /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/argobots-1.0-qra2gqxuisqqlbdfrhwm5mvq2iga3l3l
8: bolt         /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/bolt-1.0-ojy67rk47pcbqpcvuq6a4c7g7qysvndv
9: caliper      /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/caliper-2.4.0-6xzechuxs2updvdrl2tdvcym3n6nf3y3l
10: darshan-runtime /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/darshan-runtime-3.2.1-6uzihv7v75yu47c2jca4qpxqdtgptn2g
11: dyninst     /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/dyninst-10.2.1-jvqx4j3ehuh73pp67b4vdy4co3kivma5
12: faodel      /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/faodel-1.1906.1-r77asm5xb256omn4trg5hnxc3e376uy
13: flecsi       /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/flecsi-1-2kxukdrijujvbmsabmmj3um54ukhrayk
14: flit         /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/flit-2.1.0-tepzltg6kmefdg4eo2rbzwmjeca56bmc
15: gasnet       /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/gasnet-2020.3.0-uynuhs6itzczkfpgbnlm2xgotvqmmeb6
16: ginkgo        /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/ginkgo-1.3.0-dodvdbixjpdg5ci5xrgomjeqybiob33i
17: globalarrays   /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/globalarrays-5.7-3zbsvrakwto5jc454jl3l36rpvray25h
18: gotcha        /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/gotcha-1.0.3-pvjdzcg3fggpagjcsorwidsslflmomnz
19: hdf5          /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/hdf5-1.10.6-arkkhmy4auglzqndt7xraupyvgkrpv7o
20: hpctoolkit    /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/hpctoolkit-2020.08.03-yqayfprp2aleaxtzq543c75lcvcviso7
21: hpx           /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/hpx-1.5.1-tzfs3nkgsacequjxflokgwjzabybk
22: hypre          /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/hypre-2.20.0-ewmv445dkzmju4upg4rreq7apgkcdbu
23: kokkos         /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/kokkos-3.2.00-3qzjrzoxl5lpqgtaq4atid6ylgkko3uk
24: kokkos-kernels /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/kokkos-kernels-3.2.00-n4trpqbmxqahdy4tolj6nhfml5j4v6
25: legion         /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/legion-20.03.0-xsotehq7eg77hcguvqx5qymfhimgtuic
26: libnrm         /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/libnrm-0.1.0-q67khfosljacbl3djdg5jeh4ths15p5f
27: libquo        /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/libquo-1.3.1-syjf6c3adia34wlneacynrwkh72i3u
28: magma          /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/magma-2.5.4-fzeektdrkybbuo6i6niikzglcwln2jx
29: mercury        /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/mercury-1.0.1-ufxkkvb7osjnwgbfedhtrmtuoj6dfbz
30: mfem           /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/mfem-4.1.0-qrepufdzopbphsyuyc6npn7k2tpprd5w
31: mpich          /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/mpich-3.2.1-5m7ofmtvtov45hcudrm3qvd2dyheunyv
32: mpifileutils   /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/mpifileutils-develop-rd5xj2pmx5vdd7fddrhbrvn2uykg4uay
33: ninja          /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/ninja-1.10.1-cr2ada5fjgvkvdtmxel4zj6venfiif5e
```

E4S v1.2 GPU Release: 67 E4S Products (ppc64le)

```
34: omega-h      /opt/spack/opt/spack/linux-ubuntu18.04-power9le/gcc-7.3.0/omega-h-9.29.0-ziz55mnp5r7l4kuhx4zqmpj2imjdvrk5
35: openmpi       /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/openmpi-3.1.6-utceq6uech6rgnabxevau4lhtrwbaol
36: openpmd-api    /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/openpmd-api-0.12.0-szt65gmbfb76iwdbcfkhryfztg5jwjd7g
37: papi          /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/papi-6.0.0.1-xu35qtffffq2ofyjic3fafmj6yeijoih
38: papyrus        /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/papyrus-develop-2zopf6p3ha4v7ijxslxskrf2qyhpt3py
39: parallel-netcdf /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/parallel-netcdf-1.12.1-svuejkorgi2bzvhgq4wts72bcjfn426r
40: pdt            /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/pdt-3.25.1-opxwliyf5vqgt3hbla7qspf3laaqbt74
41: petsc          /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/petsc-3.14.0-phaqc52ryvhcib37qqjg2lmqdebql2uo
42: plasma         /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/plasma-20.9.20-vc40lrzgwsvxq7mevom2j7mhsgb6ynam
43: precice        /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/precice-2.1.1-qlitin5qdhtz3n7rg4jjzxkdss4qocvn
44: pumi           /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/pumi-2.2.2-m4uipa7yh632dftix4kzyxcz3pm3fasv
45: py-jupyterhub   /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/py-jupyterhub-1.0.0-gzzlyaf4gr2xgsgpndmbp2pkffm3tuc
46: py-libensemble  /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/py-libensemble-0.7.1-oee4zlxigkj5nnkr6fyu7thzsntfvvu
47: py-petsc4py    /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/py-petsc4py-3.13.0-g2rp2v37qbp5fo5fm6c4xtrj6shsbz
48: qthreads        /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/qthreads-1.14-bdxpllr2gf7knpek4vo5sjvzh5py5fdaf
49: raja            /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/raja-0.12.1-q32nuymeowavkwzmoiwx6f5md246tw66
50: rempi           /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/rempi-1.1.0-h3x5q2rwwsv34v7e4ricjw65wcd5mvkg
51: scr              /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/scr-2.0.0-2okrlxki5b63gzakjy2x4sbovrmegmcx
52: slate            /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/slate-develop-2jp7v35nifhyucbf4vmi3mjsernm5t26
53: slepc            /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/slepc-3.14.0-7qn6k5qxzf32tc2cnuk2mknlvqv6hfw
54: strumpack        /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/strumpack-5.0.0-gy5opc36suubh6uoijy4l223psdyrilg
55: sundials          /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/sundials-5.4.0-wonraynurs6xhyv6m6bc7o4grlwchlnp
56: superlu-dist     /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/superlu-dist-6.3.1-poufv43kq7tw2rw6upldbpcpbkpbdta
57: swig              /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/swig-4.0.2-3bddrfojvkrowa43v5so3ongbmhzxx5s
58: sz   /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/sz-2.1.10-fld5xazn2spjg46yaaaam5gftgyb5loa
59: tasmanian        /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/tasmanian-7.3-zbz26kn2yabritfi2wsbqv5raexgi4p3
60: tau              /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/tau-2.29-zqbkmoraislptbdny6fw4pakoipm3cbv
61: trilinos         /opt/spack/opt/spack/linux-ubuntu18.04-power9le/gcc-7.3.0/trilinos-13.0.0-olf4mdmym4sjbgue66gx42k7dbeb6z27
62: turbine          /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/turbine-1.2.3-jy42tjmn7rd2ofwwb3jaanlri2hnte65
63: umpire           /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/umpire-4.0.1-ynagdhefpcujnpeybxtasoqecr2p7bxj
64: unifyfs          /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/unifyfs-0.9.0-sxswh3b5upcys4bxc5wdzczvwvxvn6emg
65: upcxx            /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/upcxx-2020.3.0-i6hf7mat23um3fz5wexqswvn6mm4o7zp
66: veloc            /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/veloc-1.4-7ygadmpwv2zr26ec6opicysts4mxkwym
67: zfp              /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/zfp-0.5.5-3r4a4s3qdeqbdabvlwlswrgig62yc6yj
```

E4S Support for Singularity Container Runtime [Sylabs.io]

Docker images are available on the [E4S Docker Hub](#) and in compressed XZ format on E4S servers.

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Container
Releases

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[Singularity ppc64le Download](#)

[CharlieCloud Download](#)

[OVA Download](#)



From source with
Spack

[Visit the Spack Project](#)

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- `wget http://oaciss.uoregon.edu/e4s/images/ubuntu18.04-e4s-gpu-ppc64le_1.2.simg`
- `singularity exec --nv ubuntu18.04-e4s-gpu-ppc64le_1.2.simg /bin/bash --rcfile /etc/bashrc`
- `spack find; module avail`

E4S v1.2 GPU Support

```
alias runsi='singularity exec --nv /home/users/sameer/images/ubuntu18.04-e4s-gpu-ppc64le_1.2.simg /bin/bash --rcfile /etc/bashrc'  
[sameer@gorgon ~]$ runsi  
Singularity> python  
Python 3.6.10 |Anaconda, Inc.| (default, Jan  7 2020, 21:47:07)  
[GCC 7.3.0] on linux  
Type "help", "copyright", "credits" or "license" for more information.  
>>> import tensorflow  
>>> import torch  
>>> import cv2  
>>> import matplotlib  
>>> import numpy  
>>> tensorflow.test.is_gpu_available()  
2020-11-05 17:09:35.705979: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1433] Found device 0 with properties:  
name: Tesla V100-SXM2-32GB major: 7 minor: 0 memoryClockRate(GHz): 1.53  
pciBusID: 0004:04:00.0  
totalMemory: 31.75GiB freeMemory: 12.35GiB  
2020-11-05 17:09:35.778351: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1433] Found device 1 with properties:  
name: Tesla V100-SXM2-32GB major: 7 minor: 0 memoryClockRate(GHz): 1.53  
pciBusID: 0004:05:00.0  
totalMemory: 31.75GiB freeMemory: 31.44GiB  
2020-11-05 17:09:35.907371: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1433] Found device 2 with properties:  
name: Tesla V100-SXM2-32GB major: 7 minor: 0 memoryClockRate(GHz): 1.53  
pciBusID: 0035:03:00.0  
totalMemory: 31.75GiB freeMemory: 883.50MiB  
2020-11-05 17:09:35.989499: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1433] Found device 3 with properties:  
name: Tesla V100-SXM2-32GB major: 7 minor: 0 memoryClockRate(GHz): 1.53  
pciBusID: 0035:04:00.0  
totalMemory: 31.75GiB freeMemory: 31.44GiB  
2020-11-05 17:09:35.989594: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1512] Adding visible gpu devices: 0, 1, 2, 3  
2020-11-05 17:09:45.948104: I tensorflow/core/common_runtime/gpu/gpu_device.cc:984] Device interconnect StreamExecutor with strength 1 ed  
ge matrix:  
2020-11-05 17:09:45.948182: I tensorflow/core/common_runtime/gpu/gpu_device.cc:990]      0 1 2 3  
2020-11-05 17:09:45.948199: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1003] 0:   N Y Y Y  
2020-11-05 17:09:45.948210: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1003] 1:   Y N Y Y  
2020-11-05 17:09:45.948222: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1003] 2:   Y Y N Y  
2020-11-05 17:09:45.948232: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1003] 3:   Y Y Y N  
2020-11-05 17:09:45.950552: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1115] Created TensorFlow device (/device:GPU:0 with 11587  
MB Snapz Pro X physical GPU (device: 0, name: Tesla V100-SXM2-32GB, pci bus id: 0004:04:00.0, compute capability: 7.0)
```

E4S: ppc64le Base Container Images

The screenshot shows the Docker Hub interface with the search bar set to 'ecpe4s' and the query 'ppc64le'. The results list three public repositories:

- ecpe4s / ubuntu1804_ppc64le_base** (Updated 2 days ago)
- ecpe4s / ubi7_ppc64le_base** (Updated 2 days ago)
- ecpe4s / centos7_ppc64le_base** (Updated 2 days ago)

A tip at the bottom left suggests switching namespaces via the dropdown menu.

The right sidebar shows the user's organizations: **ecpcontainers**, **ecpe4s**, and **ecpsdk**. It also features links for **Download Docker Desktop** and **Secure, Private Repo Pricing**.

- Hub.docker.com
- ecpe4s
- Ubuntu 18.04
- RHEL/UBI 7.6
- Centos 7.6

Multi-platform E4S Docker Recipes

The screenshot shows a GitHub repository page for 'UO-OACISS / e4s'. The 'Code' tab is selected. The 'e4s / docker-recipes /' folder is expanded, showing a list of files and their descriptions. The files are organized into several groups:

- centos7-base-ppc64le: base recipes: standardize + improve parameterization (4 months ago)
- centos7-base-x86_64: base recipes: standardize + improve parameterization (4 months ago)
- centos7-e4s-ppc64le: remove old recipes (10 months ago)
- centos7-e4s-x86_64: remove old recipes (10 months ago)
- centos7-runner-ppc64le: runners: use base images from 2020-09-01 (4 months ago)
- centos7-runner-x86_64: runners: use base images from 2020-09-01 (4 months ago)
- centos7-spack-ppc64le: new spack ppc64le recipes (5 months ago)
- centos7-spack-x86_64: new spack x86_64 recipes (5 months ago)
- centos8-base-ppc64le: base recipes: standardize + improve parameterization (4 months ago)
- centos8-base-x86_64: base recipes: standardize + improve parameterization (4 months ago)
- centos8-e4s-ppc64le: remove old recipes (10 months ago)
- centos8-e4s-x86_64: remove old recipes (10 months ago)
- centos8-runner-ppc64le: runners: use base images from 2020-09-01 (4 months ago)
- centos8-runner-x86_64: runners: use base images from 2020-09-01 (4 months ago)
- centos8-spack-ppc64le: new spack ppc64le recipes (5 months ago)
- centos8-spack-x86_64: new spack x86_64 recipes (5 months ago)
- rhel7-base-ppc64le: base recipes: standardize + improve parameterization (4 months ago)
- rhel7-base-x86_64: base recipes: standardize + improve parameterization (4 months ago)

At the top right of the code listing, there are 'Go to file' and 'Add file' buttons.

10 lines (6 sloc) | 178 Bytes

```
1 FROM ecpe4s/ubuntu18.04-spack-x86_64:0.14.1
2
3 WORKDIR /e4s-env
4
5 COPY /spack.yaml .
6
7 RUN spack install --cache-only \
8   && spack clean -a && rm -rf /tmp/root/spack-stage
9
10 WORKDIR /
```

E4S: Multi-platform Reproducible Docker Recipes

https://github.com/UO-OACISS/e4s/tree/master/docker-recipes/ubi7/ppc64le/base

UO-OACISS / e4s

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

Branch: master e4s / docker-recipes / ubi7 / ppc64le / base / Create new file Upload files Find file History

eugenewalker use spack.lock in ubi7 ppc64le base recipe Latest commit 079af58 18 hours ago

..

modules update ppc64le recipes to 1.3: use spack 0.13.1 + use base env + add ... 9 days ago

Dockerfile use spack.lock in ubi7 ppc64le base recipe 18 hours ago

README.md add README for UBI7 ppc64le base 2 days ago

build.sh update ppc64le recipes to 1.3: use spack 0.13.1 + use base env + add ... 9 days ago

packages.yaml v1.2 of ubi7 ppc64le base recipe 29 days ago

spack.lock use spack.lock in ubi7 ppc64le base recipe 18 hours ago

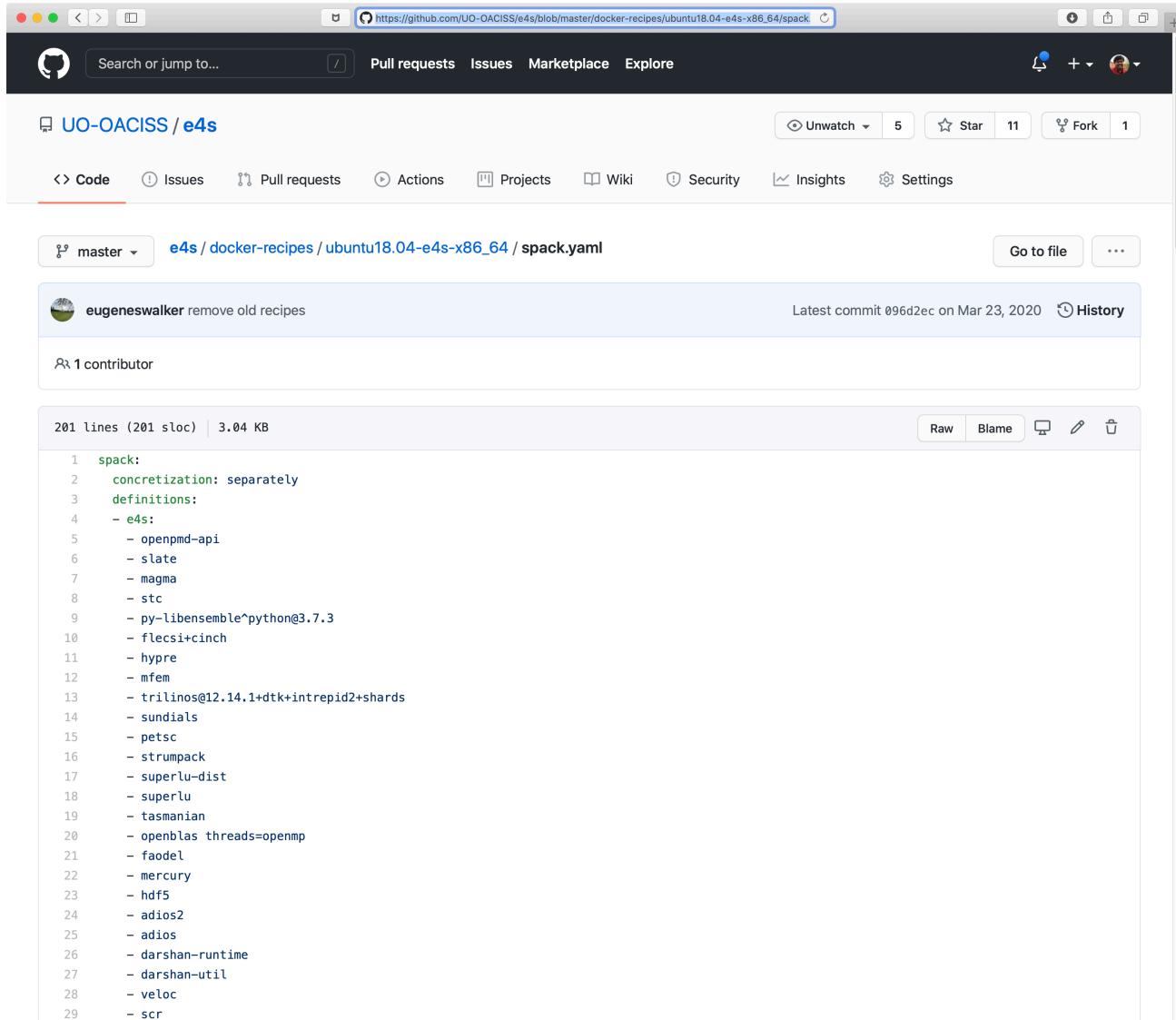
spack.yaml update ppc64le recipes to 1.3: use spack 0.13.1 + use base env + add ... 9 days ago

README.md

E4S

- x86_64
- ppc64le
- aarch64

E4S Spack environment spack.yaml



The screenshot shows a GitHub repository page for the `e4s/docker-recipes/ubuntu18.04-e4s-x86_64` branch. The file being viewed is `spack.yaml`. The code listing shows a single-level dependency graph where `spack` depends on numerous scientific and engineering libraries. The code is as follows:

```
1 spack:
2   concretization: separately
3   definitions:
4     - e4s:
5       - openpmd-api
6       - slate
7       - magma
8       - stc
9       - py-libensemble^python@3.7.3
10      - flecs+cinch
11      - hypre
12      - mfem
13      - trilinos@12.14.1+dtk+intrepid2+shards
14      - sundials
15      - petsc
16      - strumpack
17      - superlu-dist
18      - superlu
19      - tasmanian
20      - openblas threads=openmp
21      - faodel
22      - mercury
23      - hdf5
24      - adios2
25      - adios
26      - darshan-runtime
27      - darshan-util
28      - veloc
29      - scr
```

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

- Docker build:

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

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

E4S: Spack Build Cache at U. Oregon

The screenshot shows a web browser window displaying the E4S Build Cache for Spack 0.16.0 inventory page. The URL in the address bar is <https://oaciss.uoregon.edu/e4s/inventory.html>. The page title is "E4S Build Cache for Spack 0.16.0". A sub-instruction says "To use this build cache, just add it to your Spack" followed by three command-line examples:

```
spack mirror add E4S https://cache.e4s.io  
wget https://oaciss.uoregon.edu/e4s/e4s.pub  
spack gpg trust e4s.pub
```

Below these are two sections: "Click on one of the packages below to see a list of all available variants." and "Last updated: 12-15-2020 14:22 PST". The first section contains several filter buttons:

- All Architectures PPC64LE X86_64
- All Operating Systems Centos 7 Centos 8 RHEL 7 RHEL 8 Ubuntu 18.04 Ubuntu 20.04

The second section shows the last update time: "Last updated: 12-15-2020 14:22 PST". Below this is a count: "27435 Spack packages". There is also a search input field labeled "Search".

The main content area displays a list of packages. One package, "amrex@20.12", is highlighted with a yellow background. A link "Click on the full spec link to find out more." is present above the table for this package. The table has columns: Link, Arch, OS, Compiler, Created, and Full Hash. The data for "amrex@20.12" is as follows:

Link	Arch	OS	Compiler	Created	Full Hash
Full Spec	ppc64le	rhe18	gcc@8.3.1	12-14-2020 12:04 PST	q7fbvowel3gusfypqv5j54au4zj7fvb6
Full Spec	ppc64le	ubuntu18.04	gcc@7.5.0	12-14-2020 12:06 PST	xskw37zx2qvrfrgtm7fmw2ipnxzucr
Full Spec	ppc64le	ubuntu20.04	gcc@9.3.0	12-14-2020 12:08 PST	h6xbsawr23rsfxm4ikwbp67fmve6dtcb
Full Spec	x86_64	ubuntu18.04	gcc@7.5.0	12-14-2020 12:07 PST	ngwoej4enmp2gzshys26d635kvhpco7
Full Spec	x86_64	ubuntu20.04	gcc@9.3.0	12-14-2020 12:08 PST	etostybexmyty43kflvoyevdvh4vxoyd

Below the highlighted package, there is a list of other packages: ant@1.10.0, ant@1.10.7, arborx@0.9-beta, argobots@1.0, argobots@1.0rc1, argobots@1.0rc2, arpack-ng@3.7.0, arpack-ng@3.8.0, ascent@develop, assimp@4.0.1, autoconf-archive@2019.01.06, autoconf@2.69, automake@1.16.1, automake@1.16.2, axl@0.1.1, axl@0.3.0, axom@0.3.3, axom@0.4.0, bash@5.0, bdftopcf@1.0.5, berkeley-db@18.1.40, berkeley-db@6.2.32, binutils@2.31.1.

- 27,000+ binaries
- S3 mirror
- No need to build from source code!

WDMApp: Speeding up bare-metal installs using E4S build cache

The screenshot shows a web browser displaying the WDMApp documentation at <https://wdmapp.readthedocs.io/en/latest/machines/rhea.html>. The page includes the ECP logo and navigation links for WDMApp, WDMApp on Rhea, WDMApp on Longhorn, WDMApp on AiMOS, and generic instructions.

Note: The E4S project has created a build cache for Rhea. This provides many packages as precompiled binaries, so will reduce the installation time. To use it:

```
$ wget https://oaciss.uoregon.edu/e4s/e4s.pub
$ spack gpg trust e4s.pub
$ spack mirror add E4S https://cache.e4s.io/e4s
```

Building WDMApp

You should be able to just follow the generic instructions from [Building WDMAPP](#).

Using E4S WDMApp docker container

Alternatively, the E4S project has created a docker image that mirrors the Rhea environment, which can be used for local development and debugging. To run this image, you need to have docker installed and then do the following:

```
$ docker pull ecpe4s/ubi7.7_x86_64_base_wdm:1.0
$ docker run -rm -it ecpe4s/ubi7.7_x86_64_base_wdm:1.0
```

In order for the image to get the access controlled components, you need to provide it with your private SSH key that provides access to the respective private github repos. In the image, do the following in the docker image:

```
# cat > .ssh/id_rsa # Then copy&paste your private key
# chmod 600 .ssh/id_rsa
```

This provides an development environment with everything but the private codes preinstalled. All that's needed to complete building and installing them is:

```
# spack install wdmapp target=x86_64
```

- E4S Spack build cache
- Adding E4S mirror
- WDMApp install speeds up!

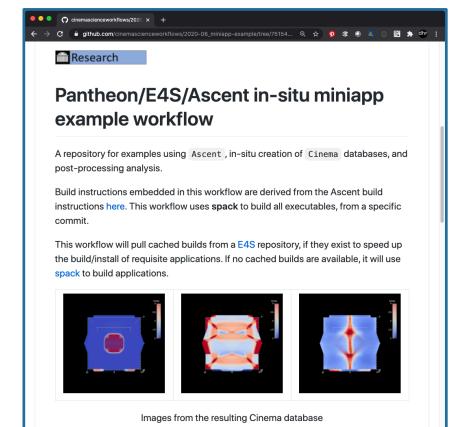
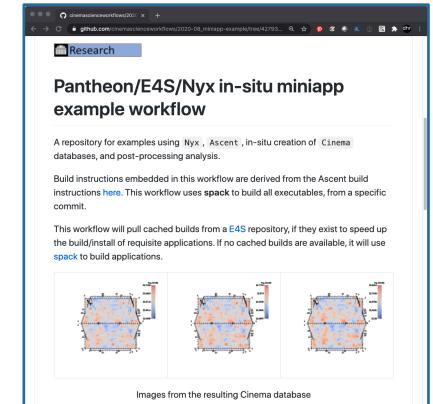
Pantheon and E4S build cache support end-to-end ECP examples

Overview: The Exascale Computing Project (ECP) is a complex undertaking, involving a myriad of technologies working together. An outstanding need is a way to capture, curate, communicate and validate workflows that cross all of these boundaries.

The **Pantheon** and **E4S** projects are collaborating to advance the integration and testing of capabilities, and to promote understanding of the complex workflows required by the ECP project. Utilizing a host of ECP technologies (spack, Ascent, Cinema, among others), this collaboration brings curated workflows to the fingertips of ECP researchers.

Contributions

- Curated end-to-end application/in-situ analysis examples can be run quickly by anyone on Summit. (<https://github.com/pantheonscience/ECP-E4S-Examples>)
- Pantheon/E4S integration speeds up build/setup times over source builds due to cached binaries (approx.10x speed up).



Instructions page for (top) Nyx, Ascent and Cinema workflow repository, and (bottom) Cloverleaf3d, Ascent, Cinema workflow. These curated workflows use Pantheon, E4S and spack to provide curated workflows for ECP.

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E4S Validation Test Suite

- Provides automated build and run tests
- Validate container environments and products
- New LLVM validation test suite for DOE LLVM

The screenshot shows a GitHub repository page for `E4S-Project / testsuite`. The repository has 8 pull requests, 2 stars, and 0 forks. The current branch is `master`, specifically the `testsuite / validation_tests / magma` directory. A commit by `eugenewalker` is shown, which uses `bash -xe` in `compile/run.sh`. The commit message indicates it uses env variables set by `spack load`. The commit was made 9 hours ago. Below the commit, there is a list of files: `Makefile`, `README.txt`, `clean.sh`, `compile.sh`, `example_f.F90`, `example_sparse.c`, `example_sparse_operator.c`, `example_v1.c`, `example_v2.c`, `run.sh`, and `setup.sh`. The `README.txt` file contains instructions for getting started with MAGMA, mentioning the MAGMA header and legacy interface details.

- `git clone https://github.com/E4S-Project/testsuite.git`

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 by `sameershende` on `a0b948d` 10 days ago, and both have 1 contributor.

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 ecpe4s/ubi7_x86_64_base:1.1
2
3 ENV FORCE_UNSAFE_CONFIGURE=1 \
4     XSDK_ENV_ROOT="/xsdk-env" \
5     EAS_GROUP="xsdk" \
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 has Spack build cache mirror and GPG key installed.
- Base image has GCC and MPICH configured for MPICH ABI level replacement (with system MPI).
- **Customized container build using binaries from E4S Spack build cache for fast deployment.**
- **No need to rebuild packages from the source code.**
- Same recipe for container and native bare-metal builds with Spack!

E4S: GitLab Runner Images

The screenshot shows a Dockerhub search results page. The search bar at the top has 'ecpe4s' in the main field and 'ppc64le' in the dropdown field. Below the search bar, there is a 'Create Repository' button. The search results list several Docker images from the 'ecpe4s' repository, all tagged with 'ppc64le' and marked as 'Not Scanned'. The images are:

- ecpe4s / **ubuntu18.04-e4s-gpu-ppc64le** Updated an hour ago
- ecpe4s / **centos7-runner-ppc64le** Updated a month ago
- ecpe4s / **centos8-runner-ppc64le** Updated a month ago
- ecpe4s / **ubuntu20.04-runner-ppc64le** Updated a month ago
- ecpe4s / **rhel8-runner-ppc64le** Updated a month ago
- ecpe4s / **ubuntu18.04-runner-ppc64le** Updated a month ago
- ecpe4s / **rhel7-runner-ppc64le** Updated a month ago

Each image entry includes a star icon (0 stars), a download count (e.g., 61, 2.9K, 37, 575, 477, 3.9K, 3.8K), and a 'Public' badge.

- Dockerhub
- Bare-bones
- Multi-platform
- Build E4S

University of Oregon GitLab CI

The screenshot shows the GitLab interface for the project **e4s**. The sidebar on the left is collapsed, and the main area displays a **Pipeline** with 18 jobs. The pipeline is organized into three columns: **Concretize**, **Trigger Builds**, and **Downstream**.

- Concretize:** Contains 10 jobs: centos7-amd64-0, centos8-amd64-0, rhel7-amd64-0, rhel7-ppc64le-0, rhel8-amd64-0, ubuntu18.04-a..., ubuntu18.04-p..., ubuntu20.04-a..., and ubuntu20.04-p... Each job has a green checkmark and a circular refresh icon.
- Trigger Builds:** Contains 9 jobs: centos7-amd64..., centos8-amd64..., rhel7-amd64-1, rhel7-ppc64le-1, rhel8-amd64-1, ubuntu18.04-a..., ubuntu18.04-p..., ubuntu20.04-a..., and ubuntu20.04-p... Each job has a green checkmark and a circular refresh icon.
- Downstream:** Contains 9 boxes, each labeled **e4s • #881** through **e4s • #889**, followed by the word **Child**. Each box contains a green checkmark and a blue "Child" button.

E4S Builds:

- Ubuntu 18.04
- Ubuntu 20.04
- RHEL 7.6
- RHEL 8
- CentOS 7
- CentOS 8

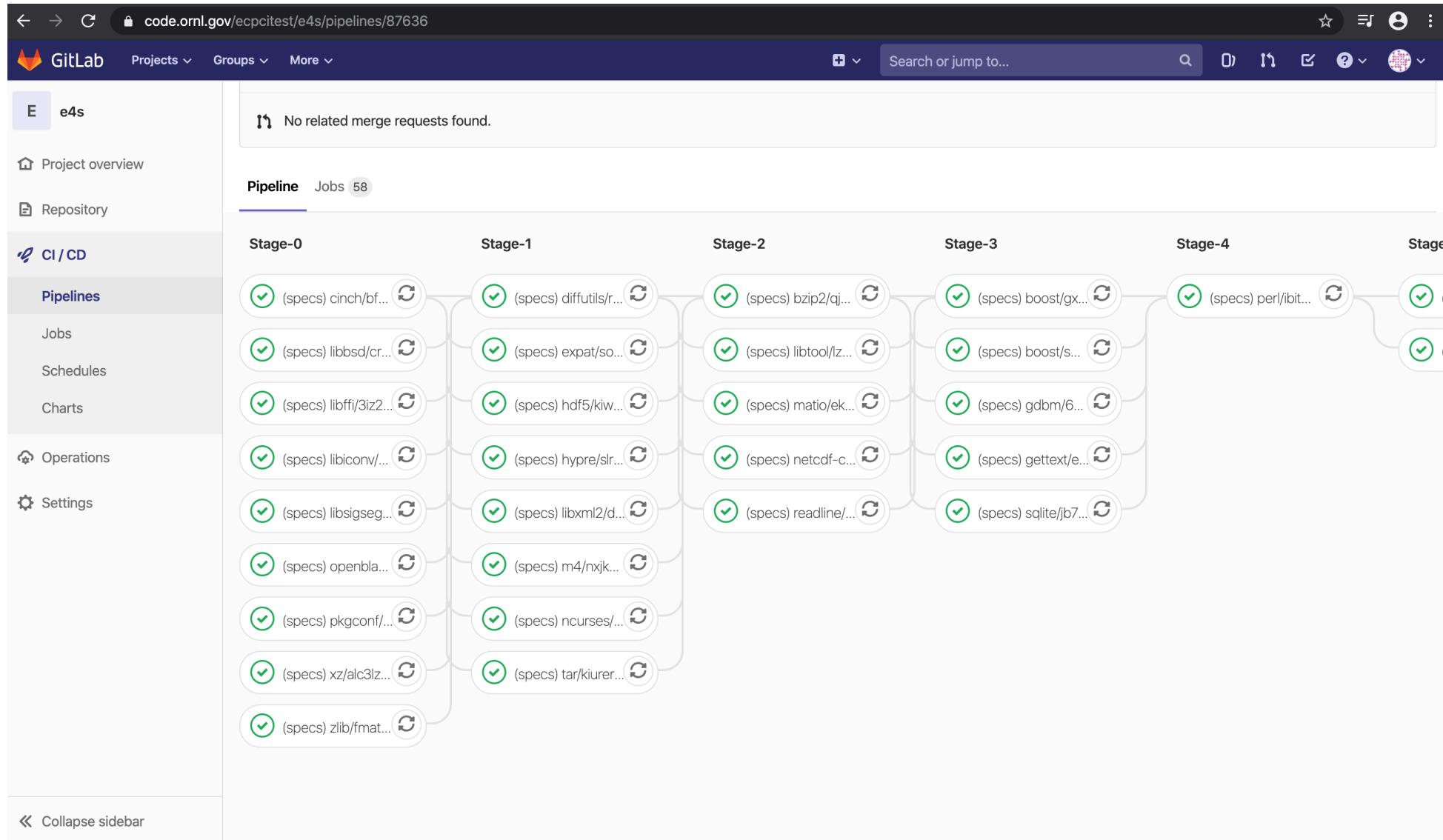
Architectures:

ppc64le and x86_64

- <https://gitlab.e4s.io>

Multi-stage E4S CI Build Pipeline on Cori, NERSC

ORNL GitLab Build Pipeline for E4S Spack Build Cache



- ppc64le (Ascent @ ORNL)
- Reproducible container builds

E4S DocPortal

- Provide a single online location for *accurate* product descriptions for ECP software products.
- Derived requirements:
 - Sustainable: Must be integrated into software team workflows.
 - Incremental: Must build on community approaches to providing this kind of information.
 - Extensible: Must be usable by any open source software team.
- Strategy:
 - Use the open source community approach of specially-name files in software repositories.
 - Adopt commonly used file names when available.
 - Identify new information items not already being requested.
 - Develop new special file names for information beyond what is already captured.
 - Create web-based raking tool to capture information from product repositories and present in summary form on a webpage.
 - Aggregates and summarizes documentation and metadata for E4S products
 - Regularly updates information directly from product repositories
 - Prototype: <https://e4s-project.github.io/DocPortal.html>

E4S DocPortal

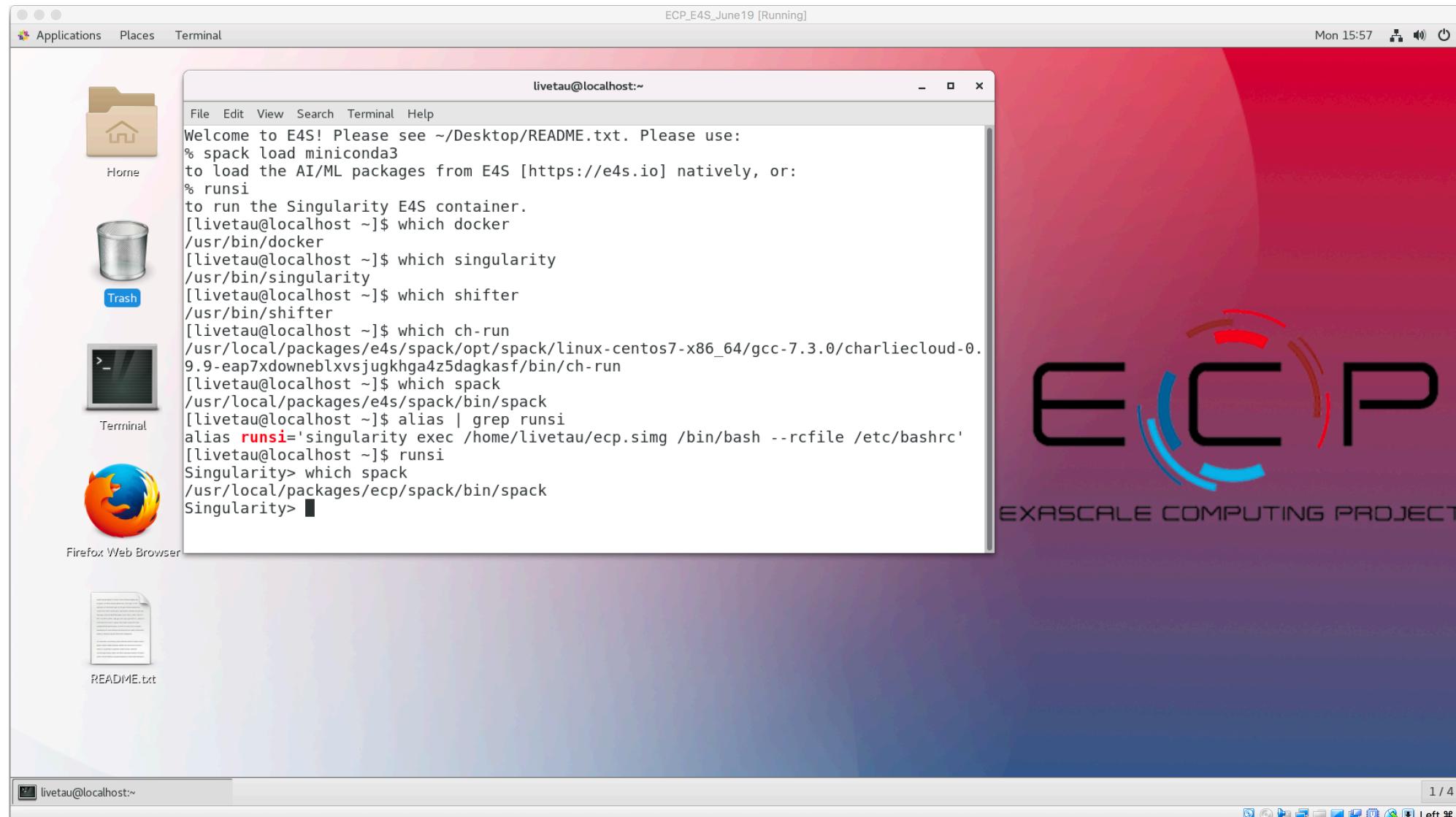
The screenshot shows the E4S DocPortal homepage. At the top, there is a navigation bar with links: HOME, EVENTS, ABOUT, DOCPORTAL (which is the active page), POLICIES, CONTACT US, JOIN, FAQ, and DOWNLOAD. Below the navigation bar, the main content area has a title "E4S Products". There is a note ": Member Product" and a search bar labeled "Search: []". A table lists three products: ADIOS2, AML, and AMREX. The table columns are Name, Area, Description, and Latest Doc Update. The table is sorted by Area (Data & Viz, PMR, PMR) and Latest Doc Update (2020-07-16, 2019-04-25, 2021-01-02). The "Description" column for AMREX includes a detailed description of the framework.

Name	Area	Description	Latest Doc Update
ADIOS2	Data & Viz	I/O and data management library for storage I/O, in-memory code coupling and online data analysis and visualization workflows.	2020-07-16 16:36:11
AML	PMR	Hierarchical memory management library from Argo.	2019-04-25 13:03:01
AMREX	PMR	A framework designed for building massively parallel block-structured adaptive mesh refinement applications.	2021-01-02 17:25:05

Description: AMReX is a publicly available software framework designed for building massively parallel block-structured adaptive mesh refinement (AMR) applications.

<https://e4s-project.github.io/DocPortal.html>

E4S VirtualBox Image

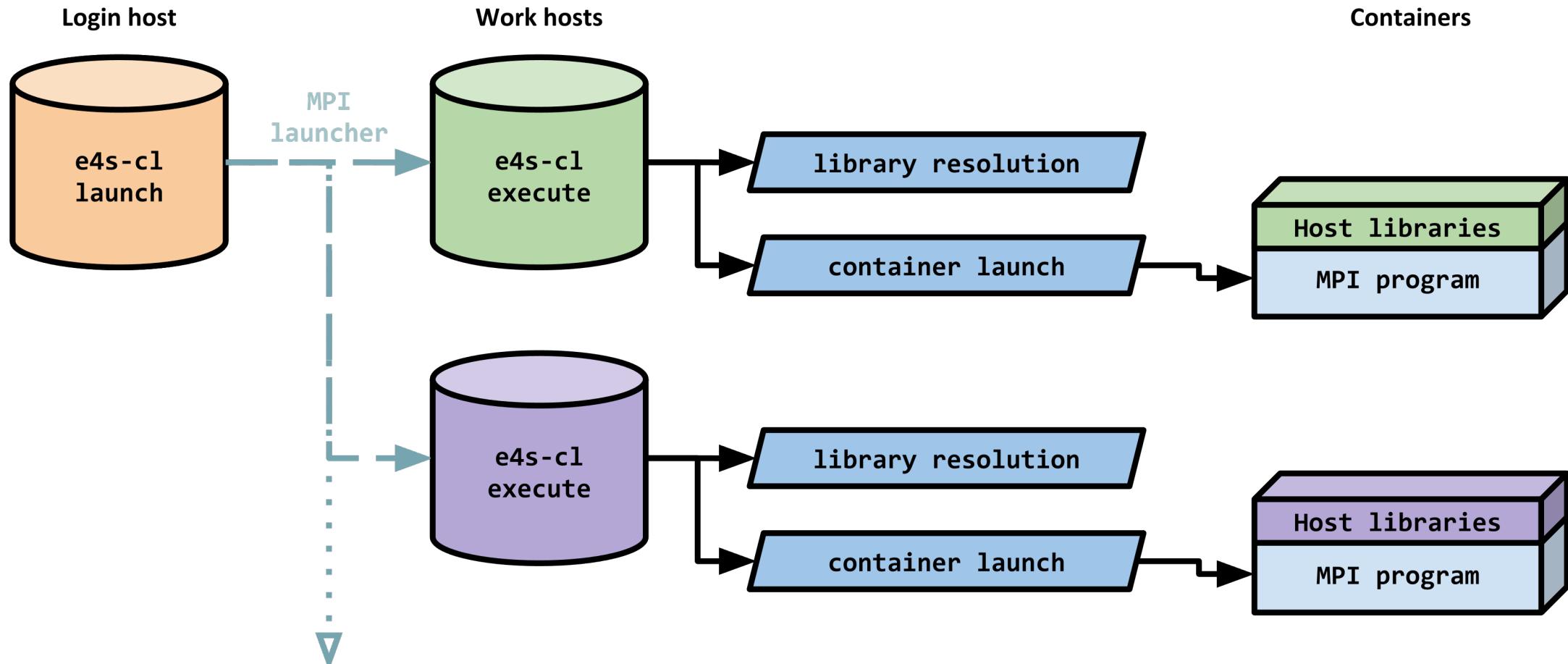


- ## Container Runtimes
- Docker
 - Shifter
 - Singularity
 - Charliecloud

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

- E4S containers support replacement of MPI libraries using MPICH ABI compatibility layer.
- Applications binaries built using E4S can be launched with Singularity using MPI library substitution for efficient inter-node communications.
- e4s-cl is a new tool that simplifies the launch and MPI replacement.
- Under development. Usage:
 1. `e4s-cl profile detect -o <profile> <MPI executable>`
 2. `e4s-cl profile select <profile>`
 3. `e4s-cl launch mpirun -np <> -hosts <> <command>`

e4s-cl Container Launcher



E4S Summary

What E4S is not

A closed system taking contributions only from DOE software development teams.

A monolithic, take-it-or-leave-it software behemoth.

A commercial product.

A simple packaging of existing software.

• What E4S is

Extensible, open architecture software ecosystem accepting contributions from US and international teams.
Framework for collaborative open-source product integration.

A full collection of compatible software capabilities **and**
A manifest of a la carte selectable software capabilities.

Vehicle for delivering high-quality reusable software products in collaboration with others.

The conduit for future leading edge HPC software targeting scalable next-generation computing platforms.
A hierarchical software framework to enhance (via SDKs) software interoperability and quality expectations.

Future work, issues...

- Improved support for GPUs and visualization tools
- DOE LLVM
- Addition of CI testing
- Facility deployment
- Scalable startup with full-featured “Supercontainers”
- Improving the launch of MPI applications
- From-source builds assisted by a binary build cache or containers
- Docker and Singularity images are available for download
 - <https://e4s.io>

Performance Research Laboratory, University of Oregon, Eugene



Acknowledgment



“This research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of two U.S. Department of Energy organizations (Office of Science and the National Nuclear Security Administration) responsible for the planning and preparation of a capable exascale ecosystem, including software, applications, hardware, advanced system engineering, and early testbed platforms, in support of the nation’s exascale computing imperative.”

