E4S Overview and Demo

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2nd E4S Forum Workshop at EuroMPI/USA 2020
via Zoom

Sameer Shende
Performance Research Laboratory, OACISS, University of Oregon

https://e4s.io

ECP EXASCALE COMPUTING PROJECT
NNSA National Nuclear Security Administration
U.S. DEPARTMENT OF ENERGY | Office of Science

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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 (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

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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.

https://e4s.io

Spack

- E4S uses the Spack package manager for software delivery
- Spack provides the ability to specify versions of software packages that are and are not interoperable.
- Spack is a build layer for not only E4S software, but also a large collection of software tools and libraries outside of ECP ST.
- Spack supports achieving and maintaining interoperability between ST software packages.
- https://spack.io

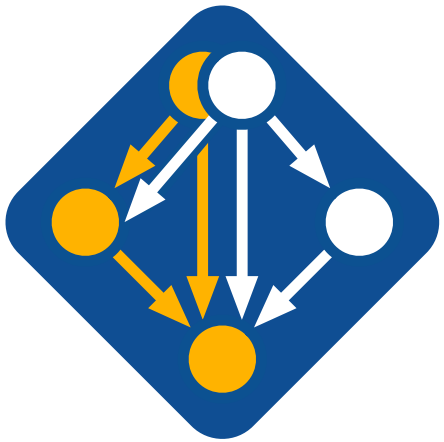
Spack enables software distribution for HPC

No installation required: clone and go

```
$ git clone https://github.com/spack/spack
$ spack install tau
```

```
$ spack install tau                                                  unconstrained
$ spack install tau@2.29.1                                           @ custom version
$ spack install tau@2.29.1 %gcc@7.3.0                                % custom compiler
$ spack install tau@2.29.1 %gcc@7.3.0 +mpi+python+pthreads           +/- build option
$ spack install tau@2.29.1 %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



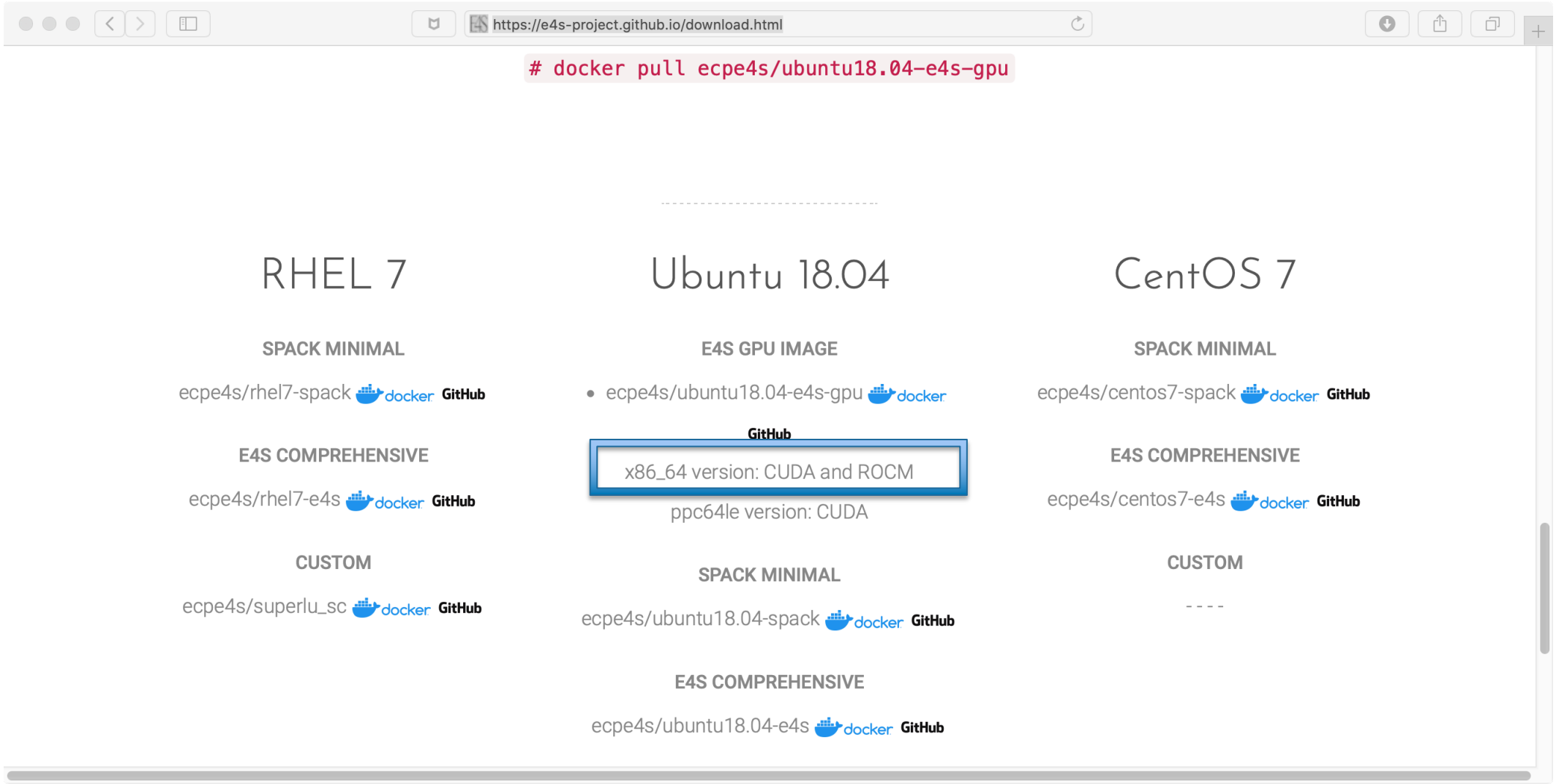
github.com/spack/spack

E4S Components

- E4S is a curated release of ECP ST products based on Spack [http://spack.io].
- E4S Spack cache to support bare-metal installs at facilities and custom container builds:
  - x86_64, ppc64le, and aarch64
- Container images on DockerHub and E4S website of pre-built binaries of ECP ST products.
- Base images and full featured containers with support for GPUs.
- GitHub recipes for creating custom images from base images.
- e4s-cl for container launch and for replacing MPI in application with system MPI libraries.
- Validation test suite on GitHub provides automated build and run tests.
- Automates build process via GitLab Continuous Integration to ensure packages can be built.
- E4S Doc Portal aggregates and summarizes documentation and metadata by raking product repos.
- E4S VirtualBox image with support for Docker, Shifter, Singularity, and Charliecloud runtimes.
- AWS image to deploy E4S on EC2.
- GCP image to deploy E4S.

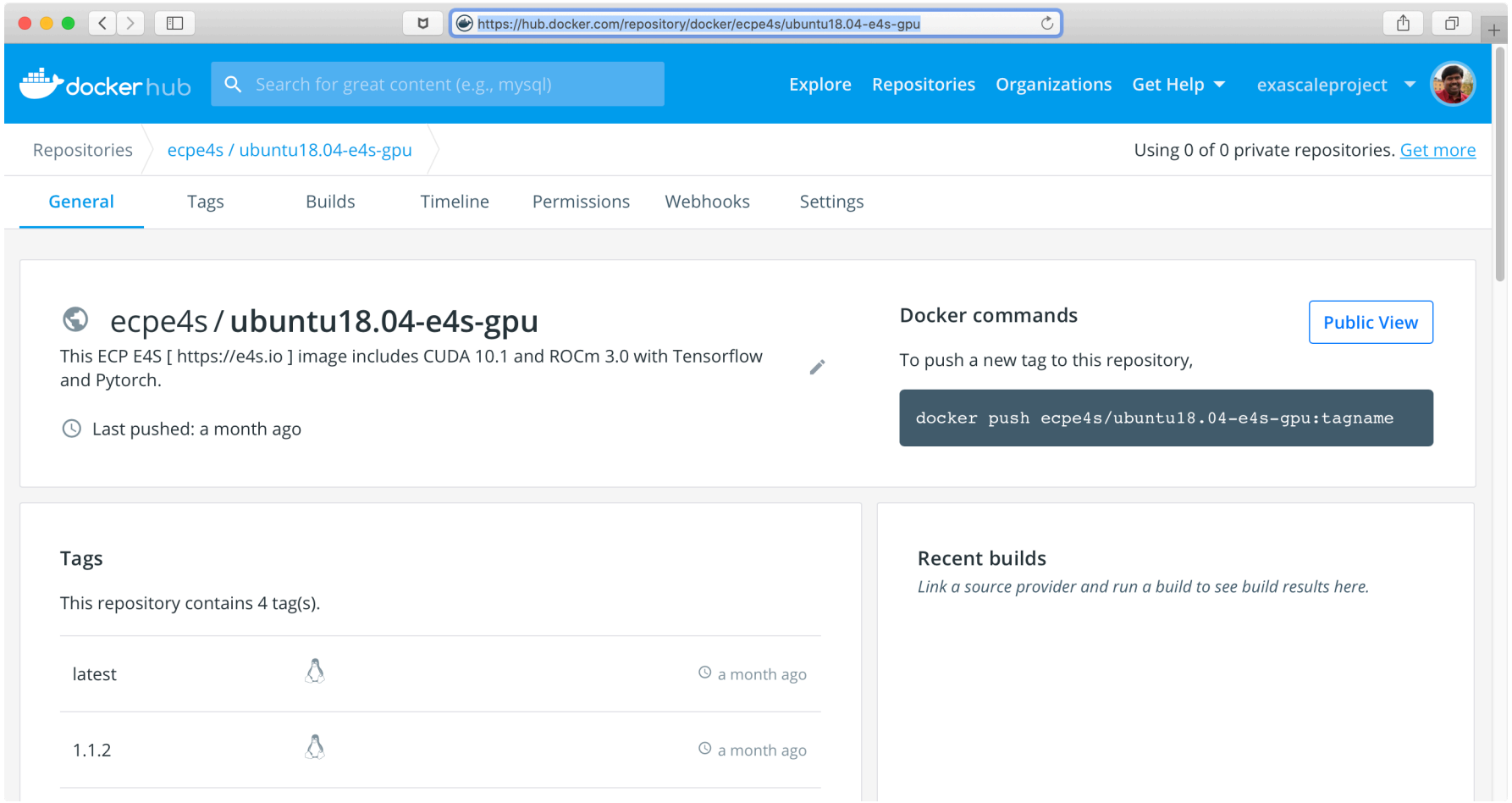
https://e4s.io

Download E4S v1.1 GPU image



https://e4s.io

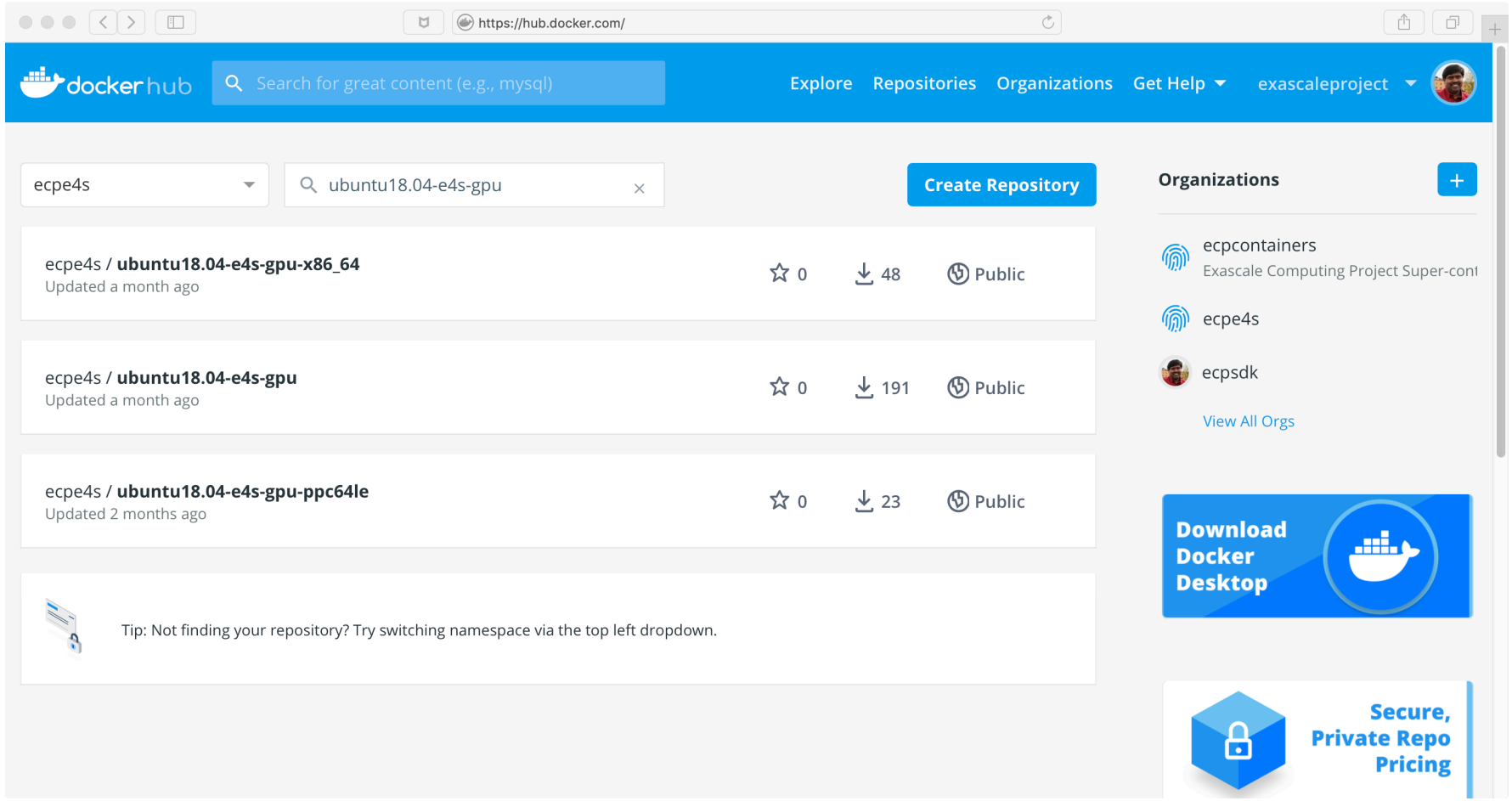
E4S v1.1 Release Available at DockerHub



- 50 ECP ST Products
- Support for GPUs
  - AMD (ROCm 3.0)
  - NVIDIA (CUDA 10.1)
  - x86_64

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

E4S v1.1 Release at DockerHub: GPU Support



- 45+ ECP ST Products
- Support for GPUs
  - NVIDIA (CUDA 10.1.243)
  - ppc64le

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

E4S v1.1.2 GPU Release for x86_64

```
1: adios        /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/adios-1.13.1-debxolyd5skx27s6ngtacb7enrcsfq64
2: aml  /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/aml-0.1.0-xdrekw6u7gr556xd6amyxcerhg5v4wcs
3: argobots     /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/argobots-1.0rc1-yrhx37ohi2vlxai6vcmtznqttletxejs
4: bolt         /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/bolt-1.0rc2-danzb3khhuosggmdjqpux4424rqr7zpa
5: caliper      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/caliper-2.0.1-hzze6uvf5e2eklzebxyzatjuxo3xgwkr
6: darshan-runtime      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/darshan-runtime-3.1.7-wscbtntqfiupsp7edyqsibhvm55a6vse
7: dyninst      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/dyninst-10.1.0-fttqy2zoqsbpcqil6ur5cevssashha2c
8: faodel       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/faodel-1.1906.1-ky5irwwreweac2bsml7w7x2szsvkkhz7
9: flecsi       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/flecsi-develop-fxq6sbr5oryertnaf4brpzs2ejshevbt
10: gasnet      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/gasnet-2019.3.0-47idkg4gcemcvtejschfcjka6cz7l64n
11: geopm       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/geopm-1.0.0-rc2-chxnuparg2hhaw4yworkqfhp36n7kxgk
12: globalarrays        /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/globalarrays-5.7-bl4hhz32b2yw64wjtoan3fafjkkj7nqk
13: gotcha      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/gotcha-1.0.2-gggazxidw2wbolux7q7n2m53nxccu3i2
14: hdf5        /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/hdf5-1.10.5-qdkkei6imkjoma5nd4jwbm6xphlkm4yp
15: hpctoolkit  /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/hpctoolkit-2019.08.14-2iwddpemc4q64pvxmd6ys5oicmyr3lyr
16: hypre       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/hypre-2.18.1-3sh6dcavpdxwd4ddykp4zer7fmqhay54
17: kokkos      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/kokkos-2.9.00-jp35xv6moqehjrynzoenj2kzpxski6cz
18: legion      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/legion-19.06.0-yf6lxznv47faxs2jf3etl74roskksvum
19: libnrm      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/libnrm-0.1.0-e7eixtdo6bz7o4dervwvpo3sb2jqfxud
20: libquo      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/libquo-1.3-l67575wypddpd5tigchg2iu4kkacmj3r
21: magma       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/magma-2.5.1-mtqtn6ad3qtfwwf5fvdc2igzccu43yhk
22: mercury     /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/mercury-1.0.1-nena7d7vhigm56abtr44jospgoymau4t
23: mfem        /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/mfem-4.0.0-ef2xjvix7qkbd6tmcith3yailtwjviul
24: mpich       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/mpich-3.2.1-yi7oup5retdgtafg3hyhrixwdjdnaxtg
25: mpifileutils        /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/mpifileutils-develop-4lo3yspw6662oc2o6oj7iv77kdnh6vtt
26: ninja       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/ninja-1.9.0-rtsvo2vqkm5dscr3sbszigdsqybm5f6c
27: openmpi     /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/openmpi-3.1.4-suwdembrvnjs6zj7roh4577ggk2wnnpc
28: papi        /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/papi-5.7.0-bdebmghm5lypkvzv3av4fmy2idvqsemb
29: papyrus     /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/papyrus-develop-bknq744bwrf4g24ucqhqk5o4bonwi4ws
30: parallel-netcdf     /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/parallel-netcdf-1.11.2-lmkvcp7xspmgob2a6v4mgoso5whlxtg4
31: pdt         /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/pdt-3.25.1-qn7v7q63nj4dxruluce7m2bqk4xatel2
32: petsc       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/petsc-3.12.1-u3ejzehj42b2t7s5xuictuhn7xxs5rxi
33: py-jupyter-notebook         /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/py-jupyter-notebook-4.2.3-styyzua7dtfm2bysot62suev4k4ezube
34: py-libensemble      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/py-libensemble-0.5.2-esfqkggd3gzpntocgoiwbgygxig5kbhy
35: qthreads    /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/qthreads-1.14-wdbuioiajj4j6pmw656nfy7qm3n7le6e
36: raja        /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/raja-0.8.0-fojlfngsdkl53id5ennuioxy52y36sdp
37: rempi       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/rempi-1.1.0-lpcvnsu5oo77uubhqrcbjrs3c5clfo3x
38: scr         /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/scr-1.2.2-u3wzsilfsyh3qqpnxpiqxs22iqxwfuis
39: strumpack   /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/strumpack-3.1.1-qrutcou5g3mf2efluktbmybcjdxu2crv
40: sundials    /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/sundials-5.0.0-4sx2ndxfzgwexxkn72mqrsu6ouoetf33
41: superlu-dist        /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/superlu-dist-6.1.1-sp4dikmr6lhmm5vlemwhx6snsudxlm62
42: sz  /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/sz-2.0.2.0-tvqs6j3rlfpl66kdwf5in3ofgdylqsmw
43: tasmanian   /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/tasmanian-7.0-ls2iqflhjstlrx5jqyfy5gvj6qbz7k7d
44: tau         /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/tau-2.29-2eoqgqfon3bjop6qd7tinrjd3wydc6jj
45: trilinos    /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/trilinos-12.14.1-zurt5mzx456bhtb2pc3w3na5atbqm6u3
46: umpire      /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/umpire-0.3.3-om5obb6t6lu7xbksrcfhhitzzt62mzgl
47: unifyfs     /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/unifyfs-develop-hlev5zptypluz37rkkeqgmxwifdkplrr
48: upcxx       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/upcxx-2019.9.0-54ryimkhwwecrhmsmgweev5ku5zvsdf7
49: veloc       /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/veloc-1.1-j2x7hcglj6grgi3w5kgcq6lomdvace3q
50: zfp         /spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.3.0/zfp-0.5.5-tlhrqw3ogejcrizc54kja3xruyrdvlwd
```

- 50 ECP ST products
- Ubuntu v18.04 x86_64
- 5.3 GB compressed image
- AI/ML package support
  - TensorFlow
  - PyTorch
- Support for GPUs
  - AMD ROCm 3.1
  - NVIDIA CUDA 10.1.248

E4S v1.1 GPU Release for ppc64le

```
1: adios        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/adios-1.13.1-ryfsxpqaab6rkefscdy3qdba47eeh5fe
2: aml  /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/aml-0.1.0-ftizegmvpbweuyzg75g3ndzhdyjx37op
3: argobots     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/argobots-1.0rc1-xjjrxwo2molgdesfwjyojaiwj24rxp3h
4: caliper      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/caliper-2.0.1-lzff2xp2eg7jqrmgy4k2ifbiii7zmpas
5: darshan-runtime      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/darshan-runtime-3.1.7-jgyzjuukvxpwjrzeaweaukygyg7q6jxz
6: dyninst      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/dyninst-10.1.0-2ayefefqh74xwuadlbs3d6p2zyammmsf
7: flecsi       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/flecsi-develop-3v4qqtzsnja6dt4lr5pps3cxv3hy6to2
8: gasnet       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/gasnet-2019.3.0-n4tdzzd4hvy6zexy7bhe4qryzbcfkoif
9: globalarrays         /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/globalarrays-5.7-ilibm5yzx6draxpkfo5t3d4csx5g64nu
10: gotcha      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/gotcha-1.0.2-h3qq2jz6a2ihwibdqndbfehh4pnmjr3z
11: hdf5        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/hdf5-1.10.5-lgnifkbzs3p6ojothkjg53wf6hut4xqv
12: hpctoolkit  /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/hpctoolkit-2019.08.14-vljantrum36jbdlzz37tynacw3ee2yhk
13: hypre       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/hypre-2.18.1-pj2krvlyc5bnjpq742a5xvk6k53r5ita
14: kokkos      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/kokkos-2.9.00-7h2cg7o3kdu23qymnfyqwsewruvwkxgr
15: legion      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/legion-19.06.0-7ksiuqzq57y24t5kl6s2n4ffqdpnlupg
16: libnrm      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/libnrm-0.1.0-5yet3aafh2rp3wuapixphq3mwykiqyqn
17: libquo      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/libquo-1.3-ul26vaqh6kl6vmqh4pj4esm7ztelbpfo
18: mercury     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/mercury-1.0.1-akxk7fk6mdbp2m5wxdaum3lehlb7dt24
19: mfem        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/mfem-4.0.0-bdte6oktrcnaktwi7qjj72pisial5krb
20: mpich       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/mpich-3.2.1-sb2fna3i4s4feofy6swrr6wivzyyu7he
21: mpifileutils        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/mpifileutils-develop-r3s7t6qzgqb4y4hpd5mzldbtskhvlqfj
22: ninja       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/ninja-1.9.0-pxjz2hyrn24ar65hqwcou7rvgafvylos
23: openmpi     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/openmpi-3.1.4-cty2bl5wikxipkgzlpu32xtmpqxzua2v
24: papi        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/papi-5.7.0-eaabymcif7c5dvjdejevnqkgat7recfp
25: papyrus     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/papyrus-develop-nu56mejweub56zjuexidml2t4o664zug
26: parallel-netcdf     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/parallel-netcdf-1.11.2-zxyjkdz4yxmyxcgyarcym5fqec4paj56
27: pdt         /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/pdt-3.25.1-czegb3ismtstyml2wugkifojybw4cacs
28: petsc       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/petsc-3.12.1-q6pm6wyb43hlc6ndpvrkphvwntbt3xul
29: py-jupyter-notebook         /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/py-jupyter-notebook-4.2.3-qky73g3q6kapsva7ishirewe3qtapxhk
30: py-libensemble      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/py-libensemble-0.5.2-gz4rxbjd5lku5lt6ji6lyf2f6qoafuzt
31: qthreads    /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/qthreads-1.14-jjpfrqevnacp6dhd5or6vz4obckmy4ah
32: raja        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/raja-0.8.0-mhamgpur67esmyekjpclfvlv6fdngod6
33: rempi       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/rempi-1.1.0-feg2oeofieeanoloaxulawxdeaqnqftj
34: scr         /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/scr-1.2.2-5sepujyr7dp5eioymphnqva4atcjfc4e
35: strumpack   /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/strumpack-3.1.1-jd7ytfdr4saggdbxx3khjy2jamlfbru4
36: sundials    /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/sundials-5.0.0-cjkp7zluit5jtm6eqd74mavwko5thr2w
37: superlu-dist        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/superlu-dist-6.1.1-6gklgz5snhaipunjjtirlo46zq76zd2d
38: sz  /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/sz-1.4.12.3-7bnst7vnpuajazlagxtot46oih4caoqa
39: tasmanian   /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/tasmanian-7.0-e3r2dvv5nnpg7yafs5hzcocvkmxaf7pn
40: tau         /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/tau-2.29-3eb5tlvcnukpkd2pls4z7ivhtc2ld7jm
41: trilinos    /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/trilinos-12.14.1-jcikf6anps63huaohpymnm4xohgrrral
42: umpire      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/umpire-0.3.3-bnxsv2cla4yc42mvfhvwlk7suylmbcou
43: unifyfs     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/unifyfs-develop-fqzlm2dhtbnb2aeggadfcue2mkv74sco
44: upcxx       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/upcxx-2019.9.0-ndrqyemtolmjk7i3dduekjbt4i3uo2jz
45: veloc       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/veloc-1.1-h723o37b5mowzewdzqburtrawnb5ynhi
46: zfp         /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/zfp-0.5.5-3r4a4s3qdeqbdabvlwlswrgig62yc6yj
```

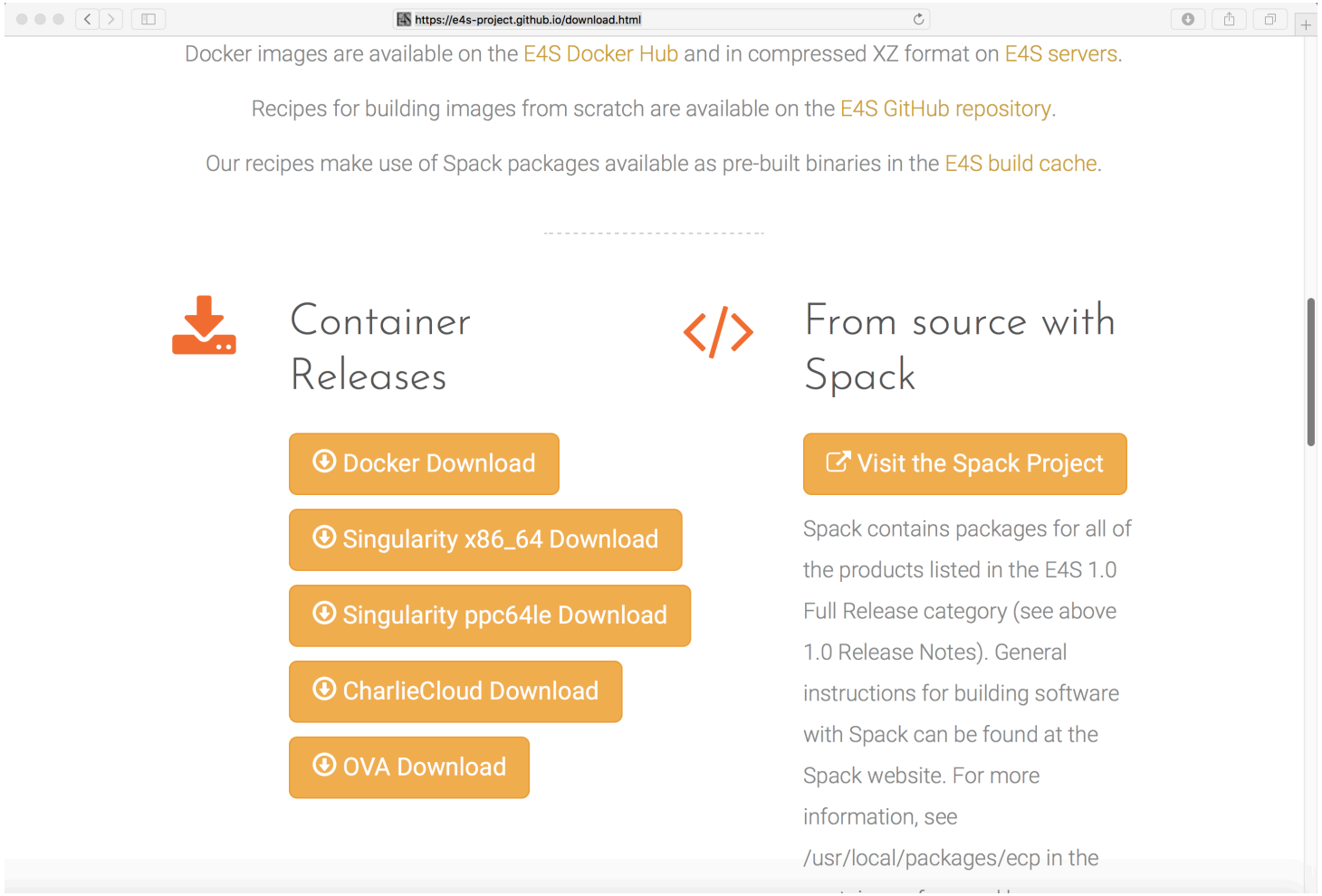
- 46 ECP ST products
- Ubuntu v18.04 ppc64le
- AI/ML package support
  - TensorFlow
  - PyTorch
- Support for GPUs
  - NVIDIA CUDA 10.1

`spack find` shows what is installed

```
5. root@3b983c57f123: / (ssh)
sameer@minotaur:~$ docker run -v $HOME:/home/sameer -it ecpe4s/ubuntu18.04-ppc64le-e4s
root@3b983c57f123:/# which spack
/spack/bin/spack
root@3b983c57f123:/# spack find
==> 235 installed packages
-- linux-ubuntu18.04-ppc64le / gcc@7.3.0 ------------------------
adios@1.13.1            hdf5@1.10.5             lua-luafilesystem@1_7_0_2  py-async-generator@1.10  py-pexpect@4.6.0          raja@0.8.0
aml@0.1.0               hdf5@1.10.5             lua-luaposix@33.4.0        py-babel@2.7.0           py-pickleshare@0.7.4      rankstr@0.0.2
argobots@1.0rc1         hdf5@1.10.5             lwgrp@1.0.2                py-backcall@0.1.0        py-pillow@6.2.0           readline@8.0
autoconf@2.69           hpctoolkit@2019.08.14   lz4@1.9.2                  py-blinker@1.4           py-prometheus-client@0.7.1 redset@0.0.3
automake@1.16.1         hwloc@1.11.11           lzo@2.10                   py-certifi@2019.9.11     py-prompt-toolkit@2.0.9   rempi@1.1.0
axl@0.1.1               hypre@2.18.1            m4@1.4.18                  py-certipy@0.1.3         py-ptyprocess@0.5.1       scr@1.2.2
binutils@2.32           intel-tbb@2019.4        margo@0.4.3                py-cffi@1.13.0           py-py@1.8.0               shuffile@0.0.3
bmi@develop             kokkos@2.7.00           matio@1.5.13               py-chardet@3.0.4         py-pycparser@2.19         snappy@1.1.7
boost@1.70.0            kokkos@2.9.00           mercury@1.0.1              py-cryptography@2.3.1    py-pygments@2.4.2         sqlite@3.30.1
boost@1.70.0            kokkos-kernels@2.7.00   mercury@1.0.1              py-cycler@0.10.0         py-pyjwt@1.7.1            strumpack@3.1.1
boost@1.70.0            kvtree@1.0.2            metis@5.1.0                py-cython@0.29.13        py-pyopenssl@19.0.0       suite-sparse@5.3.0
bzip2@1.0.8             leveldb@1.22            mfem@4.0.0                 py-decorator@4.4.0       py-pyparsing@2.4.2        sundials@5.0.0
c-blosc@1.17.0          libarchive@3.3.2        mpich@3.2.1                py-entrypoints@0.3       py-python-dateutil@2.8.0  superlu@5.2.1
caliper@2.0.1           libbsd@0.9.1            mpifileutils@develop       py-idna@2.8              py-python-dateutil@2.8.0  superlu-dist@6.1.1
cmake@3.15.4            libcircle@0.2.1-rc.1    mumps@5.2.0                py-ipykernel@5.1.0       py-python-editor@1.0.4    sz@1.4.12.3
curl@7.63.0             libdwarf@20180129       nasm@2.14.02               py-ipython@7.3.0         py-python-oauth2@1.1.1    tar@1.32
darshan-runtime@3.1.7   libfabric@1.8.1         ncurses@6.1                py-ipython-genutils@0.2.0 py-pytz@2019.3           tasmanian@7.0
darshan-util@3.1.7      libffi@3.2.1            netcdf@4.7.1               py-jinja2@2.10.3         py-requests@2.22.0        tcl@8.6.8
diffutils@3.7           libiberty@2.31.1        netlib-scalapack@2.0.2     py-joblib@0.14.0         py-scikit-learn@0.21.3    texinfo@6.5
dtcmp@1.1.0             libiconv@1.16           nettle@3.4.1               py-jsonschema@2.6.0      py-scikit-optimize@0.5.2  trilinos@12.14.1
dyninst@10.1.0          libjpeg-turbo@2.0.3     ninja@1.9.0                py-jupyter-client@4.4.0  py-scipy@1.3.1            umpire@0.3.3
elfutils@0.177          libmonitor@2018.07.18   numactl@2.0.12             py-jupyter-console@5.2.0 py-setuptools@41.4.0      unifyfs@develop
emacs@26.2              libnrm@0.1.0            openblas@0.3.7             py-jupyter-core@4.4.0    py-setuptools@41.4.0      unzip@6.0
er@0.0.3                libpciaccess@0.13.5     openmpi@3.1.4              py-jupyter-notebook@4.2.3 py-simplegeneric@0.8.1   upcxx@2019.9.0
expat@2.2.9             libpfm4@4.10.1          openssl@1.1.1d             py-jupyterhub@1.0.0      py-six@1.12.0             util-macros@1.19.1
findutils@4.6.0         libpng@1.6.37           papi@5.7.0                 py-kiwisolver@1.1.0      py-six@1.12.0             veloc@1.1
flatcc@0.5.3            libpthread-stubs@0.4    papyrus@develop            py-libensemble@0.5.2     py-sqlalchemy@1.3.9       xerces-c@3.2.2
flecsi@develop          libquo@1.3              parallel-netcdf@1.11.2     py-mako@1.0.4            py-tornado@6.0.3          xz@5.2.4
freetype@2.10.1         libsigsegv@2.12         parmetis@4.0.3             py-markupsafe@1.1.1      py-traitlets@4.3.3        zeromq@4.3.2
gdbm@1.18.1             libsodium@1.0.17        pcre@8.42                  py-matplotlib@3.1.1      py-urllib3@1.25.6         zfp@0.5.5
gettext@0.20.1          libtool@2.4.6           pcre@8.42                  py-mistune@0.7.1         py-vcversioner@2.16.0.0   zlib@1.2.11
git@2.21.0              libunwind@1.2.1         pdsh@2.31                  py-mpi4py@3.0.1          py-wcwidth@0.1.7          zstd@1.4.3
glm@0.9.7.1             libunwind@2018.10.12    perl@5.30.0                py-nbconvert@4.2.0       py-ytopt@0.1.0
globalarrays@5.7        libxml2@2.9.9           petsc@3.12.1               py-nbformat@4.4.0        py-zmq@17.1.2
gmp@6.1.2               libyogrt@1.24           pkgconf@1.6.3              py-numpy@1.17.3          python@3.7.3
gotcha@0.0.2            lmod@8.1.5              py-alembic@1.0.7           py-oauthlib@3.1.0        python@3.7.4
gotcha@1.0.2            lua@5.3.5               py-asn1crypto@0.22.0       py-pamela@1.0.0          qthreads@1.14
```

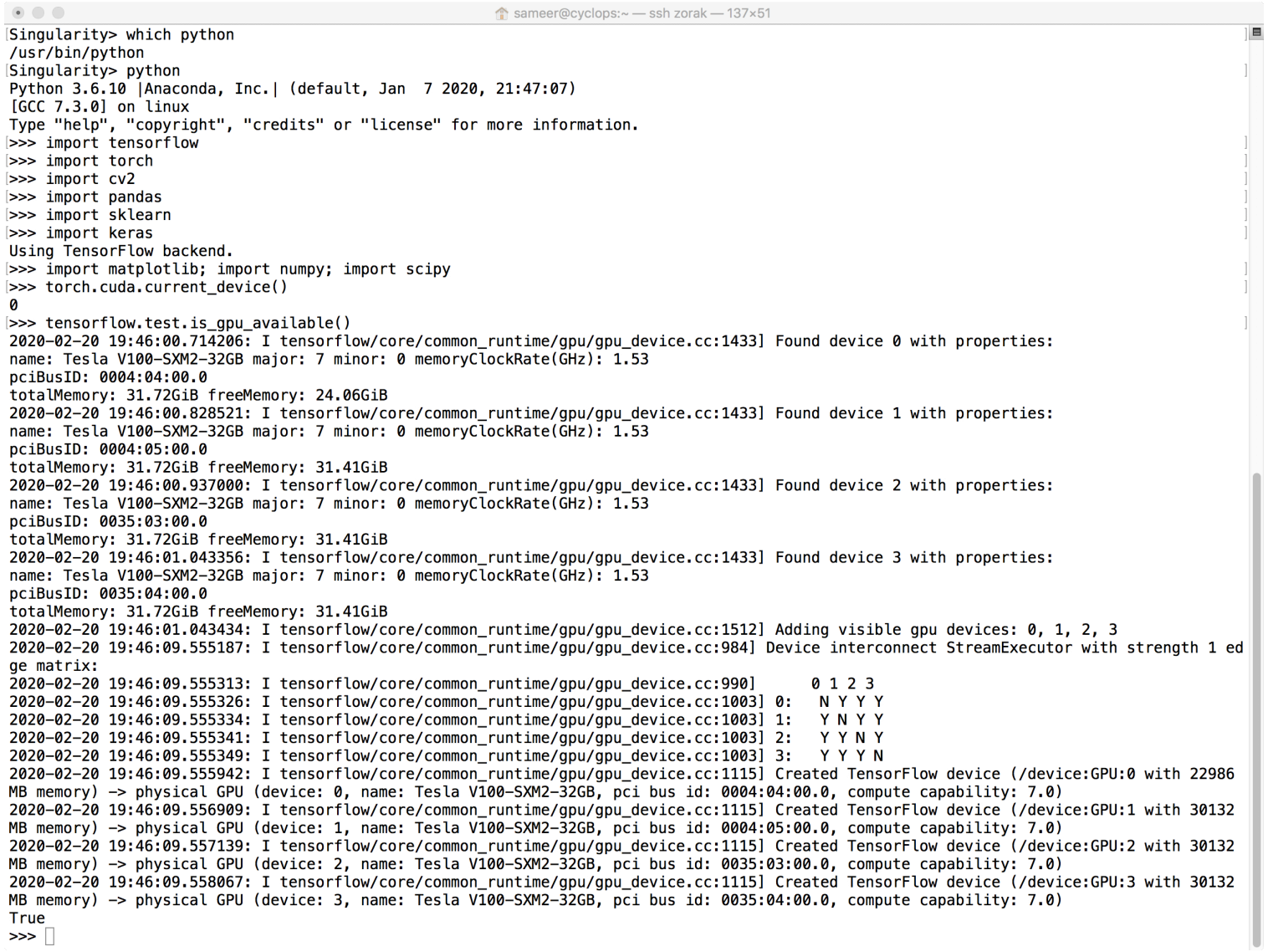
- All the versions coexist!
  - Multiple versions of same package are ok.
- Packages are installed to automatically find correct dependencies.
- Binaries work *regardless of user's environment*.
- Spack also generates module files.
  - Don't *have* to use them.

E4S Support for Singularity Container Runtime [Sylabs.io]



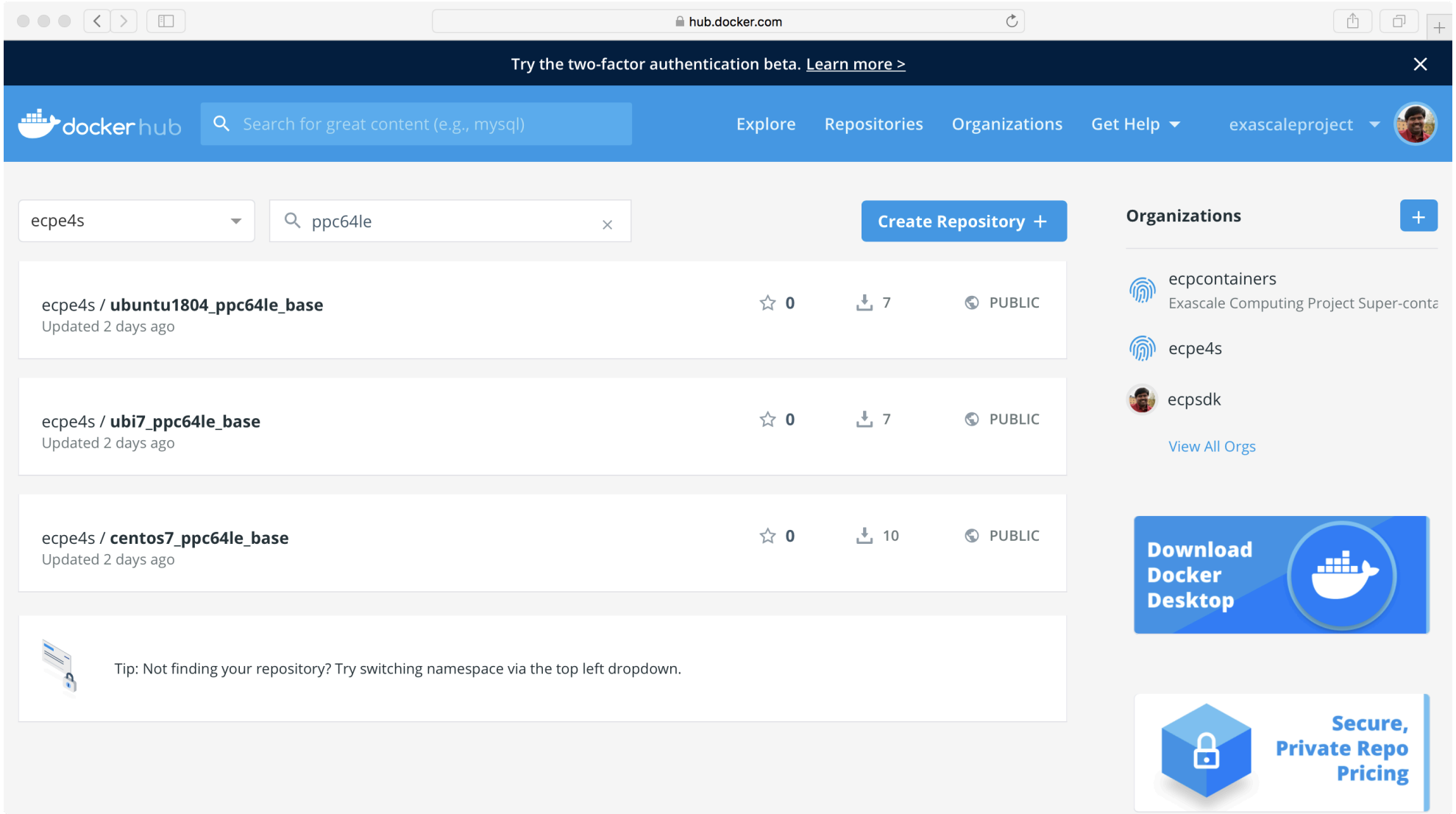
- wget http://oaciss.uoregon.edu/e4s/images/e4s_ubuntu1804_gpu_ppc64le_1.1.simg
- singularity exec --nv e4s_ubuntu1804_gpu_ppc64le_1.1.simg /bin/bash --rcfile /etc/bashrc
- spack find

E4S v1.1 GPU Support for ppc64le



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

E4S: ppc64le Base Container Images



- Hub.docker.com
- ecpe4s

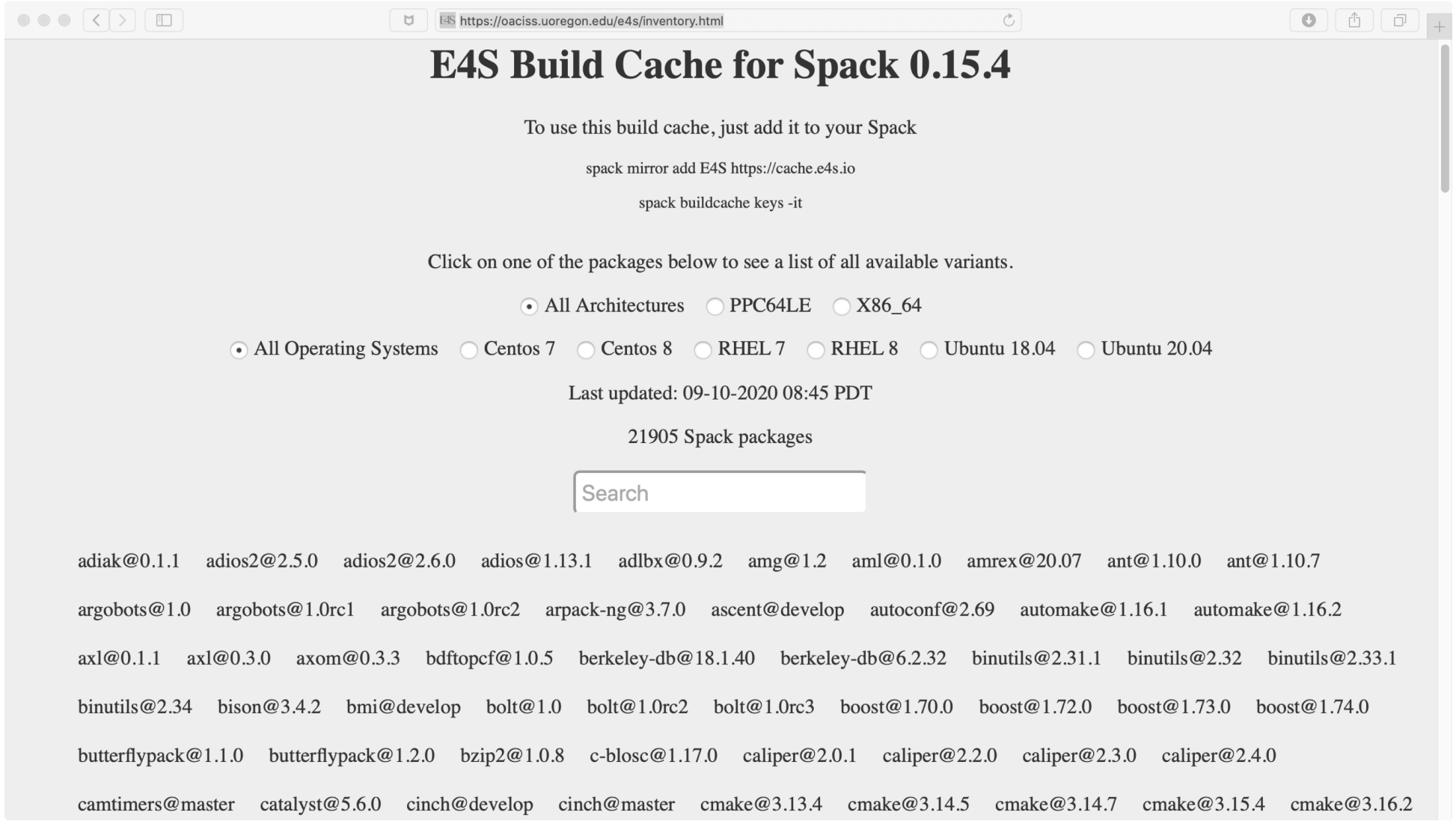
- Ubuntu 18.04
- RHEL/UBI 7.6
- Centos 7.6

E4S Spack Build Cache and Container Build Pipeline

Reproducible, Customizable Container Builds & Spack Mirrors

- E4S provides base images and recipes for building Docker containers based on SDKs
  - Git: https://github.com/UO-OACISS/e4s
  - E4S provides build caches for Spack for native bare-metal as well as container builds based installation of ST products
  - Build caches: https://oaciss.uoregon.edu/e4s/inventory.html
    - The build cache model can be extended to target platforms, and can be managed by facilities staff when appropriate.

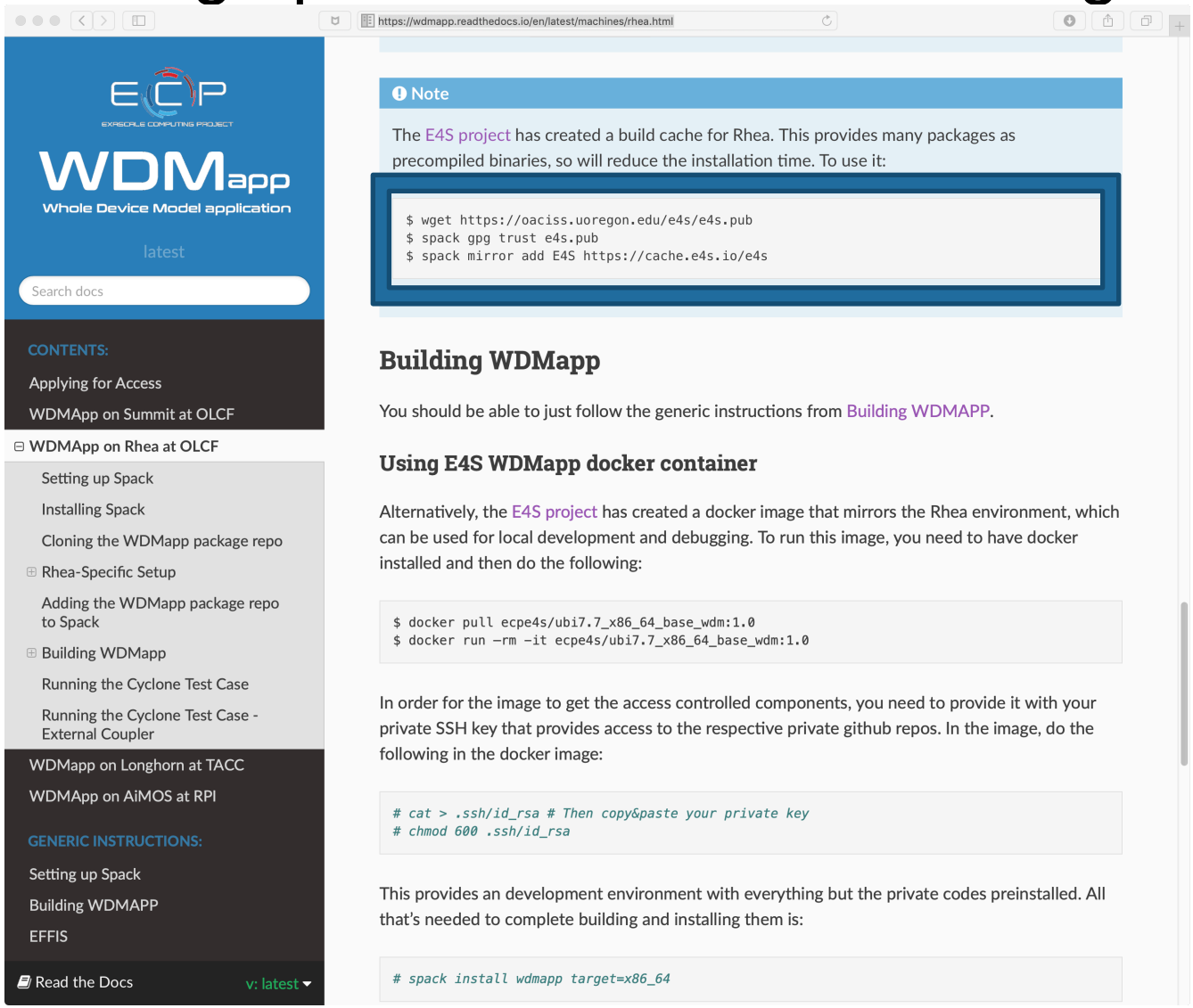
E4S: Spack Build Cache at U. Oregon



- 20,000+ binaries!
- S3 mirror
- No need to build from source code!

- https://oaciss.uoregon.edu/e4s/inventory.html

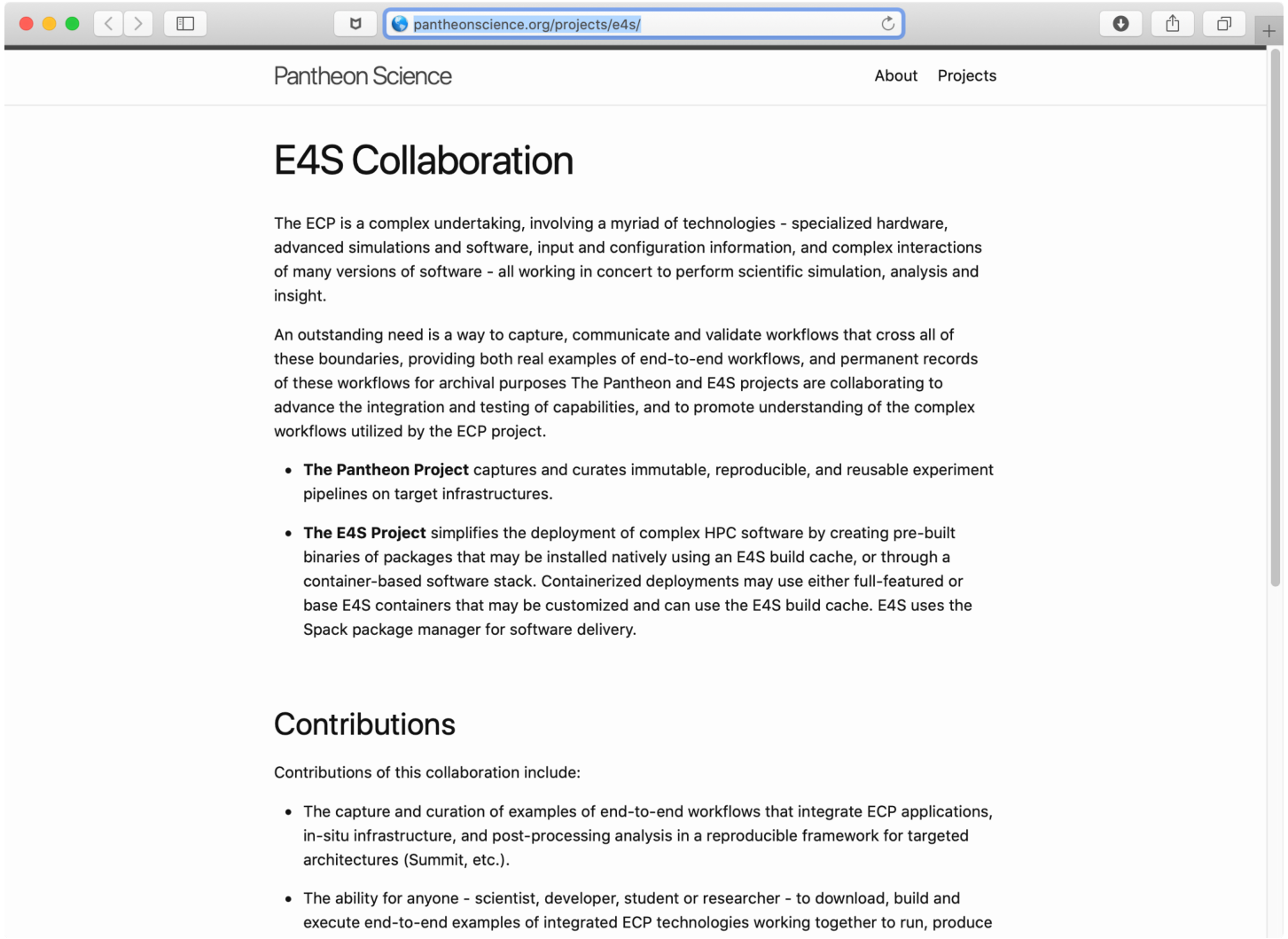
WDMapp: Speeding up bare-metal installs using E4S build cache



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

- https://wdmapp.readthedocs.io/en/latest/machines/rhea.html

Pantheon Science at LANL

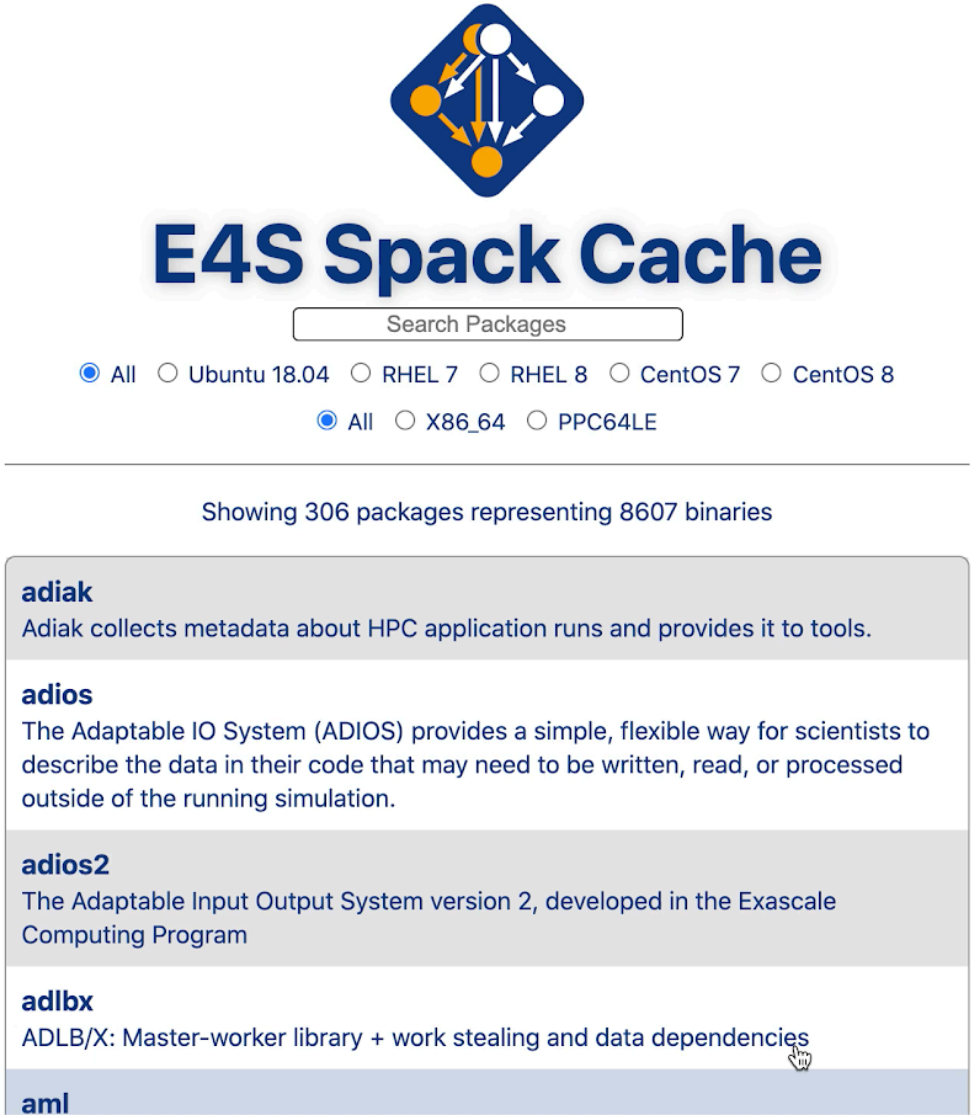


PANTHEON

- E4S Spack build cache
- Adding E4S mirror
- Pantheon spack install 10x speedup!

- https://pantheonscience.org/projects/e4s/

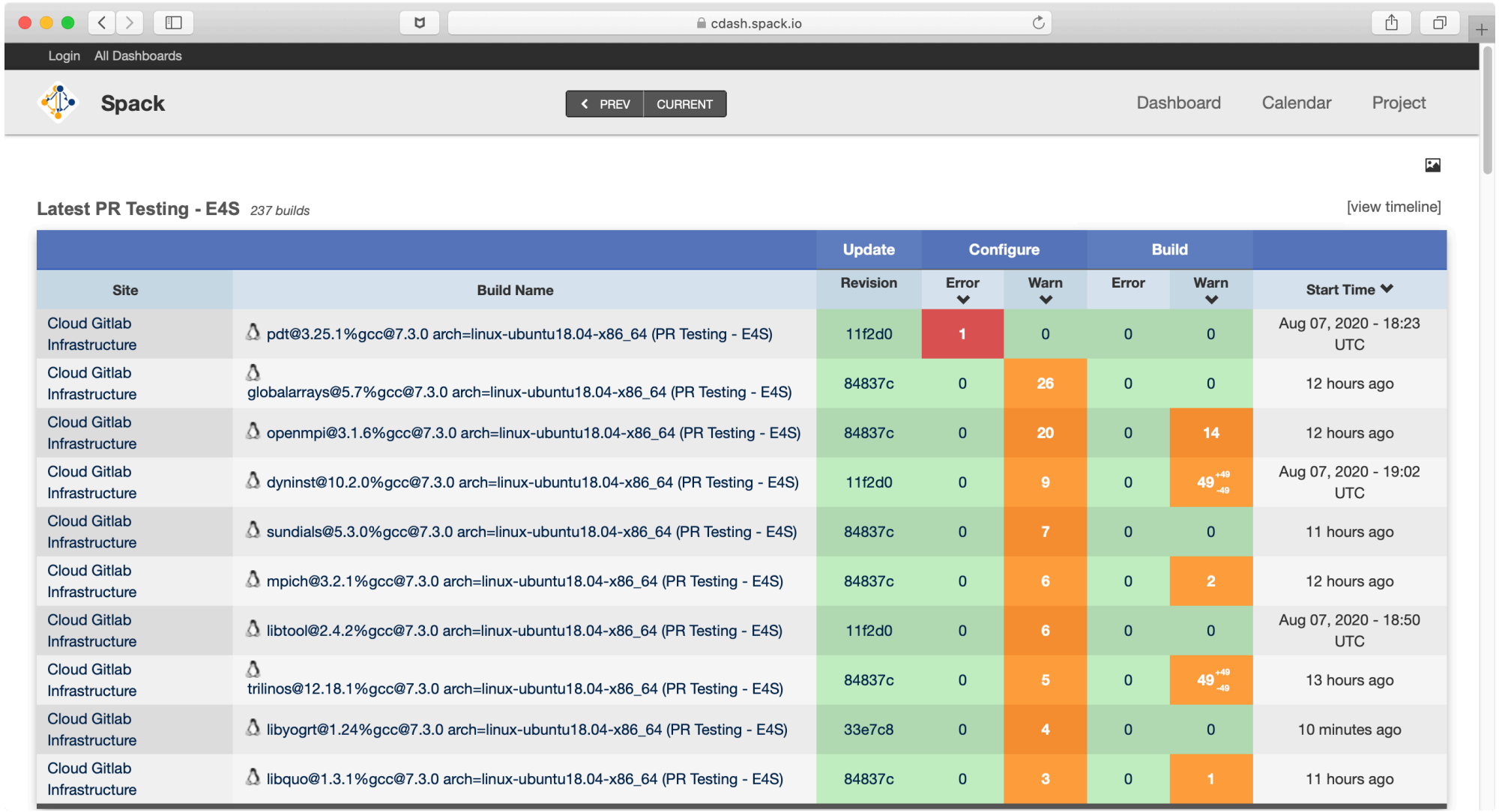
New E4S Spack Cache Website (under development)



E4S Spack Environment - Current Examples

- Building on **AWS Cloud** as part of Spack PR and Release Testing
  - CI Dashboard available @ https://cdash.spack.io
- Building at **University of Oregon**
  - ppc64le and x86/64 systems with mpich
- Building at **OLCF Ascent**
- Working on **NERSC Cori** and **ALCF Theta** currently
- See examples of how the environment is tailored for existing sites:
  - https://github.com/UO-OACISS/e4s/tree/master/e4s-facility-environments
- Binaries available in the E4S Build Cache
  - https://oaciss.uoregon.edu/e4s/inventory.html
  - Improved inventory page currently under development
- Google Cloud Platform (GCP) integration

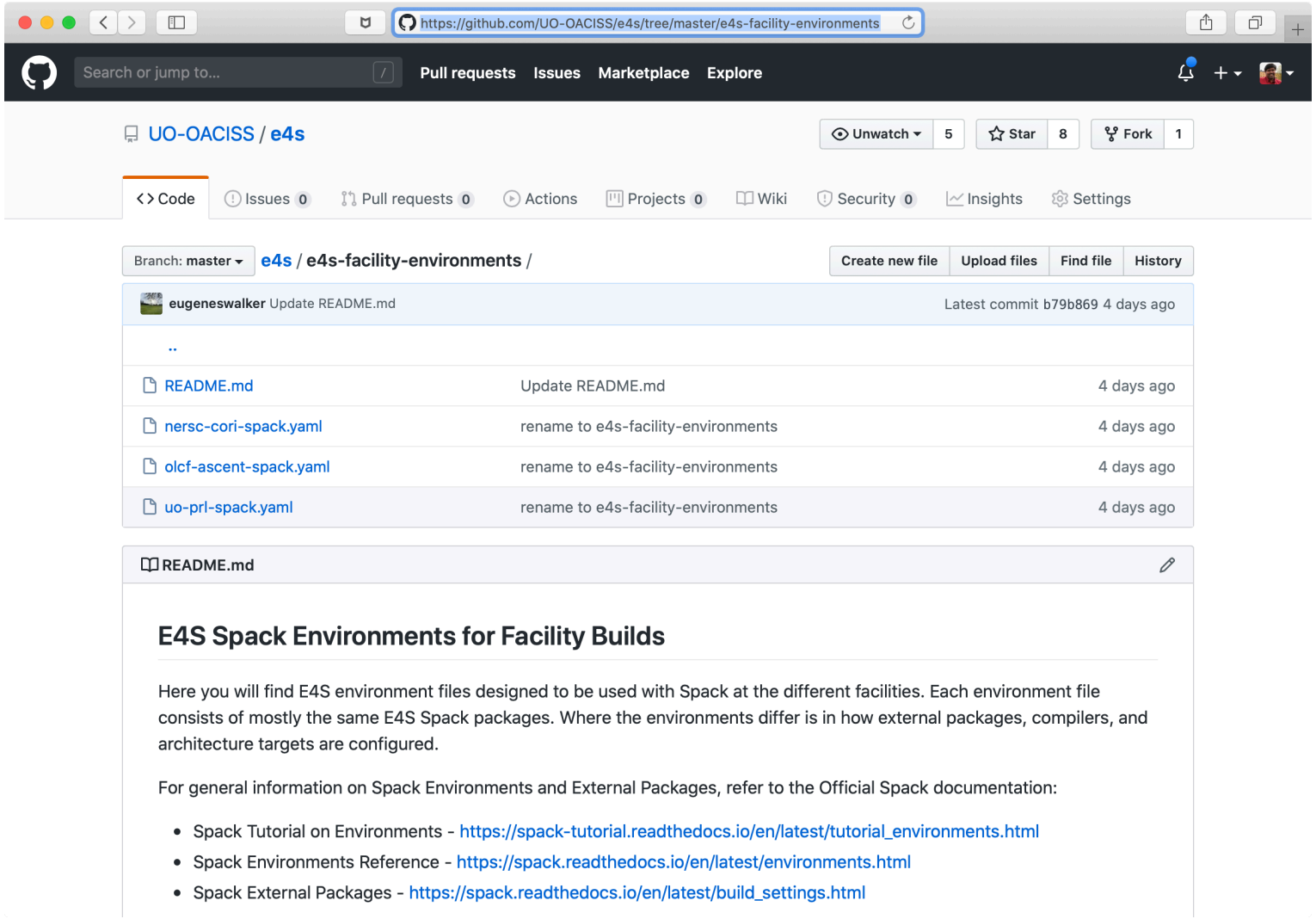
E4S Dashboard for Spack Pull Request (PR) testing



		Update	Configure		Build		
Site	Build Name	Revision	Error	Warn	Error	Warn	Start Time
Cloud Gitlab Infrastructure	pdt@3.25.1%gcc@7.3.0 arch=linux-ubuntu18.04-x86_64 (PR Testing - E4S)	11f2d0	1	0	0	0	Aug 07, 2020 - 18:23 UTC
Cloud Gitlab Infrastructure	globalarrays@5.7%gcc@7.3.0 arch=linux-ubuntu18.04-x86_64 (PR Testing - E4S)	84837c	0	26	0	0	12 hours ago
Cloud Gitlab Infrastructure	openmpi@3.1.6%gcc@7.3.0 arch=linux-ubuntu18.04-x86_64 (PR Testing - E4S)	84837c	0	20	0	14	12 hours ago
Cloud Gitlab Infrastructure	dyninst@10.2.0%gcc@7.3.0 arch=linux-ubuntu18.04-x86_64 (PR Testing - E4S)	11f2d0	0	9	0	49 +49 -49	Aug 07, 2020 - 19:02 UTC
Cloud Gitlab Infrastructure	sundials@5.3.0%gcc@7.3.0 arch=linux-ubuntu18.04-x86_64 (PR Testing - E4S)	84837c	0	7	0	0	11 hours ago
Cloud Gitlab Infrastructure	mpich@3.2.1%gcc@7.3.0 arch=linux-ubuntu18.04-x86_64 (PR Testing - E4S)	84837c	0	6	0	2	12 hours ago
Cloud Gitlab Infrastructure	libtool@2.4.2%gcc@7.3.0 arch=linux-ubuntu18.04-x86_64 (PR Testing - E4S)	11f2d0	0	6	0	0	Aug 07, 2020 - 18:50 UTC
Cloud Gitlab Infrastructure	trilinos@12.18.1%gcc@7.3.0 arch=linux-ubuntu18.04-x86_64 (PR Testing - E4S)	84837c	0	5	0	49 +49 -49	13 hours ago
Cloud Gitlab Infrastructure	libyogrt@1.24%gcc@7.3.0 arch=linux-ubuntu18.04-x86_64 (PR Testing - E4S)	33e7c8	0	4	0	0	10 minutes ago
Cloud Gitlab Infrastructure	libquo@1.3.1%gcc@7.3.0 arch=linux-ubuntu18.04-x86_64 (PR Testing - E4S)	84837c	0	3	0	1	11 hours ago

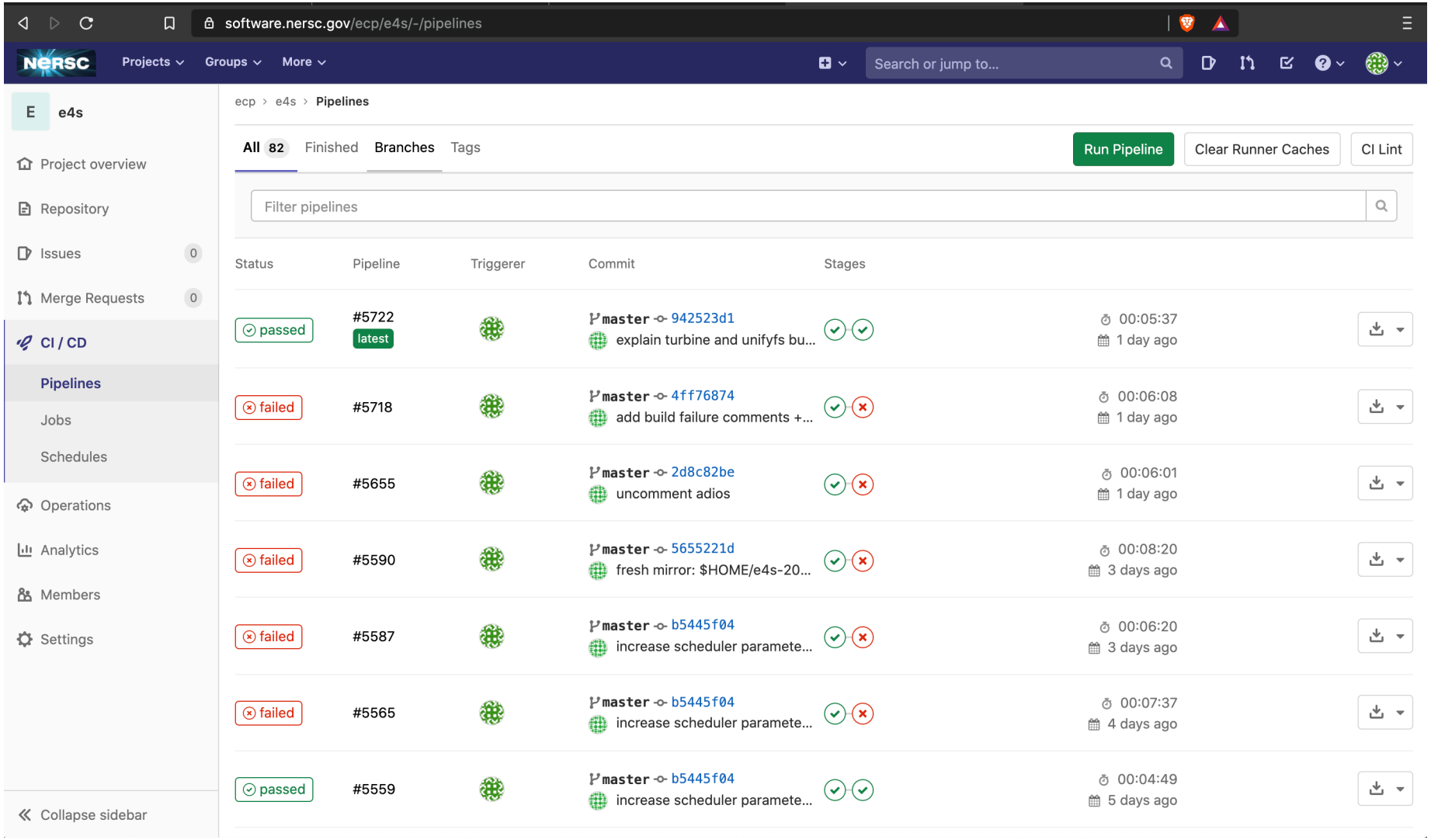
https://cdash.spack.io

E4S Tailored to DOE Facility Environments

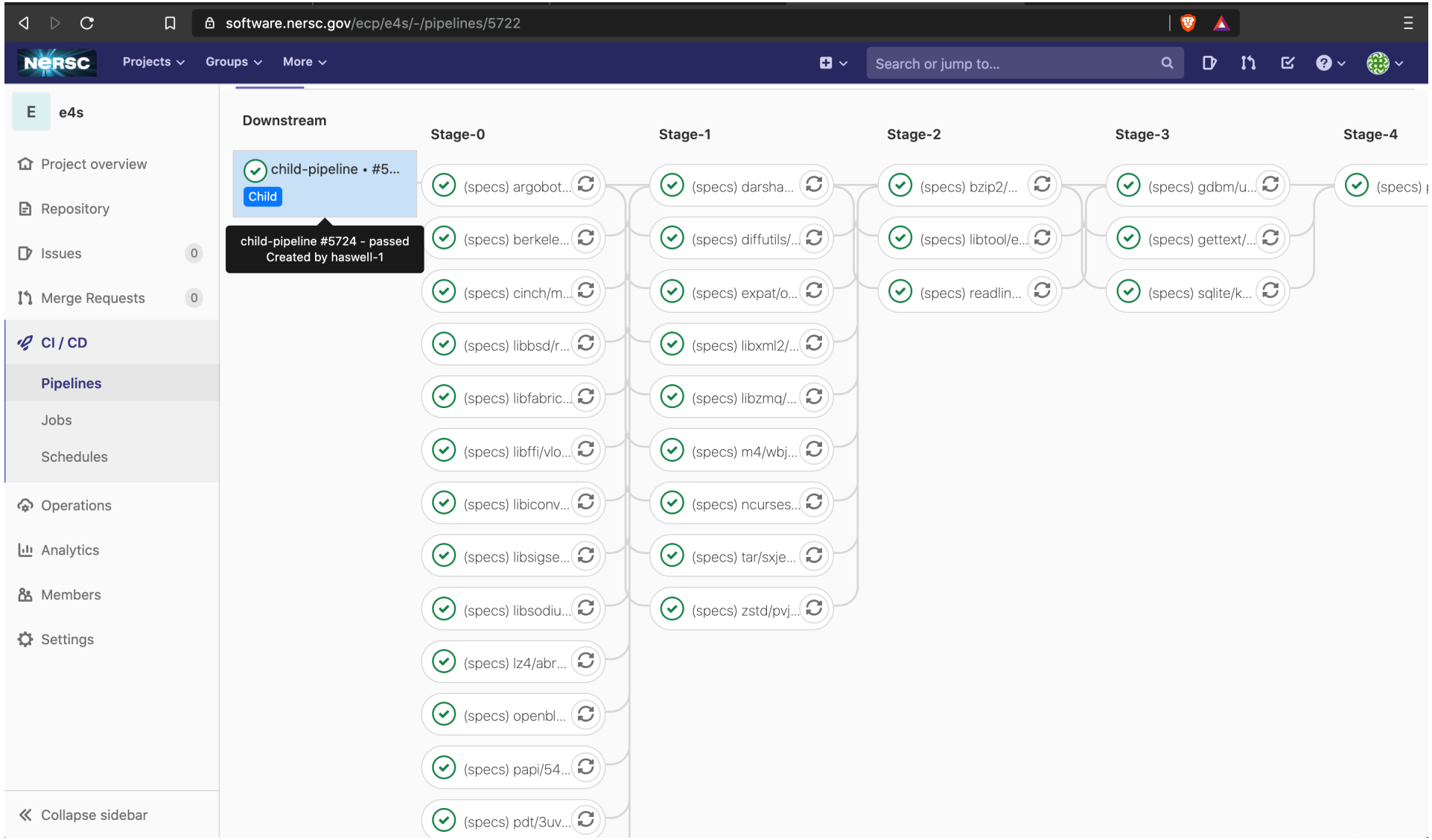


https://github.com/UO-OACISS/e4s/tree/master/e4s-facility-environments

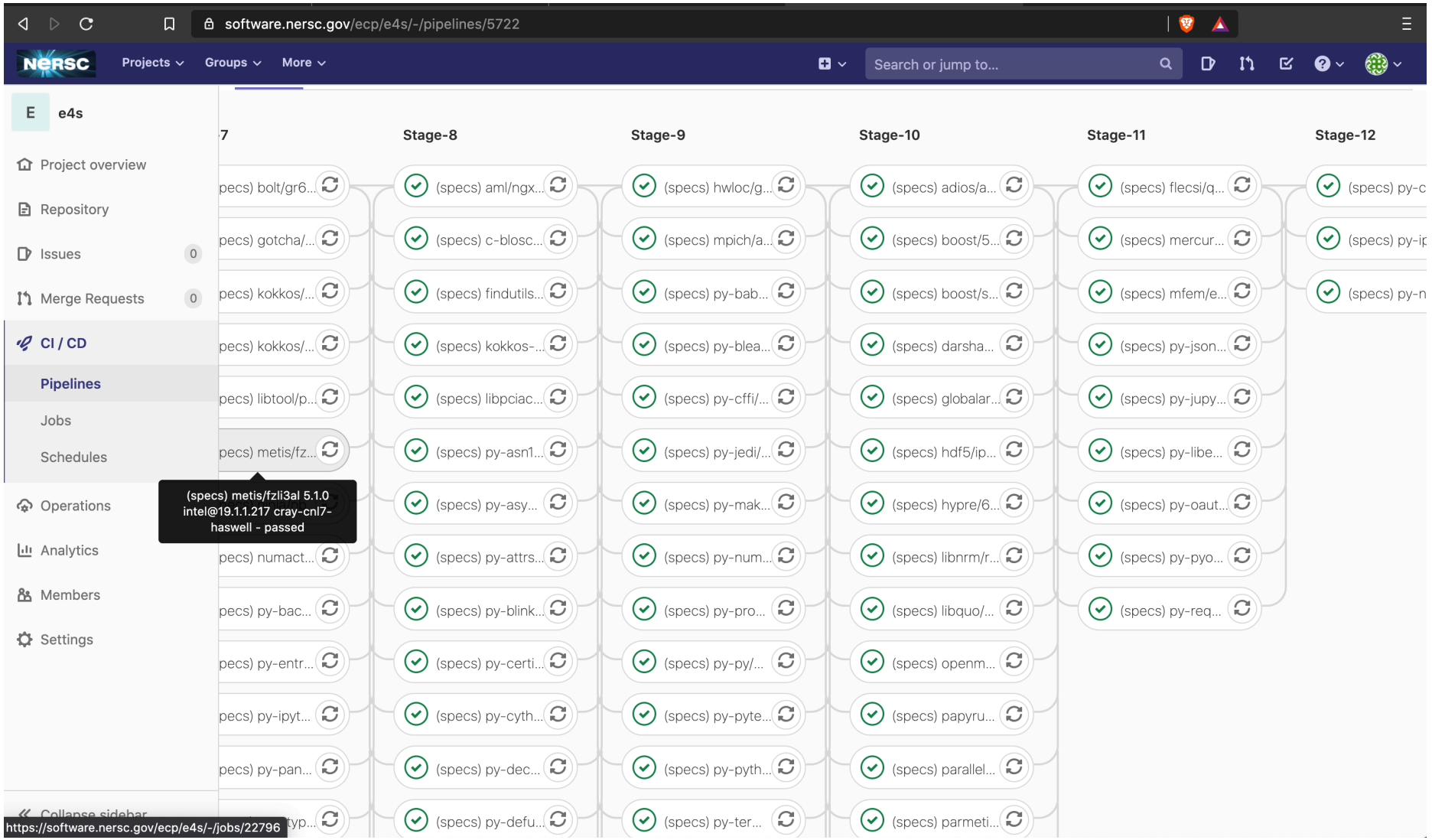
E4S Build Pipeline Summary on Cori, NERSC



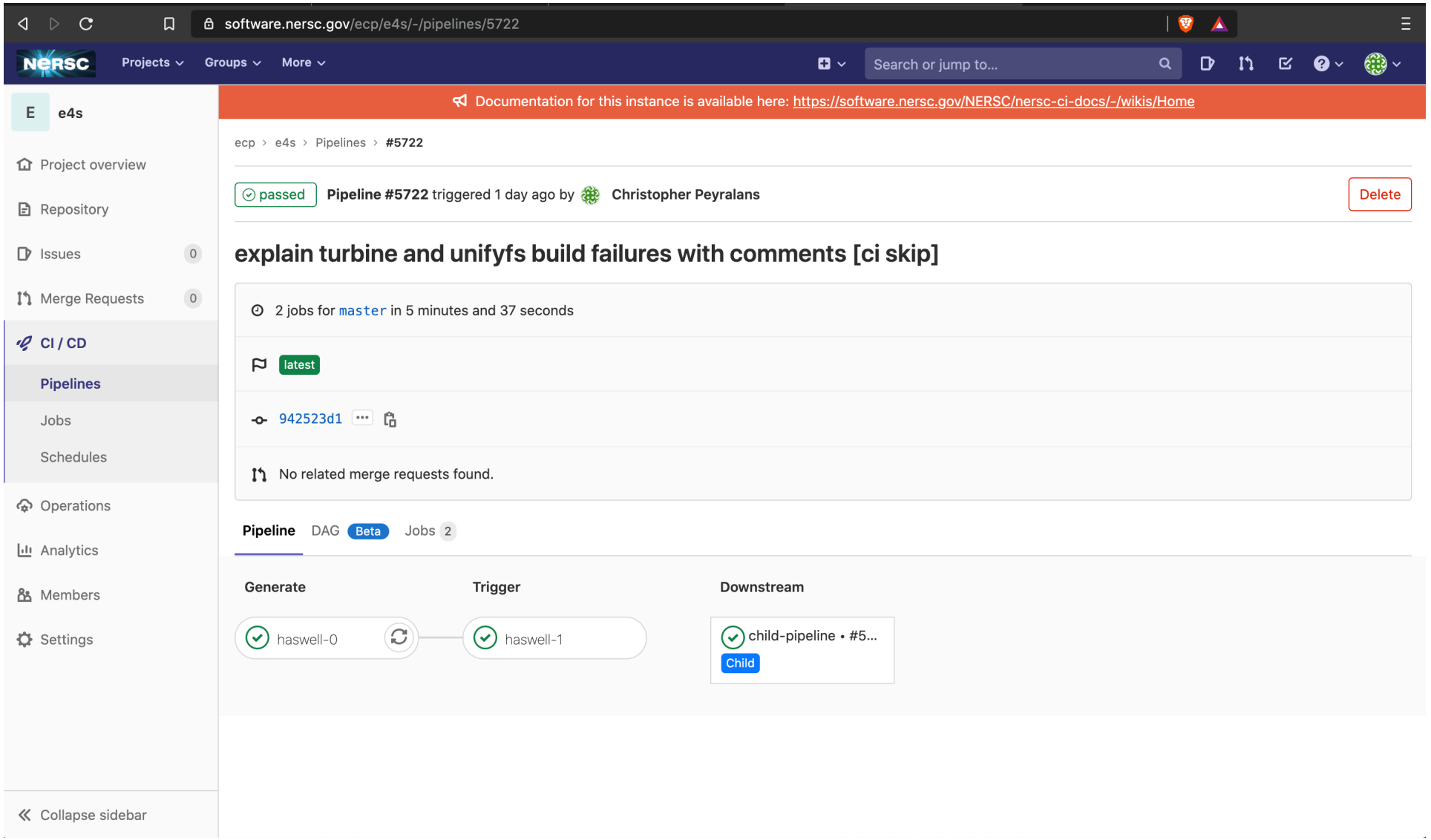
Multi-stage E4S CI Build Pipeline on Cori, NERSC



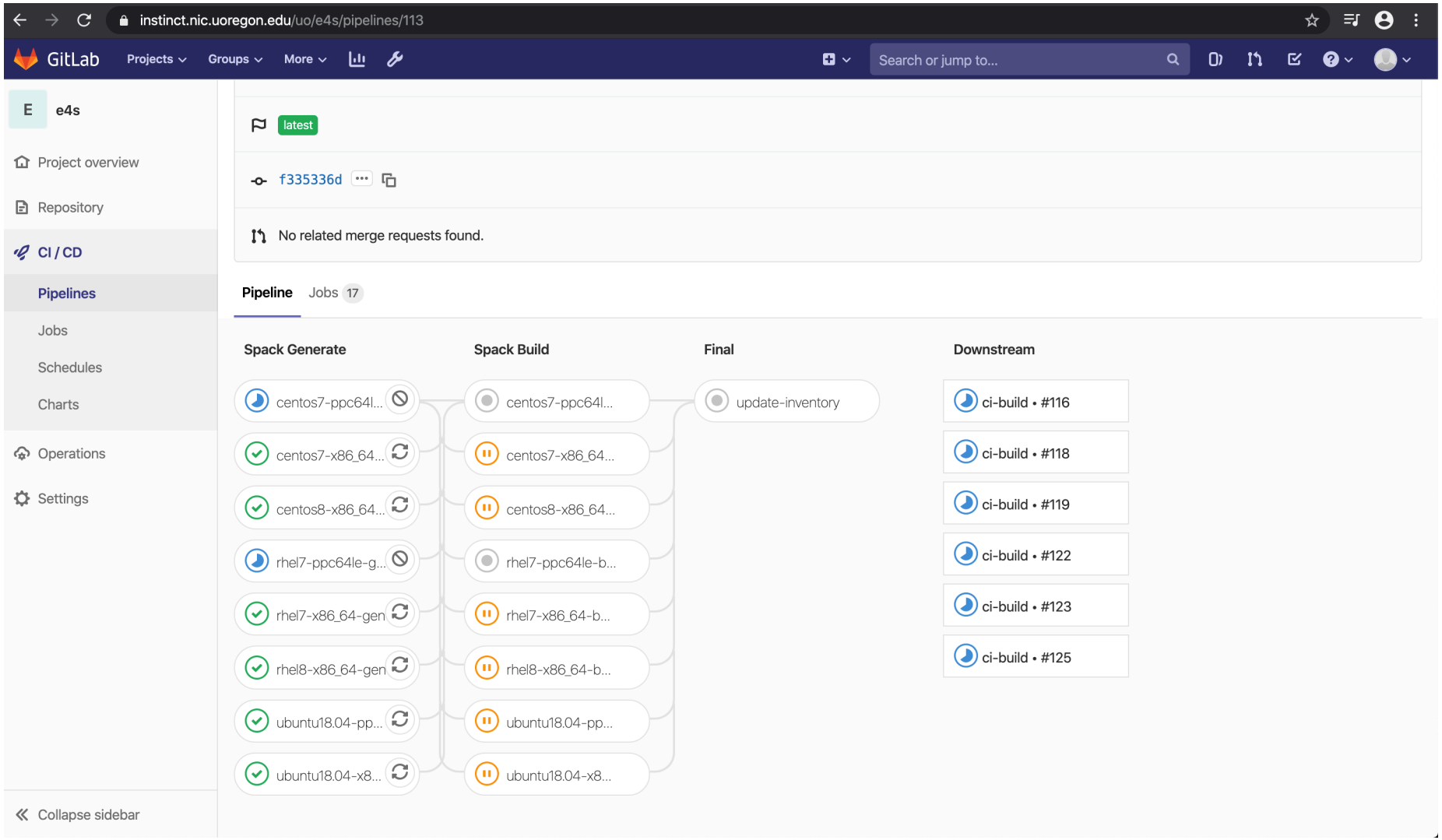
E4S CI on Cori, NERSC



E4S CI on Cori, NERSC

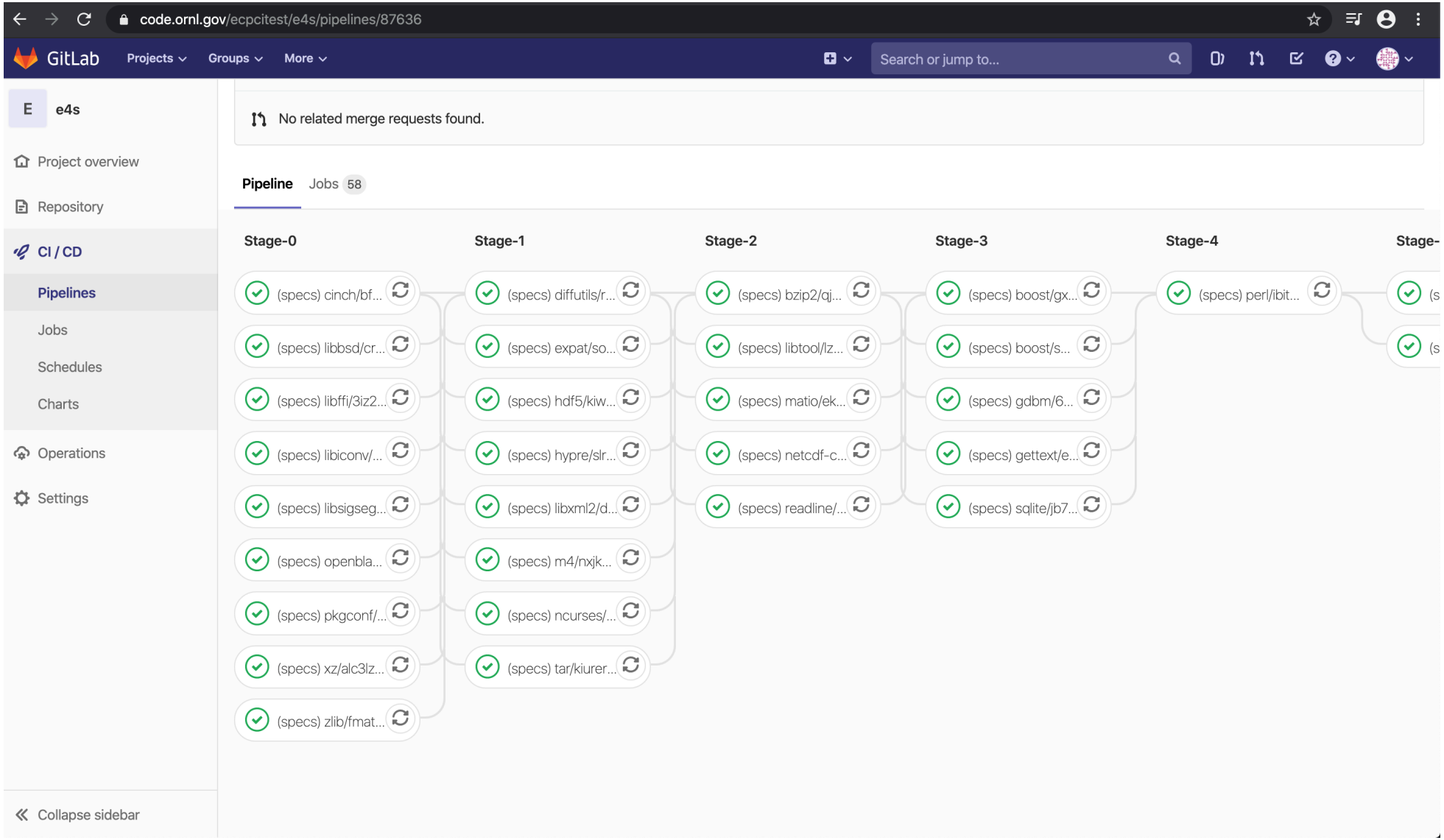


E4S: Build Pipeline for Creating Spack Build Cache at U. Oregon



- GitLab
- Multi-platform builds

ORNL GitLab Build Pipeline for E4S Spack Build Cache



- ppc64le (Ascent @ ORNL)
- Reproducible container builds

E4S VM Image for Google Cloud Project (GCP)

- VM Image for Google Compute Engine
  - Ubuntu 18.04
  - Intel Cascade Lake
- Spack v0.15.4
- Pre-configured to use E4S Cloud Build Cache
- 53 E4S Packages
  - SuperLU
  - Sundials
  - Trilinos
  - UPCXX
  - … and more

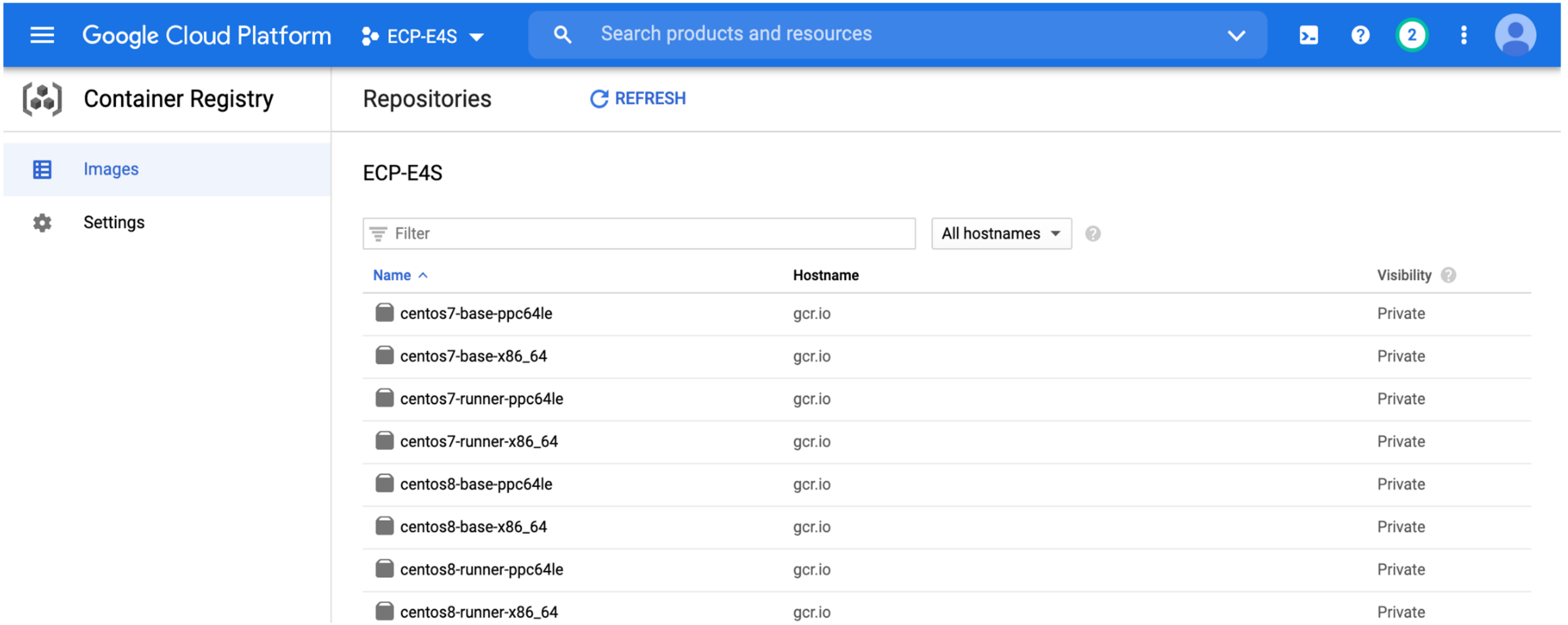
E4S GitLab via Google Kubernetes Engine

- E4S GitLab running via Google Kubernetes Engine (GKE)
  - GitLab Version 13.3.5 with updates deployed via Helm Chart
- GitLab Continuous Integration (CI)
  - Build E4S Spack packages using University of Oregon runners
- E4S package binaries automatically pushed to E4S Cloud Build Cache upon successful build
  - Spack mirror URL: https://cache.e4s.io
  - Spack mirror inventory: https://oaciss.uoregon.edu/e4s/inventory.html

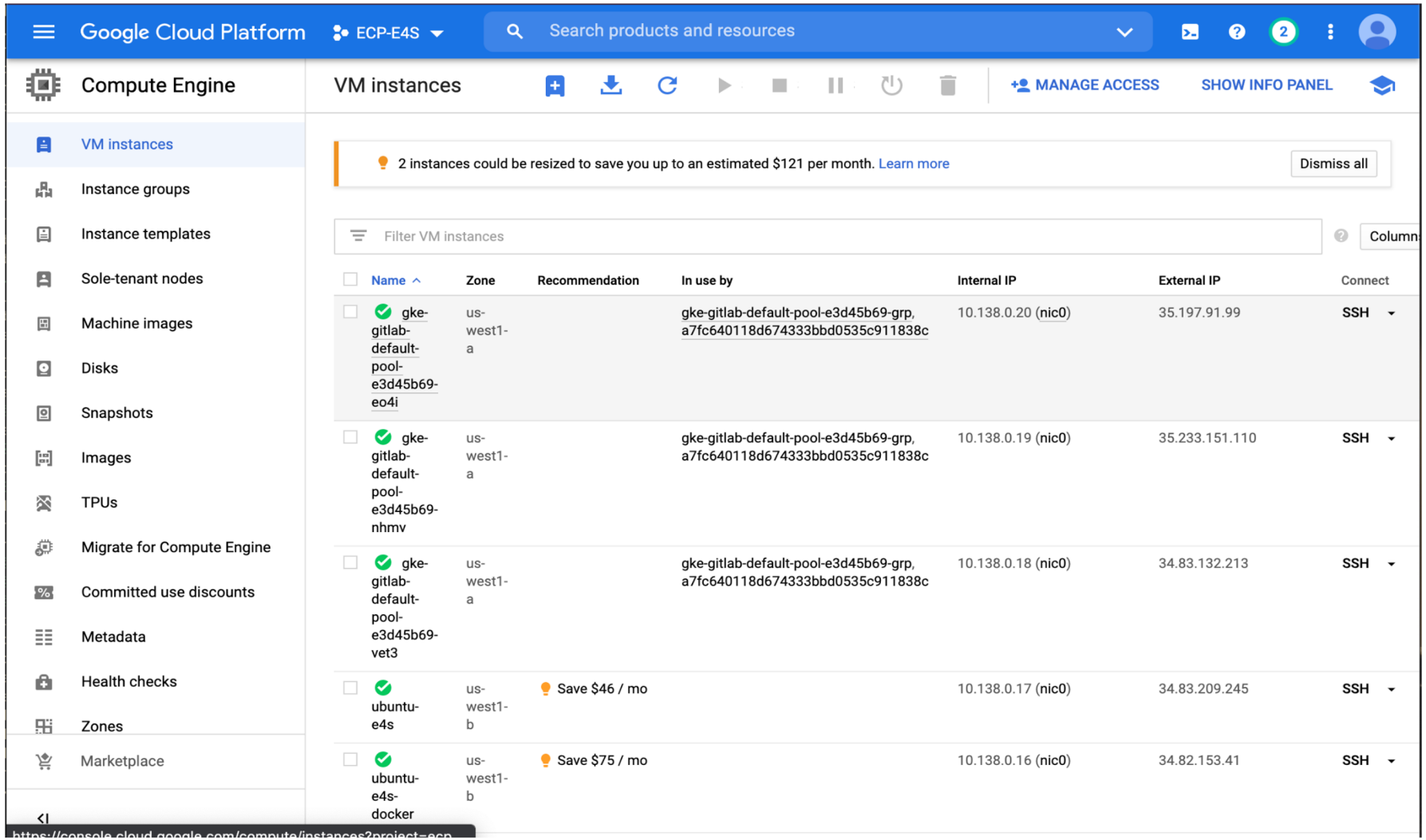
E4S Container Images via gcr.io

- Pre-release container images deployed to Google Container Registry (gcr.io)
- Use of private registry eases collaboration burden during pre-release testing
- Shields end-users from potential bugs
- Image types:
  - Base layers
  - Base Spack images
  - GitLab CI Runner images
  - Full E4S images

E4S Repositories on GCP



E4S VM Instances on GCP used by GitLab

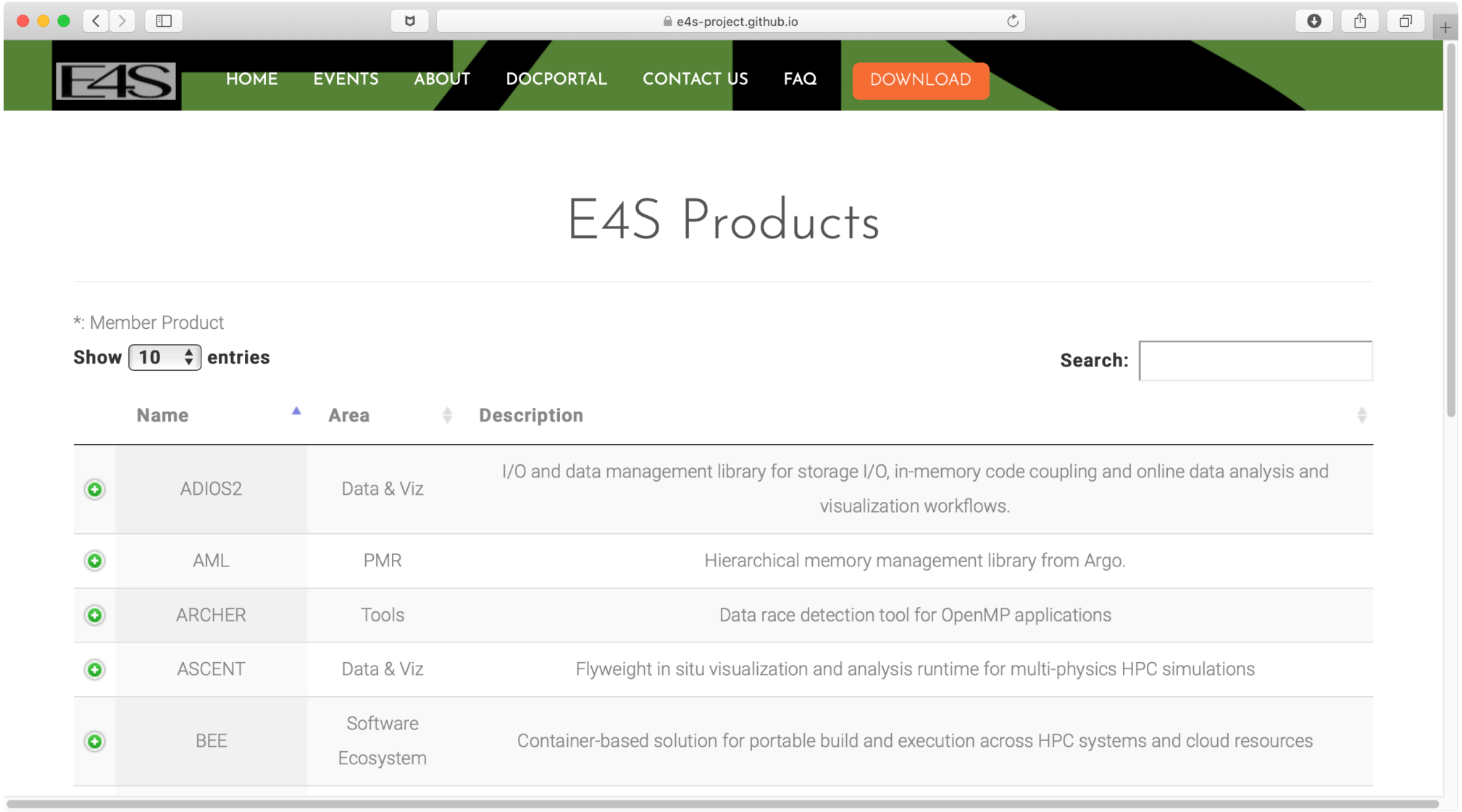


E4S Components

E4S DocPortal

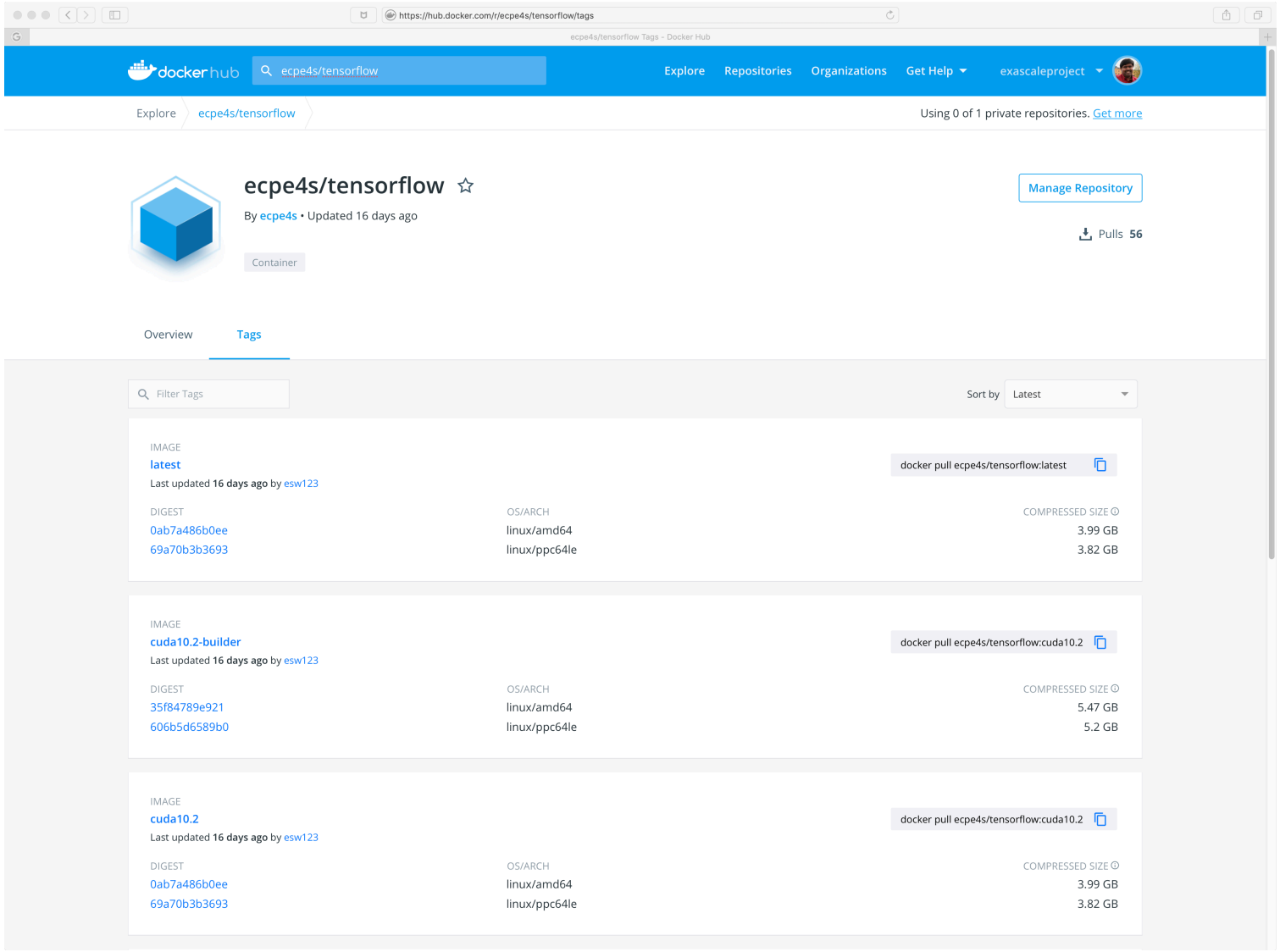
- Provide a single online location for *accurate* product descriptions for ECP software products.
- Derived requirements:
  - Sustainable: Must be integrated into software team workflows.
  - Incremental: Must build on community approaches to providing this kind of information.
  - Extensible: Must be 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



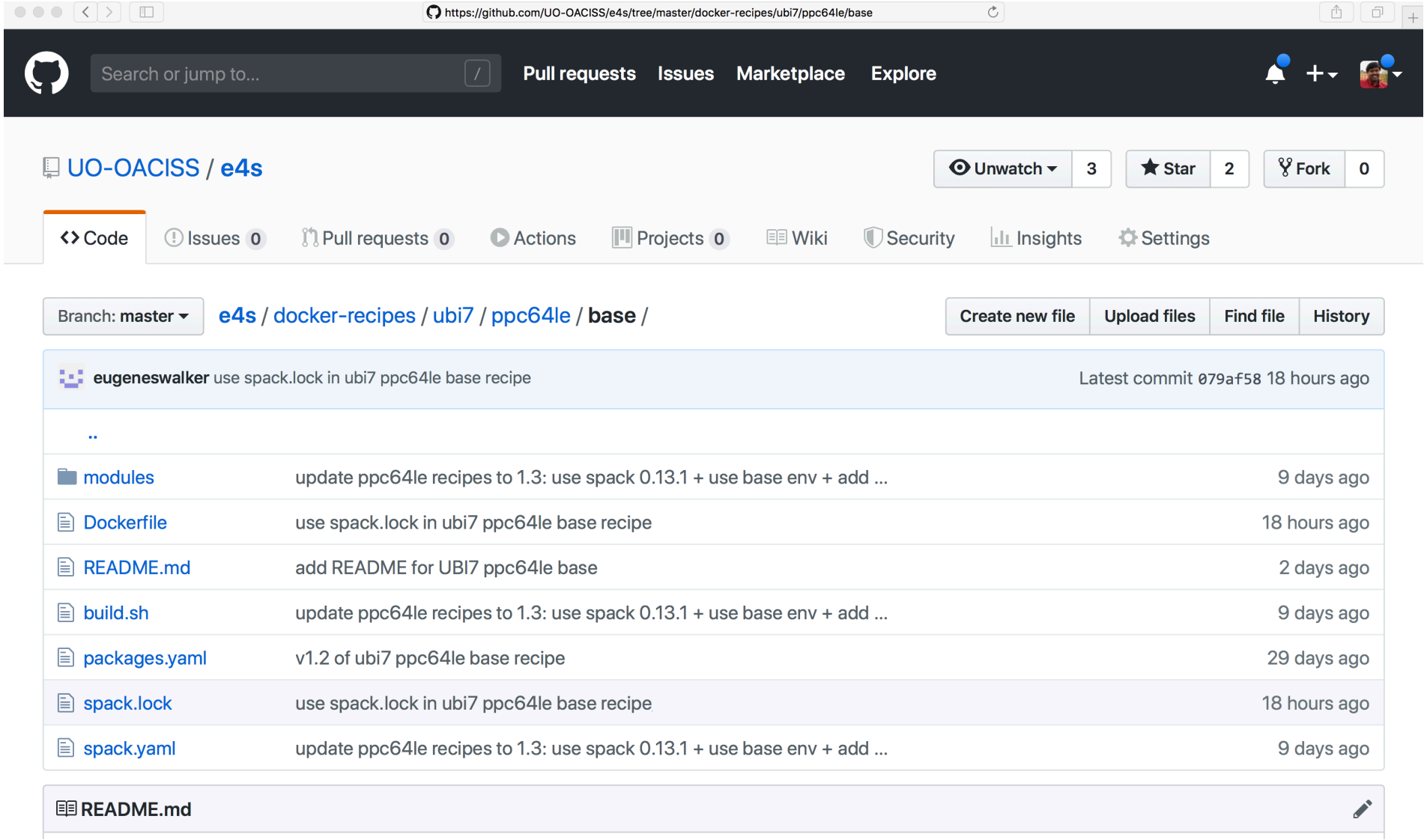
https://e4s-project.github.io/DocPortal.html

E4S: DockerHub Images: ecpe4s



- Dockerhub
- Tensorflow 2.2
- CUDA 10.2
- ppc64le

E4S: Multi-platform Reproducible Docker Recipes



E4S base images

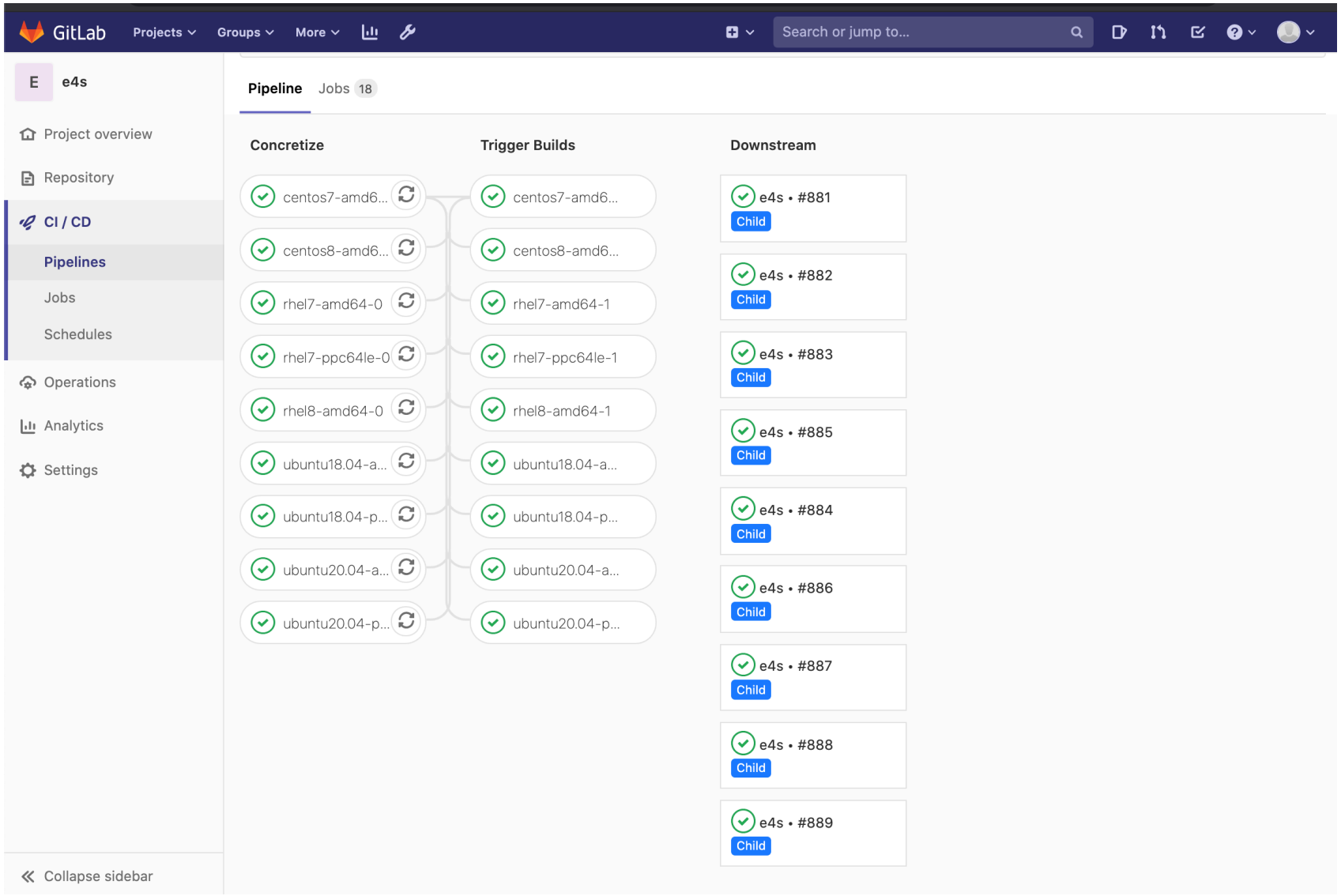
- x86_64
- ppc64le
- aarch64

https://e4s.io

University of Oregon GitLab CI

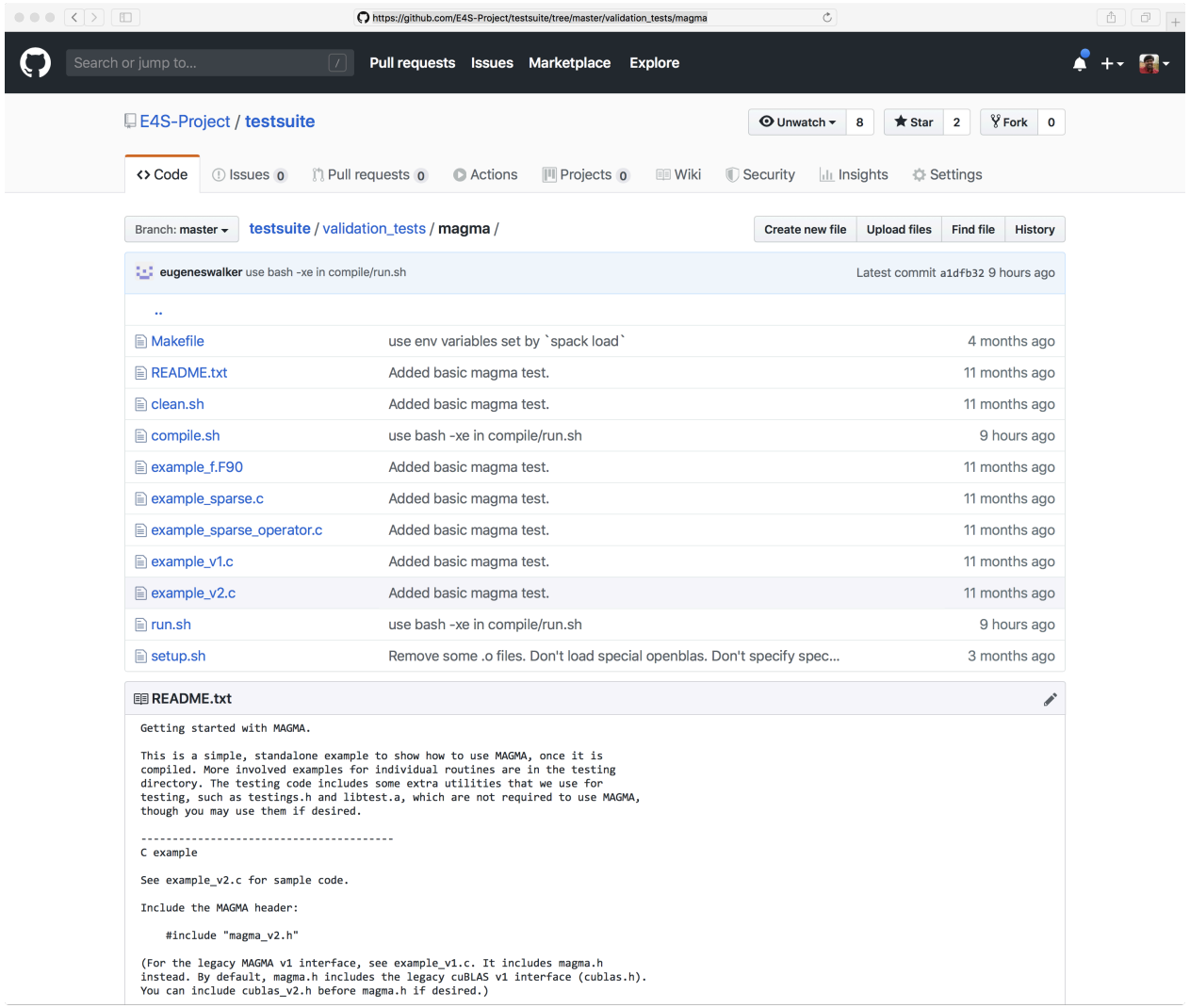
August 10, 2020
E4S Builds:
- Ubuntu 18.04
- Ubuntu 20.04
- RHEL 7.6
- RHEL 8
- CentOS 7
- CentOS 8

Architectures:
ppc64le and x86_64



E4S Validation Test Suite

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



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

Reproducible Container Builds using E4S Base Images

UO-OACISS / e4s

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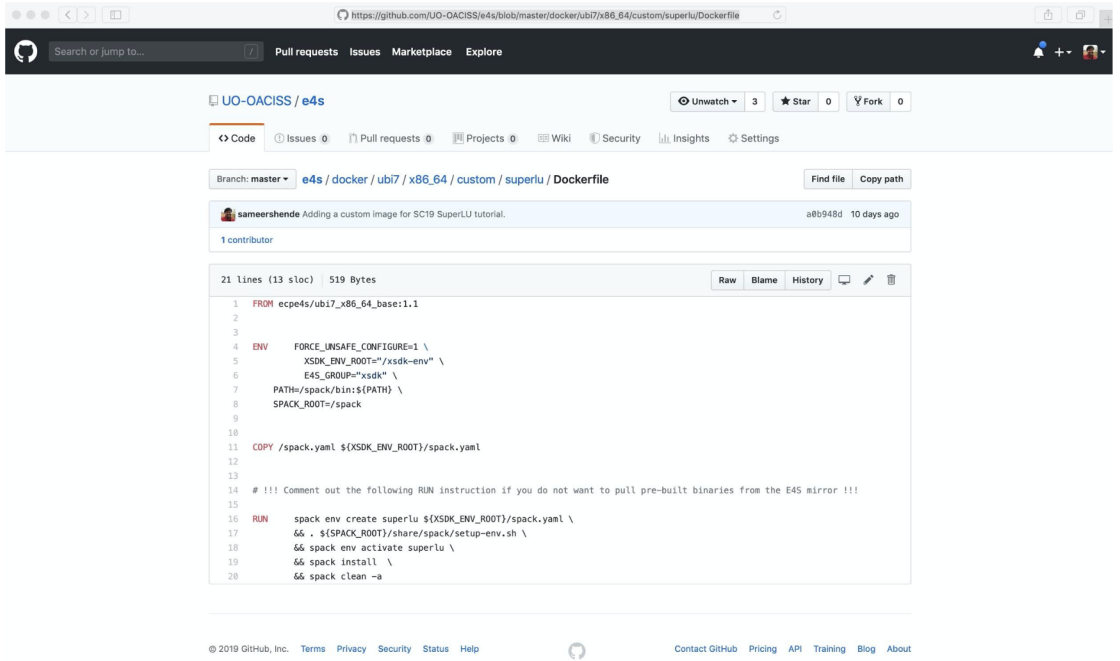
Branch: master — e4s / docker / ubi7 / x86_64 / custom / superlu / **spack.yaml** — Find file | Copy path

sameershende Adding a custom image for SC19 SuperLU tutorial. a0b948d 10 days ago

1 contributor

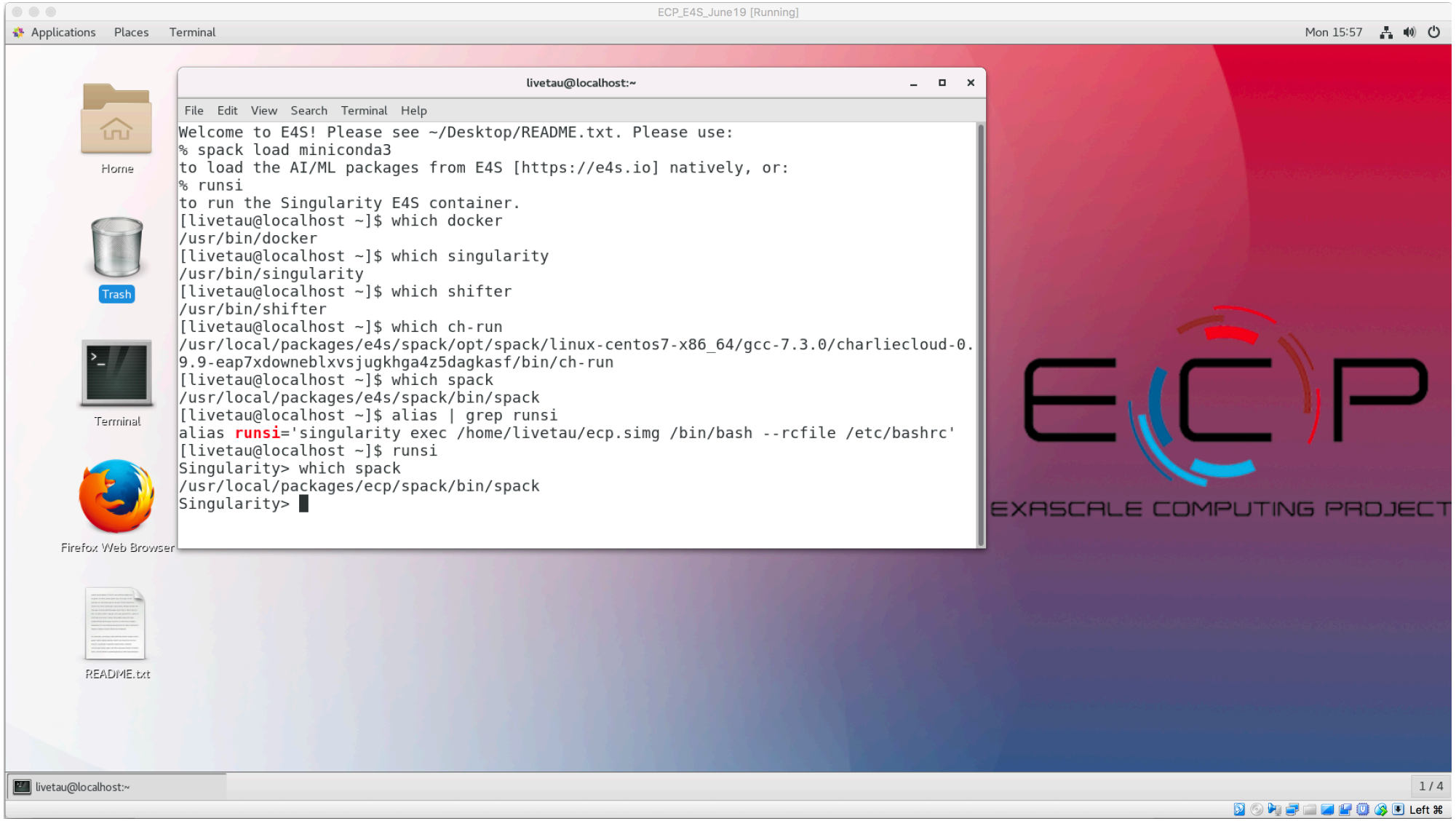
35 lines (34 sloc) | 579 Bytes — Raw | Blame | History

```
spack:
  packages:
    all:
      compiler: [gcc@7.3.0]
      variants: +mpi
      providers:
        mpi: [mpich]
      buildable: true
      version: []
      paths: {}
      modules: {}
    mpich:
      version: [3.2.1]
      variants: ~wrapperrpath
      buildable: true
      providers: {}
      paths: {}
      modules: {}
      compiler: []
    gcc:
      version: [7.3.0]
      buildable: true
      providers: {}
      paths: {}
      modules: {}
      compiler: []
  specs:
  - superlu-dist
  - petsc
  - mfem
  - strumpack
  - butterflypack
  - openblas
  view: false
```



- 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 VirtualBox Image



Container Runtimes

- Docker
- Shifter
- Singularity
- Charliecloud

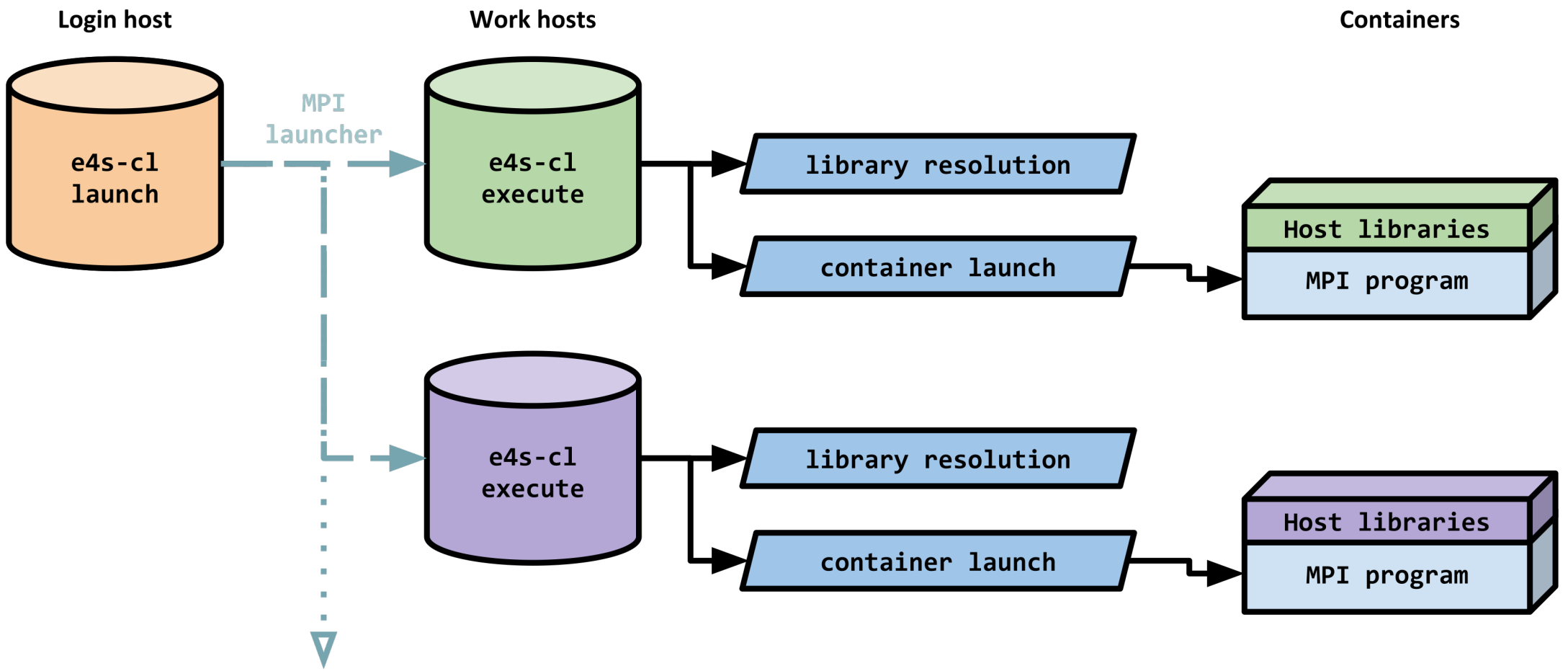
https://e4s.io

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



https://e4s.io

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