

# Using Trilinos with E4S



Trilinos Users Group Meeting 2021, Thursday, Dec. 2, 2021, 10am MST/9am PST

[https://trilinos.github.io/trilinos\\_user-developer\\_group\\_meeting\\_2021.html](https://trilinos.github.io/trilinos_user-developer_group_meeting_2021.html)

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[https://e4s.io/talks/E4S\\_TUG\\_Dec21.pdf](https://e4s.io/talks/E4S_TUG_Dec21.pdf)



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U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science

# E4S: Extreme-scale Scientific Software Stack

- Curated, Spack based software distribution
- Spack binary build caches for bare-metal installs
- 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-cl container launcher tool for MPI substitution in applications
- E4S VirtualBox image with support for container runtimes
  - Docker
  - Singularity
  - Shifter
  - Charliecloud
- AWS and GCP images to deploy E4S

# Extreme-scale Scientific Software Stack (E4S)



- E4S: HPC Software Ecosystem – a curated software portfolio
- A **Spack-based** distribution of software tested for interoperability and portability to multiple architectures
- Available from **source, containers, cloud, binary caches**
- Leverages and enhances SDK interoperability thrust
- Not a commercial product – an open resource for all
- 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
- Feb 2020: E4S 1.1 - 61 full release products
- Nov 2020: E4S 1.2 (aka, 20.10) - 67 full release products
- Feb 2021: E4S 21.02 - 67 full release, 4 partial release
- May 2021: E4S 21.05 - 76 full release products
- Aug 2021: E4S 21.08 - 88 full release products
- Nov 2021: E4S 21.11 - 91 full release products



<https://e4s.io>

Also include other products .e.g.,  
AI: PyTorch, TensorFlow (CUDA, ROCm)  
Co-Design: AMReX, Cabana, MFEM

# E4S Outreach Activities



## E4S HACKATHON

January 12

WHEN: January 12, 2021 @ 10:00 am – 10:00 pm ET

CONTACT: Sameer Shende  
[Email](#)

### E4S Hackathon

We encourage ECP ST and related team members to attend the E4S Hackathon on January 12, 2021. The hackathon will focus on the porting of numerical tools, libraries, and applications to three different GPU architectures — NVIDIA, Intel, AMD — and making them available through Spack. The hackathon will also help developers update their product repositories to better map files for updating the content in the [E4S DocPortal](#). The Spack and E4S teams will be available to answer questions and help ECP software and application developers. The hackathon will be a virtual Zoom based event. The Spack and E4S teams will enable access to a testbed at the University of Oregon featuring the three GPU architectures with a common filesystem for porting and testing.

*Important: Participants are required to enter a temporary password when registering (through "Tickets"). Please do not use any important password and immediately change the password when logging in for the first time on the testbed at the University of Oregon.*



## GETTING STARTED WITH E4S FOR INDUSTRY AND AGENCIES WORKSHOP

June 14 – June 15

WHEN: June 14, 2021 @ 11:00 am – June 15, 2021 @ 2:00 pm ET

CONTACT: David Martin  
[Email](#)

### Getting Started with E4S for Industry and Agencies Workshop

The Extreme-scale Scientific Software Stack (E4S) project aims to tame both the complexity and portability problems by creating an ecosystem of numerical libraries, runtime systems, and tools that lowers the barrier for entry for the HPC and AI/ML developer communities. E4S is a community effort to provide open source software packages for developing, deploying, and running scientific applications on HPC platforms. It aims to deliver a modular, interoperable, and deployable software stack based on the Spack package manager. The "Getting Started with E4S for Industry and Agencies" workshop was held on June 14-15, 2021. The intended audience was technical people from companies and US government agencies that are considering using E4S in their environment.

### Workshop Agenda ([Slides](#))

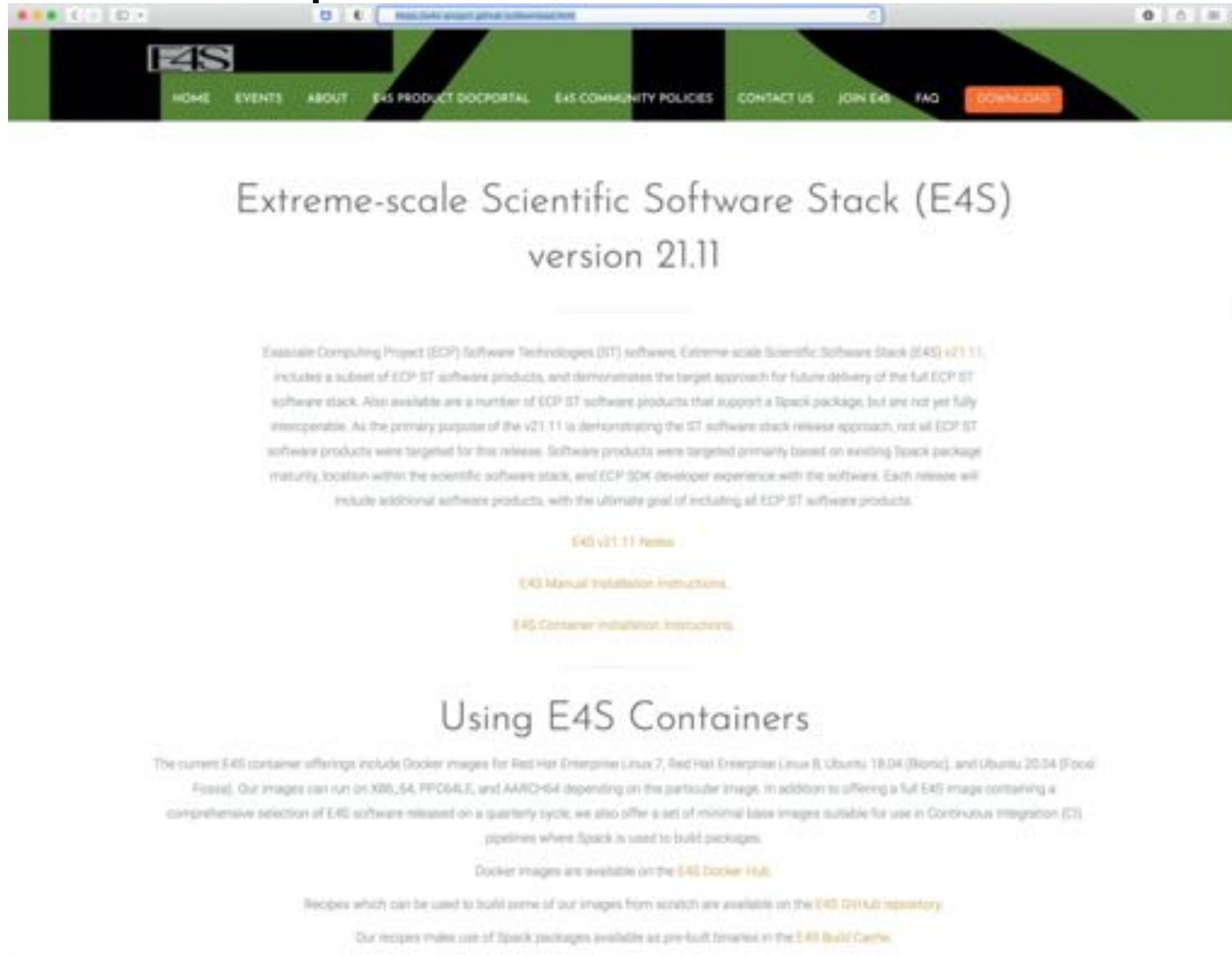
Day 1: Monday, June 14

8:00 AM – 9:30 AM – **OVERVIEW E4S**, MIKE HEROUX, DIRECTOR OF ECP SOFTWARE TECHNOLOGY ([VIDEO](#))

- *Who should attend*
  - Technical Leaders and developers who may or may not be familiar with E4S.
  - Prospective and first-time developers using E4S.
- *Topics addressed* This overview will discuss the philosophy behind E4S, the E4S components, and why industry should understand and consider adopting some of these components.

10:00 AM – 12:00 PM – **GETTING STARTED WITH E4S FOR INDUSTRY AND AGENCY TUTORIAL**, SAMEER SHENDE (ECP TECHNICAL LEAD FOR E4S)

# E4S Download from <https://e4s.io>



The screenshot shows the homepage of the Extreme-scale Scientific Software Stack (E4S) website. The header features a navigation bar with links: HOME, EVENTS, ABOUT, E4S PRODUCT DOCPORTAL, E4S COMMUNITY POLICIES, CONTACT US, JOIN E4S, and a prominent orange DOWNLOAD button. The main heading reads "Extreme-scale Scientific Software Stack (E4S) version 21.11". Below this, a paragraph explains that E4S v21.11 is a subset of ECP ST software products, demonstrating the target approach for future delivery. It notes that while some ECP ST products support a Spack package, not all are fully interoperable. The primary purpose of v21.11 is to demonstrate the ST software stack release approach, with products targeted based on existing Spack package maturity, location within the scientific software stack, and ECP SDK developer experience. Each release will include additional software products, with the ultimate goal of including all ECP ST software products. Three links are provided: [E4S v21.11 Files](#), [E4S Manual Installation Instructions](#), and [E4S Container Installation Instructions](#). A section titled "Using E4S Containers" follows, stating that current E4S container offerings include Docker images for Red Hat Enterprise Linux 7, Red Hat Enterprise Linux 8, Ubuntu 18.04 (Bionic), and Ubuntu 20.04 (Focal Fossa). These images can run on x86\_64, PPC64LE, and AARCH64 depending on the image. In addition to offering a full E4S image containing a comprehensive selection of E4S software released on a quarterly cycle, a set of minimal base images suitable for use in Continuous Integration (CI) pipelines where Spack is used to build packages is also offered. Docker images are available on the [E4S Docker Hub](#). Recipes which can be used to build some of our images from scratch are available on the [E4S GitHub repository](#). The recipes make use of Spack packages available as pre-built binaries in the [E4S Build Cache](#).

# Download E4S 21.11 GPU Container Image: NVIDIA, AMD, Intel



- Full featured Singularity image
- GPU base images for
  - x86\_64 (Intel, AMD, NVIDIA)
  - ppc64le
  - aarch64
- Packages with support for all three GPU runtimes:
  - Kokkos
  - TAU



# 21.11 Release: 91 Official Products + dependencies (gcc, x86\_64)

```
1: adios2 /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/adios2-2.7.1-4qzf7mzvghree7vzhia5homece6jzc2k
2: alquimia /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/alquimia-1.0.9-m2seuqbzraqqesmpqeyyiwlqdeihsq3r
3: aml /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/aml-0.1.0-52bcp4rwi6xzk1r2qpl3a3huqle6sszh
4: amrex /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/amrex-21.11-7bb5j5a6ozsgddf2eyrffpy2brqknewq
5: arborx /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/arborx-1.1-qdabctwt5xpyip12kdfn53ueifpy3mw5i
6: argobots /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/argobots-1.1-6vbx4fbx3ert23po2fzeuddnyal2wmiy
7: ascent /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/ascent-0.7.1-aijl3oqrcrdoz2bpabeyvtg6uzc4seob
8: axom /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/axom-0.5.0-xaa26pwr3yr625ums6b4p6uxobmrgzkh
9: bolt /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/bolt-2.0-fh7dq6fzfeie5fl3nqzindyzvggges6v
10: butterflypack /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/butterflypack-2.0.0-otoimkvs5kwd7fool3uqf5574dysb7ud
11: cabana /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/cabana-0.4.0-hczsjbp2bke3b2ovuvyubr6f4kfzwdt
12: caliper /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/caliper-2.7.0-6wyi2jsiepczmulgxtzjjiaopqr26iy
13: catalyst /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/catalyst-5.6.0-h77spazrgb6ydf765iyuglvqdivvook
14: chai /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/chai-2.4.0-cvcmt7qh457whlgo46z73avoiz3wdsxy
15: charliecloud /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/charliecloud-0.25-dtxafv2422vaxp7ihqmc332yt5v6mzt
16: conduit /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/conduit-0.7.2-kx4lp6skbe7sstmulhzzszusw37yfwdq
17: darshan-runtime /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/darshan-runtime-3.3.1-6zcvdaohaersjbt2cuandyqgbfwn7dnn
18: datatransferkit /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/datatransferkit-3.1-rc3-53dtzpnkqhndejqjptw4j6wqijjsjo26u
19: dyninst /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/dyninst-11.0.1-r63gihwhdsrehmchw45duykrueggor23
20: faodel /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/faodel-1.2108.1-gocysw2xc4rjp3av2rfokhu4dvrn2ml
21: flecsi /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/flecsi-2.1.0-iuolizsdjxiuknomqpehlnte2asi54r
22: flit /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/flit-2.1.0-ywc5thidgsdtg6474uxgqkdnefyax75l
23: flux-sched /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/flux-sched-0.19.0-cc5zm4atwcpkoybepcc4r3khkdxh3mtj
24: fortrilinos /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/fortrilinos-2.0.0-ywy56z7j1haxgy3vvcerc67i7vjbelczc
25: gasnet /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/gasnet-2021.9.0-37bcasne2t26z4f7rju7fy52eeqoolx
26: ginkgo /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/ginkgo-1.4.0-7b5gicftkdjme5vi5phvymtw5ichochk
27: globalarrays /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/globalarrays-5.0-bv7uslrymise7kjadm72okt26yziyo47
28: gotcha /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/gotcha-1.0.3-u6tтыkuc7w75fpckuy4piy72uhdxvdx
29: hdf5 /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/hdf5-1.12.1-h2uwi5y62osghdrb6xsgdt3lmo6h2ylj
30: heffte /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/heffte-2.2.0-eri5pxovnynn557l2nurwddxmepvrsth
31: hpctoolkit /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/hpctoolkit-2021.10.15-vbfmr3qvlzfzafyn21olb3hkclsq5v
32: hpx /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/hpx-1.7.1-tdou2dmt5p4nbcrtbuyi35exzvr5ldi
33: hypre /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/hypre-2.23.0-h5cudf346j2hti7exgdrbxku4pwt46ii
34: kokkos /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/kokkos-3.4.01-klsmq76webvynj3helrcfacc3lcuucmb
35: kokkos-kernels /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/kokkos-kernels-3.4.01-sd4zmqbi4i67tc77lzapltak6tnchasn
36: legion /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/legion-21.03.0-aipgy23rif36pv4u4pivatzuqhvrg4jf
37: libnm /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/libnm-0.1.0-mjn3bmqp5ub7ooz35qnooartbjnnoqx
38: libquo /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/libquo-1.3.1-pah7fsgud2hpwdbnaap7jam337kxtul
39: loki /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/loki-0.1.7-2zpo6dh6bdrko47n4gziacm6xteoflm
40: magma /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/magma-2.6.1-hzi3pvxdl7k6fgupj4laagcfc1i3zwr5
41: mercury /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/mercury-2.0.1-jbzjyopvabgyzwy3ne75nlsv7wl4etwh
42: metall /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/metall-0.17-dd7fzx7g34o7ggiituwpgw6aqendc4ul
43: mfem /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/mfem-4.3.0-emaug2hgogpviw2ov5y4lw7rsybtzliw
44: mpich /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/mpich-3.4.2-bfamq5fmi7yh3fdkwr4vw6xn7rr5lc75
45: mpifileutils /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/mpifileutils-0.11-onrcotnug776fzd55av3xoyw7d5wmwt
```

## GPU runtimes

- Intel (oneAPI)
  - 2021.4
- AMD (ROCm)
  - 4.3
- NVIDIA (CUDA)
  - 11.4
- NVHPC
  - 2021.9



# 21.11 Release: 91 Official Products + dependencies (contd.)

```
46: mpifileutils /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mpifileutils-0.11-ajx7675xid7lvcfk4u4ifbunshdqzz7k
47: netlib-scalapack /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/netlib-scalapack-2.1.0-xn73q57pjteeundik4shoezrlo2g6mrq
48: ninja /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/ninja-1.10.2-txpvjbtkrq7ovnuLuobagoqgn5gabq3d
49: nrm /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/nrm-0.1.0-yyrb64omok3tyqh6gzolo3k3h34y5rpj
50: omega-h /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/omega-h-9.34.1-gaulvevjniqaw16fbazyknuqfinffnjw
51: openpmd-api /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/openpmd-api-0.14.3-mnziagkceftx7m3kwzc4pk7dmkrqk5q
52: openmpi /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/openmpi-4.1.1-uw4owrxv26x3ygr5q7udhme3freqwzl
53: papi /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/papi-6.0.0.1-ehedapozusx3i7lfpichari5atqvmh74
54: papyrus /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/papyrus-1.0.1-dl6ak3mnzrltiwusuriolnfl5ks2wxx
55: parallel-netcdf /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/parallel-netcdf-1.12.2-nxbqhe3qkzdxu6o4hsk2vqnpq3mswqjg
56: paraview /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/paraview-5.9.1-xixczmqgghdx2x5dyzgp532zua2jwow
57: parsec /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/parsec-3.0.2012-h2m2judrwzxiqevr6q3j7wnrqct67sfh
58: pdt /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/pdt-3.25.1-dfzobkfuiqcrpxae5hnfezqm6gpqi3wk
59: petsc /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/petsc-3.16.1-vtjfiqa2amthfcd5hbgphy5l7snp2i4
60: plasma /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/plasma-21.8.29-xdwx32rgusitrac72mqkurknhrsbzof
61: precice /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/precice-2.3.0-mxwok2fd6meuzcv6v5lmd5bv4zpuqrk5
62: pumi /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/pumi-2.2.6-b7ydidbb45jo3kkced2kjahpnqtg4qt1
63: py-jupyterhub /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-jupyterhub-1.4.1-3515htiyp6a64azpehogjt4vf2f2no67
64: py-libensemble /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-libensemble-0.8.0-f27asumkzcgzbxhnrknsyoyxy3sfpq1
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66: py-radical-saga /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-radical-saga-1.8.0-lbuszbgvc3lbbqwhrldcurhpk1roco7f
67: py-radical-pilot /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-radical-pilot-1.8.0-wkjrzkqe2v2dpdvapay7emxj2jtaif2f4
68: qthreads /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/qthreads-1.16-kcir2bkoatobn4e2qz7fncrffs7pgn4v
69: raja /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/raja-0.14.0-ns3dxuqr5fbufgvhyxqe3ydi6ip7mbr
70: rempi /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/rempi-1.1.0-ib2lnlqhr3zvmrnbgatgbcu7fjnw6vzv
71: scr /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/scr-3.0rc2-gb3auatilui4yrlo4cjgvhabwve254id
72: slate /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/slate-2021.05.02-wb4vyncciraa7dqksegnhvkk7kx64frhy
73: slepc /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/slepc-3.16.0-hgn6jvzk2oo5q5cdiybvulurjmmvdf2k
74: strumpack /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/strumpack-6.1.0-i7t4sy35etpvmzajlyljvp4ncgf3g5
75: sundials /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/sundials-5.8.0-q4wq3fsvsa7ml3xjstb3nmsc4sb2pdb7
76: superlu-dist /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/superlu-dist-7.1.1-hft52tkp3cbvl7c6ushtpp566iad72qk
77: stc /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/stc-0.9.0-w2ubukpoj7ouvf5wrxmwvxfm225nsx7
78: swig /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-11.1.0/swig-4.0.2-tlf7zp6ptp7vx66s5dsy2ujx57lt6qne
79: sz /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/sz-2.1.12-n5wqbtryijanb6p6qh27p36daq4y2mce
80: tasmanian /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/tasmanian-7.7-i6urkzufeppq6yygpr2upj2j2lwbphh1
81: tau /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/tau-2.31-ceaf0a37nxemdsio6c21xr3knu54nidr
82: trilinos /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/trilinos-13.2.0-7tqdn7m6rhct4jxuwjinkhubas54sw
83: turbine /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/turbine-1.3.0-ur5he6cmg73k6doLxsbaysvfaunceua
84: umap /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/umap-2.1.0-7sqykikt6qkgfbgnxgwbjwy2ia47cc5d
85: umpire /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/umpire-6.0.0-qy2li7mkl4wgbbplga6gqudrw3pl64mw
86: unifyfs /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/unifyfs-0.9.1-xdusd5vqnurbrl3priwyjutxbq3cpki
87: upcxx /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/upcxx-2021.9.0-nb32n2wmpjqos77untzfkfte15426e4o
88: velox /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/velox-1.5-tl435lrbllqcw746hq32aan6frmoq5gi
89: vtk-m /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/vtk-m-1.6.0-yw4rayrgc3foebzaunuptat4urdu5js3
90: warpx /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/warpx-21.11-5vf3w65haj2jydmr34bcjhx54u4oce25
91: zfp /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/zfp-0.5.5-o2thmry2kturpuooiprs75wjmlieixk7b
```



# E4S 21.11: Trilinos configurations cuda\_arch=80 and cuda\_arch=70

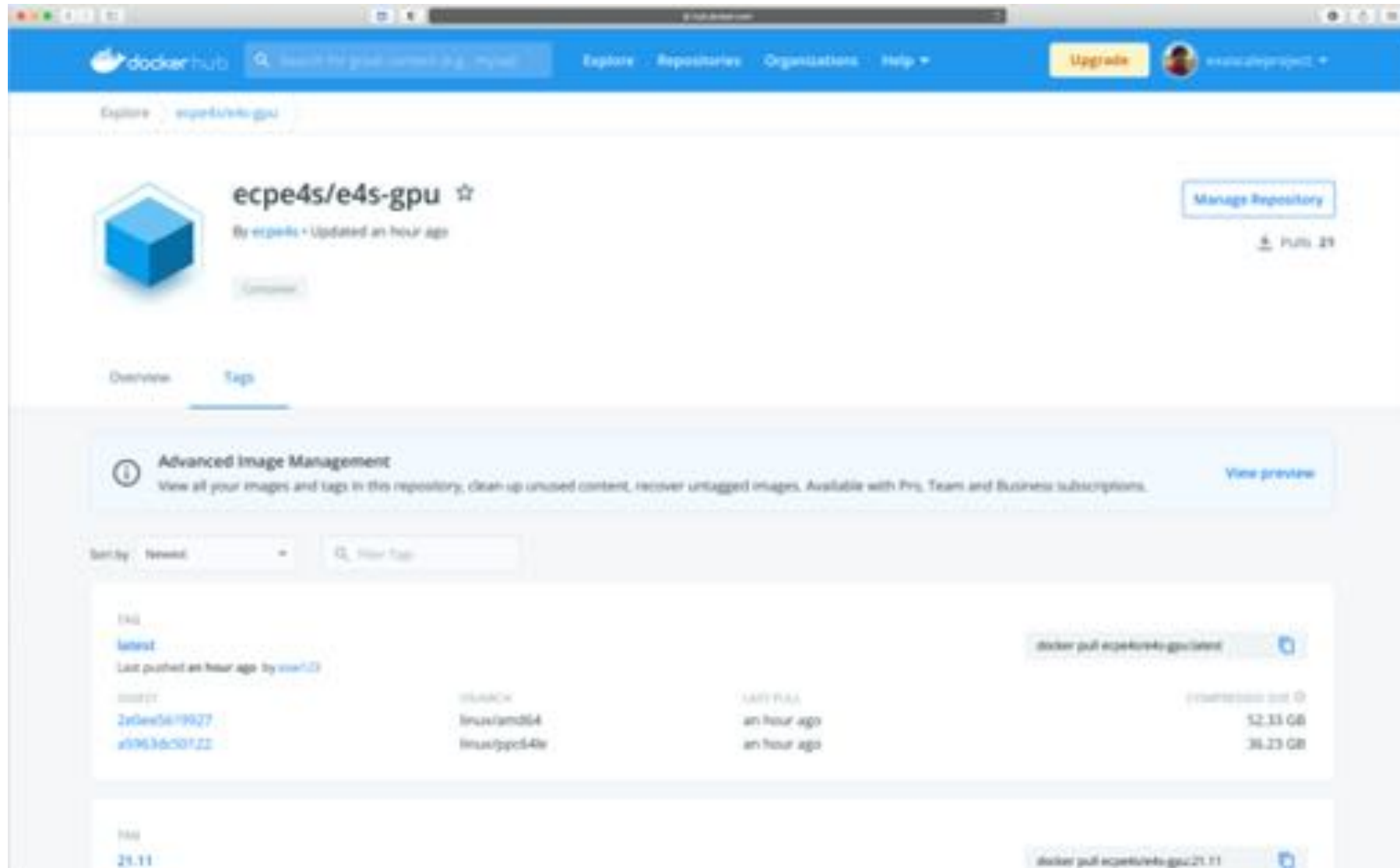
```
Singularity> spack find -dl -v trilinos@13.0.1
==> 1 installed package
-- linux-ubuntu20.04-x86_64 / gcc@9.3.0 -----
xmx42u4 trilinos@13.0.1~adios2+amesos+amesos2+anasazi+artec-basker+belos+boost+chaco+complex+cuda+cuda_rdc+debug+dtk+epetra+epetraext+epetraextbtf+epetraextexper
imental+epetraextgraphreorderings+exodus+explicit_template_instantiation+float+fortran+gtest+ hdf5+hypre+ifpack+ifpack2+intrepid+intrepid2+ipo+isorropia+kokkos+me
suite+minitensor+nl+mpi+mu2u+mumps+nox+openmp+phalanx+piro+python+rol+rythmos+sacado+scorec+shards+shared+shylu+stk+stektos+stratimikos+strumpack+suite-sparse+
superlu+superlu-dist+teko+tempus+tpetra+trilinoscouplings+wrapper+xi+zeitan+zeitan2 build_type=RelWithDebInfo cuda_arch=none cxxstd=14 gotype=long_long
ghlyle6 boost@1.77.0+atomic+chrono+clanglibc++-container-context-coroutine+date_time+debug+exception+fiber+filesystem+graph+icu+iostreams+locale+log+math+mpi
+multithreaded+numpy-pic+program_options+python+random+regex+serialization+shared+signals+singlethreaded+system+taggedlayout+test+thread+timer+versionedlayout+wa
ve cxxstd=98 patches=93f4aad8f88d1437c58d95a2d866398ef3753b99ef5de24f7a46bc883bd5df86 visibilityglobal
acrn735 bzip2@1.0.8~debug-pic+shared
ufqpnq zlib@1.2.11+optimize+pic+shared
blvhc36 hwloc@2.4.0~cairo+cuda-glibc+libudev+libxml2+netloc+nvml+opencl+pci+rocm+shared
4jbn7uz libpciaccess@0.16
xlbisrk libxml2@2.9.12~python
zth4obv libiconv@1.16 libs=shared,static
mq4ikt5 xz@5.2.5+pic libs=shared,static
nxjjpha ncurses@6.2+symlinks+termlib abi=none
vds2a7e metis@5.1.0~gdb-int64-real64+shared build_type=Release patches=4991da938cd3a1d3dea78e49b6ebecba80273f98df2a656e38b83d55b281da1,b1225da886685ea558db7
ac88dd8854742ea5afe5ed61ad4d8fe7a495b1278d2
jpicv6o mpich@3.4.2~argobots+fortran+hwloc+hydra+libxml2+pci+rocm+slurm+verbs+wrapper+path device=ch4 netmod=ofi pmix=pmi
uz3fmys libfabric@1.13.2~debug+kdreg fabric=ram,sockets,tcp,udp
xsf3dfi openblas@0.3.10~bignuma-consistent_fpcsr+ilp64+locking+pic+shared threads=openmp
vhu5a7 parmetis@4.0.3~gdb-int64-ipo+shared build_type=RelWithDebInfo patches=4f892531eb0a807eb1b82e683a416d3e35154a455274cf9b162fb02854d1a5b,50ed2801bc9392
69689789942067c58b3e522c269269a438d5d34c80edbc5878,784b84f7c7444d4372cb59ccae1289d4ef3b8833bc4ee3cf58f369bce972a9d
lvlywfg superlu-dist@7.1.1~cuda-int64-ipo+openmp+shared build_type=RelWithDebInfo cuda_arch=none

Singularity> spack find -dl -v trilinos@13.2.0 +cuda cuda_arch=80
==> 1 installed package
-- linux-ubuntu20.04-x86_64 / gcc@9.3.0 -----
lvlywfg trilinos@13.2.0~adios2+amesos+amesos2+anasazi+artec-basker+belos+boost+chaco+complex+cuda+cuda_rdc+debug+dtk+epetra+epetraext+epetraextbtf+epetraextexper
imental+epetraextgraphreorderings+exodus+explicit_template_instantiation+float+fortran+gtest+ hdf5+hypre+ifpack+ifpack2+intrepid+intrepid2+ipo+isorropia+kokkos+me
suite+minitensor+nl+mpi+mu2u+mumps+nox+openmp+phalanx+piro+python+rol+rythmos+sacado+scorec+shards+shared+shylu+stk+stektos+stratimikos+strumpack+suite-sparse+
superlu+superlu-dist+teko+tempus+tpetra+trilinoscouplings+wrapper+xi+zeitan+zeitan2 build_type=RelWithDebInfo cuda_arch=80 cxxstd=14 gotype=long_long
ghlyle6 boost@1.77.0+atomic+chrono+clanglibc++-container-context-coroutine+date_time+debug+exception+fiber+filesystem+graph+icu+iostreams+locale+log+math+mpi
+multithreaded+numpy-pic+program_options+python+random+regex+serialization+shared+signals+singlethreaded+system+taggedlayout+test+thread+timer+versionedlayout+wa
ve cxxstd=98 patches=93f4aad8f88d1437c58d95a2d866398ef3753b99ef5de24f7a46bc883bd5df86 visibilityglobal
acrn735 bzip2@1.0.8~debug-pic+shared
ufqpnq zlib@1.2.11+optimize+pic+shared
t2yzj1 cuda@11.4.2~dev
4jbn7uz hwloc@2.4.0~cairo+cuda-glibc+libudev+libxml2+netloc+nvml+opencl+pci+rocm+shared
libpciaccess@0.16
libxml2@2.9.12~python
libiconv@1.16 libs=shared,static
xz@5.2.5+pic libs=shared,static
ncurses@6.2+symlinks+termlib abi=none
kokkos+nvcc-wrapper@1.2.0~mpi
mpich@3.4.2~argobots+fortran+hwloc+hydra+libxml2+pci+rocm+slurm+verbs+wrapper+path device=ch4 netmod=ofi pmix=pmi
libfabric@1.13.2~debug+kdreg fabric=ram,sockets,tcp,udp
metis@5.1.0~gdb-int64-real64+shared build_type=Release patches=4991da938cd3a1d3dea78e49b6ebecba80273f98df2a656e38b83d55b281da1,b1225da886685ea558db7
ac88dd8854742ea5afe5ed61ad4d8fe7a495b1278d2
xsf3dfi openblas@0.3.10~bignuma-consistent_fpcsr+ilp64+locking+pic+shared threads=openmp
vhu5a7 parmetis@4.0.3~gdb-int64-ipo+shared build_type=RelWithDebInfo patches=4f892531eb0a807eb1b82e683a416d3e35154a455274cf9b162fb02854d1a5b,50ed2801bc9392
69689789942067c58b3e522c269269a438d5d34c80edbc5878,784b84f7c7444d4372cb59ccae1289d4ef3b8833bc4ee3cf58f369bce972a9d
Scxxgku superlu-dist@7.1.1~cuda-int64-ipo+openmp+shared build_type=RelWithDebInfo cuda_arch=none

Singularity> 
```

- Trilinos 13.2.0
- CUDA 11.4.2
- cuda\_arch=80 (for A100)

# E4S v2021-02 Release: GPU, ppc64le for Docker Containers



- 91 E4S Products
- Support for GPUs
  - ppc64le and x86\_64

• `docker pull ecpe4s/e4s-gpu`



# E4S 21.11 GPU Release: 91 E4S Products (ppc64le)

```
1: adios2 /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/adios2-2.7.1-ldgyyfdotfy6gpxlcr7ukcd2zqy7dtk
2: alquimia /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/alquimia-1.0.9-sba2gv6bnjr7x6cvscivj7udb6ql4s4k
3: aml /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/aml-0.1.0-dvzmjczox3ubd7lnxdgaggoksk5v43k
4: amrex /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/amrex-21.11-bochehw3hziv3hvpjfgzk4gzukpub434
5: arborx /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/arborx-1.1-2ocu7oexml06bbr6ki7nhcqzphvsf7di
6: argobots /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/argobots-1.1-trhfaqcm2lib5tsw4axzqls4tbbxt45
7: ascent /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/ascent-0.7.1-b4h5qerq2jeb2sfqjtrbttzt5t5zpz7e
8: axom /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/axom-0.5.0-bmdk6urkjs6ustj7ubmm4vp4uo2cwa
9: bolt /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/bolt-2.0-lfkm2qifo3qdvddgdcqeq2b7rgv3yesq
10: butterflypack /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/butterflypack-2.0.0-qxe43g2fxpw5h4bzttdzjptlp27idy7
11: cabana /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/cabana-0.4.0-vgtzjwojg6hljiki15o4qwybvbtpt274
12: caliper /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/caliper-2.7.0-ssibgi4tqiioyedewfxj7jcxlju67gdw
13: chai /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/chai-2.4.0-c6aszygyyexbc6yedmgfwb7hujtmc1
14: charliecloud /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/charliecloud-0.25-45c55u3sg54qt3u5zvpa3leyin57rn2f
15: conduit /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/conduit-0.7.2-gtel3lgyuoc2v4emndmhgbbi2bn3zfa
16: darshan-runtime /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/darshan-runtime-3.3.1-dtybw7bvkl4otzpdliout456zjv3cya5
17: datatransferkit /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/datatransferkit-3.1-rc3-lexrtrlqlbpywagagneq6tinikqft515
18: dyninst /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/dyninst-11.0.1-6kmzpsa5uurubuefeo2463gvua4x3oej
19: exaworks /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/exaworks-0.1.0-ibfujbaymzdnvx4rxtx5hnfv6kgyegy
20: faodel /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/faodel-1.2108.1-ierf32uf3dninjzbrqr3fhic3pkfti5
21: flecsi /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/flecsi-1.4.2-j6eul76nv3jwum6g2ifh7x3lacedn2u3i
22: flit /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/flit-2.1.0-lbkrrpmiawtvljllak5w7oycyakujjz
23: flux-sched /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/flux-sched-0.19.0-azlepgnf4x3szj74ttgx5aqtzbyl5gxa
24: fortrilinos /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/fortrilinos-2.0.0-cg346iqfzjupsa37whrn4tvpjbgxxnd
25: gasnet /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/gasnet-2021.9.0-vov6viwltjtd2xdcjebkcuyds22yk4f
26: ginkgo /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/ginkgo-1.4.0-isjktvku6r65marjrdrep2cjphyu6d2
27: globalarrays /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/globalarrays-5.0-ue7lygmoqeznr14zonekhkpc7qo46xdb
28: gotcha /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/gotcha-1.0.3-nyelkzzogqa4ca4lug5wj12jkhibrvpq
29: hdf5 /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/hdf5-1.12.1-dscpp3b5u3k3nusfoh3d4zvc2fdbndqm
30: heffte /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/heffte-2.2.0-cbijfxgg77w3nfpri4szl2mghl7lrnhs
31: hpctoolkit /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/hpctoolkit-2021.10.15-racjlvq2z3d13euln7ybh6nmjwjghja
32: hpx /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/hpx-1.7.1-wtti5py323torlms07g6bfrgrh4bo6d4
33: hypre /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/hypre-2.23.0-q5zfpxllicqe4sgsu6433hunaa7sqvzbz
34: kokkos /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/kokkos-3.4.01-7bopbt2jv34cvnucpmfbw3npggotwvl
35: kokkos-kernels /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/kokkos-kernels-3.4.01-xhkhohrzepfvxwkiaeqmwiylbjxd4daa
36: legion /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/legion-21.03.0-t6fsvautw2h6cbv4neab3phbssebo1nm
37: libnm /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/libnm-0.1.0-jsse7qvcjj4opsa7avql2dkogwqzm5m
38: libquo /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/libquo-1.3.1-klnddbwro2x46jfc2ystw5sm6ds43cvl
39: loki /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/loki-0.1.7-ggwkzpwjztzrps5x2fnimeesu5i6un
40: magma /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/magma-2.6.1-df5ncmusf6viglrdfo6ladkyltxgcxe
41: mercury /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mercury-2.0.1-nblhmpo2yjt4nj572uq5vkkzlwzebd5
42: metall /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/metall-0.17-7fomntjjbwhldxq5hfocv5vmfignp6t
43: mfem /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mfem-4.3.0-lbm2ladjftanl5qbu5orcfciwj3u5zrm
44: mpark-variant /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mpark-variant-1.4.0-xyf5xrvdszmtlswk35ayonajo2falqg5
45: mpich /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mpich-3.4.2-i2roe5wfv4uhmbqzxcj4rvhx3ugev
```

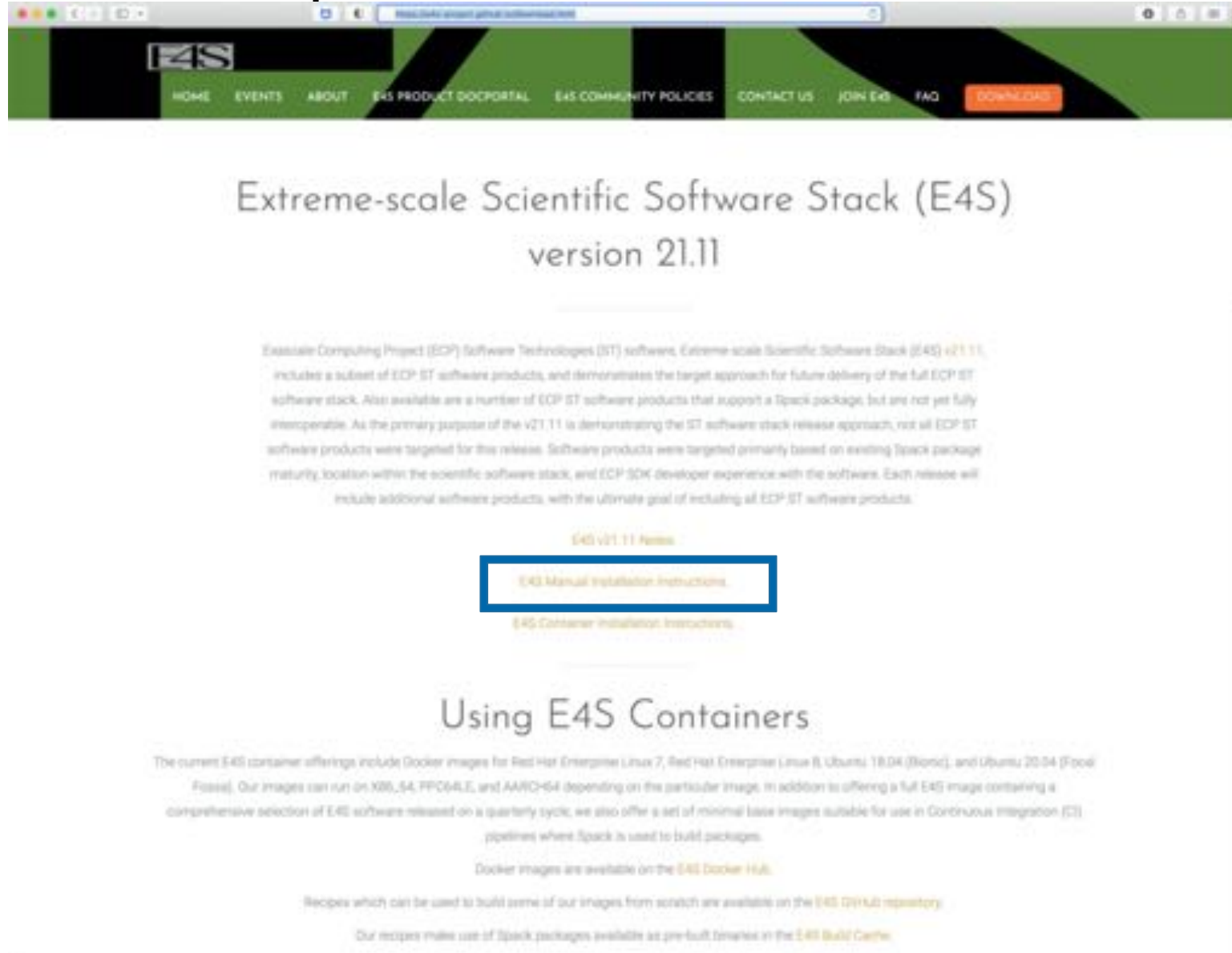
- 91 E4S products
- Ubuntu v18.04 ppc64le
- Support for GPUs
  - NVIDIA CUDA
  - NVHPC 21.9

# E4S 21.11 ppc64le Singularity image

```
46: mpifileutils /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mpifileutils-0.11-ajx7675xid7lvcfk4u4ifbunshdqqz7k
47: netlib-scalapack /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/netlib-scalapack-2.1.0-xn73q57pjteeundik4shoezrlo2g6mrq
48: ninja /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/ninja-1.10.2-tpxvjbtkrq7ovmuluobagoqgn5gabg3d
49: nrm /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/nrm-0.1.0-yyrb64omok3tyqh6gzolo3k3h54y5rpj
50: omega-h /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/omega-h-9.34.1-gaulvevjniqawi6fbazyknuqfinffnjw
51: openpmc-api /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/openpmc-api-0.14.3-mnziagkceftx7wm3kwzc4pk7dnkrqk5q
52: openmpi /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/openmpi-4.1.1-uw4owrxv26x3ygr5q7udhme3freqwz1
53: papi /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/papi-6.0.0.1-ehedapozusx3i7lfpichari5atqvmh74
54: papyrus /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/papyrus-1.0.1-dl6ak3mzzltiwsuriolnfl5ks2wxxw
55: parallel-netcdf /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/parallel-netcdf-1.12.2-nxbqhe3qkzdxu6o4hsk2vqnpq3mswqj
56: paraview /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/paraview-5.9.1-xixczmqggnhdx2x5dyzgp532zua2jwow
57: parsec /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/parsec-3.0.2012-h2m2judrwxigevr6q3j7wnrqct67sfb
58: pdt /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/pdt-3.25.1-dfzobkfuiqcrpxae5hnfezqm6ppqi3wk
59: petsc /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/petsc-3.16.1-vtjfiqia2anthfcd5hbgphy5i7snp2i4
60: plasma /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/plasma-21.8.29-xdwx3zrgusitrac72mqkurknhrsbzof
61: precice /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/precice-2.3.0-mxwok2fd6meuzcv6v5lmd5bv4zpuqrk5
62: pumi /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/pumi-2.2.6-b7ydidbb45jo3kkced2kjahpnqtg4qti
63: py-jupyterhub /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-jupyterhub-1.4.1-35l5htiyp6a64azpehogjt4vf2f2no67
64: py-libensemble /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-libensemble-0.8.0-f27asumkzcgbrzhonrknsyoyxy3sfpql
65: py-parsl /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-parsl-1.1.0-e3ge67qfbnhto57ubonckxoywezsyyga
66: py-radical-saga /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-radical-saga-1.8.0-lbuszbgvc3ibbqwhrlidcurhpk1roco7f
67: py-radical-pilot /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-radical-pilot-1.8.0-wkjkzqe2v2dpdvapay7emxj2jtaif2f4
68: qthreads /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/qthreads-1.16-kcir2bkoatobn4e2qz7fmcrrfs7pgn4v
69: raja /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/raja-0.14.0-ns3dxwqr5fbufgvhyxqe3ydi6ip7mbr
70: rempi /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/rempi-1.1.0-1b2lnlqhr3zvmrnrbgtgbcujfnw6vzv
71: scr /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/scr-3.0rc2-gb3auatilu4yrlo4c9gvhabwve254id
72: slate /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/slate-2021.05.02-wb4vynciraa7dqksegnhvkx7kx64frhy
73: slepc /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/slepc-3.16.0-hgn6jvzrk2oo5q5cdiybvuiurjmmvdf2k
74: strumpack /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/strumpack-6.1.0-17t4sy3setpvmzajlyljvp4ncgf3g5
75: sundials /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/sundials-5.8.0-q4wq3fsvsa7m13xjstb3nmsc4sb2pdb7
76: superlu-dist /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/superlu-dist-7.1.1-hft52tkp3cbvl7c6ushtpp566iad72qk
77: stc /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/stc-0.9.0-w2ubukpoj7ouvf5wrxmwvxfm223nsx7
78: swig /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-11.1.0/swig-4.0.2-1l7z6p6tp7vx66s5dsy2ujx57lt6qne
79: sz /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/sz-2.1.12-n5qgbtrijjanb6p6qh27p36daq4y2mce
80: tasmanian /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/tasmanian-7.7-i6urkzufeppqw6yypgz2upj2j2iwbghhi
81: tau /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/tau-2.31-cegfgg37nxemds1o6c2jxr3knu54njdr
82: trilinos /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/trilinos-13.2.0-7tgd7m6rhcc4jxuwujinkhu6as54sw
83: turbine /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/turbine-1.3.0-ur5he6cmg73k6dolxsbaysvfaunceua
84: umap /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/umap-2.1.0-7sqkyikt6qkgf6gnxgwbjwy2ia47cc5d
85: umpire /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/umpire-6.0.0-qy2li7mkl4wgbhplga6gqudrw3pl64mw
86: unifyfs /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/unifyfs-0.9.1-xdusd5vqnurbrl3priwyutxjbq3cpki
87: upcxx /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/upcxx-2021.9.0-nb32n2wmpjqos77untzfkftel5426e4o
88: veloc /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/veloc-1.5-tl435lrlblqcw746hq32aan6frqmoq5gi
89: vtk-m /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/vtk-m-1.6.0-yw4rayrgc3foebzaunuptat4urdu5js3
90: warpx /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/warpx-21.11-5vf3w65haj2jydmr34bcjhxs4u4oce25
91: zfp /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/zfp-0.5.5-o2thmry2kturpuooiprs75wjmliekk7b
```



# E4S Download from <https://e4s.io>



The screenshot shows the homepage of the Extreme-scale Scientific Software Stack (E4S) website. The header features a navigation bar with links: HOME, EVENTS, ABOUT, E4S PRODUCT DOCPORTAL, E4S COMMUNITY POLICIES, CONTACT US, JOIN E4S, and a prominent orange DOWNLOAD button. The main heading reads "Extreme-scale Scientific Software Stack (E4S) version 21.11". Below this, a paragraph explains that E4S v21.11 is a subset of ECP ST software products, demonstrating the target approach for future delivery. It notes that while some ECP ST products support a Spack package, not all are fully interoperable. The primary purpose of v21.11 is to demonstrate the ST software stack release approach, with products targeted based on existing Spack package maturity, location within the scientific software stack, and ECP SDK developer experience. Each release will include additional software products, with the ultimate goal of including all ECP ST software products.

Below the paragraph are three links: "E4S v21.11 Files", "E4S Manual Installation Instructions" (which is highlighted with a blue rectangular box), and "E4S Container Installation Instructions".

The next section is titled "Using E4S Containers". It states that the current E4S container offerings include Docker images for Red Hat Enterprise Linux 7, Red Hat Enterprise Linux 8, Ubuntu 18.04 (Bionic), and Ubuntu 20.04 (Focal Fossa). These images can run on x86\_64, PPC64LE, and AARCH64 depending on the particular image. In addition to offering a full E4S image containing a comprehensive selection of E4S software released on a quarterly cycle, the website also offers a set of minimal base images suitable for use in Continuous Integration (CI) pipelines where Spack is used to build packages.

Docker images are available on the [E4S Docker Hub](#). Recipes which can be used to build some of our images from scratch are available on the [E4S GitHub repository](#). The recipes make use of Spack packages available as pre-built binaries in the [E4S Build Cache](#).

# E4S 21.11 bare-metal installation



The screenshot shows a web browser window displaying the E4S-Project.github.io Manual Installation Instructions page. The page has a clean, minimalist design with a white background and black text. The title 'E4S-Project.github.io' is at the top in a large, bold, sans-serif font. Below it, the subtitle 'Manual Installation Instructions' is also in a large, bold, sans-serif font. The page is divided into two main sections: 'References' and 'Instructions'. The 'References' section contains a list of links: 'Spack General Documentation', 'Spack Environments Documentation', 'Spack Build Cache Documentation', 'E4S Model Environment Repository', 'E4S 21.11 Model Environments', and 'E4S Homepage'. The 'Instructions' section contains a paragraph of text and a code block with terminal commands. The text explains that if you want to use Spack's Clingo-based concretizer, you can either let Spack bootstrap Clingo for you, or you can install it manually via pip, in which case Spack will not need to bootstrap it. The code block shows the commands to install pip and Clingo, clone the Spack repository, checkout the e4s-21.11 branch, and source the setup-env.sh script. Below the code block, there is a paragraph explaining how to configure Spack to know where the E4S Build Cache is located, mentioning both release-specific and mixed build caches.

E4S-Project.github.io

## Manual Installation Instructions

### References

- [Spack General Documentation](#)
- [Spack Environments Documentation](#)
- [Spack Build Cache Documentation](#)
- [E4S Model Environment Repository](#)
- [E4S 21.11 Model Environments](#)
- [E4S Homepage](#)

### Instructions

If you want to use Spack's Clingo-based concretizer, you can either let Spack bootstrap Clingo for you, or you can install it manually via pip, in which case Spack will not need to bootstrap it. To install it via pip

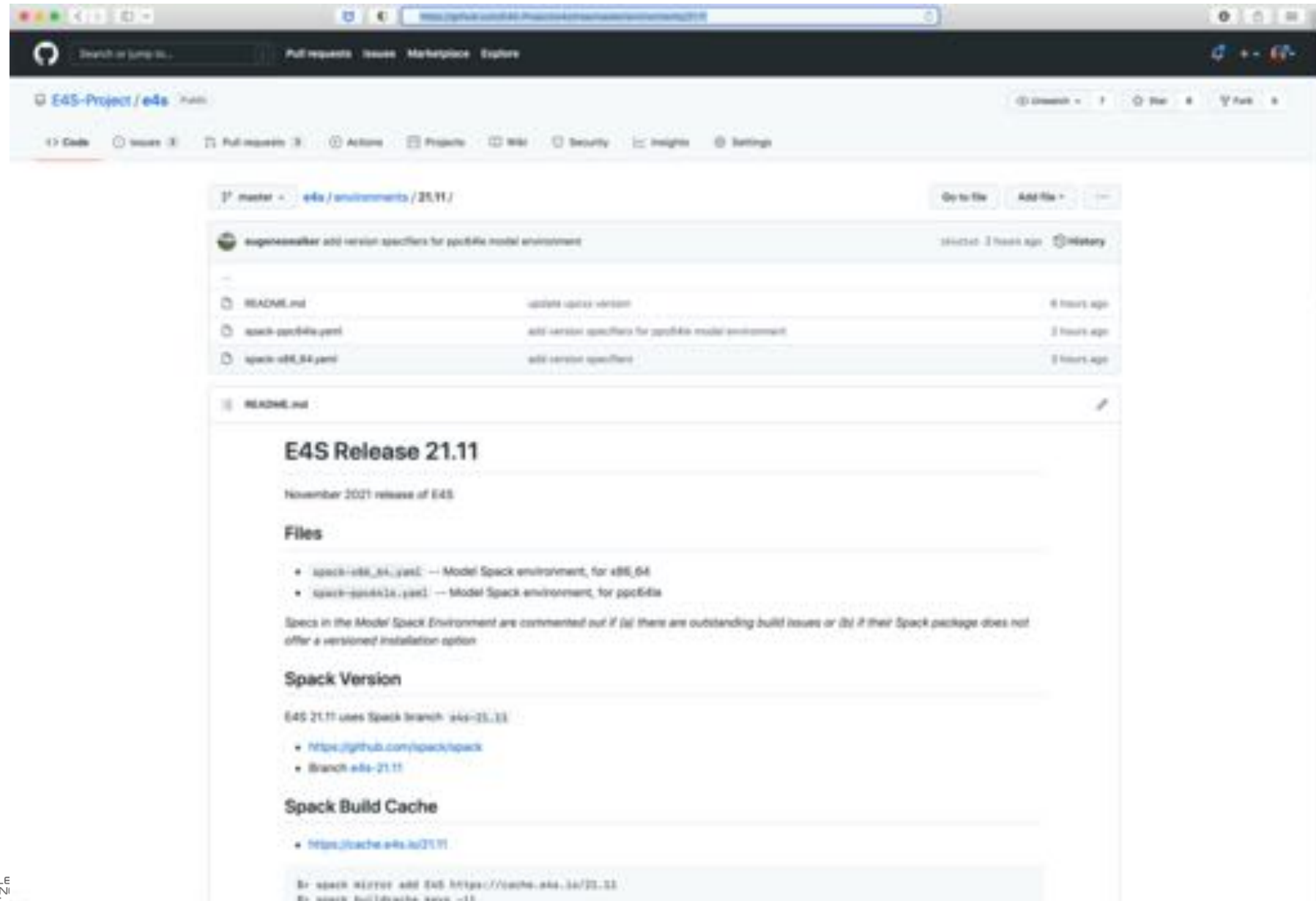
```
$> pip install --user --upgrade pip
$> pip install --user clingo
```

Clone Spack, checkout the appropriate release branch, if desired, and source the Spack setup-env.sh script.

```
$> git clone https://github.com/spack/spack
$> (cd spack && git checkout e4s-21.11)
$> . spack/share/spack/setup-env.sh
```

Configure Spack to know where the E4S Build Cache is located. You can use either a release specific build cache, or the mixed build cache. The release specific build cache contains only binaries from the particular release, whereas the mixed build cache contains binaries from all releases and from in between releases.

# E4S 21.11 bare-metal Spack installation environments on GitHub



The screenshot shows the GitHub interface for the E4S-Project repository, specifically the `e4s/environments/21.11` directory. The commit history table is as follows:

| Commit               | Message  | Author       | Time        |
|----------------------|--|--------------|-------------|
| <code>8f8f8f8</code> | update spack version                                 | eugenewalker | 6 hours ago |
| <code>7d7d7d7</code> | add version specifiers for ppc64le model environment | eugenewalker | 2 hours ago |
| <code>6e6e6e6</code> | add version specifier                                | eugenewalker | 2 hours ago |

The README content for the 21.11 release is as follows:

## E4S Release 21.11

November 2021 release of E4S

### Files

- `spack-e4s_64.yaml` — Model Spack environment, for x86\_64
- `spack-ppc64le.yaml` — Model Spack environment, for ppc64le

Specs in the Model Spack Environment are commented out if (a) there are outstanding build issues or (b) if their Spack package does not offer a versioned installation option

### Spack Version

E4S 21.11 uses Spack branch `e4s-21.11`

- <https://github.com/spack/spack>
- Branch `e4s-21.11`

### Spack Build Cache

- <https://cache.e4s.io/21.11>

```
Br spack mirror add E4S https://cache.e4s.io/21.11
Br spack buildcache keys --11
```

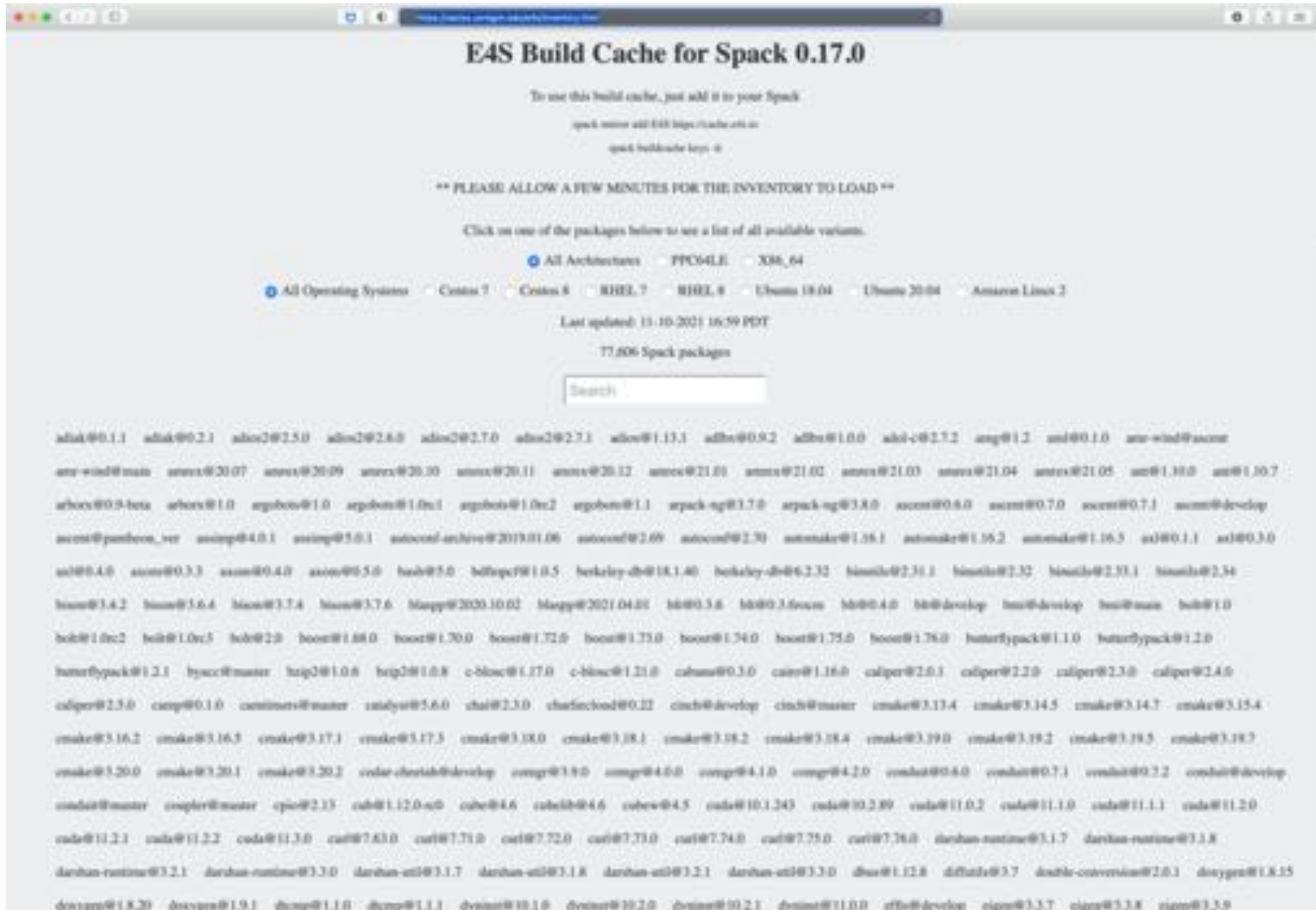
# E4S 21.11 bare-metal installation spack.yaml recipe

```
01  # Trilinos
02  variants: +openmpi +mpi +serial +cuda +cuda_arch=00
03  # FFTW
04  variants: +openmpi
05  # FFTW
06  variants: +openmpi +mpi +serial +cuda
07  # FFTW
08  variants: +openmpi +mpi +serial +cuda
09  # FFTW
10  variants: +openmpi +mpi +serial +cuda
11  # FFTW
12  variants: +openmpi +mpi +serial +cuda
13  # FFTW
14  variants: +openmpi +mpi +serial +cuda
15  # FFTW
16  variants: +openmpi +mpi +serial +cuda
17  # FFTW
18  variants: +openmpi +mpi +serial +cuda
19  # FFTW
20  variants: +openmpi +mpi +serial +cuda
21  # FFTW
22  variants: +openmpi +mpi +serial +cuda
23  # FFTW
24  variants: +openmpi +mpi +serial +cuda
25  # FFTW
26  variants: +openmpi +mpi +serial +cuda
27  # FFTW
28  variants: +openmpi +mpi +serial +cuda
29  # FFTW
30  variants: +openmpi +mpi +serial +cuda
31  # FFTW
32  variants: +openmpi +mpi +serial +cuda
33  # FFTW
34  variants: +openmpi +mpi +serial +cuda
35  # FFTW
36  variants: +openmpi +mpi +serial +cuda
37  # FFTW
38  variants: +openmpi +mpi +serial +cuda
39  # FFTW
40  variants: +openmpi +mpi +serial +cuda
41  # FFTW
42  variants: +openmpi +mpi +serial +cuda
43  # FFTW
44  variants: +openmpi +mpi +serial +cuda
45  # FFTW
46  variants: +openmpi +mpi +serial +cuda
47  # FFTW
48  variants: +openmpi +mpi +serial +cuda
49  # FFTW
50  variants: +openmpi +mpi +serial +cuda
51  # FFTW
52  variants: +openmpi +mpi +serial +cuda
53  # FFTW
54  variants: +openmpi +mpi +serial +cuda
55  # FFTW
56  variants: +openmpi +mpi +serial +cuda
57  # FFTW
58  variants: +openmpi +mpi +serial +cuda
59  # FFTW
60  variants: +openmpi +mpi +serial +cuda
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70  variants: +openmpi +mpi +serial +cuda
71  # FFTW
72  variants: +openmpi +mpi +serial +cuda
73  # FFTW
74  variants: +openmpi +mpi +serial +cuda
75  # FFTW
76  variants: +openmpi +mpi +serial +cuda
77  # FFTW
78  variants: +openmpi +mpi +serial +cuda
79  # FFTW
80  variants: +openmpi +mpi +serial +cuda
81  # FFTW
82  variants: +openmpi +mpi +serial +cuda
83  # FFTW
84  variants: +openmpi +mpi +serial +cuda
85  # FFTW
86  variants: +openmpi +mpi +serial +cuda
87  # FFTW
88  variants: +openmpi +mpi +serial +cuda
89  # FFTW
90  variants: +openmpi +mpi +serial +cuda
91  # FFTW
92  variants: +openmpi +mpi +serial +cuda
93  # FFTW
94  variants: +openmpi +mpi +serial +cuda
95  # FFTW
96  variants: +openmpi +mpi +serial +cuda
97  # FFTW
98  variants: +openmpi +mpi +serial +cuda
99  # FFTW
100 variants: +openmpi +mpi +serial +cuda
```

- Trilinos variants
- Built with CUDA



# E4S: Spack Build Cache at U. Oregon to speed up installation



- 75,000+ binaries
- S3 mirror
- No need to build from source code!

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

# E4S Frank build statistics, monitoring failure of jobs

Summary

Period Beginning: 2023-09-22 07:48:34.825+00

Period Ending: 2023-11-24 20:25:43.62+00

Number of Jobs: 193014

Number of Failed Jobs, all types: 9601

Number of Failed Jobs, system failures only: 876

Node Descriptions

• UD Frank Node Descriptions

Shortcuts

• Job Times, Last 4 Hours

• Job Times, Overview, All

• Job Times, Detailed, All

• Runner System Failures, by Runner, Last 4 Hours

• Runner System Failures, by Runner, All

• Runner System Failures, by Type, Last 4 Hours

• Runner System Failures, by Type, All

• Runner System Failures, Last 20

Job Times, Last 4 Hours

| name     | total_runtime | avg_runtime     | n   | pct_uo | pct_aws |
|----------|---------------|-----------------|-----|--------|---------|
| rebuild  | 23:14:32.5    | 00:11:49.088983 | 118 | 100%   | 0%      |
| generate | 01:41:42.054  | 00:02:02.04108  | 50  | 100%   | 0%      |
| service  | 00:52:17.515  | 00:00:51.434672 | 61  | 97%    | 3%      |

Job Times, Overview

| name     | total_runtime   | avg_runtime     | n      | pct_uo | pct_aws |
|----------|-----------------|-----------------|--------|--------|---------|
| rebuild  | 16605:48:23.241 | 00:06:16.086963 | 158955 | 60%    | 40%     |
| generate | 2320:23:16.239  | 00:08:33.202449 | 16277  | 67%    | 33%     |
| service  | 305:14:02.474   | 00:01:02.215065 | 17662  | 81%    | 19%     |
| other    | 00:49:16.909    | 00:00:24.640908 | 120    | 98%    | 2%      |

Job Times, Detailed

| name                           | total_runtime   | avg_runtime     | n      | pct_uo | pct_aws |
|--------------------------------|-----------------|-----------------|--------|--------|---------|
| rebuild                        | 16605:48:23.241 | 00:06:16.086963 | 158955 | 60%    | 40%     |
| e4s-pr-generate                | 1203:50:57.253  | 00:22:00.090543 | 3283   | 66%    | 34%     |
| radius-pr-generate             | 370:30:59.29    | 00:06:57.483346 | 3195   | 65%    | 35%     |
| e4s-develop-generate           | 201:14:29.111   | 00:22:44.348608 | 531    | 85%    | 15%     |
| rebuild-index                  | 188:27:27.859   | 00:02:44.871898 | 4115   | 86%    | 14%     |
| data-vis-sdk-pr-generate       | 144:55:12.951   | 00:02:41.022516 | 3240   | 64%    | 36%     |
| build_systems-pr-generate      | 134:54:25.661   | 00:02:26.284838 | 3320   | 66%    | 34%     |
| e4s-on-power-pr-generate       | 111:39:57.649   | 00:26:41.584259 | 251    | 95%    | 0%      |
| cleanup                        | 59:17:42.459    | 00:00:51.83644  | 4118   | 84%    | 16%     |
| no-specs-to-rebuild            | 57:28:52.156    | 00:00:21.946352 | 9429   | 77%    | 23%     |
| radius-develop-generate        | 55:23:44.022    | 00:06:25.733118 | 517    | 82%    | 18%     |
| tutorial-pr-generate           | 48:41:52.415    | 00:03:45.627304 | 777    | 52%    | 48%     |
| data-vis-sdk-develop-generate  | 20:32:30.767    | 00:02:23.038234 | 517    | 80%    | 20%     |
| build_systems-develop-generate | 19:14:09.214    | 00:02:13.171565 | 520    | 83%    | 17%     |
| tutorial-develop-generate      | 05:35:00.044    | 00:02:48.907933 | 119    | 58%    | 42%     |
| e4s-on-power-develop-generate  | 03:49:57.882    | 00:32:51.126    | 7      | 71%    | 0%      |
| other                          | 00:49:16.909    | 00:00:24.640908 | 120    | 98%    | 2%      |

Runner System Failures, by Runner, Last 4 Hours

| runner | n_jobs | n_system_failures | system_failure_rate | facility |
|--------|--------|-------------------|---------------------|----------|
| empty  |        |                   |                     |          |

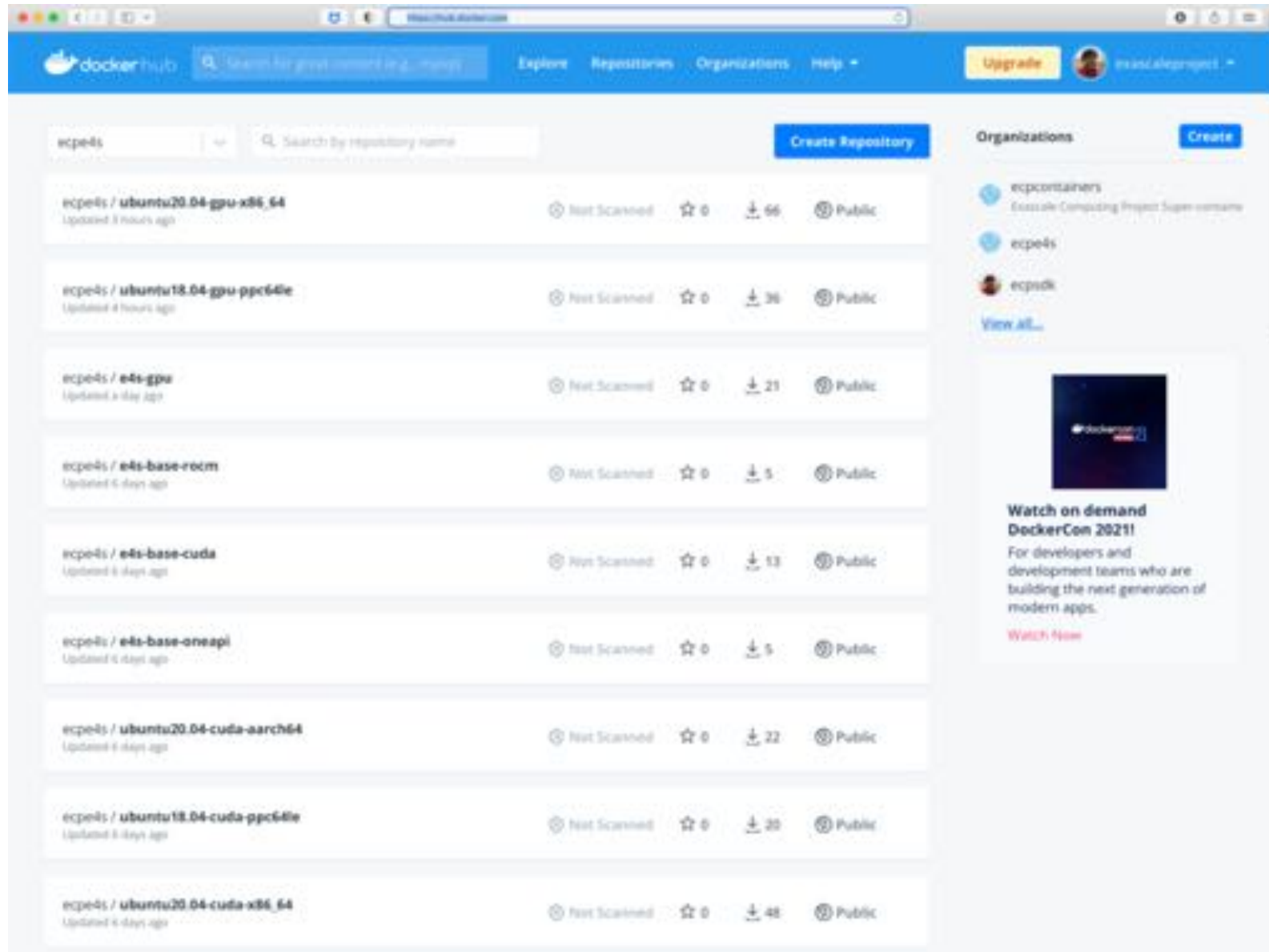
Runner System Failures, by Runner

| runner  | n_jobs | n_system_failures | pct_system_failures | facility |
|---|--------|-------------------|---------------------|----------|
| large-x86-pub-gitlab-runner-64lcfb66b-u2gnl   | 41727  | 50                | 0.12%               | AWS      |
| large-x86-pub-gitlab-runner-64lcfb66b-28pd5   | 16326  | 277               | 1.70%               | AWS      |
| medium-x86-pub-gitlab-runner-5b4dd9758-kxjvf  | 4002   | 110               | 2.75%               | AWS      |
| xlarge-x86-pub-gitlab-runner-7c58cc9d47-k87vf | 3870   | 120               | 3.10%               | AWS      |
| medium-x86-pub-gitlab-runner-5b4dd9758-nf2pg  | 3272   | 4                 | 0.12%               | AWS      |
| xlarge-x86-pub-gitlab-runner-7c58cc9d47-6eh2n | 1802   | 106               | 5.88%               | AWS      |
| medium-x86-pub-gitlab-runner-5b4dd9758-9qjtp  | 1400   | 114               | 8.14%               | AWS      |
| large-x86-pub-gitlab-runner-658c98576-k7czw   | 174    | 1                 | 0.57%               | AWS      |
| uo-jupiter                                    | 26154  | 0                 | 0.00%               | UD       |
| uo-iristinct                                  | 21024  | 0                 | 0.00%               | UD       |
| uo-illyad                                     | 17826  | 0                 | 0.00%               | UD       |
| uo-godzilla                                   | 13993  | 43                | 0.31%               | UD       |
| uo-gilgamesh                                  | 12620  | 0                 | 0.00%               | UD       |
| uo-delphi                                     | 12444  | 5                 | 0.04%               | UD       |
| uo-nature                                     | 5887   | 4                 | 0.07%               | UD       |
| uo-eagle                                      | 3369   | 1                 | 0.03%               | UD       |
| uo-vina                                       | 3207   | 0                 | 0.00%               | UD       |
| uo-minotaur                                   | 1815   | 12                | 0.66%               | UD       |
| uo-centaur                                    | 1671   | 29                | 1.74%               | UD       |
| uo-typhon                                     | 13     | 0                 | 0.00%               | UD       |
| uo-medusa                                     | 9      | 0                 | 0.00%               | UD       |

Runner System Failures, by Type, Last 4 Hours

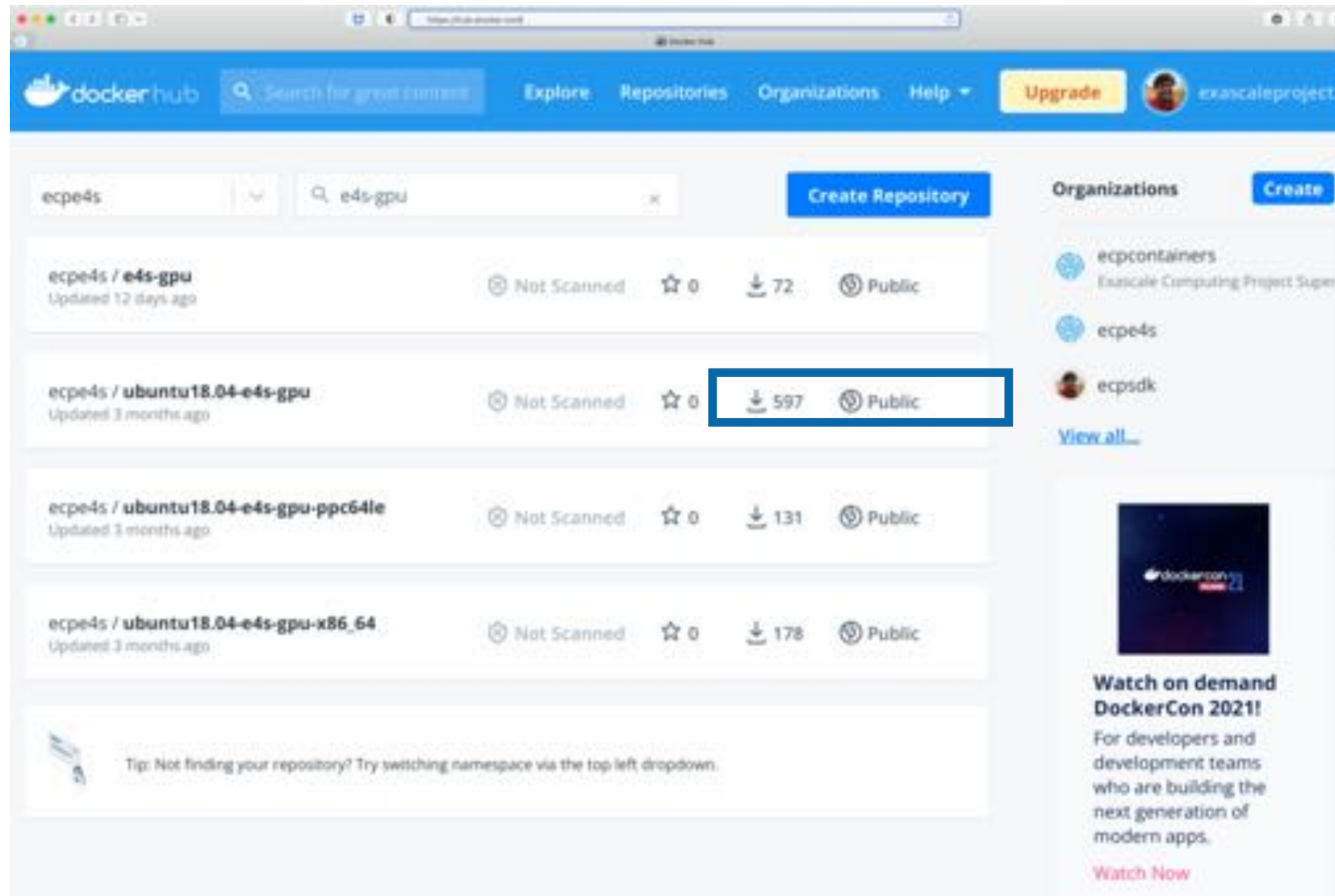
| failure_type | n | n_aws | n_uo | percent |
|--------------|---|-------|------|---------|
| empty        |   |       |      |         |

# E4S Base Container Images for x86\_64, ppc64le, and aarch64



- Hub.docker.com
- ecpe4s
- Platforms:
  - x86\_64
  - Ppc64le
  - aarch64
- GPU runtimes:
  - Cuda
  - ROCm
  - oneAPI

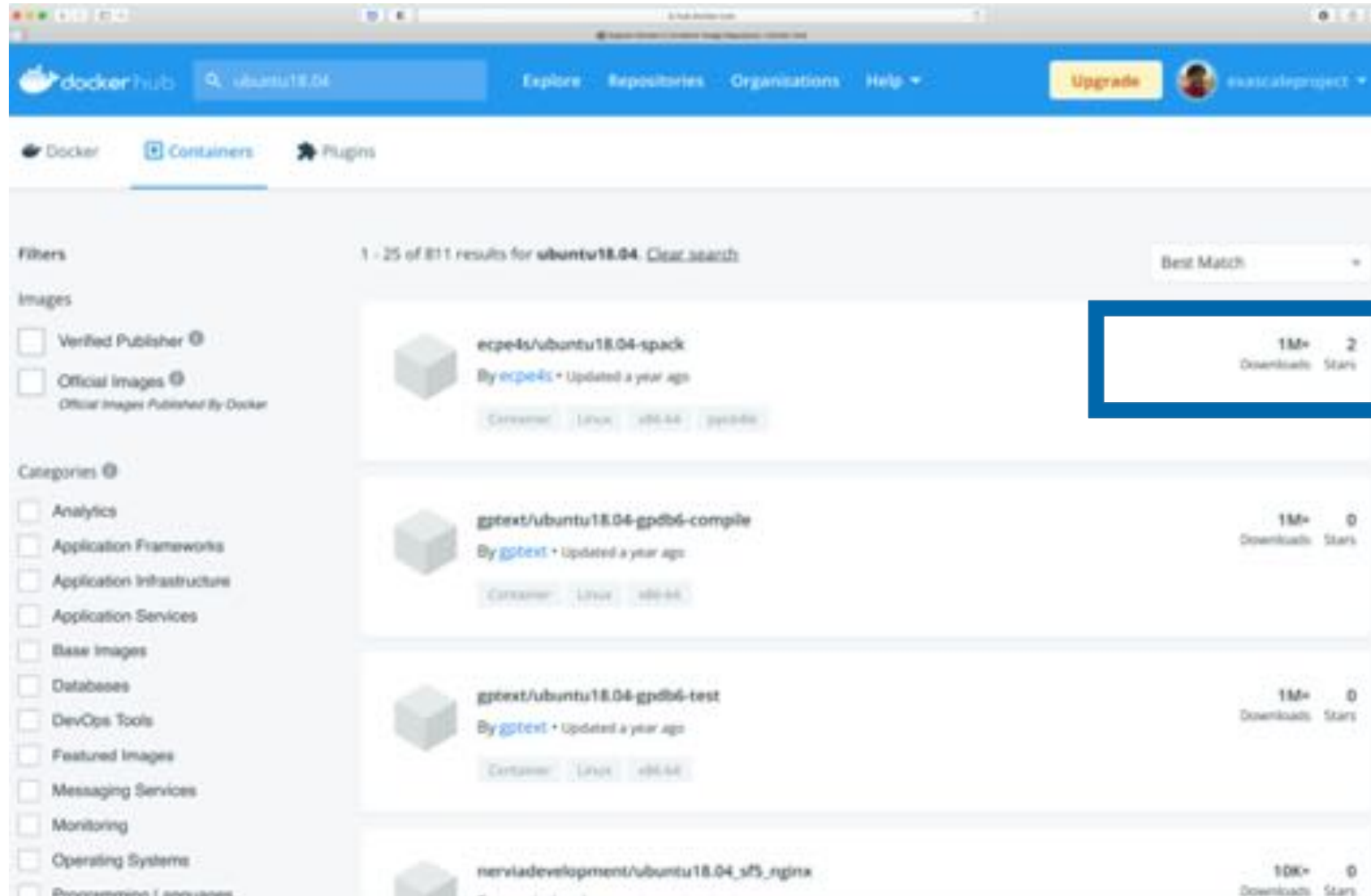
# E4S Full Featured Container GPU image for x86\_64 and ppc64le



- Hub.docker.com
- ecpe4s
- Platforms:
  - x86\_64
  - ppc64le
- GPU runtimes:
  - Cuda
  - ROCm
  - oneAPI

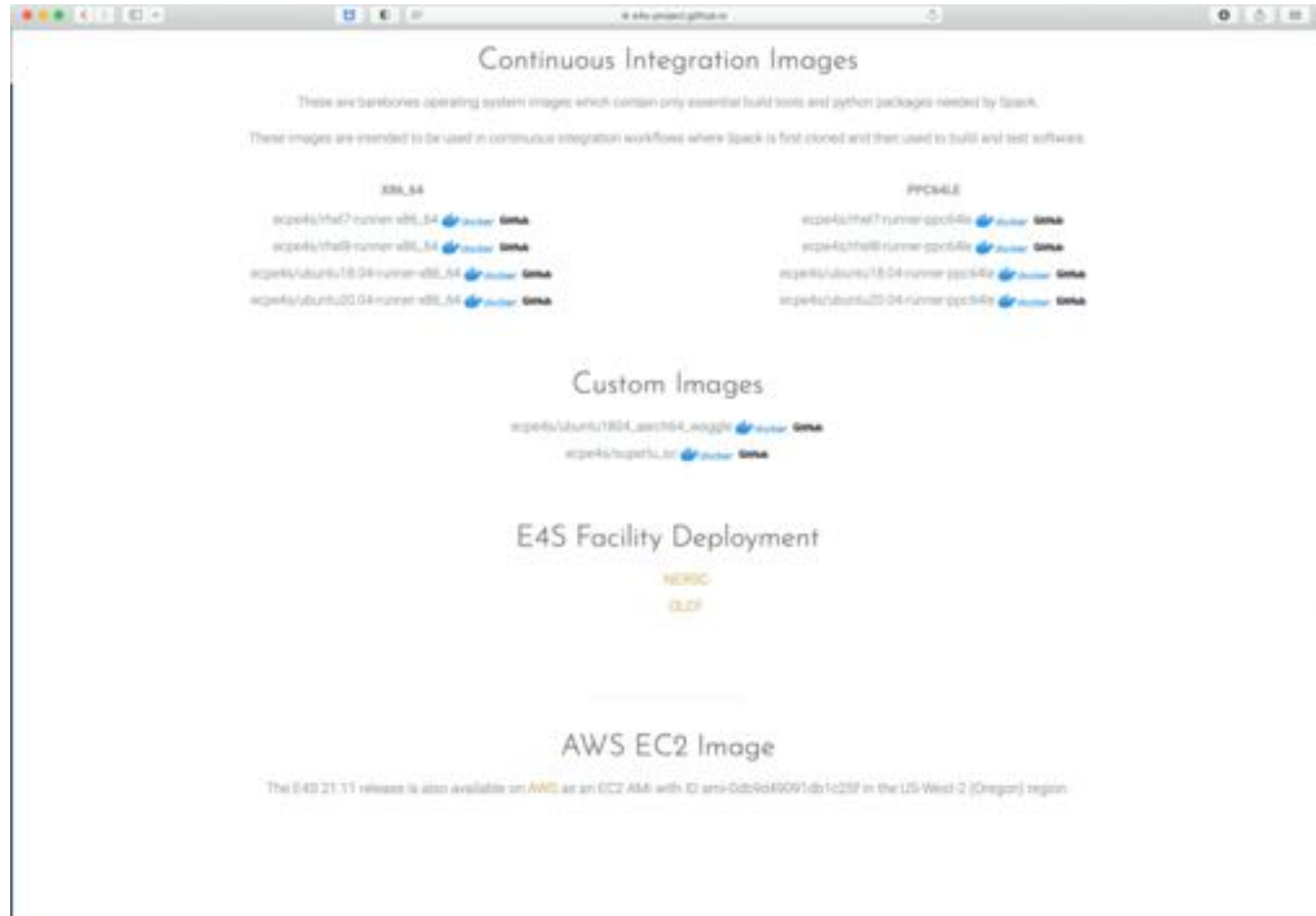


# E4S Base Container Images for x86\_64 with Spack (no GPU)



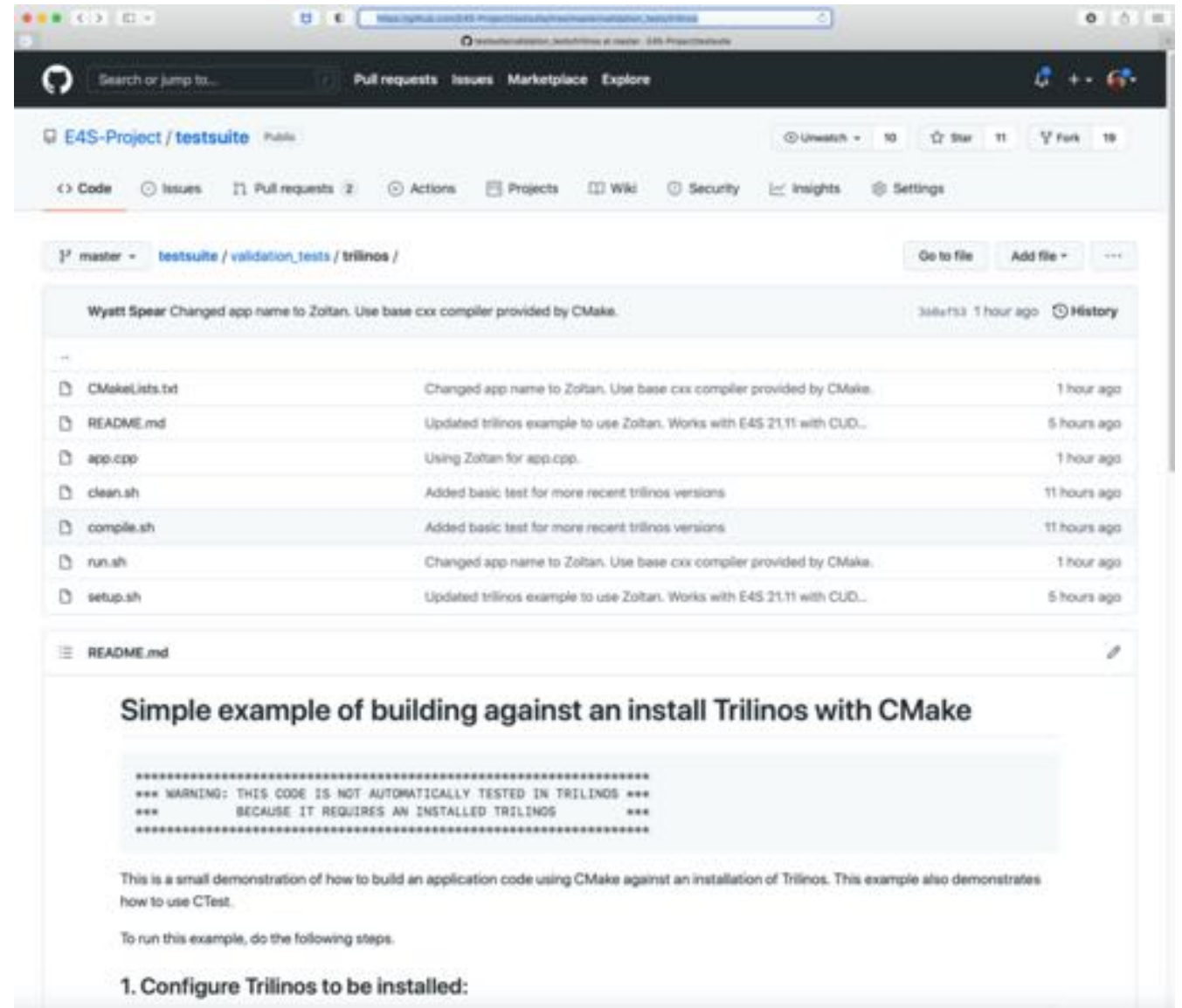
- Popular Ubuntu18.04
- 1M+ downloads!
- 2 stars

# E4S 21.11 Cloud, CI, and Custom images



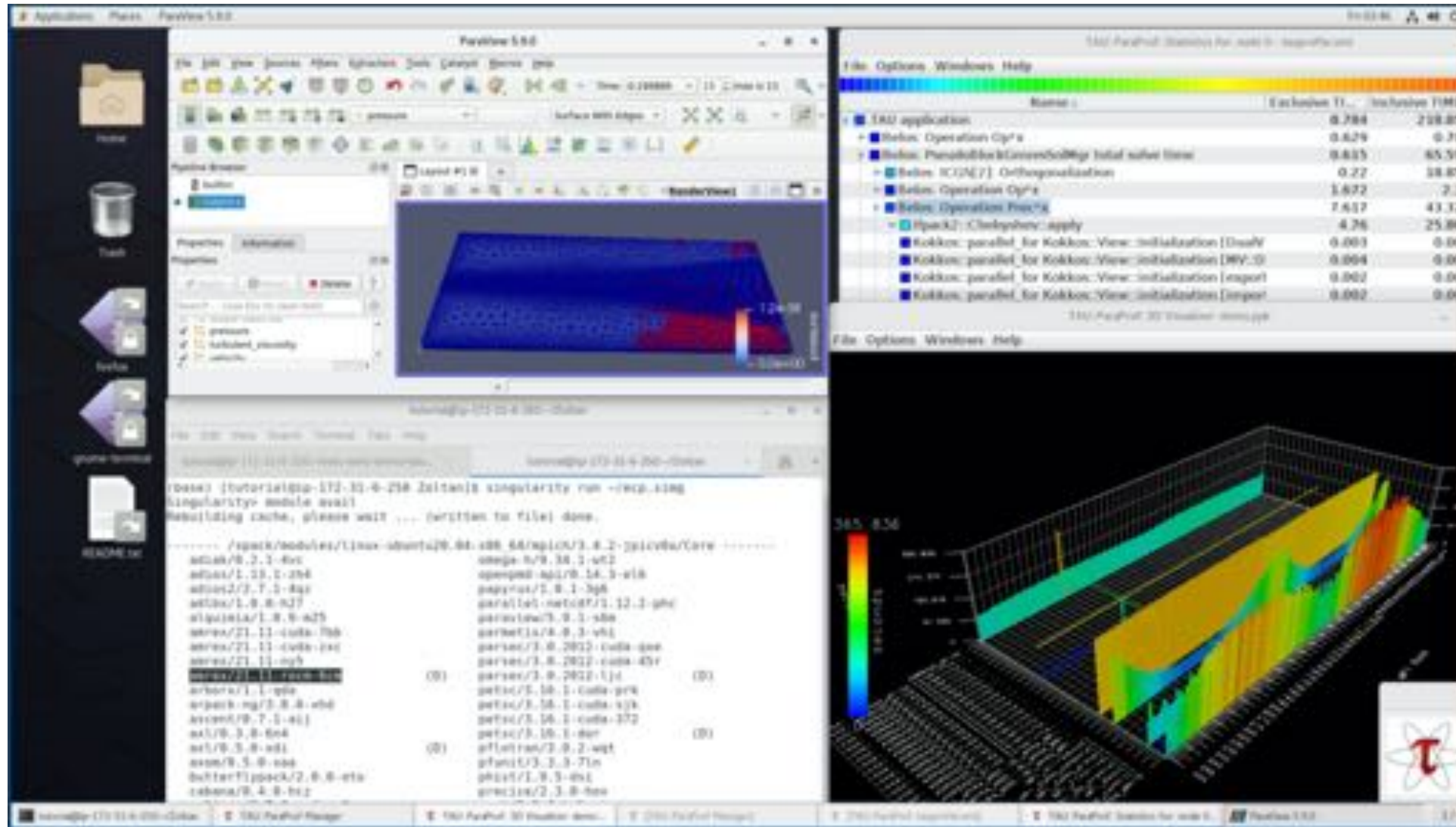
# E4S Validation Test Suite: Trilinos

- Provides automated build and run tests
- Validate container environments and products



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

E4S 21.11 AWS image: US-West2 (OR) ami-0db9d49091db1c25f



## E4S 21.11 AWS

- Intel oneAPI
- CUDA
- NVHPC
- ROCm
- AWS DCV
- Spack Build Cache
- ECP: Nalu-Wind
- Trilinos 13.2.0
- OpenFOAM
- ParaView
- TAU
- Docker
- Shifter
- Charliecloud
- E4S Singularity...



# 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 and Wi4MPI [CEA] for OpenMPI replacement.
- 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.
  - `e4s-cl init --backend [singularity|shifter] --image <file> --source <startup_cmds.sh>`
  - `e4s-cl mpirun -np <N> <command>`

- Usage:

```
. /opt/intel/oneapi/setvars.sh
```

```
e4s-cl init --backend singularity --image ~/images/e4s-gpu-x86.sif --source ~/source.sh
```

```
cat ~/source.sh
```

```
. /spack/share/spack/setup-env.sh
```

```
spack load trilinos+cuda cuda_arch=80
```

```
spack unload mpich
```

```
e4s-cl mpirun -np 4 ./a.out
```

<https://github.com/E4S-Project/e4s-cl>

# Quickstart Guide: Using E4S 21.11 Singularity container

## Setup:

```
% cd; wget https://oaciss.uoregon.edu/e4s/images/21.11/e4s-gpu-x86\_64.sif
```

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

## Using Singularity container:

```
% singularity run --nv e4s-gpu-x86_64.sif
```

```
Singularity> cd testsuite/validation_tests/trilinos
```

```
Singularity> ./clean.sh
```

```
Singularity> ./compile.sh
```

```
Singularity> ./run.sh
```

```
Singularity> exit
```

```
%
```

# Using Intel MPI with E4S 21.11 Singularity container with e4s-cl

## Setup:

```
% cd; git clone https://github.com/E4S-Project/e4s-cl; cd e4s-cl; make INSTALLDIR=`pwd`;
```

## Substituting MPICH in Trilinos application with Intel MPI using e4s-cl:

```
% cat ~/source.sh
. /spack/share/spack/setup-env.sh
spack load trilinos+cuda cuda_arch=80
spack unload mpich
$ cd ~/testsuite/validation_tests/trilinos; cat run_e4s-cl.sh
#!/bin/bash
export PATH=$HOME/e4s-cl/bin:$PATH
source /opt/intel/oneapi/setvars.sh
which e4s-cl
which mpirun
/bin/rm -f *.log
e4s-cl init --source $HOME/source.sh \
    --backend singularity \
    --image $HOME/e4s-gpu-x86_64.sif
e4s-cl mpirun -np 4 ./build/Zoltan

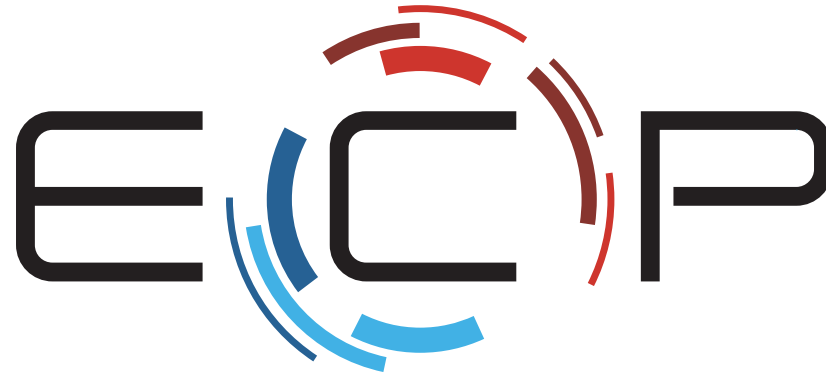
e4s-cl profile delete `e4s-cl profile list -s`

% ./run_e4s-cl.sh
```

# Thank you

<https://www.exascaleproject.org>

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EXASCALE COMPUTING PROJECT

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