

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

Wednesday, January 13<sup>th</sup>, 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

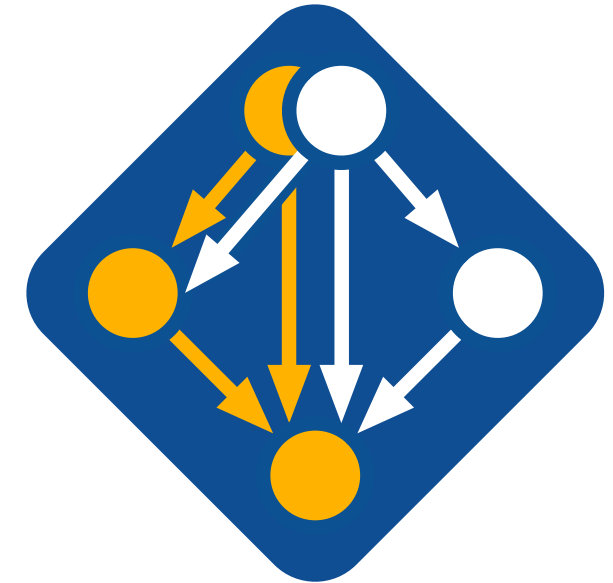
- How to install Spack (works out of the box):

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

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

 [@spackpm](https://twitter.com/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+threads +/- 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@2.6.9    diffutils@3.7    libiconv@1.16    m4@1.4.18        ncurses@6.2      openssl@1.1.1g   texinfo@6.5
automake@1.16.2  findutils@4.6.0  libpciaccess@0.16 matio@1.5.17     netcdf-c@4.7.4   parmetis@4.0.3  trilinos@13.0.0
boost@1.74.0     glm@0.9.7.1      libsigsegv@2.12  metis@5.1.0     netlib-scalapack@2.1.0 perl@5.26.1     util-macros@1.19.1
bzip2@1.0.8     hdf5@1.10.7     libtool@2.4.6   mpich@3.2.1     omega-h@9.29.0  pkgconf@1.7.3   xz@5.2.5
cmake@3.18.4    hypre@2.20.0    libxml2@2.9.10  numpys@5.3.3   openblas@0.3.10  suite-sparse@5.7.2  zlib@1.2.11

-- linux-ubuntu18.04-ppc64le / gcc@7.3.0 -----
adiak@0.1.1      flit@2.1.0       libpfm4@4.11.0   papyrus@develop  py-more-itertools@7.2.0  qthreads@1.14
adios@1.13.1    gasnet@2020.3.0  libpng@1.6.37    parallel-netcdf@1.12.1  py-mpi4py@3.0.3          raja@0.12.1
adios2@2.6.0    gasnet@2020.3.0  libpthread-stubs@0.4  parmetis@4.0.3      py-nbclient@0.5.0       rankstr@0.0.2
adlbx@0.9.2     gdbm@1.18.1      libquo@1.3.1     pcre@8.44          py-nbconvert@6.0.1      readline@8.0
aml@0.1.0       gettext@0.20.2   libsigsegv@2.12  pcre2@10.35        py-nbformat@5.0.7       redset@0.0.3
amrex@20.10     gettext@0.21     libsodium@1.0.18  pdsh@2.31          py-nest-asyncio@1.4.0   rempi@1.1.0
arborx@0.9-beta  ginkgo@1.3.0    libtool@2.4.6    pdt@3.25.1         py-notebook@6.1.4       scr@2.0.0
argobots@1.0    git@2.28.0      libunistring@0.9.10  perl@5.26.1        py-numpy@1.19.2        shuffle@0.0.3
arpack-ng@3.7.0  git@2.28.0      libunwind@1.4.0   petsc@3.13.6       py-oauthlib@3.1.0       slate@develop
ascent@develop  glm@0.9.7.1     libunwind@1.4.0   petsc@3.14.0       py-pamela@1.0.0         slepc@3.14.0
autoconf@2.6.9  globalarrays@5.7  libuuid@1.0.3    pkgconf@1.7.3     py-pandocfilters@1.4.2  snappy@1.1.8
automake@1.16.2  gmake@4.2.1     libyogrt@1.24    plasma@20.9.20    py-pandocfilters@1.4.2  sqlite@3.31.1
axl@0.3.0       gmp@6.1.2       libzmq@4.3.2     precice@2.1.1     py-parso@0.6.1          strumpack@5.0.0
axom@0.3.3      googletest@1.10.0  lmod@8.3         pumi@2.2.2        py-petsc4py@3.13.0     suite-sparse@5.7.2
bash@5.0        gotcha@0.0.2    lua@5.3.5        py-alembic@1.0.7   py-pexpect@4.7.0       sundials@5.4.0
binutils@2.33.1  gotcha@1.0.3    lua-luafilesystem@1_7_0_2  py-argon2-cffi@20.1.0  py-pickleshare@0.7.5   superlu@5.2.1
bmi@develop     gperftools@2.7  lua-luaposix@33.4.0  py-asn1crypto@0.24.0  py-prompt-toolkit@2.0.9  superlu-dist@6.3.0
bolt@1.0        hdf5@1.8.21     lwgrp@1.0.3      py-async-generator@1.10  py-psutil@5.7.2        superlu-dist@6.3.1
boost@1.73.0    hdf5@1.8.21    lz4@1.9.2        py-attrs@19.3.0    py-ptyprocess@0.6.0     swig@4.0.2
boost@1.73.0    hdf5@1.10.6    lzo@2.10         py-babel@2.7.0     py-py@1.8.0            sz@1.4.12.3
boost@1.73.0    hdf5@1.10.6    m4@1.4.18        py-backcall@0.1.0   py-pycparser@2.20      sz@2.0.2.0
boost@1.73.0    hpctoolkit@2020.08.03  magma@2.5.4     py-bleach@3.1.0    py-pyelftools@0.26     tar@1.32
butterflypack@1.2.0  hpx@1.5.1      margo@0.4.3     py-blinker@1.4     py-pygments@2.6.1     tasmanian@7.3
bzip2@1.0.8     hwloc@1.11.11  matio@1.5.17    py-certifi@2020.6.20  py-pyjwt@1.7.1         tau@2.29
c-blosc@1.17.0  hwloc@2.2.0    mbedtls@2.16.7  py-certipy@0.1.3   py-pyopenssl@19.0.0    tcl@8.6.10
caliper@2.4.0   hypre@2.18.2   mercury@1.0.1   py-cffi@1.14.3     py-pyrsistent@0.15.7  texinfo@6.5
cinch@master    hypre@2.20.0   mercury@1.0.1   py-chardet@3.0.4   py-pytest-runner@5.1   turbine@1.2.3
cmake@3.17.3    intel-tbb@2020.3  kokkos@3.2.0    py-cryptography@2.7  py-python-dateutil@2.8.0  umap@2.1.0
conduit@master  kokkos-kernels@3.2.0.0  mfem@4.1.0     py-cython@0.29.21  py-python-editor@1.0.4  umpire@4.0.1
conduit@master  kvtree@1.0.2   metis@5.1.0     py-decorator@4.4.2  py-python-oauth2@1.1.1  unifyfs@0.9.0
cuda@10.2.89   legion@20.03.0  mpark-variant@1.4.0  py-defusedxml@0.6.0  py-pytz@2020.1         unzip@6.0
curl@7.72.0    leveldb@1.22   mpi4py@3.2.1    py-difflib@0.9.0   py-requests@2.24.0     upcxx@2020.3.0
darshan-runtime@3.2.1  libarchive@3.4.1  mpich@3.2.1    py-entrypoints@0.3  py-send2trash@1.5.0    util-macros@1.19.1
di... Snapz Pro X 3.2.1  libbsd@0.10.0  ncurses@6.2    py-idna@2.8        py-setuptools@50.1.0
di...
```

All the versions coexist!

- Multiple versions of same package are ok.

Packages are installed to automatically find correct dependencies.

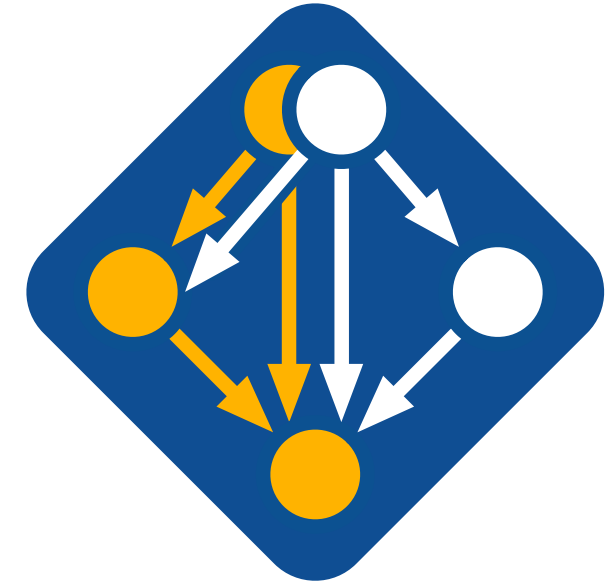
Binaries work *regardless of user's environment*.

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](https://spack.io)

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

 [@spackpm](https://twitter.com/spackpm)



# Download E4S v1.2 GPU Container Image

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

OS	Variant	Image Name
RHEL 7	SPACK MINIMAL	ecpe4s/rhel7-spack
	E4S COMPREHENSIVE	ecpe4s/rhel7-e4s
	CUSTOM	ecpe4s/superlu_sc
Ubuntu 18.04	E4S GPU IMAGE	ecpe4s/ubuntu18.04-e4s-gpu
	E4S GPU IMAGE	x86_64 version: CUDA and ROCM
	E4S GPU IMAGE	ppc64le version: CUDA
	SPACK MINIMAL	ecpe4s/ubuntu18.04-spack
CentOS 7	SPACK MINIMAL	ecpe4s/centos7-spack
	E4S COMPREHENSIVE	ecpe4s/centos7-e4s

# E4S v1.2 GPU Release for x86\_64

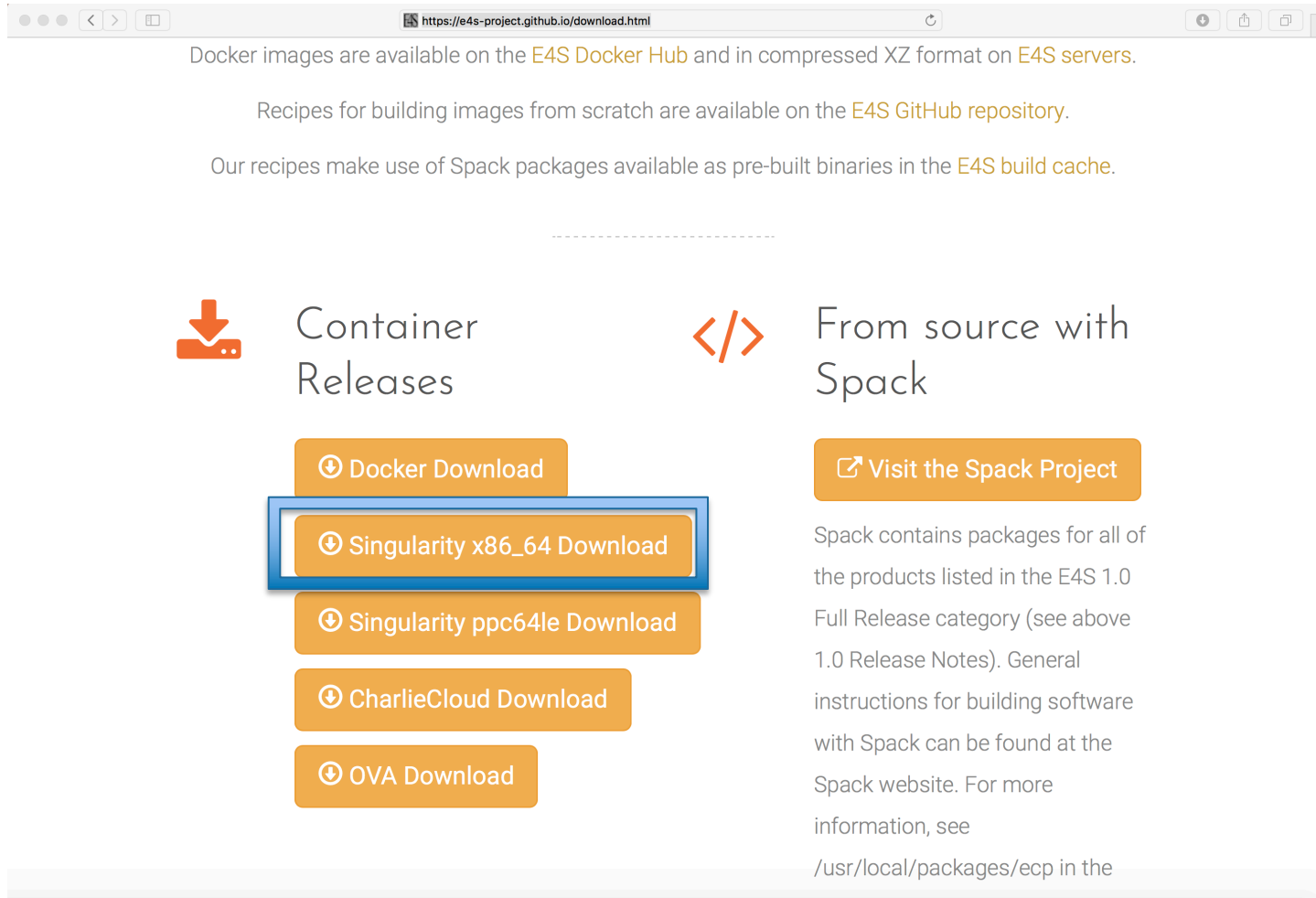
```
1: adios2 /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/adios2-2.6.0-nkp24j7enorn3dt7626chuqm3pbkrvfe
2: aml /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/aml-0.1.0-3mwyb6cf6ervfnruqb5u33v46buyuqth
3: arborx /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/arborx-0.9-beta-qjzxlkcgplto6pnpjwejh5xpoik3adr
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-ciwwqg6lh6unww3hjsnu47wr7cpqptqgy
6: axom /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/axom-0.3.3-tzyejxpy3p3ekaev35k2bhpkr74cnuhh
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-jqugqxx2uunyaduoe3owhd2snves6mlr
10: dyninst /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/dyninst-10.2.1-xad3v6rvosm6qfai5fc7d4nn33svtzzf
11: faodel /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/faodel-1.1906.1-ijilel2vjionmj56mscqkw2hpecfsuym
12: flecsi /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/flecsi-1-c7sevlnc2ak4pf2jgg6wh3mwictch5l2
13: flit /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/flit-2.1.0-yvvog7kmax22ei2yyrwxj3heimz5am
14: gasnet /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/gasnet-2020.3.0-ufraq5hym67eq3jsg4jtttjqqo4i6hmq
15: ginkgo /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/ginkgo-1.2.0-r6lorgchpr5qrcwyqqxtewqdhtpi4rmt
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-1.0.3-7n7bjnzsnf5w5tnihiok3otbaewdhjmu
18: hdf5 /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/hdf5-1.10.6-k74avubedd5knvlc73dr3ib5oyw6bcwn
19: hpctoolkit /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/hpctoolkit-2020.08.03-wck4g3h3jhfvzvxorelxqunbe3xsesry
20: hpx /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/hpx-1.5.0-pynmocntkmuwkoyo5jxtycvg34w6kue
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-pqv3uugd6cv3qftyr3rx6dm2gao2tg3
23: kokkos-kernels /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/kokkos-kernels-3.1.00-y4veufypftworlbehxusg4yzh6n7anhp
24: legion /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/legion-20.03.0-zkbz7h2wuze4dgbwcb04w5fvqltugmog
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-w45wcw6dqbiajeeauj3ryaeskqu7bzx6
27: magma /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/magma-2.5.3-yksxthffslhjrhwgxcx7smz2tca6ojfn
28: mercury /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/mercury-1.0.1-ppledsr3drk2upciyftsuawfxrtjp73q
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-kgwtpelzobpkrvg24ct6padfbhw7nene
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-eln73w7ytpvgqtkmkqyjmg4gsabsu2w4p
```

- 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-gorrfrvrik575lldzgg46qmmu63kxl7x
37: papyrus          /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/papyrus-develop-iu3dgpmmwyykgv5mpw2dwcrol4wbwbai
38: parallel-netcdf /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/parallel-netcdf-1.12.1-tmmkzibn43xr7su76msxxusyzzrphdtn5
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-2.2.2-52czzdbxeg7pmjkd55nub5jgxzodcprh
44: py-jupyterhub    /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/py-jupyterhub-1.0.0-tr3wcolaij3kbzb6xm4mbbvackstws3
45: py-libensemble   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/py-libensemble-0.7.0-mxvqxhiiblqnmhlfepbxboyiskqyvbej
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-q3lalpbqoshiyvjjgrnhb2iqiisvnrp
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-o2hkund66coxn2rrbtalda2vq35uu7j
55: stc              /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/stc-0.8.3-oxfik7nsmgufogy7xilzsrct7it63ej
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-tcatyiuzh6quctrgd2g3dcli7xa7gvtj
58: tasmanian        /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/tasmanian-7.1-quo3grs5kb2xrvjufpi7vn66cpjfnadv
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-13.0.0-6xfnp44g5xm7gpn2en6gkwzfcykd3x
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-3.0.0-6woo2uuvazcucxikc6xad6g3zksu2ygi
64: unifyfs          /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/unifyfs-0.9.0-be7mqbng7kdeewdlglhdm4jknquiiil
65: upcxx            /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/upcxx-2020.3.0-pshe62qyvnmrvesqa4pkj6bdq3fxucf
66: veloc            /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/veloc-1.4-gk3iwfjhmglawp7rmxf2eh37rqpqm2
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]



The screenshot shows a web browser window with the URL `https://e4s-project.github.io/download.html`. The page content includes:

- 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](#).

---

The page is divided into two main sections:

- Container Releases** (indicated by a download icon):
  - [Docker Download](#)
  - [Singularity x86\\_64 Download](#) (highlighted with a blue border)
  - [Singularity ppc64le Download](#)
  - [CharlieCloud Download](#)
  - [OVA Download](#)
- From source with Spack** (indicated by a code icon):
  - [Visit the Spack Project](#)

Below the 'From source with Spack' section, there is text explaining that Spack contains packages for all products listed in the E4S 1.0 Full Release category, and provides instructions for building software with Spack, including a reference to the Spack website and a path: `/usr/local/packages/ecp`.



- `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 repository is public and was last pushed 2 minutes ago. It contains 7 tags. The 'Tags and Scans' section lists the following tags and their push times:

TAG	OS	PUSHED
latest	ppc64le	2 minutes ago
2020-11-04	ppc64le	a day ago
2020-11-01	ppc64le	4 days ago
2020-10-27	ppc64le	9 days ago

The 'Recent builds' section is currently empty, with a link to view build results. The 'Docker commands' section provides the command to push a new tag to the repository:

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

- 67 ECP Products
- Support for GPUs
  - NVIDIA (CUDA 10.2)
  - ppc64le and x86\_64

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

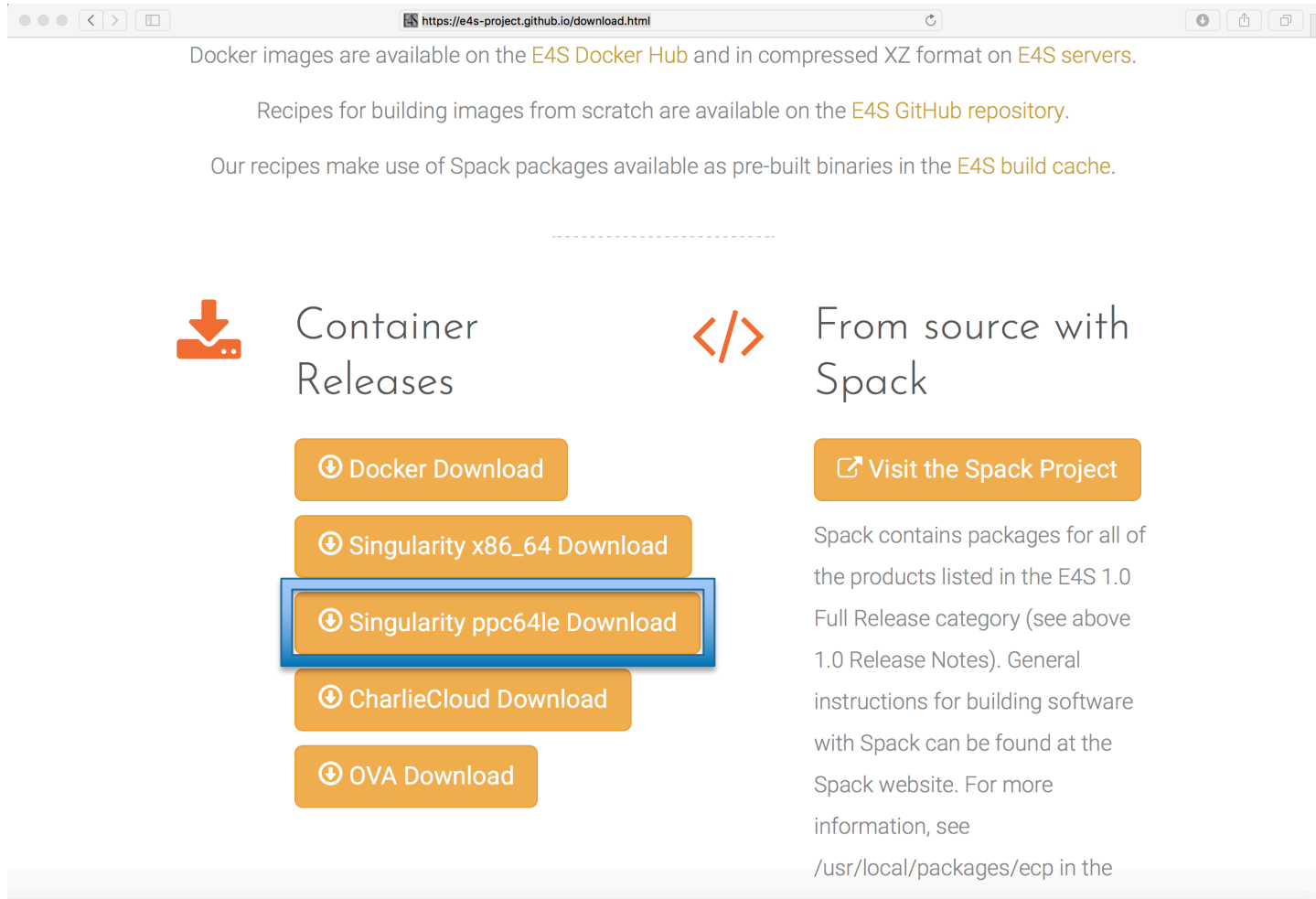
# E4S v1.2 GPU Release: 67 E4S Products (ppc64le)

```
1: adios2 /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/adios2-2.6.0-veoqi5iqkx4kbeddhxoroggvxqbtvos
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-20.10-4z5quvltq3fbzv5n6rrjv5byq7472emy
4: arborx /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/arborx-0.9-beta-p7lw7eobsrdpqwhb7ispxgphng2tn4nt
5: ascent /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/ascent-develop-7ktzsmvluqvd4xzoop7hjwddyjetn2ai
6: axom /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/axom-0.3.3-zfgqs6qa6vxlodjnaoeffmyl26czmp5
7: argobots /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/argobots-1.0-qra2gqxuisqqldbfrhwm5mvq2iga3l3l
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-2.4.0-6xzehuxs2updvdl2tdvcym3n6nf3y3l
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-r77asm5xkb256omn4trg5hnx3e376uy
13: flecsi /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/flecsi-1-2kxukdrijujvmsabmmj3um54ukhrayk
14: flit /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/flit-2.1.0-tepzltg6kmeffd4eo2rbzwmjeca56bmc
15: gasnet /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/gasnet-2020.3.0-uynuhs6itczckfpgbnlm2xgotvqmmeb6
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-pvjdzcg3fggpajcsorwidslflmomnz
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-yqayfprp2aleaxtzq543c75lcvcvviso7
21: hpx /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/hpx-1.5.1-tzfs3nkglsacequjxflokigwgjzabybk
22: hypre /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/hypre-2.20.0-ewmv445dkzmju4upg4rregq7apgkcdbu
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-q67khfosljacbl3djdj5jeh4thsl5p5f
27: libquo /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/libquo-1.3.1-syjf6c3adia34wlwneacynrwkhh72i3u
28: magma /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/magma-2.5.4-fzeektdrkybbuo6i6niikzglcwlnt2jx
29: mercury /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/mercury-1.0.1-ufxkkvb7osjnwgbfevdhtrmtuoj6dfbz
30: mfem /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/mfem-4.1.0-qrepufdzopbphsyuyc6nfn7k2tpprd5w
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-cr2ada5fjgkvdtmxel4zj6venfiif5e
```

# 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-ziz55mnp5r7l4kuhx4zqmjp2imjdvrk5
35: openmpi      /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/openmpi-3.1.6-utceq6uech6rgnabxevau4lhtzrwbaol
36: openpmd-api  /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/openpmd-api-0.12.0-szt65gmfb76iwdbcfkhryfztg5jwjd7g
37: papi         /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/papi-6.0.0.1-xu35qtffffq2ofyjjc3fafmj6yeijoih
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-svuejkorgi2bzhvghq4wts72bcjfn426r
40: pdt         /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/pdt-3.25.1-opxwliy5vqgt3hbla7qspf3laaqbt74
41: petsc       /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/petsc-3.14.0-phaqc52ryvhcib37qqjg2lmqdeqbl2uo
42: plasma     /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/plasma-20.9.20-vc4olrzgwsvx7mevom2j7mhsgb6ynam
43: precice    /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/precice-2.1.1-qlitin5qdhtz3n7rg4jjzxkds4qocvn
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-gzzlya6f4gr2xgsgpndmbp2pkffm3tuc
46: py-libensemble /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/py-libensemble-0.7.1-oe4zlxigkjc5nnkr6fyu7thzsnftvvu
47: py-petsc4py  /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/py-petsc4py-3.13.0-g2rp2v37qbp5fo5fmg6c4xtrj6shsbz
48: qthreads   /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/qthreads-1.14-bdpxlr2gf7knpek4vo5sjvzh5py5fdaf
49: raja       /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/raja-0.12.1-q32nuxmeowavkwzmoiw6f5md246tw66
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-2.0.0-2okrlxki5b63gzakjy2x4sbovrmeqmcx
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-gy5opc36suubh6uoiqy4l223psdyrilg
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-poufv43kq7tw2rw6upldbpcpabkpbdt
57: swig      /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/swig-4.0.2-3bdrfojvkrowa43v5so3ongbmhzzx5s
58: sz       /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/sz-2.1.10-fl5xazn2spjg46yaaaam5gftgyb5loa
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-olf4mdmym4sjobgue66gx42k7dbeb6z27
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-ynagdhefpcujnpeybxtaoqecr2p7bxj
64: unifyfs  /opt/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/unifyfs-0.9.0-sxsw3b5upcys4bxc5wdzcwvxn6emg
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-0.5.5-3r4a4s3qdeqbdabvwlswrgig62yc6yj
```

# 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

- [Container 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://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 edge 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. At the top, there's a navigation bar with 'docker hub' logo, a search bar containing 'ppc64le', and links for 'Explore', 'Repositories', 'Organizations', and 'Get Help'. The user profile 'exascaleproject' is visible. Below the navigation, a dropdown menu shows 'ecpe4s' and a search bar contains 'ppc64le'. A 'Create Repository +' button is present. The main content area lists three repositories:

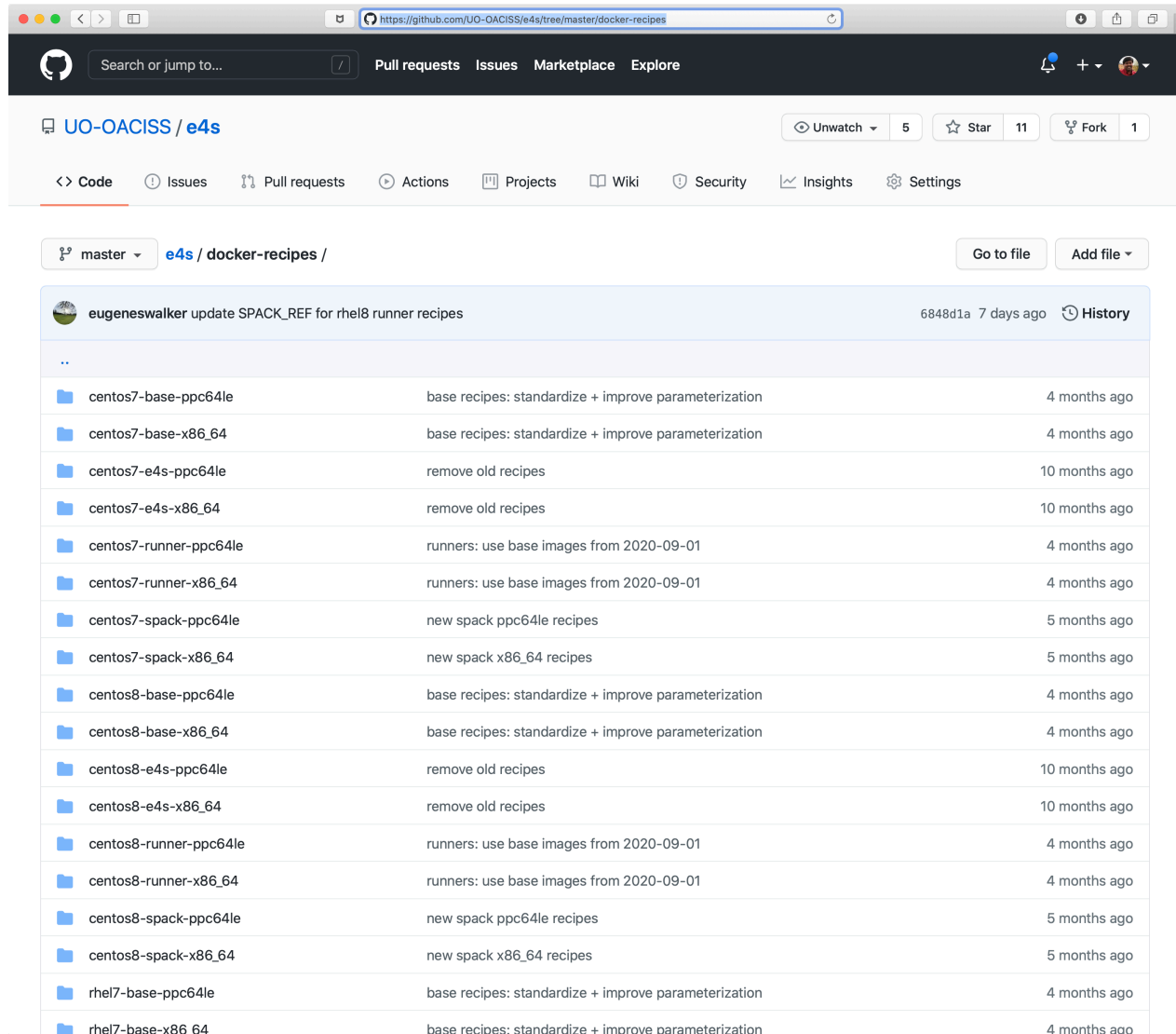
Repository Name	Stars	Downloads	Visibility
ecpe4s / <b>ubuntu1804_ppc64le_base</b> Updated 2 days ago	0	7	PUBLIC
ecpe4s / <b>ubi7_ppc64le_base</b> Updated 2 days ago	0	7	PUBLIC
ecpe4s / <b>centos7_ppc64le_base</b> Updated 2 days ago	0	10	PUBLIC

Below the list is a tip: "Tip: Not finding your repository? Try switching namespace via the top left dropdown." On the right side, there's an 'Organizations' section listing 'ecpcontainers', 'ecpe4s', and 'ecpsdk'. At the bottom right, there are two promotional banners: '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 repository has 5 pull requests, 11 stars, and 1 fork. The file tree view shows a directory structure for 'e4s / docker-recipes /'. The files are organized by platform and architecture, with descriptions and commit dates.

File Name	Description	Commit Date
..		
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-spacak-ppc64le	new spack ppc64le recipes	5 months ago
centos7-spacak-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-spacak-ppc64le	new spack ppc64le recipes	5 months ago
centos8-spacak-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

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 /
```

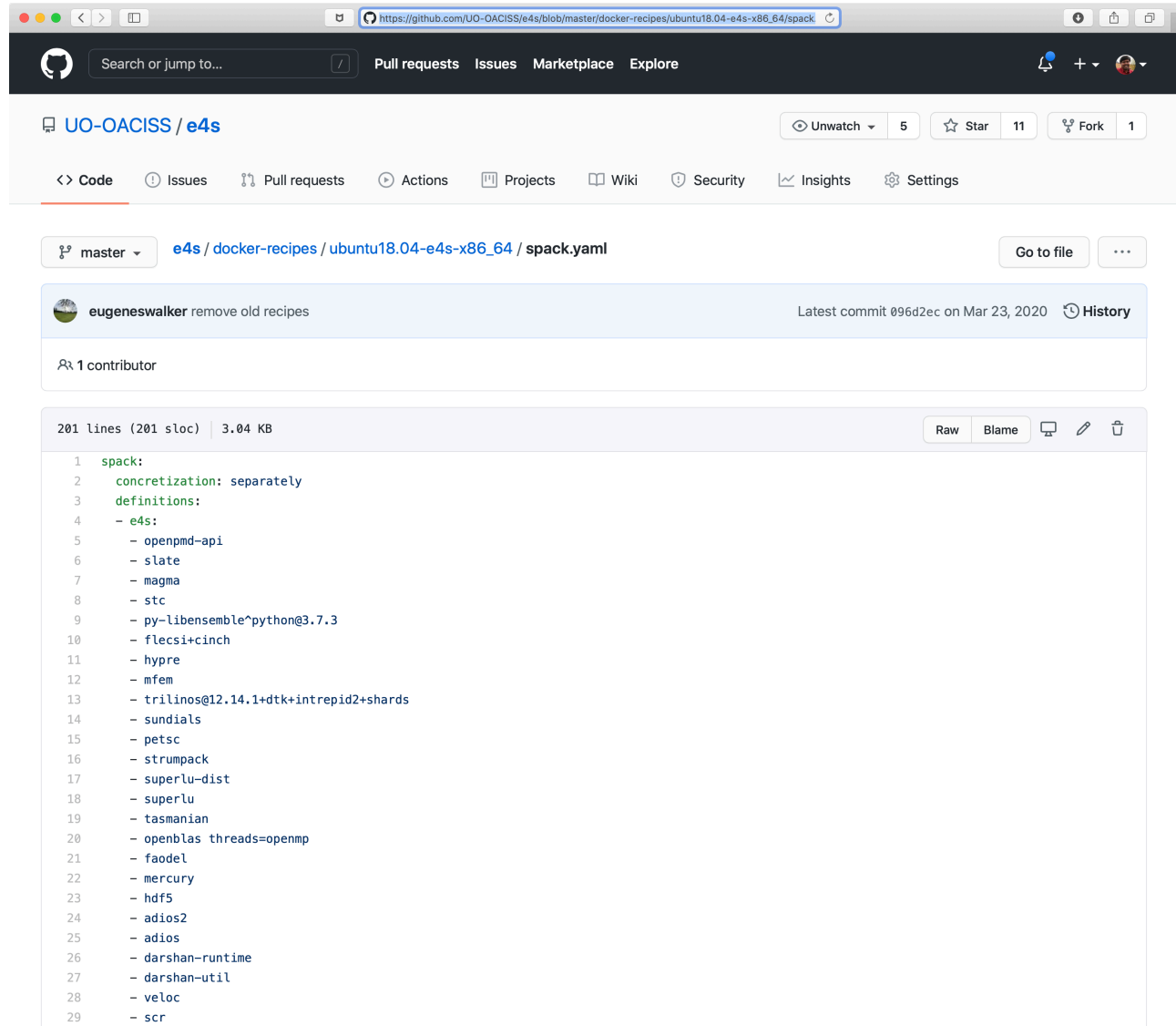
# E4S: Multi-platform Reproducible Docker Recipes

The screenshot shows a GitHub repository page for 'UO-OACISS / e4s'. The repository is located at <https://github.com/UO-OACISS/e4s/tree/master/docker-recipes/ubi7/ppc64le/base>. The repository has 3 pull requests, 2 stars, and 0 forks. The file structure is as follows:

File/Folder	Description	Last Commit
..		
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

- E4S
- x86\_64
  - ppc64le
  - aarch64

# E4S Spack environment spack.yaml



The screenshot shows a GitHub repository page for 'UO-OACISS / e4s'. The file 'spack.yaml' is selected, showing its content. The file is 201 lines long (201 sloc) and 3.04 KB. The content is a Spack environment definition for E4S on Ubuntu 18.04. The file lists various software packages to be installed, including openmpi, slate, magma, stc, py-libensemble, flecsi, cinch, hypre, mfem, trilinos, sundials, petsc, strumpack, superlu-dist, superlu, tasmanian, openblas, faodel, mercury, hdf5, adios2, adios, darshan-runtime, darshan-util, veloc, and scr.

```
1 spack:
2   concretization: separately
3   definitions:
4     - e4s:
5       - openmpi
6       - slate
7       - magma
8       - stc
9       - py-libensemble^python@3.7.3
10      - flecsi+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

**E4S Build Cache for Spack 0.16.0**

To use this build cache, just add it to your Spack

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

Click on one of the packages below to see a list of all available variants.

All Architectures
  PPC64LE
  X86\_64

All Operating Systems
  Centos 7
  Centos 8
  RHEL 7
  RHEL 8
  Ubuntu 18.04
  Ubuntu 20.04

Last updated: 12-15-2020 14:22 PST

27435 Spack packages

Search

adiak@0.1.1 adios2@2.5.0 adios2@2.6.0 adios@1.13.1 adlbox@0.9.2 adol-c@2.7.2 amg@1.2 aml@0.1.0 amrex@20.07  
 amrex@20.09 amrex@20.10 amrex@20.11  
**amrex@20.12**

Click on the full spec link to find out more.

Link	Arch	OS	Compiler	Created	Full Hash
<a href="#">Full Spec</a>	ppc64le	rhel8	gcc@8.3.1	12-14-2020 12:04 PST	q7fbvowel3gusfypqv5j54au4zj7fvb6
<a href="#">Full Spec</a>	ppc64le	ubuntu18.04	gcc@7.5.0	12-14-2020 12:06 PST	xskw37zx2qvrfigtm7fmw2ipnxzxucr
<a href="#">Full Spec</a>	ppc64le	ubuntu20.04	gcc@9.3.0	12-14-2020 12:08 PST	h6xbsawr23rsfxm4ikwbp67fmve6dtcb
<a href="#">Full Spec</a>	x86_64	ubuntu18.04	gcc@7.5.0	12-14-2020 12:07 PST	ngwoej4enmp2gzshys26d635kvpcog7
<a href="#">Full Spec</a>	x86_64	ubuntu20.04	gcc@9.3.0	12-14-2020 12:08 PST	etostybexmyty43kflvoyevdvh4vxoyd

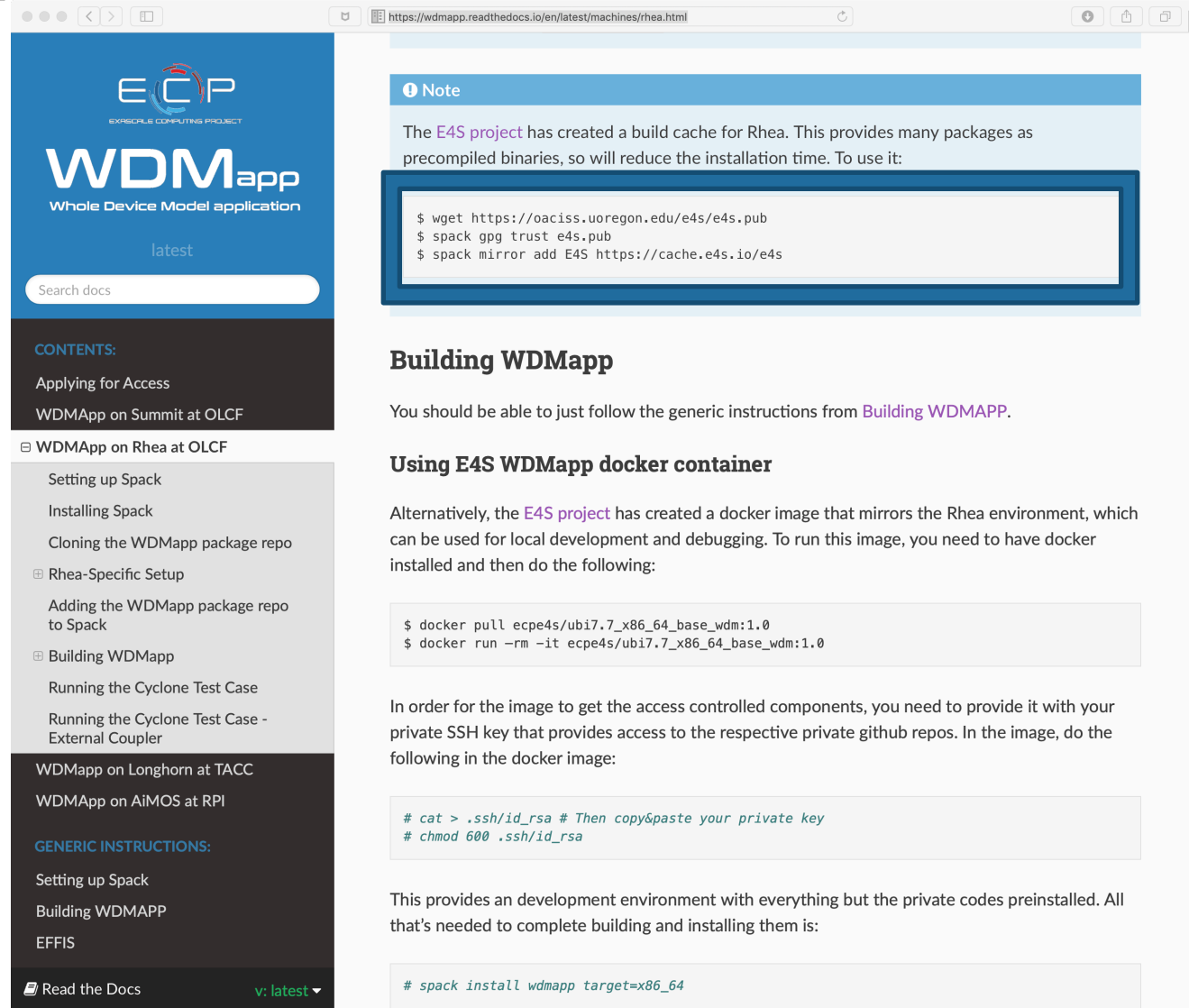
ant@1.10.0 ant@1.10.7 arborx@0.9-beta argobots@1.0 argobots@1.0rc1 argobots@1.0rc2 arpack-ng@3.7.0 arpack-ng@3.8.0  
 ascent@develop assimp@4.0.1 autoconf-archive@2019.01.06 autoconf@2.69 automake@1.16.1 automake@1.16.2 axl@0.1.1  
 axl@0.3.0 axom@0.3.3 axom@0.4.0 bash@5.0 bdfpcf@1.0.5 berkeley-db@18.1.40 berkeley-db@6.2.32 binutils@2.31.1

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

• <https://oaciss.uoregon.edu/e4s/inventory.html>



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



The screenshot shows the WDMApp documentation website. The left sidebar contains a navigation menu with sections like 'CONTENTS:', 'WDMApp on Rhea at OLCF', and 'GENERIC INSTRUCTIONS:'. The main content area features a 'Note' section with a blue header, followed by a terminal code block containing three commands for setting up the E4S build cache. Below this, there are sections for 'Building WDMApp' and 'Using E4S WDMApp docker container', each with a terminal code block showing Docker commands and SSH key setup instructions.

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

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

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

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

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

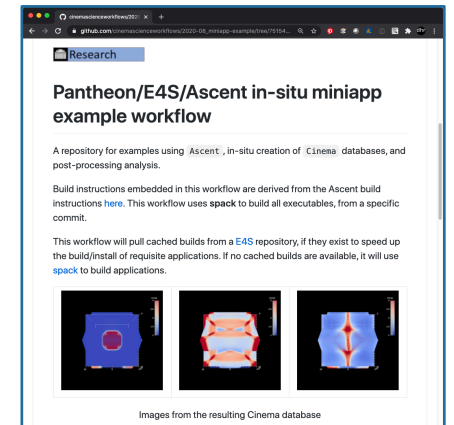
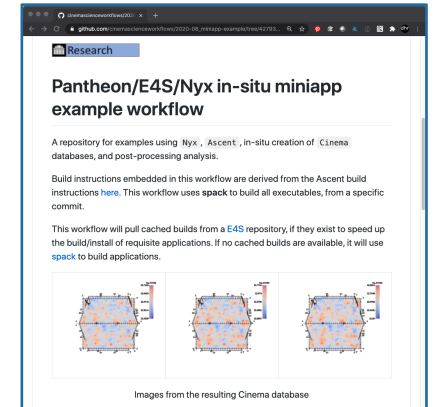
# Pantheon and E4S build cache support end-to-end ECP examples

**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.

LA-UR-20-27327 1/13/21



# 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 the GitHub repository page for `E4S-Project/testsuite`. The repository is on the `master` branch, and the current view is the `validation_tests/magma` directory. The file tree shows the following files and their commit history:

File	Description	Commit Time
..		
Makefile	use env variables set by `spack load`	4 months ago
README.txt	Added basic magma test.	11 months ago
clean.sh	Added basic magma test.	11 months ago
compile.sh	use bash -xe in compile/run.sh	9 hours ago
example_f.F90	Added basic magma test.	11 months ago
example_sparse.c	Added basic magma test.	11 months ago
example_sparse_operator.c	Added basic magma test.	11 months ago
example_v1.c	Added basic magma test.	11 months ago
example_v2.c	Added basic magma test.	11 months ago
run.sh	use bash -xe in compile/run.sh	9 hours ago
setup.sh	Remove some .o files. Don't load special openblas. Don't specify spec...	3 months ago

The `README.txt` file content is as follows:

```
Getting started with MAGMA.

This is a simple, standalone example to show how to use MAGMA, once it is
compiled. More involved examples for individual routines are in the testing
directory. The testing code includes some extra utilities that we use for
testing, such as testings.h and libtest.a, which are not required to use MAGMA,
though you may use them if desired.

-----
C example

See example_v2.c for sample code.

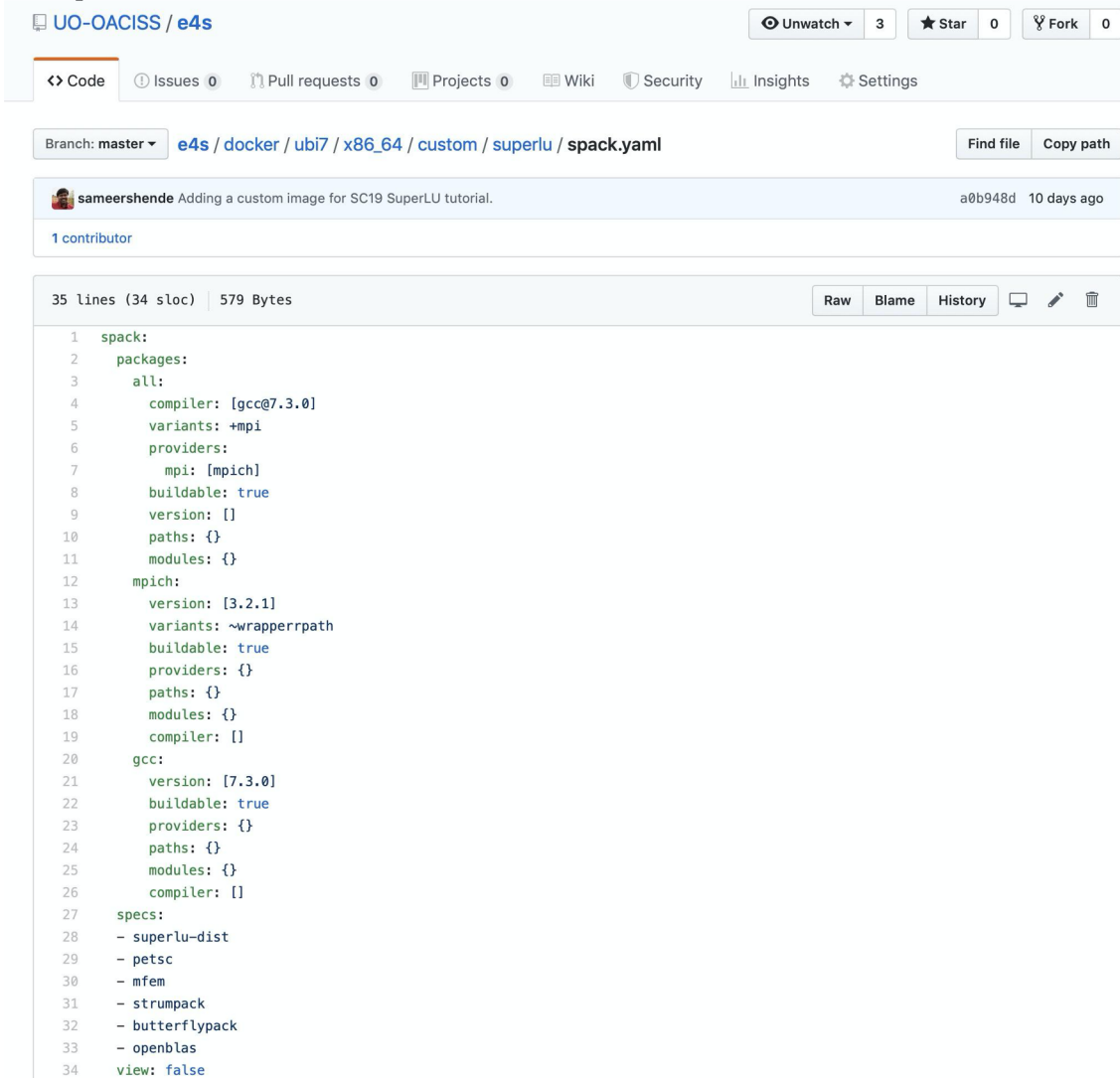
Include the MAGMA header:

#include "magma_v2.h"

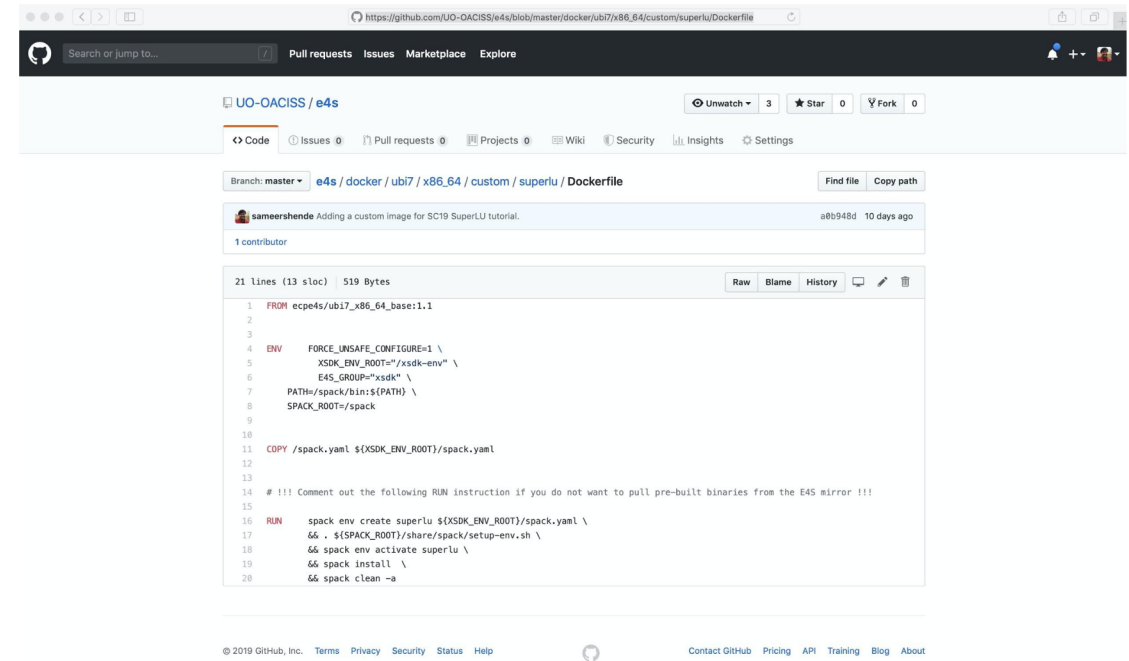
(For the legacy MAGMA v1 interface, see example_v1.c. It includes magma.h
instead. By default, magma.h includes the legacy cuBLAS v1 interface (cublas.h).
You can include cublas_v2.h before magma.h if desired.)
```

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

# Reproducible Container Builds using E4S Base Images



```
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    mpich:
13      version: [3.2.1]
14      variants: ~wrapperrpath
15      buildable: true
16      providers: {}
17      paths: {}
18      modules: {}
19      compiler: []
20    gcc:
21      version: [7.3.0]
22      buildable: true
23      providers: {}
24      paths: {}
25      modules: {}
26      compiler: []
27  specs:
28  - superlu-dist
29  - petsc
30  - mfem
31  - strumpack
32  - butterflypack
33  - openblas
34  view: false
```



```
1 FROM ecpe4s/ubi7_x86_64_base:1.1
2
3
4 ENV FORCE_UNSAFE_CONFIGURE=1 \
5     XSDK_ENV_ROOT="/xsdk-env" \
6     E4S_GROUP="xsdk" \
7     PATH="/spack/bin:${PATH}" \
8     SPACK_ROOT="/spack"
9
10
11 COPY /spack.yaml ${XSDK_ENV_ROOT}/spack.yaml
12
13
14 # !!! Comment out the following RUN instruction if you do not want to pull pre-built binaries from the E4S mirror !!!
15
16 RUN spack env create superlu ${XSDK_ENV_ROOT}/spack.yaml \
17     && . ${SPACK_ROOT}/share/spack/setup-env.sh \
18     && spack env activate superlu \
19     && spack install \
20     && spack clean ->
```

- 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 the Docker Hub interface with search filters for 'ecpe4s' and 'ppc64le'. A list of seven repositories is displayed, each with its name, update time, scan status, star count, download count, and visibility.

Repository Name	Updated	Not Scanned	Stars	Downloads	Visibility
ecpe4s / ubuntu18.04-e4s-gpu-ppc64le	Updated an hour ago	Not Scanned	0	61	Public
ecpe4s / centos7-runner-ppc64le	Updated a month ago	Not Scanned	0	2.9K	Public
ecpe4s / centos8-runner-ppc64le	Updated a month ago	Not Scanned	0	37	Public
ecpe4s / ubuntu20.04-runner-ppc64le	Updated a month ago	Not Scanned	0	575	Public
ecpe4s / rhel8-runner-ppc64le	Updated a month ago	Not Scanned	0	477	Public
ecpe4s / ubuntu18.04-runner-ppc64le	Updated a month ago	Not Scanned	0	3.9K	Public
ecpe4s / rhel7-runner-ppc64le	Updated a month ago	Not Scanned	0	3.8K	Public

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

# University of Oregon GitLab CI

### E4S Builds:

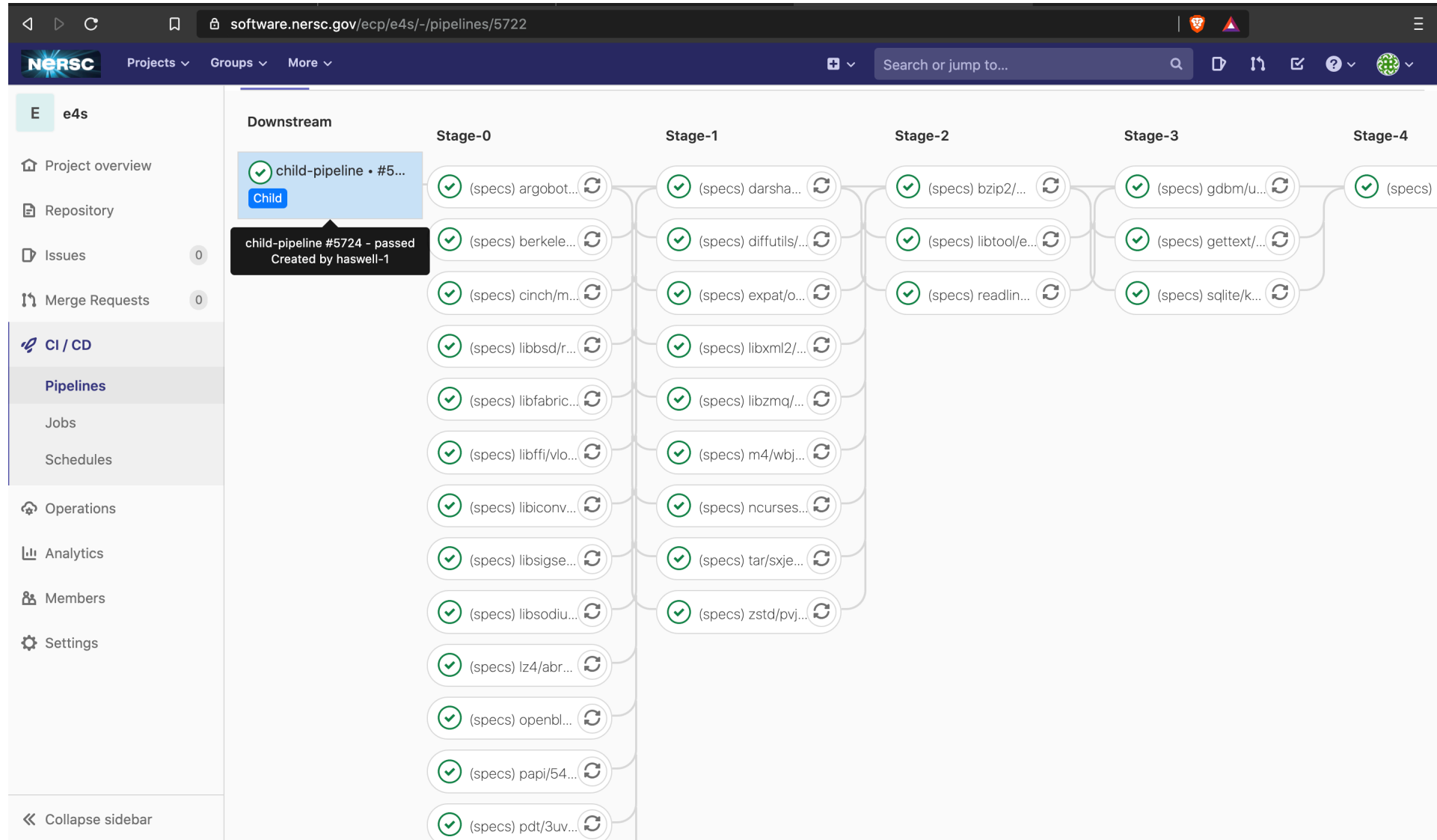
- Ubuntu 18.04
- Ubuntu 20.04
- RHEL 7.6
- RHEL 8
- CentOS 7
- CentOS 8

Architectures:  
ppc64le and x86\_64

The screenshot shows the GitLab CI interface for a pipeline. The left sidebar contains navigation options: Project overview, Repository, CI / CD (selected), Pipelines, Jobs, Schedules, Operations, Analytics, and Settings. The main area displays the pipeline stages: Concretize, Trigger Builds, and Downstream. Each stage contains a list of jobs with their names and status (all are successful, indicated by green checkmarks). The Downstream stage shows a vertical list of jobs, each labeled as a 'Child'.

Stage	Job Name	Status
Concretize	centos7-amd64-0	Success
	centos8-amd64-0	Success
	rhel7-amd64-0	Success
	rhel7-ppc64le-0	Success
	rhel8-amd64-0	Success
	ubuntu18.04-amd64-0	Success
	ubuntu18.04-ppc64le-0	Success
	ubuntu20.04-amd64-0	Success
Trigger Builds	centos7-amd64-1	Success
	centos8-amd64-1	Success
	rhel7-amd64-1	Success
	rhel7-ppc64le-1	Success
	rhel8-amd64-1	Success
	ubuntu18.04-amd64-1	Success
	ubuntu18.04-ppc64le-1	Success
	ubuntu20.04-amd64-1	Success
Downstream	e4s #881	Success
	e4s #882	Success
	e4s #883	Success
	e4s #885	Success
	e4s #884	Success
	e4s #886	Success
	e4s #887	Success
	e4s #888	Success
	e4s #889	Success

# Multi-stage E4S CI Build Pipeline on Cori, NERSC



# ORNL GitLab Build Pipeline for E4S Spack Build Cache

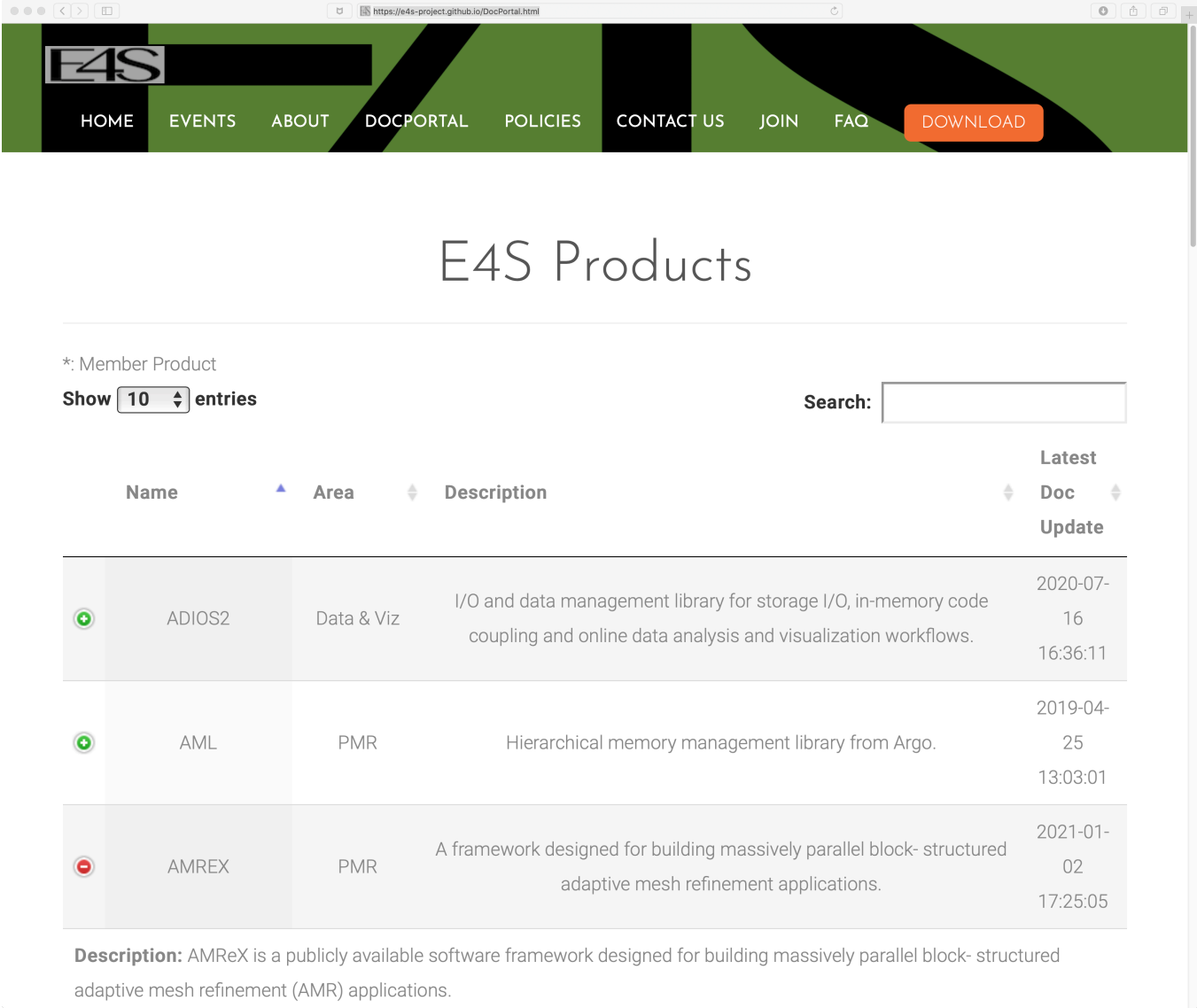
The screenshot shows a GitLab CI/CD pipeline for the 'e4s' project. The pipeline is organized into five stages, each containing multiple jobs. All jobs are marked with a green checkmark, indicating successful completion. The jobs are arranged in a grid-like structure, with each job in a stage depending on the completion of jobs in the previous stage. The jobs are labeled with their names and IDs, such as '(specs) cinch/bf...', '(specs) libbsd/cr...', etc. The pipeline is titled 'Pipeline Jobs 58'.

- 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 website. At the top is a navigation bar with the E4S logo and links for HOME, EVENTS, ABOUT, DOCPORTAL, POLICIES, CONTACT US, JOIN, FAQ, and a DOWNLOAD button. The main heading is "E4S Products". Below this, there is a search bar and a "Show 10 entries" dropdown. A table lists three products: ADIOS2, AML, and AMREX. Each row includes a status icon (green plus for ADIOS2 and AML, red minus for AMREX), the product name, area, description, and the latest document update date and time.

\*: Member Product

Show  entries

Search:

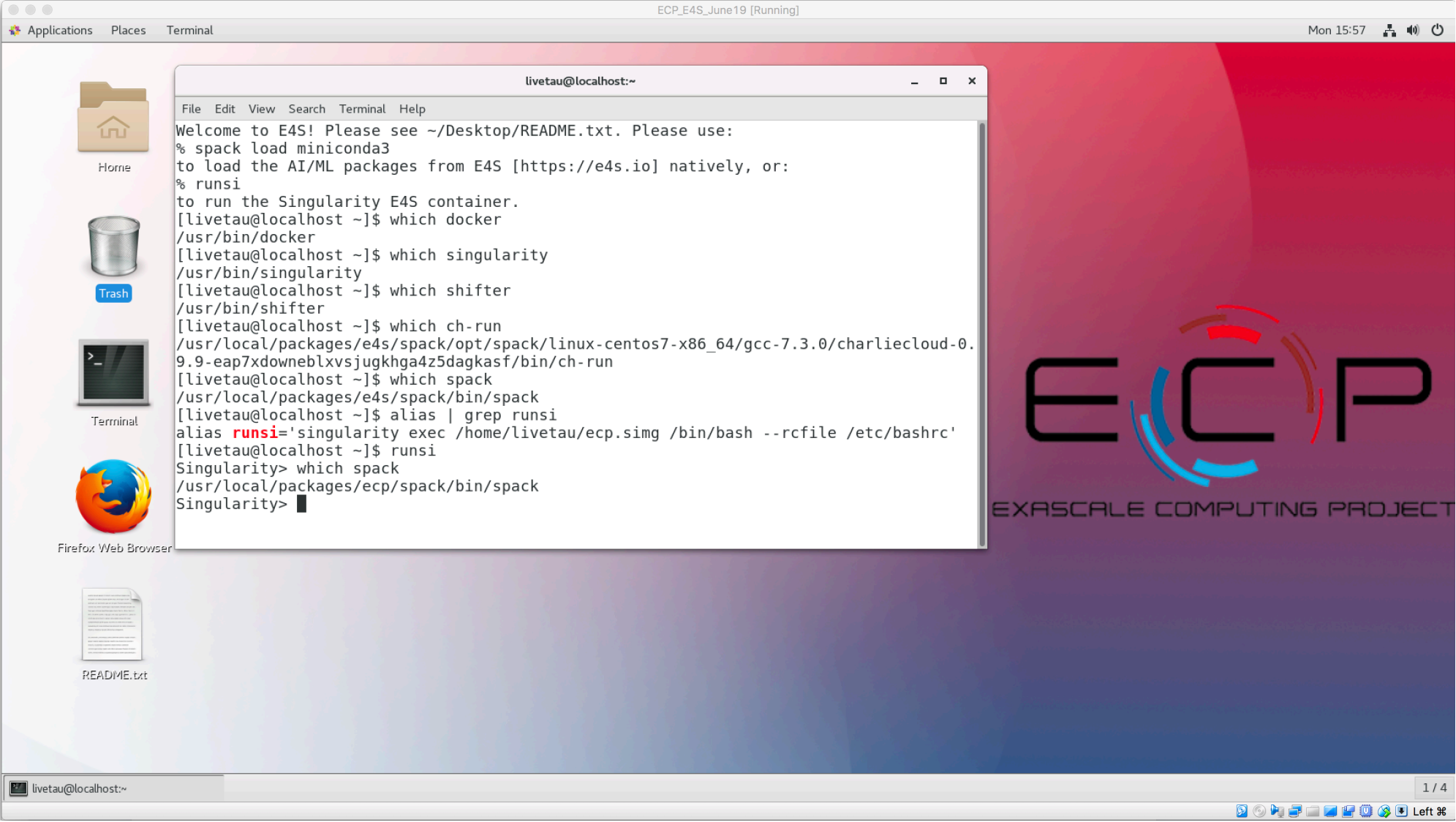
	Name	Area	Description	Latest Doc Update
	ADIOS2	Data & Viz	I/O and data management library for storage I/O, in-memory code coupling and online data analysis and visualization workflows.	2020-07-16 16:36:11
	AML	PMR	Hierarchical memory management library from Argo.	2019-04-25 13:03:01
	AMREX	PMR	A framework 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

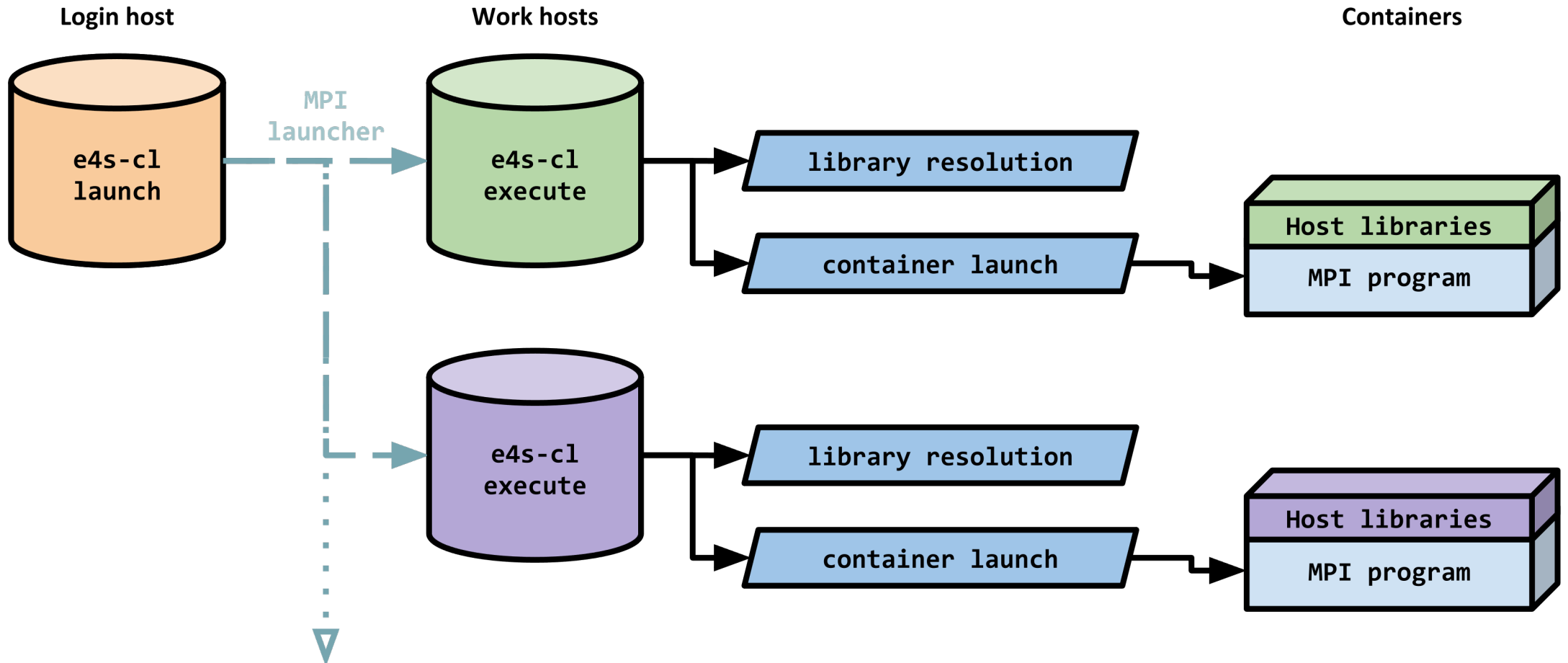


- Container Runtimes
- Docker
  - Shifter
  - Singularity
  - Charliecloud

# 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



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