E4S: The Extreme-scale Scientific Software Stack Release 24.05

Release 24.05 notes

May 9, 2024

E4S 24.05: What's New?

- E4S includes 129+ HPC packages on ARM, x86_64, and ppc64le platforms, 128K+ binaries in E4S build Cache.
- E4S includes a comprehensive suite of AI/ML packages including DeepHyper, Google.generativeai (Gemini API), along with previously supported OpenAI (API), TorchBraid, Pandas, Scikit-Learn, JAX, PyTorch, TensorFlow, Horovod, OpenCV, and LBANN with support for GPUs.
- VSCodium (MIT License) Integrated Development Environment GUI now supported in containers and CSPs.
- E4S DocPortal updated with AI/ML tools.
- OS upgrade for containers: Ubuntu 22.04 LTS.
- Upgraded CUDA from version 11 to 12, ROCm upgraded from version 5.4 to 5.7.1.
- New tools: Laghos, Glvis, netcdf-fortran, fpm, e4s-cl, and e4s-alc.
- E4S includes new applications: Nek5000, Nekbone, Laghos and previously supported GROMACS, CP2K, Xyce, Quantum Espresso, ExaGo, LAMMPS, WARPX, Dealii, and OpenFOAM.
- Adaptive Computing's HPC Cloud on demand data center (ODDC) web-based platform for multi-user, multi-node ParaTools Pro for E4S images on AWS marketplace with support for aarch64 (Graviton) as well as x86_64 with NVIDIA GPUs with VNC based remote desktop and torque (qsub) for multi-node execution:
  - https://adaptivecomputing.com/

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E4S: Extreme-scale Scientific Software Stack

- E4S is a community effort to provide open-source software packages for developing, deploying and running scientific applications on HPC platforms.
- E4S has built a comprehensive, coherent software stack that enables application developers to productively develop highly parallel applications that effectively target diverse exascale architectures.
- E4S provides a curated, Spack based software distribution of 125+ HPC, EDA (e.g., Xyce), and AI/ML packages (e.g., DeepHyper, TorchBraid, Scikit-Learn, Pandas, TensorFlow, PyTorch, JAX, Horovod, and LBANN).
- With E4S Spack binary build caches, E4S supports both bare-metal and containerized deployment for GPU based platforms.
  - X86_64, ppc64le (IBM Power 10), aarch64 (ARM64) with support for GPUs from NVIDIA, AMD, and Intel
  - HPC and AI/ML packages are optimized for GPUs and CPUs.
- Container images on DockerHub and E4S website of pre-built binaries of ECP ST products.
- Base images and full featured containers (with GPU support) and DOE LLVM containers.
- Commercial support for E4S through ParaTools, Inc. for installation, maintaining an issue tracker, and ECP AD engagement.
  - https://dashboard.e4s.io https://e4s.io/talks/E4S_Support_Dec23.pdf
- E4S for commercial cloud platforms: AWS image supports MPI implementations and containers with remote desktop (DCV).
  - Intel MPI, NVHPC, MVAPICH2, MPICH, MPC, OpenMPI
- e4s-cl container launch tool allows binary distribution of applications by substituting MPI in the containerized app with the system MPI. A-la-carte tool to customize container images: e4s-alc.
- Quarterly releases: E4S 24.05 released on May 9, 2024: https://e4s.io/talks/E4S_24.05.pdf

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https://e4s.io

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 with support for GPUs from NVIDIA, AMD, and Intel in each release
- 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
- Feb 2022: E4S 22.02 – 100 full release products
- May 2022: E4S 22.05 – 101 full release products
- August 2022: E4S 22.08 – 102 full release products
- November 2022: E4S 22.11 – 103 full release products
- February 2023: E4S 23.02 – 106 full release products
- May 2023: E4S 23.05 – 109 full release products
- Aug 2023: E4S 23.08 – 115 full release products
- Nov 2023: E4S 23.11 – 120 full release products
- Feb 2024: E4S 24.02 – 122 full release products
- May 9, 2024: E4S 24.05 – 125 full release products

https://e4s.io

Lead: Sameer Shende (U Oregon)

Also include other products .e.g.,
AI: DeepHyper, TorchBraid, Scikit-Learn, JAX, PyTorch, TensorFlow, Horovod, LBANN
Co-Design: AMReX, Cabana, MFEM
EDA: Xyce

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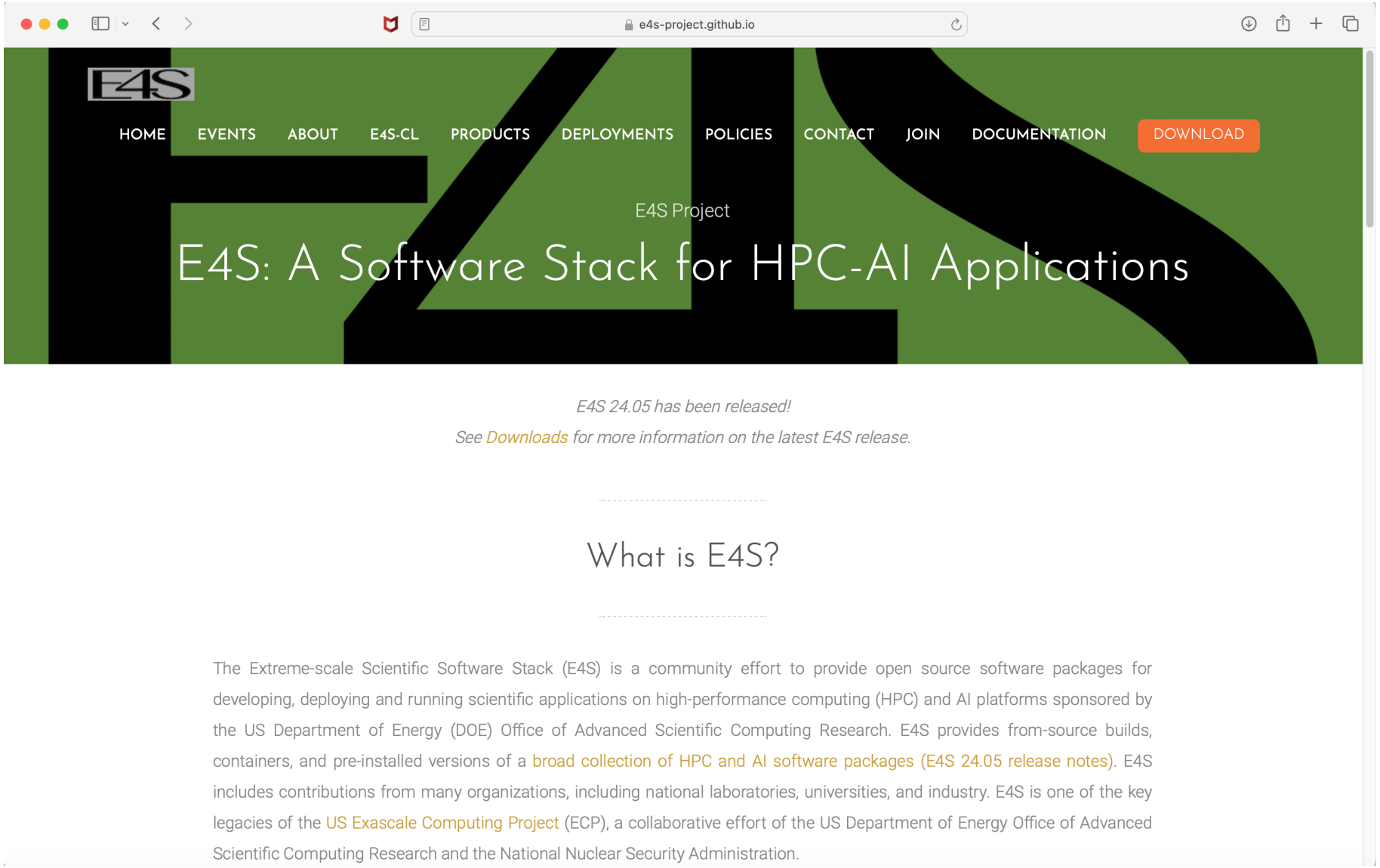
E4S Download from https://e4s.io



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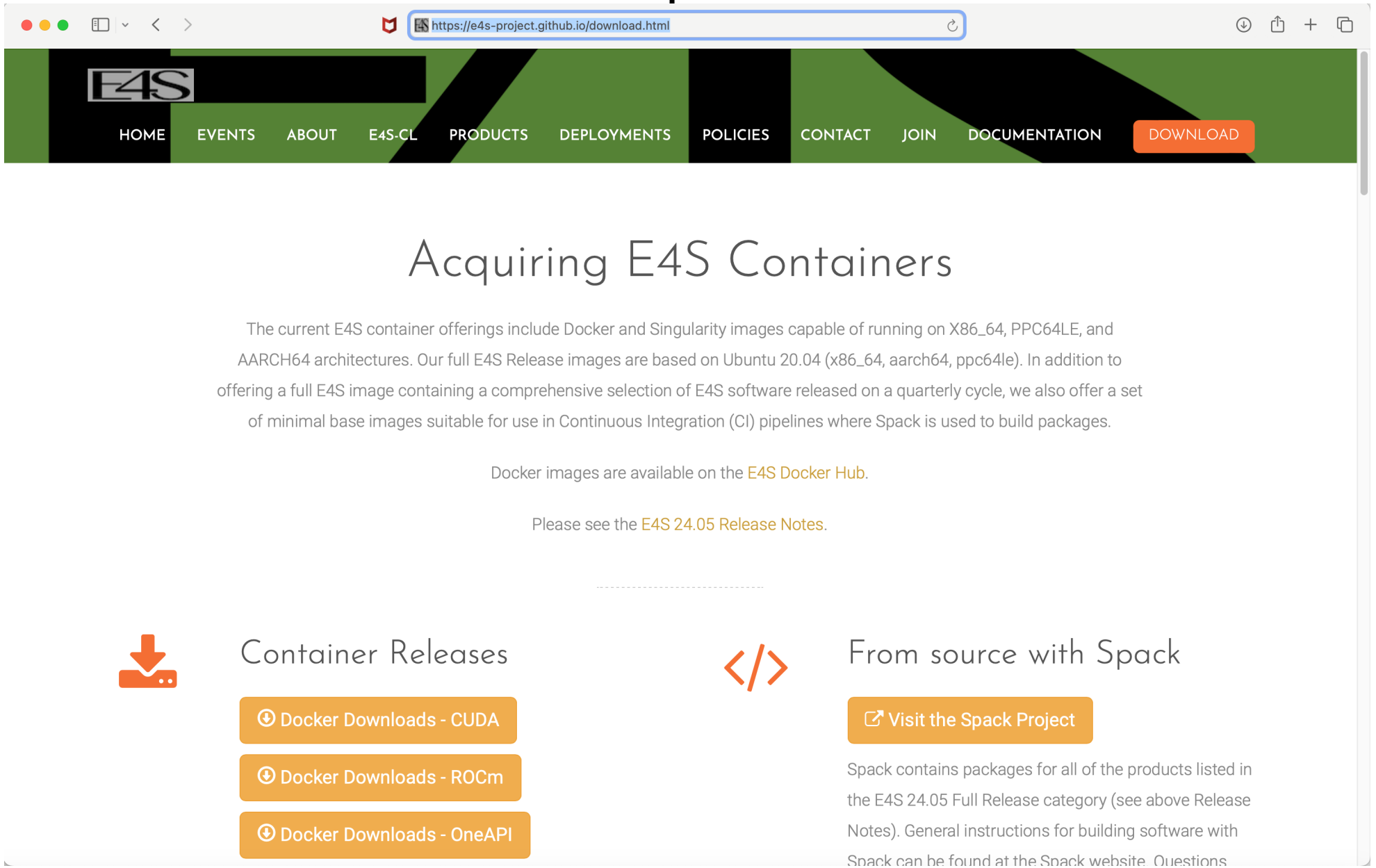
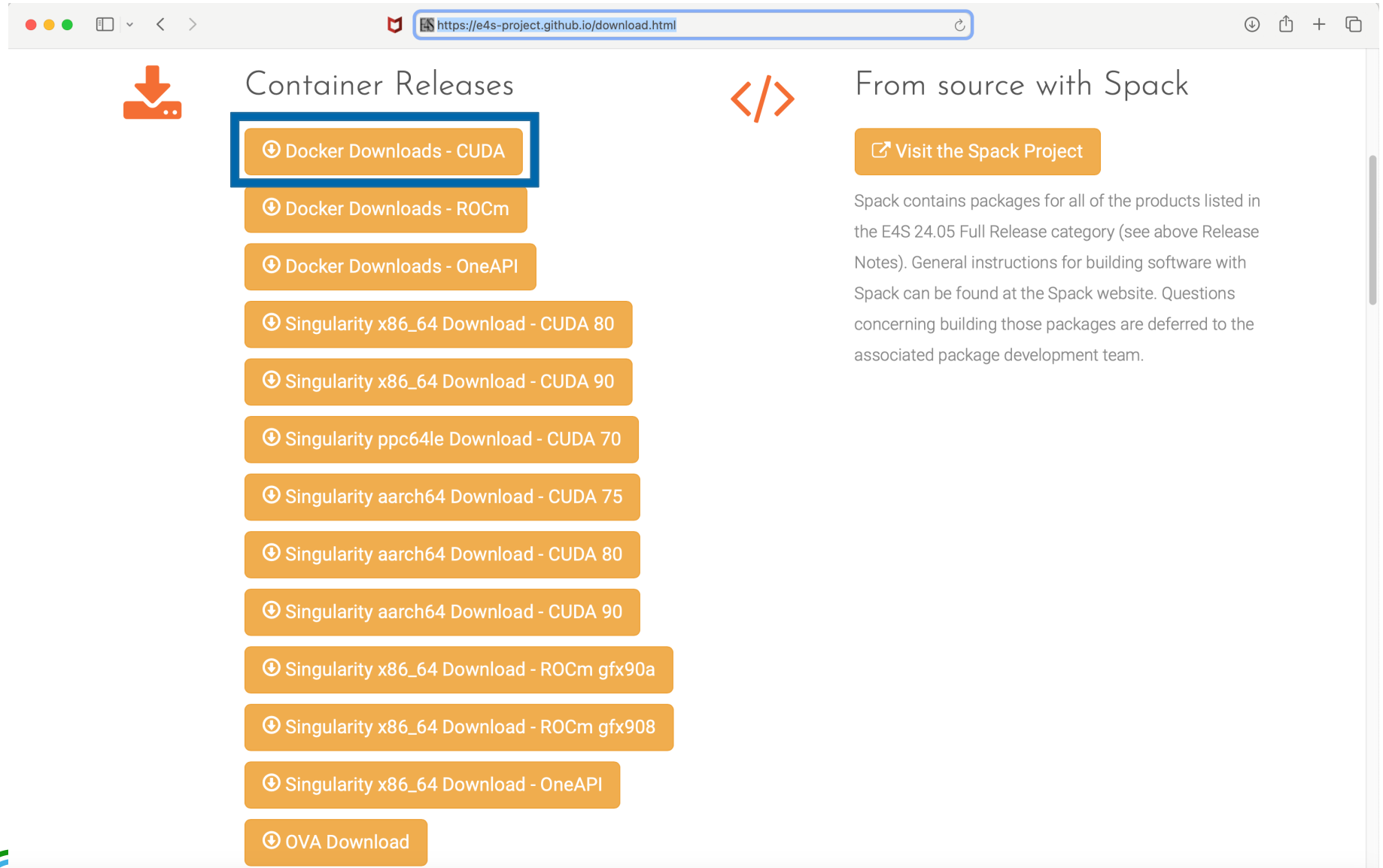
E4S Container Download from https://e4s.io



E4S Container Download from https://e4s.io



- Separate full featured Singularity images for 3 GPU architectures
- GPU full featured images for
  - x86_64 (Intel, AMD, NVIDIA)
  - ppc64le (NVIDIA)
  - aarch64 (NVIDIA)
- Full featured images available on Dockerhub
- 125+ products on 3 architectures

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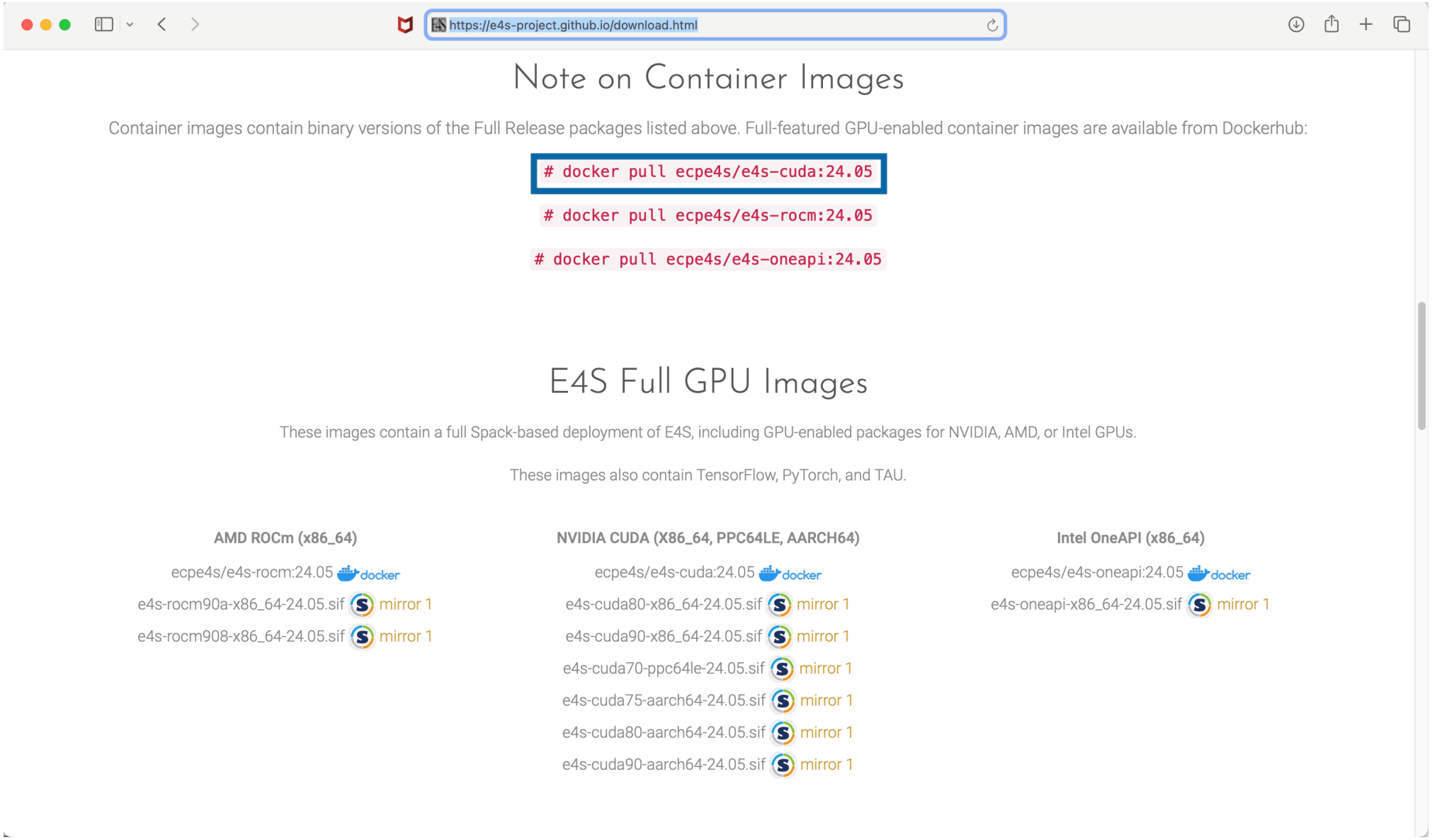
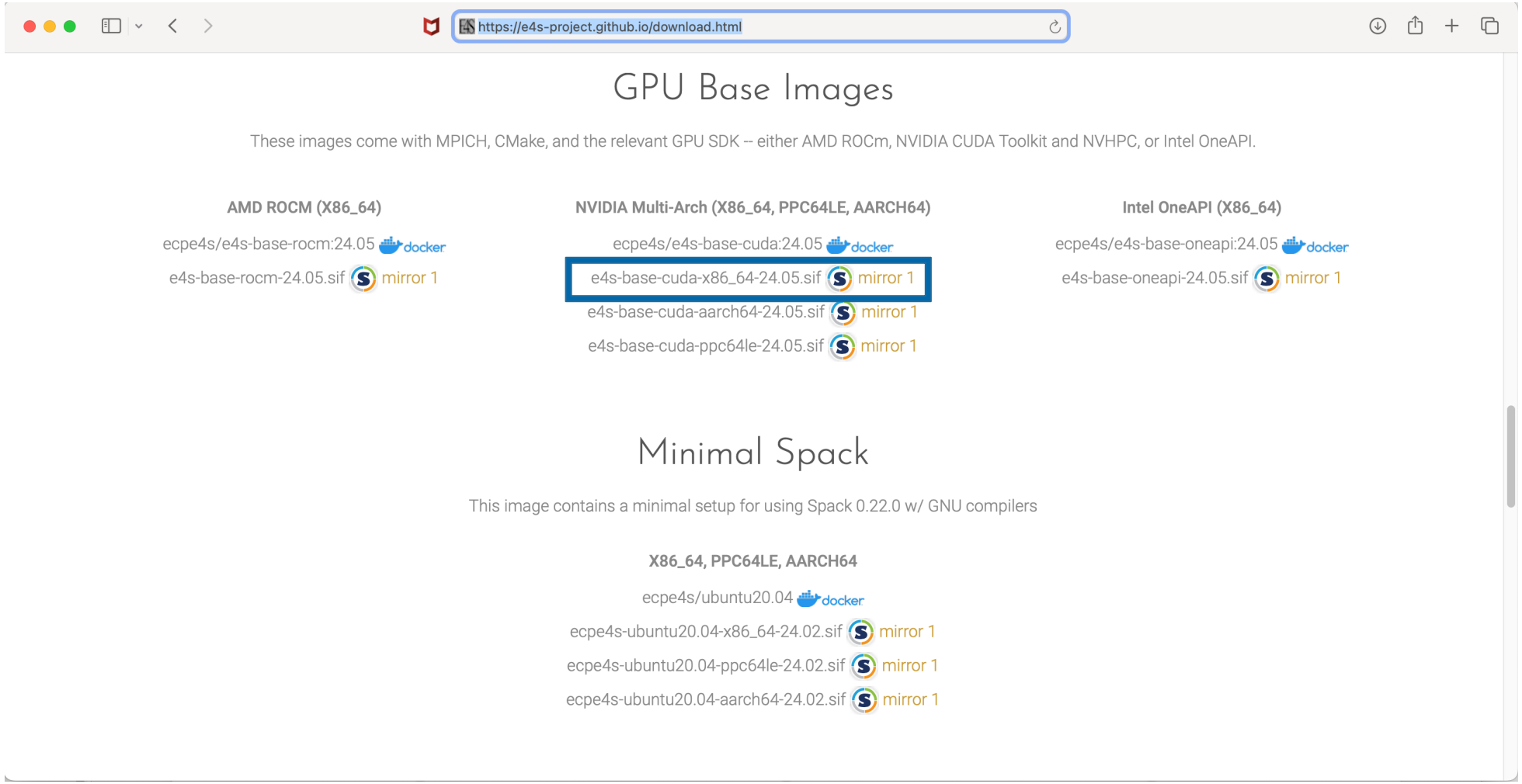
Download E4S 24.02 GPU Container Images: AMD, Intel, and NVIDIA



https://e4s.io

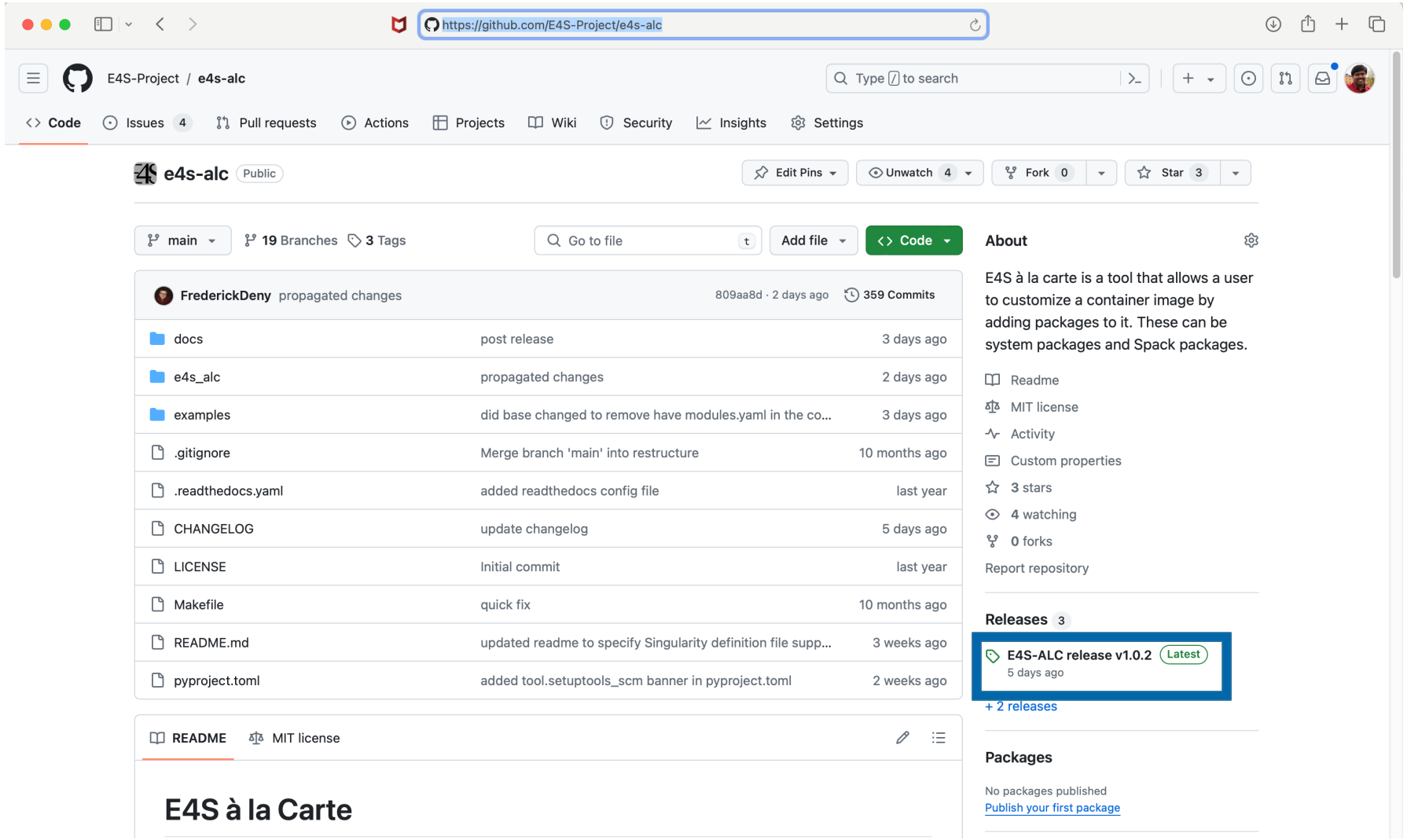
E4S base container images allow users to customize their containers



- Intel oneAPI
- AMD ROCm
- NVIDIA NVHPC and CUDA

https://e4s.io

e4s-alc: a new tool to customize container images. Version 1.0.2

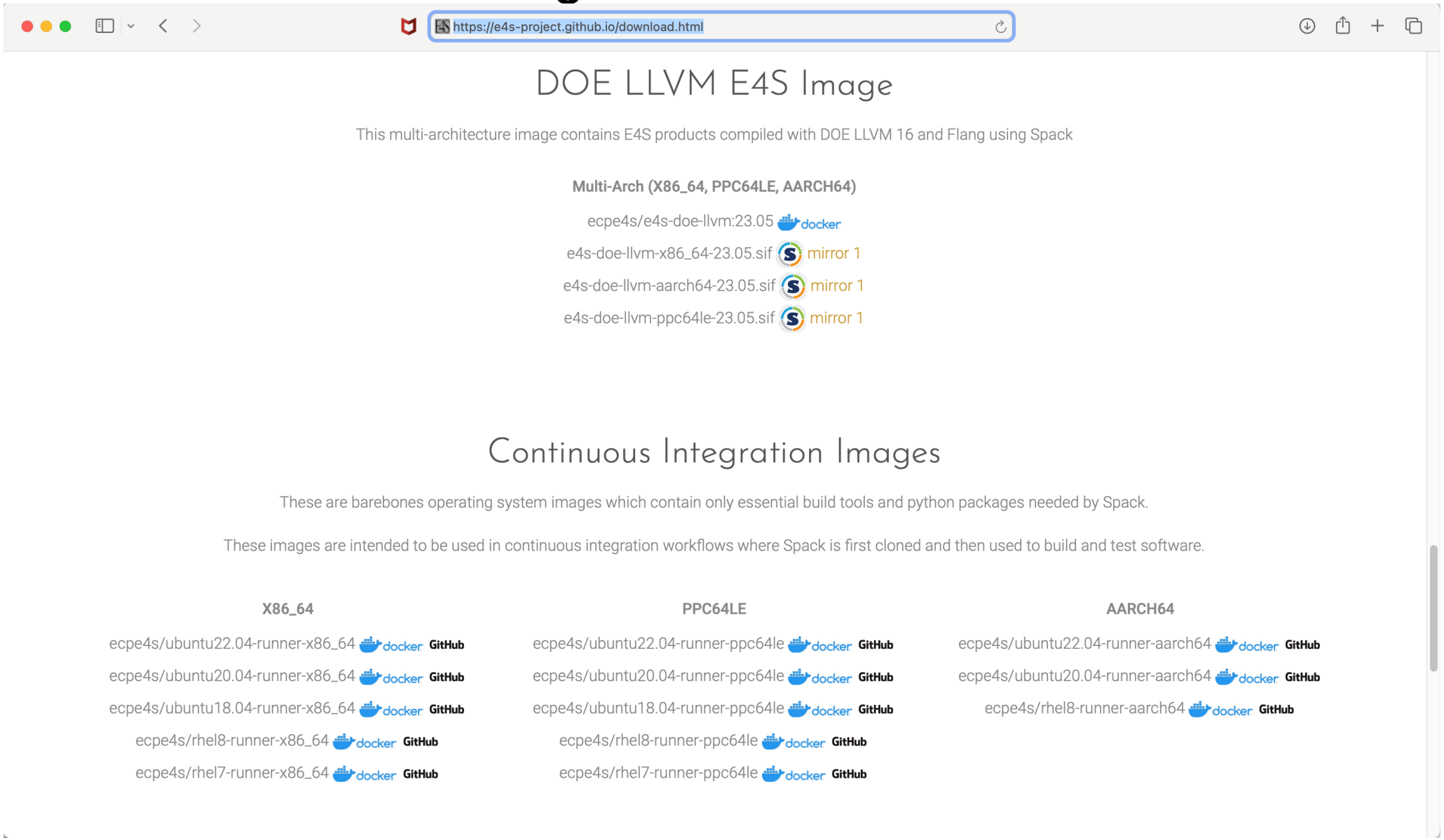


Add to a base image:

- Spack packages
- OS packages
- Tarballs
- Can create a Dockerfile
- Can create Singularity definition file

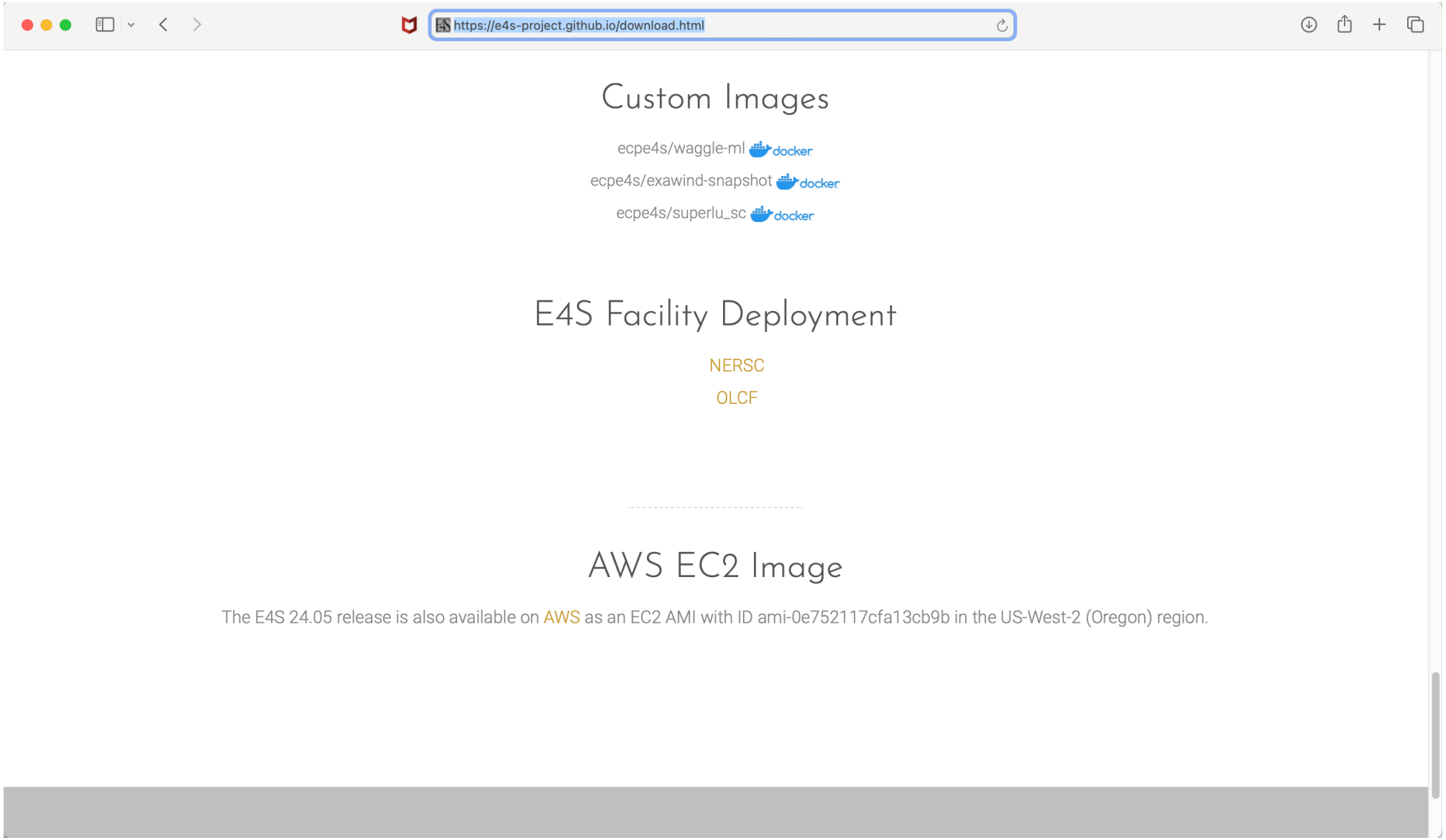
https://github.com/E4S-Project/e4s-alc

E4S DOE LLVM and CI images



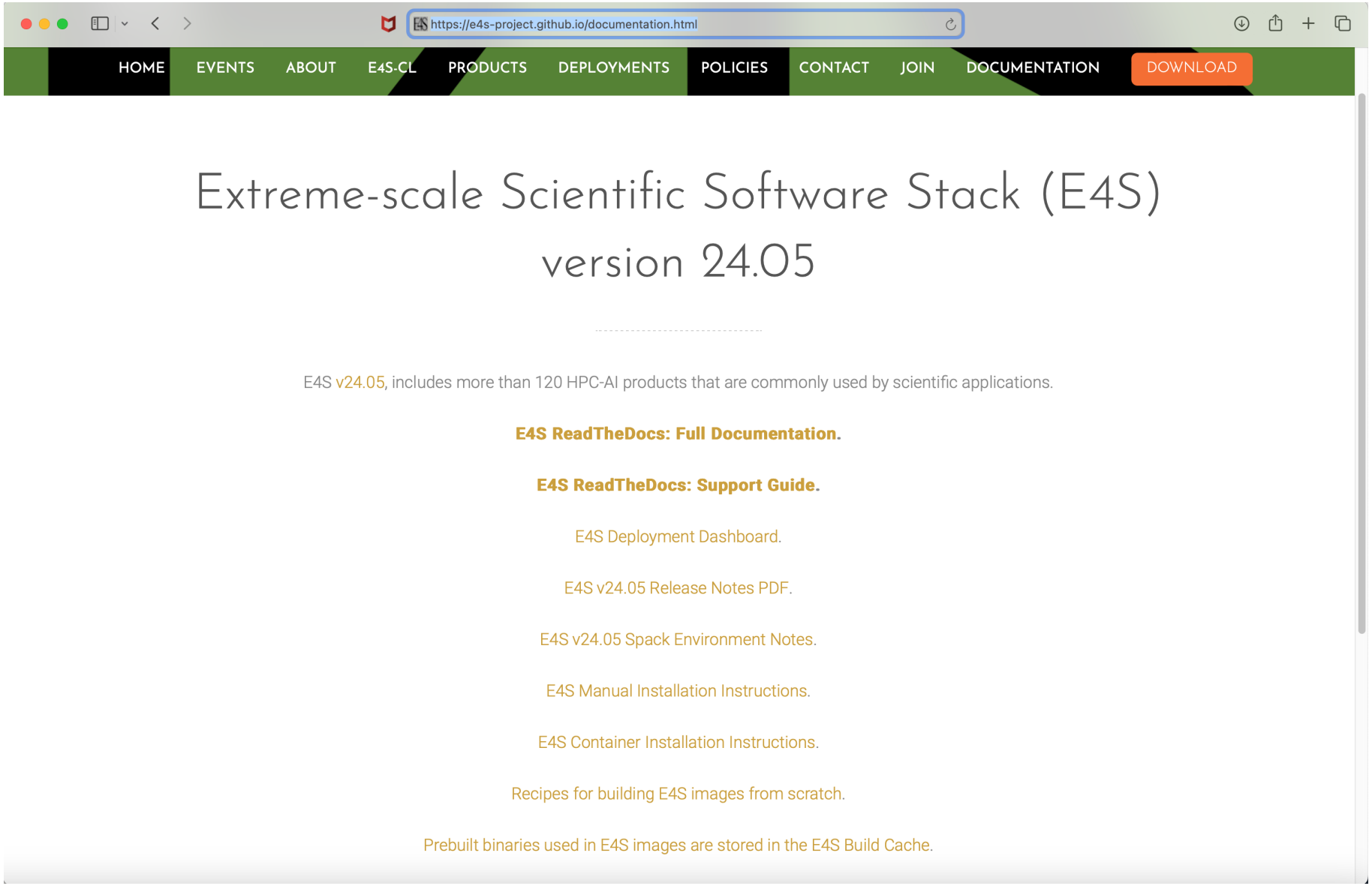
https://e4s.io

E4S Facility Deployment and AWS EC2 Image



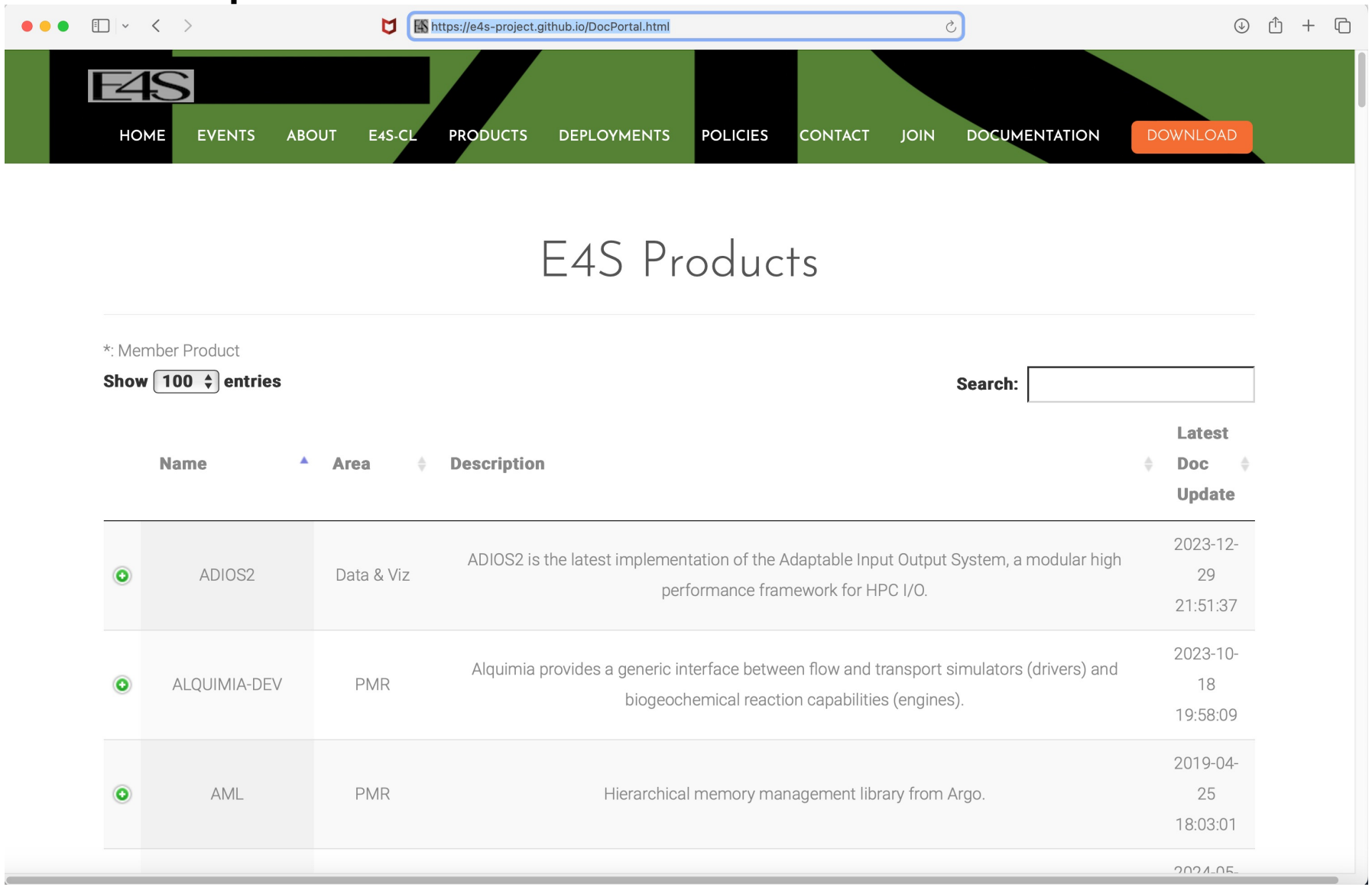
DOE Facility Deployment Dashboard: https://dashboard.e4s.io

E4S 24.05 Detailed Documentation for Bare-metal Installation



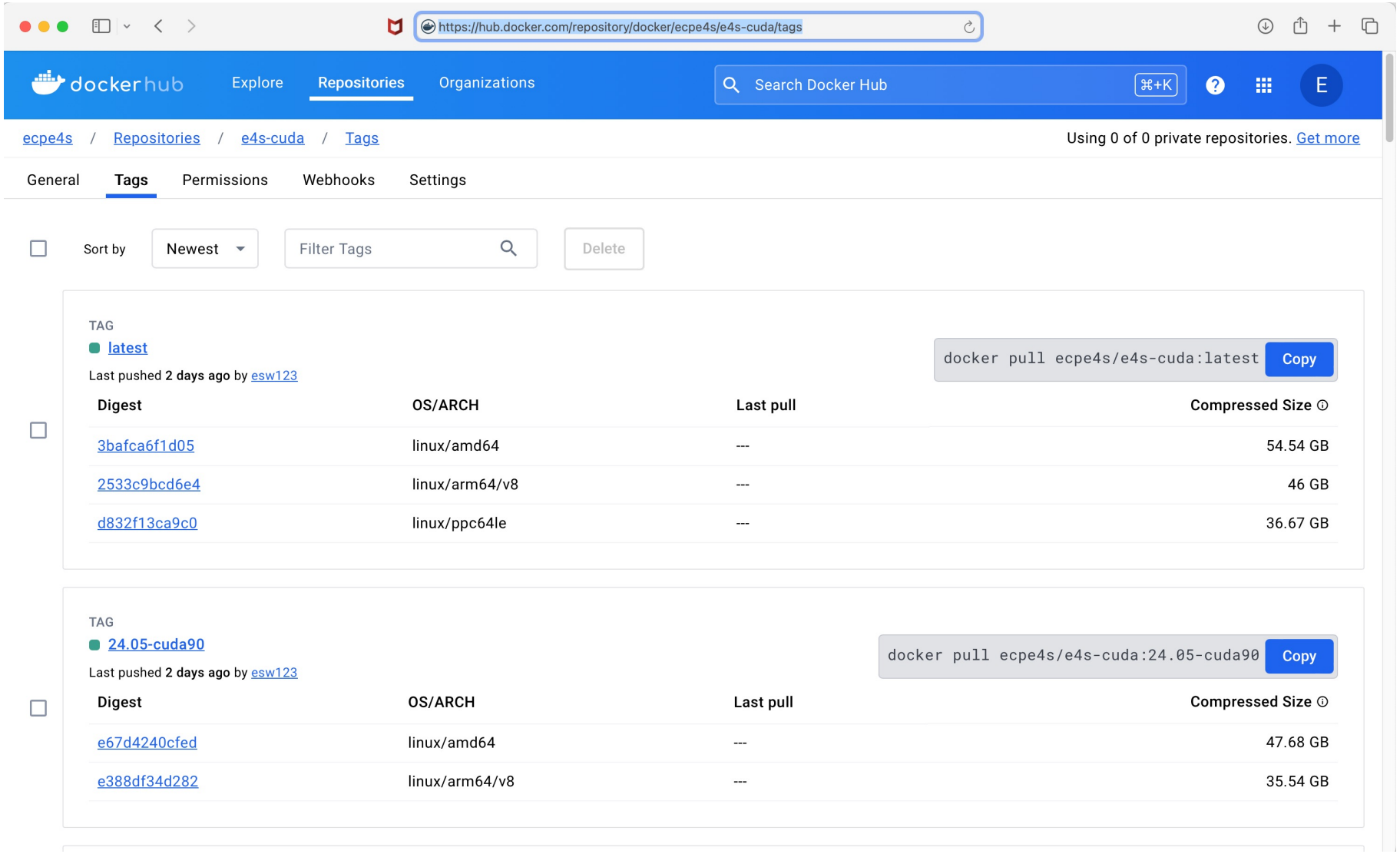
https://e4s.io

E4S DocPortal Updated with AI/ML tools



https://e4s.io

E4S 24.05 full featured container release on Dockerhub



Architectures:

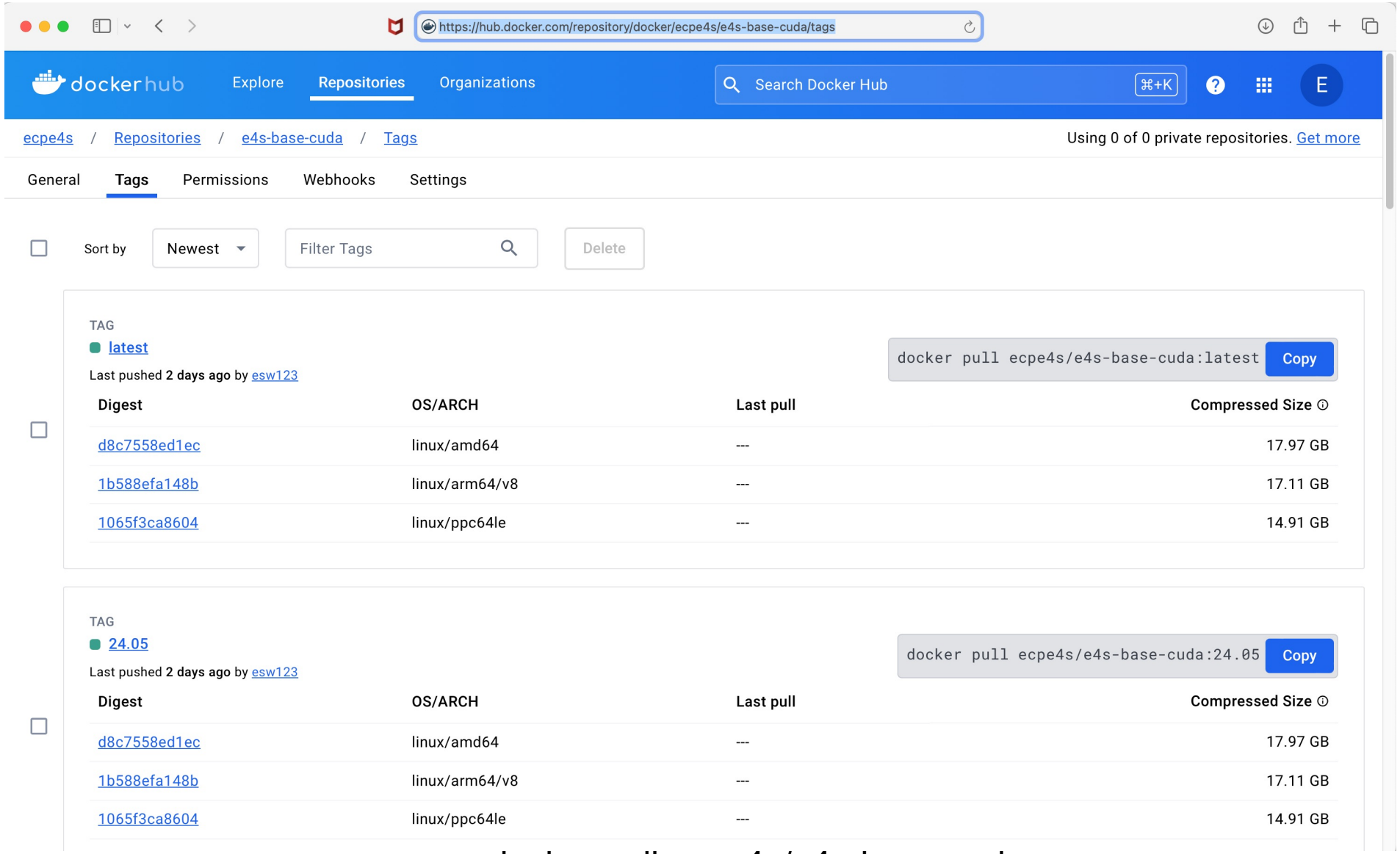
- x86_64
- aarch64
- ppc64le

Software:

- CUDA 12.3
- NVHPC 24.3
- ROCm 5.7.1
- oneAPI 2024.0.2

docker pull ecpe4s/e4s-cuda:24.05

E4S 24.05 base container release on Dockerhub

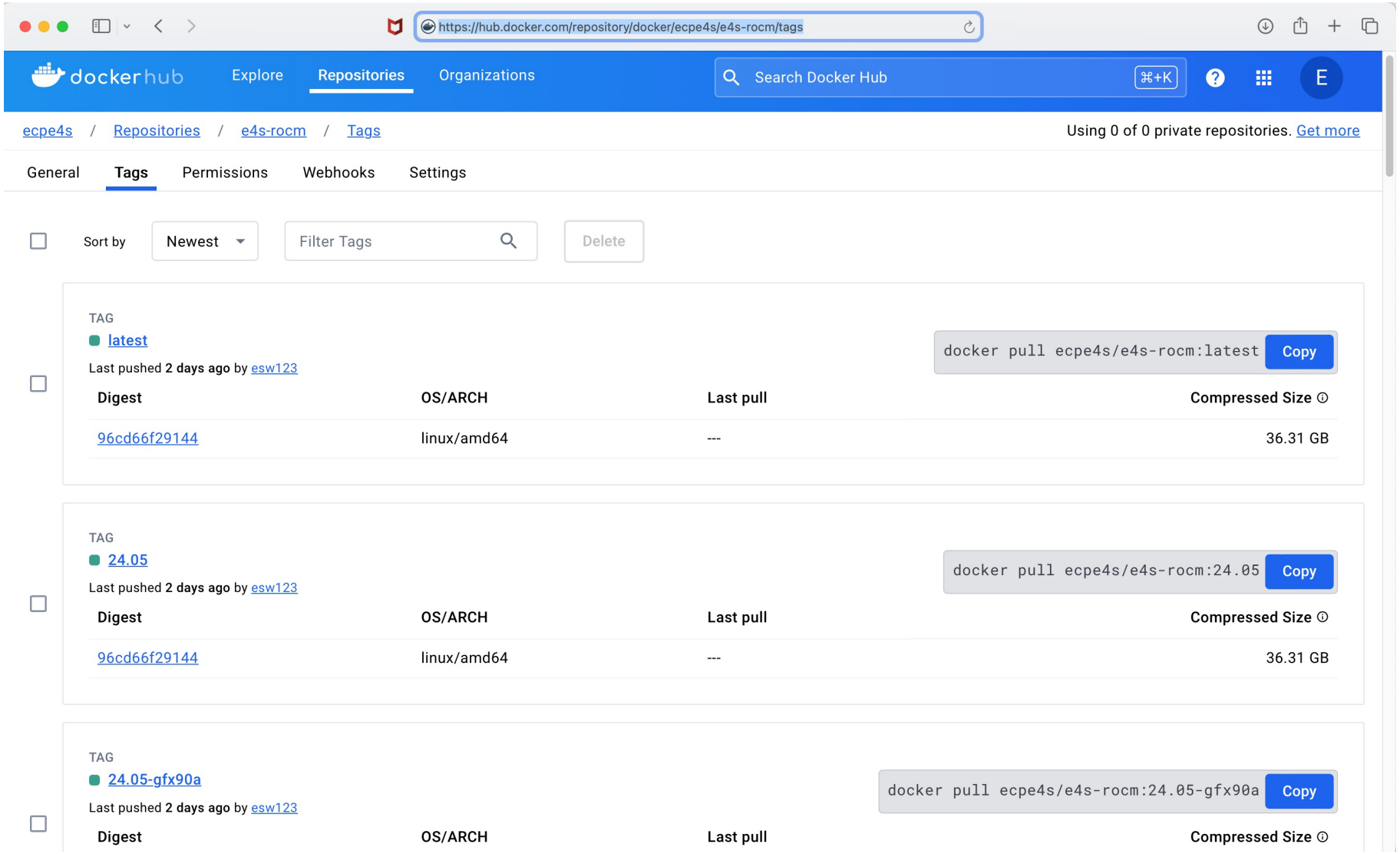


Architectures:

- x86_64
- aarch64
- ppc64le

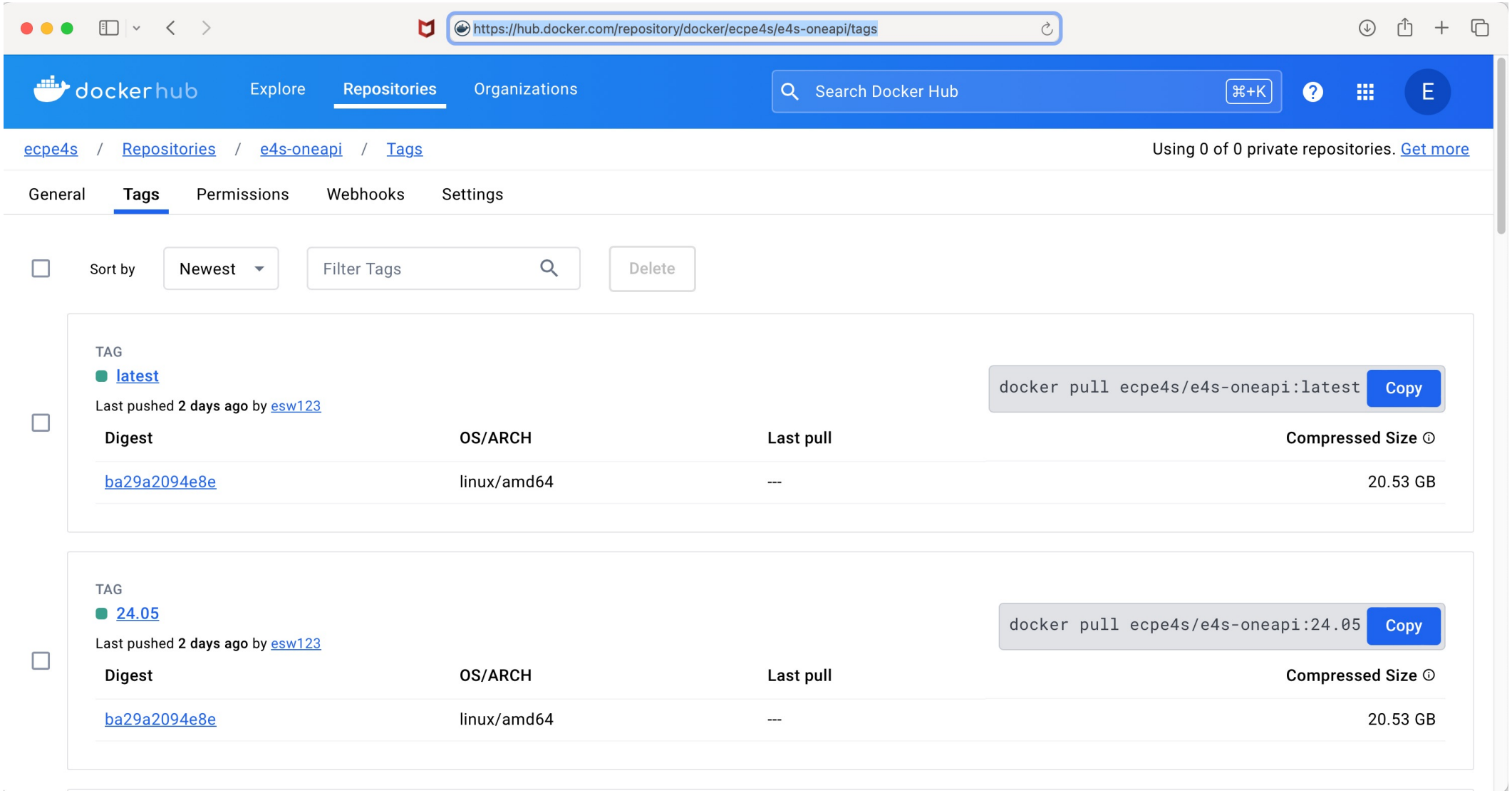
docker pull ecpe4s/e4s-base-cuda

E4S 24.05 ROCm release on Dockerhub



docker pull ecpe4s/e4s-rocm:24.05

E4S 24.05 oneAPI release on Dockerhub



docker pull ecpe4s/e4s-oneapi

24.05 Release: 129+ Official Products + dependencies (gcc, x86_64)

```
 1:  adios2            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/adios2-2.10.0-fhuiyladmsjw7zdpjd7mgamelpxmmfgs
 2:  alquimia          /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/alquimia-1.1.0-n5d3ne33zfjlogk6n7iqs6m7sfwzxasc
 3:  aml               /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/aml-0.2.1-sm2ewqj576lgrucxtmoh6gqkbjfxkiem
 4:  amrex             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/amrex-24.04-fl42ppt7g3573xeh3nnu7syg6vr6j4df
 5:  arborx            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/arborx-1.6-y7ixljvrlbc3vaelntlb5mvbkm26jzfo
 6:  argobots          /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/argobots-1.2-uyjbdlcm5wigztepqrjbwmbtg2ca6ami
 7:  ascent            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/ascent-0.9.2-dq5zu46qs5hv22wzc7e2jrozdfohevbt
 8:  axom              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/axom-0.9.0-73k3merxjlpa5v5ihcj37oq3balc3jrl
 9:  bolt              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/bolt-2.0-qpw2avwvi7tnhj47hironbi2zspkn5cx
10:  blaspp            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/blaspp-2023.11.05-pww7j6zd7msdt2ltyzmryjfu26klib6a
11:  bricks            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/bricks-2023.08.25-bfuoywxc35gkrgilfub5fjcbp3kjchng
12:  butterflypack     /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/butterflypack-2.4.0-qbytiad2aoh5ktglk4ql7rlkxtpoktxh
13:  cabana            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/cabana-0.6.0-gkqtbw66liat2ibpejcdwnm5swbhezmb
14:  caliper           /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/caliper-2.10.0-a2ep7ama3lfow5fauof7ffyhlzpcl6wq
15:  camp              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/camp-2024.02.0-pqzl2rlh3nz6hpdzpzftpxm35zsuhbvl
16:  chai              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/chai-2024.02.0-las35mttcz6kqovxiwix7py2g2z4hzqh
17:  charliecloud      /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/charliecloud-0.37-ikliebzc7m6spnzzoqqoplzav4inybt2
18:  conduit           /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/conduit-0.9.1-thvaheolv3ghtgzqu3wody6oxrwopere
19:  cp2k              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/cp2k-2024.1-xt2k55iofzvzrllcwdxd5kbckb7cih7b
20:  cusz              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/cusz-0.3.1-vfez6ufthc7mydxtmi7vpumrbzojuxct
21:  darshan-runtime   /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/darshan-runtime-3.4.4-gtl7r3zgisttljt7vxz4cdoqgtfduhln
22:  datatransferkit   /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/datatransferkit-3.1.1-y2x5h7mkzp5xezu5nown4y3j4fypxlzp
23:  dealii            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/dealii-9.5.1-z5tmzgo5qqmrigga3fevfzn2otdp3sqg
24:  dyninst           /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/dyninst-13.0.0-q27acrq3hcryhkwwu76xxd2zjhn2hjap
25:  e4s-alc           /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/e4s-alc-1.0.1-d2heapw26w5s36zangfv26wexngpvw4s
26:  e4s-cl            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/e4s-cl-1.0.3-3cvqfsyd7n7xi6qjpx5d4v3ksfo54d3e
27:  ecp-data-vis-sdk  /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/ecp-data-vis-sdk-1.0-wg5fy36scr4pkjlwpbhsqychgrjekoad
28:  exago             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/exago-1.6.0-7bkxxxgpuk5uyms5o3exqv66ode7az4n
29:  exaworks          /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/exaworks-0.1.0-mzvjjzj4vphquq5iv7tzmgnugw3i4ggx
30:  faodel            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/faodel-1.2108.1-rdjkcddli4jxng72udz42jq2mfsse2xi
31:  flecsi            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/flecsi-2.2.1-uajf4jjvy7th3srmseb2qsrzqviscd25
32:  flit              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/flit-2.1.0-cscnnxz6d45d7qpokzxp3j4agssblluv
33:  flux-core         /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/flux-core-0.61.2-aqnxfpazpprf5ws5cpmkp57qkjpchwsx
34:  flux-sched        /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/flux-sched-0.33.1-l67x2qr66uy7axlfjanjvyh64ppkm5bg
35:  fortrilinos       /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/fortrilinos-2.3.0-sjhgihagmzmjgmamuxphx4kttzahir3i
36:  gasnet            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/gasnet-2023.9.0-k7moh4hh75daydo4rwbdcuxmp73ctrft
37:  ginkgo            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/ginkgo-1.7.0-bt5qfvajamxmexjj6rzz62m4o56lchug
38:  globalarrays      /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/globalarrays-5.8.2-6ajsibvoeieueutrrgxi2deincdyruvy
39:  gotcha            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/gotcha-1.0.6-fowofvm722ho3txcctewm4rzwd7so6g3
40:  gptune            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/gptune-4.0.0-jqwwn3amkh55ae627vksisdishtwclr7
41:  gromacs           /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/gromacs-2024.1-ylm6fqy5rvm62dllqzbvywhzogvoprfn
42:  h5bench           /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/h5bench-1.4-sr3jfwtgdmekw2s2d2oaiyyv6jfn6stz
43:  hdf5              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/hdf5-1.14.3-o364hojddndkkioz3wmf3q567bcqivjo
```

GPU runtimes

- AMD (ROCm)
  - 5.7.1
- NVIDIA (CUDA)
  - 12.3
- NVHPC
  - 24.3
- Intel oneAPI 2024.0.2

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24.05 Release: 129+ Official Products + dependencies (gcc, x86_64)

```
44:  hdf5-vol-cache     /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/hdf5-vol-cache-v1.1-hlm7x7poznrjhjfgop6whzavftxlijj4
45:  hdf5-vol-async     /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/hdf5-vol-async-1.7-566thbgt7n7zi3maicubfamq3vkm4nun
46:  hdf5-vol-log       /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/hdf5-vol-log-1.4.0-b6a334oqxqbtavvwnib7wxc5tcu6xalk
47:  heffte             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/heffte-2.4.0-cekkr45afwsnn2ovtivsiiua5nrbg3w2
48:  hpctoolkit         /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/hpctoolkit-2024.01.1-p7jkx6ayo4mkivobioj4c3x2tz7dsm3k
49:  hpx                /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/hpx-1.9.1-iqhua6ztl47nz7ysyrvvqcih7e4u7jyk
50:  hypre              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/hypre-2.31.0-xxomsx3eg3q4qgd5xmui3phadg43h7nl
51:  kokkos             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/kokkos-4.3.00-fdzqphdxgo6srjcsqhwtlwrg663h4t5l
52:  kokkos-kernels     /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/kokkos-kernels-4.3.00-j4w6nmiuedb4jnhysk7c3lnmyisxcubi
53:  laghos             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/laghos-3.1-b7iajnooxa5blmufbtszvmc6rb52dvag
54:  lammps             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/lammps-20230802.3-a4dgzqvapienaliasstggpv7tdjeu3ri
55:  lapackpp           /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/lapackpp-2023.11.05-ad4fc5dkkgfggmso3esulu3ez52i6ys5
56:  lbann              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/lbann-0.104-6qylqaj2tr4favk2y5mt7clpntbmukb7
57:  legion             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/legion-24.03.0-rfinzjur4odnh3yf2tycgbi2zbuqmgn7
58:  libcatalyst        /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/libcatalyst-2.0.0-rc4-ja7hh6ezcg7rzuanbxukwbcp7o47iues
59:  libnrm             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/libnrm-0.1.0-rlzyjb5irlidq3uq2ckmdekb25pxzzdp
60:  libpressio         /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/libpressio-0.95.1-bxf5clha6zj7js26pg2uiaufnxlnsinq
61:  libquo             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/libquo-1.4-k2oy73q6fvaxoycgxrcuih2kmptxn7ho
62:  loki               /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/loki-0.1.7-4ngxknefhg3dh5mvngt2jvqlqorp5iu7
63:  magma              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/magma-2.8.0-crdwg7htvkuj6ljrlkc3uouqyhpyoojd
64:  mercury            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/mercury-2.3.1-zumkp4tcozd3qd5rjq7xmymnev2sg3sg
65:  metall             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/metall-0.25-re6fv5xk774c7sgle5bmokjv6e7dbkss
66:  mfem               /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/mfem-4.6.0-fvfh3g2vm4yl7tajdryuewnngsogkr4e
67:  mgard              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/mgard-2023-12-09-rxkl2uk3scasx6rqaiquarymwlecdheq
68:  mpark-variant      /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/mpark-variant-1.4.0-dhvuog3rhmlvh3ec4xrpkyoonpejhjdq
69:  mpich              /usr/local/mpich/install/mpich
70:  mpifileutils       /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/mpifileutils-0.11.1-5kseyh2jbrz7ksqsqsnakyyqx7nt7xme
71:  nccmp              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/nccmp-1.9.1.0-zzzpb5llrpfriwap4plxltrtmnl2l5cc
72:  nco                /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/nco-5.1.9-dfhtouuhfuvdd2qnlnyr46qchlbnlvxt
73:  nek5000            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/nek5000-19.0-2wqmvu3d5zh5hyftxvh4v2ypxprshocl
74:  nekbone            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/nekbone-17.0-emknoveznrxix76qppgwiodbjmtd6k37
75:  netcdf-fortran     /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/netcdf-fortran-4.6.1-j4bkapqsekkikoxz6v55q3u72e74njgb
76:  netlib-scalapack   /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/netlib-scalapack-2.2.0-ku2qbneae6j7eppy7cjmxccqcny7kg4f
77:  nrm                /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/nrm-0.1.0-7ro2g7vz2xw6hcbtopbmj5h6kocp5kwe
78:  omega-h            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/omega-h-9.34.13-gqp6exxu5xm2o7wb26e3kcnm3fn7ksuy
79:  openfoam           /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/openfoam-2312-omwa2qxbucnuo4taadrsgx5qsrxmnolv
80:  openmpi            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/openmpi-5.0.3-2bvhq7ow6ymrr73ksmnq3dzhmgwx4urf
81:  openpmd-api        /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/openpmd-api-0.15.2-gnfn5u42ukhb7d4rwpr2uwxf2ctlriin
82:  papi               /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/papi-7.1.0-aqrtxaaeaycqjvq7ggursnztzegwsu5d
83:  papyrus            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/papyrus-1.0.2-g7o6dht5tmvub2vtjlud2glvw5fbt5s3
84:  parallel-netcdf    /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/parallel-netcdf-1.12.3-hv5xg6awlelcv6ihffy5pfyljbat5fgt
85:  paraview           /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/paraview-5.12.0-keknhbz3xhfsdu67psbykeslkyhxzeod
86:  parsec             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/parsec-3.0.2209-vtb2hut5gwsbtvapidd2jsxbmqo5n6mv
```

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24.05 Release: 129+ Official Products + dependencies (gcc, x86_64)

```
  87:  pdt                /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/pdt-3.25.2-ntyx5npeoedhytnmp2f2fjbqsbpwowzo
  88:  petsc              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/petsc-3.21.0-qeo4b4cvo35wnmrao7hpfvuk6sqit2ay
  89:  phist              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/phist-1.12.0-mzhuo2qv7rgc3crxxbsgihvontvpgfl2
  90:  plasma             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/plasma-23.8.2-6sy2higf2u3lstk7xgnweid2gkiixili
  91:  plumed             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/plumed-2.9.0-k3gvo2opujkkiuwaymg4mpvk2c46lrm
  92:  precice            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/precice-3.1.1-wdb2xo77ds3v6zfqosrc7p4egra5rwaf
  93:  pruners-ninja      /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/pruners-ninja-1.0.1-symckmo6ooovcfagoaexjmanwf53tkxk
  94:  pumi               /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/pumi-2.2.8-aheswn3usl2uuaqyolbfjvfwbfnk7aar
  95:  py-cinemasci       /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/py-cinemasci-1.3-yxek54vn476avt4i4ffrlfw6l2m3ste5
  96:  py-deephyper       /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/py-deephyper-0.6.0-blk2nxp6cblh5tllhmloyofdjla3vfmo
  97:  py-jupyterhub      /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/py-jupyterhub-1.4.1-p3d3g7w33ka44mznqfnxgjekk7vqb4zw
  98:  py-libensemble     /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/py-libensemble-1.2.2-m4mzpifflfv7psqeaxojla672zerrxir
  99:  py-parsl           /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/py-parsl-2023.08.21-wvs7iiej4x4c3tm7rwvwi4dn5i22aozq
 100:  py-radical-saga    /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/py-radical-saga-1.47.0-6bb3j5mn4gwblawzvjjwbk6u7cytihav
 101:  qthreads           /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/qthreads-1.18-zkyzsc3ekeyd33s5k4vb4hnmk6b2fpb2
 102:  quantum-espresso   /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/quantum-espresso-7.3.1-4ifcespyaxqctcn7nvv4iozp7f2rwfhl
 103:  raja               /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/raja-2024.02.0-2njptptnlqcmofybw6vqokeca7pwl6iq
 104:  rempi              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/rempi-1.1.0-kpijbhup65kavzuxn626ix2k74c6volg
 105:  scr                /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/scr-3.0.1-nrgb7ztgti4hdaiwbaecvjgejgemy6aj
 106:  slate              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/slate-2023.11.05-p55lqsgekdwnigjpisqyt3v4stz7xkuw
 107:  slepc              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/slepc-3.21.0-tz3mwstqygi75v2cp7iv6izgh5e2p6zs
 108:  stc                /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/stc-0.9.0-6i6frt2hsdjnn7avmsuli6qjxova6ogm
 109:  strumpack          /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/strumpack-7.2.0-nnutidatsqdcs4yd4zgvszwqeha3wqth
 110:  sundials           /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/sundials-7.0.0-kae4vjqhlhsmup5gbg5fj7qhfotu7nil
 111:  superlu-dist       /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/superlu-dist-8.2.1-mpfggyo26xhcwrav3h3ggqtwtq4glgi7
 112:  swig               /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/swig-4.1.1-kxca6xdwutn47opikmgztifx7lb24wxh
 113:  sz3                /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/sz3-3.1.7-oozjyrpquv5bfyvkwtkgjcmuuek44bry
 114:  tasmanian          /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/tasmanian-8.0-neqt3xyiksojlknbm6pvsvtgdtjzjr32
 115:  tau                /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/tau-2.33.2-h7dgidkne2k3xqumof2ux5cr74qrkpvg
 116:  trilinos           /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/trilinos-15.1.1-vwvbdhmwahq5s7dxc3fc6kpbth27alun
 117:  turbine            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/turbine-1.3.0-75xp3vorpsxgufs3c2gtx64b5ua4itij
 118:  umap               /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/umap-2.1.0-qzrq5rtq4zf55sbw6ldfcvz26puhcwx3
 119:  umpire             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/umpire-2024.02.0-e4mqgdg53gnroe6lbndx53gykupxgann
 120:  unifyfs            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/unifyfs-2.0-ftlvq6v655adtpsu74sbf4mq75xgo5jd
 121:  upcxx              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/upcxx-2023.9.0-3qi64d5ssz3owl53y2tekvrnon3ev3s7
 122:  variorum           /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/variorum-0.7.0-bcjnkmkgbq7qxpwmckwlmixpusv3t3gb
 123:  veloc              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/veloc-1.7-koe3ykxgxbzalhxdhm5uyj5qvpfomts2
 124:  visit              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/visit-3.3.3-mnudpebe6ppnov54hpc53dgwnyqqz6dc
 125:  vtk-m              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/vtk-m-2.1.0-wmxwujtmduiulmxcalaznuz4cz3pymzv
 126:  wannier90          /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/wannier90-3.1.0-iqqefxuryg377waf74wpk76ra2cdey5r
 127:  warpx              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/warpx-23.08-5gt7i7cldkpm36qgal7zo6qozlhuvzr6
 128:  xyce               /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/xyce-7.8.0-a7keyuythgdlekfknkmdm7vpgguauzzc
 129:  zfp                /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/zfp-1.0.0-md2k77z73i2wvdhsxjssepmj54dyjyey
```

Languages:

- Rust
- Julia with support for MPI, and CUDA
- Python

AI products

- TensorBraid
- DeepHyper
- OpenAI
- Tensorflow
- Pytorch
- JAX
- Horovod
- LBANN

EDA Tools:

- Xyce

3D Visualization

- Paraview
- VisIt
- TAU's paraprof
- Jupyter notebook …

PESO

E4S Tools: e4s-chain-spack.sh

```
Singularity> rm -rf ~/tmp/spack
Singularity> . /etc/e4s/e4s-chain-spack.sh ~/tmp/spack
Cloning into '/home/users/sameer/tmp/spack'...
remote: Enumerating objects: 531987, done.
remote: Counting objects: 100% (180/180), done.
remote: Compressing objects: 100% (92/92), done.
remote: Total 531987 (delta 83), reused 139 (delta 60), pack-reused 531807
Receiving objects: 100% (531987/531987), 176.96 MiB | 32.95 MiB/s, done.
Resolving deltas: 100% (249575/249575), done.
Updating files: 100% (11224/11224), done.
Singularity> spack find valgrind
==> Error: No package matches the query: valgrind
Singularity> spack install valgrind
[+] /opt/intel/oneapi (external intel-oneapi-mpi-2021.11.0-2qi2xp2qs4kxwddgnibhixhgjmwvngvo)
[+] /spack/opt/spack/linux-ubuntu22.04-x86_64/oneapi-2024.0.2/gmake-4.4.1-zpg4uz3bbxf4ljfzxsm5uhhepceiwdwd
[+] /spack/opt/spack/linux-ubuntu22.04-x86_64/oneapi-2024.0.2/boost-1.84.0-zualrbbikg6f5cvkjif227s3mebjfnov
==> Installing valgrind-3.20.0-7t4aj3mw3fokiyun6ofcjgxaj6teseas [4/4]
==> No binary for valgrind-3.20.0-7t4aj3mw3fokiyun6ofcjgxaj6teseas found: installing from source
==> Fetching https://mirror.spack.io/_source-cache/archive/85/8536c031dbe078d342f121fa881a9ecd205cb5a78e639005ad570011bdb9f3c6.tar.bz2
==> Ran patch() for valgrind
==> valgrind: Executing phase: 'autoreconf'
==> valgrind: Executing phase: 'configure'
==> valgrind: Executing phase: 'build'
==> valgrind: Executing phase: 'install'
==> valgrind: Successfully installed valgrind-3.20.0-7t4aj3mw3fokiyun6ofcjgxaj6teseas
  Stage: 3.53s.  Autoreconf: 0.00s.  Configure: 45.60s.  Build: 28.97s.  Install: 3.15s.  Post-install: 1.32s.  Total: 1m 22.86s
[+] /home/users/sameer/tmp/spack/opt/spack/linux-ubuntu22.04-x86_64/oneapi-2024.0.2/valgrind-3.20.0-7t4aj3mw3fokiyun6ofcjgxaj6teseas
Singularity> spack load valgrind
Singularity> which valgrind
/home/users/sameer/tmp/spack/opt/spack/linux-ubuntu22.04-x86_64/oneapi-2024.0.2/valgrind-3.20.0-7t4aj3mw3fokiyun6ofcjgxaj6teseas/bin/valgrind
Singularity> valgrind --help | head
usage: valgrind [options] prog-and-args

  tool-selection option, with default in [ ]:
    --tool=<name>             use the Valgrind tool named <name> [memcheck]

  basic user options for all Valgrind tools, with defaults in [ ]:
    -h --help                 show this message
    --help-debug              show this message, plus debugging options
    --help-dyn-options        show the dynamically changeable options
    --version                 show version
Singularity>
```

e4s-chain-spack.sh allows a user to extend and add new tools to an existing Spack installation in a read-only filesystem in a container and chain both Spack installations!

E4S Support for AI/ML frameworks with NVIDIA GPUs

```
$ singularity run --nv e4s-24.05-cuda90-arm64.sif
Singularity> nvidia-smi
Thu May  9 10:17:49 2024
+---------------------------------------------------------------------------------------+
| NVIDIA-SMI 535.146.02             Driver Version: 535.146.02   CUDA Version: 12.2     |
|-----------------------------------------+----------------------+----------------------+
| GPU  Name                 Persistence-M | Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp   Perf          Pwr:Usage/Cap |         Memory-Usage | GPU-Util  Compute M. |
|                                         |                      |               MIG M. |
|=========================================+======================+======================|
|   0  NVIDIA GH200 480GB             Off | 00000009:01:00.0 Off |                    0 |
| N/A   23C    P0              78W / 900W |     25MiB / 97871MiB |      0%      Default |
|                                         |                      |             Disabled |
+-----------------------------------------+----------------------+----------------------+

+---------------------------------------------------------------------------------------+
| Processes:                                                                            |
|  GPU   GI   CI        PID   Type   Process name                            GPU Memory |
|        ID   ID                                                             Usage      |
|=======================================================================================|
|    0   N/A  N/A     17296      G   /usr/libexec/Xorg                             4MiB |
+---------------------------------------------------------------------------------------+
Singularity> python
Python 3.10.12 (main, Nov 20 2023, 15:14:05) [GCC 11.4.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import tensorflow
>>> import torch
>>> torch.cuda.get_device_name(0)
'NVIDIA GH200 480GB'
>>> torch.cuda.get_arch_list()
['sm_75', 'sm_80', 'sm_90']
>>> torch.__version__
'2.3.0'
>>> tensorflow.__version__
'2.16.1'
>>>
```

E4S 24.05 supports NVIDIA Grace-Hopper GH200 GPUs with TensorFlow and PyTorch

E4S Support for AI/ML and Python tools

```
$ singularity run --nv e4s-24.05-cuda90-amd64.sif
Singularity> python
Python 3.10.12 (main, Nov 20 2023, 15:14:05) [GCC 11.4.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import openai
>>> import google.generativeai
>>> import tensorflow
>>> import torch
>>> import jax
>>> import torchbraid
>>> import deephyper
>>> import pandas
>>> import cv2
>>> import sklearn
>>> import open3d
>>> import numpy
>>> import scipy
>>> import matplotlib
>>> import plotly
>>> import seaborn
>>> import mpi4py
>>>
Singularity> grep Ubuntu /etc/os-release
PRETTY_NAME="Ubuntu 22.04.4 LTS"
NAME="Ubuntu"
Singularity>
```

PESO

E4S 24.05 Support for GPUs: NVIDIA

```
$ singularity run --nv e4s-24.05-cuda90-amd64.sif
Singularity> spack find -x +cuda
-- linux-ubuntu22.04-x86_64 / gcc@11.4.0 ------------------------
adios2@2.10.0      chai@2024.02.0        gromacs@2024.1         legion@24.03.0     petsc@3.21.0       superlu-dist@8.2.1  zfp@0.5.5
amrex@24.04        cusz@0.3.1            heffte@2.4.0           libpressio@0.95.1  py-torch@2.2.2     tasmanian@8.0
arborx@1.6         ecp-data-vis-sdk@1.0  hpctoolkit@2024.01.1   magma@2.8.0        raja@2024.02.0     tau@2.33.2
axom@0.9.0         exago@1.6.0           hpx@1.9.1              mfem@4.6.0         slate@2023.11.05   trilinos@15.1.1
bricks@2023.08.25  flecsi@2.2.1          kokkos@4.3.00          mgard@2023-12-09   slepc@3.21.0       umpire@2024.02.0
cabana@0.6.0       flux-core@0.61.2      kokkos-kernels@4.3.00  papi@7.1.0         strumpack@7.2.0    upcxx@2023.9.0
caliper@2.10.0     ginkgo@1.7.0          lammps@20230802.3      parsec@3.0.2209    sundials@7.0.0     vtk-m@2.1.0
==> 43 installed packages
Singularity> spack find -x
-- linux-ubuntu22.04-x86_64 / gcc@11.4.0 ------------------------
adios@1.13.1         darshan-runtime@3.4.4  h5bench@1.4            mercury@2.3.1          petsc@3.21.0           superlu@5.3.0
adios2@2.7.1         darshan-util@3.4.4     hdf5@1.12.3            metall@0.25            phist@1.12.0           superlu-dist@8.2.1
adios2@2.10.0        datatransferkit@3.1.1  hdf5-vol-async@1.7     mfem@4.6.0             plasma@23.8.2          superlu-dist@8.2.1
alquimia@1.1.0       dealii@9.5.1           hdf5-vol-cache@v1.1    mfem@4.6.0             plumed@2.9.0           swig@4.0.2-fortran
aml@0.2.1            dyninst@13.0.0         hdf5-vol-log@1.4.0     mgard@2023-12-09       precice@3.1.1          sz@2.1.12.5
amrex@24.04          e4s-alc@1.0.1          heffte@2.4.0           mgard@2023-12-09       pruners-ninja@1.0.1    sz3@3.1.7
amrex@24.04          e4s-cl@1.0.3           heffte@2.4.0           mpark-variant@1.4.0    pumi@2.2.8             tasmanian@8.0
arborx@1.6           ecp-data-vis-sdk@1.0   hpctoolkit@2024.01.1   mpich@4.1.2            py-cinemasci@1.3       tasmanian@8.0
arborx@1.6           ecp-data-vis-sdk@1.0   hpctoolkit@2024.01.1   mpifileutils@0.11.1    py-deephyper@0.6.0     tau@2.33.2
argobots@1.2         exago@1.6.0            hpx@1.9.1              nccmp@1.9.1.0          py-h5py@3.11.0         tau@2.33.2
ascent@0.9.2         exago@1.6.0            hpx@1.9.1              nco@5.1.9              py-jupyterhub@1.4.1    trilinos@13.0.1
axom@0.9.0           exaworks@0.1.0         hypre@2.31.0           nek5000@19.0           py-libensemble@1.2.2   trilinos@15.1.1
axom@0.9.0           faodel@1.2108.1        kokkos@4.3.00          nekbone@17.0           py-petsc4py@3.21.0     trilinos@15.1.1
bolt@2.0             flecsi@2.2.1           kokkos@4.3.00          netcdf-fortran@4.6.1   py-torch@2.2.2         turbine@1.3.0
boost@1.79.0         flecsi@2.2.1           kokkos-kernels@4.3.00  netlib-scalapack@2.2.0 py-warpx@23.08         umap@2.1.0
bricks@2023.08.25    flit@2.1.0             kokkos-kernels@4.3.00  nrm@0.1.0              qthreads@1.18          umpire@2024.02.0
bricks@2023.08.25    flux-core@0.61.2       laghos@3.1             nvhpc@24.3             quantum-espresso@7.3.1 umpire@2024.02.0
butterflypack@2.4.0  flux-core@0.61.2       lammps@20230802.3      omega-h@9.34.13        raja@2024.02.0         unifyfs@2.0
cabana@0.6.0         fortrilinos@2.3.0      lammps@20230802.3      openfoam@2312          raja@2024.02.0         upcxx@2023.9.0
cabana@0.6.0         fpm@0.10.0             lbann@0.104            openmpi@5.0.3          rempi@1.1.0            upcxx@2023.9.0
caliper@2.10.0       gasnet@2023.9.0        legion@24.03.0         openpmd-api@0.15.2     scr@3.0.1              variorum@0.7.0
caliper@2.10.0       ginkgo@1.7.0           legion@24.03.0         papi@7.1.0             slate@2023.11.05       veloc@1.7
chai@2024.02.0       ginkgo@1.7.0           libcatalyst@2.0.0-rc4  papi@7.1.0             slate@2023.11.05       visit@3.3.3
chai@2024.02.0       globalarrays@5.8.2     libnrm@0.1.0           papyrus@1.0.2          slepc@3.21.0           vtk-m@2.0.0
charliecloud@0.37    glvis@4.2              libpressio@0.95.1      parallel-netcdf@1.12.3 slepc@3.21.0           vtk-m@2.1.0
conduit@0.9.1        gmp@6.2.1              libpressio@0.95.1      paraview@5.12.0        stc@0.9.0              wannier90@3.1.0
cp2k@2024.1          gotcha@1.0.6           libquo@1.4             parsec@3.0.2209        strumpack@7.2.0        xyce@7.8.0
cuda@11.8.0          gptune@4.0.0           libunwind@1.6.2        parsec@3.0.2209        strumpack@7.2.0        zfp@0.5.5
cuda@12.2.0          gromacs@2024.1         loki@0.1.7             pdt@3.25.2             sundials@7.0.0         zfp@0.5.5
cusz@0.3.1           gromacs@2024.1         magma@2.8.0            petsc@3.21.0           sundials@7.0.0
==> 179 installed packages
```

E4S 24.05 Support for GPUs: NVIDIA (modules)

```
$ singularity run --nv e4s-24.05-cuda90-amd64.sif
Singularity> module avail

------------------------------------------ /spack/share/spack/lmod/linux-ubuntu22.04-x86_64/mpich/4.1.2-w2qwypv/Core ------------------------------------------
   adios/1.13.1                      flecsi/2.2.1-cuda90                    mfem/4.6.0-cuda90                  slate/2023.11.05-cuda90-openmp
   adios2/2.7.1                      flecsi/2.2.1                    (D)    mfem/4.6.0                  (D)    slate/2023.11.05-openmp        (D)
   adios2/2.10.0-cuda90       (D)    fortrilinos/2.3.0                      mpifileutils/0.11.1                slepc/3.21.0-cuda90
   alquimia/1.1.0                    ginkgo/1.7.0-cuda90-openmp             nccmp/1.9.1.0                      slepc/3.21.0                   (D)
   amrex/24.04-cuda90                ginkgo/1.7.0-openmp             (D)    nco/5.1.9                          stc/0.9.0
   amrex/24.04                (D)    globalarrays/5.8.2                     nek5000/19.0                       strumpack/7.2.0-cuda90-openmp
   arborx/1.6-cuda90                 glvis/4.2                              nekbone/17.0                       strumpack/7.2.0-openmp         (D)
   arborx/1.6                 (D)    gptune/4.0.0                           netcdf-fortran/4.6.1               sundials/7.0.0-cuda90
   ascent/0.9.2-openmp               gromacs/2024.1-cuda90-openmp           netlib-scalapack/2.2.0             sundials/7.0.0                 (D)
   axom/0.9.0-cuda90-openmp          gromacs/2024.1-openmp           (D)    omega-h/9.34.13                    superlu-dist/8.2.1-cuda90
   axom/0.9.0-openmp          (D)    h5bench/1.4                            openfoam/2312                      superlu-dist/8.2.1             (D)
   boost/1.79.0                      hdf5-vol-async/1.7                     openpmd-api/0.15.2                 sz/2.1.12.5
   bricks/2023.08.25-cuda            hdf5-vol-cache/v1.1                    papyrus/1.0.2                      tasmanian/8.0-cuda90
   bricks/2023.08.25          (D)    hdf5-vol-log/1.4.0                     parallel-netcdf/1.12.3             tasmanian/8.0                  (D)
   butterflypack/2.4.0-openmp        hdf5/1.12.3                            paraview/5.12.0                    tau/2.33.2-cuda
   cabana/0.6.0-cuda90               heffte/2.4.0-cuda90                    parsec/3.0.2209-cuda90             tau/2.33.2                     (D)
   cabana/0.6.0               (D)    heffte/2.4.0                    (D)    parsec/3.0.2209             (D)    trilinos/13.0.1
   caliper/2.10.0-cuda90             hpctoolkit/2024.01.1-cuda              petsc/3.21.0-cuda90                trilinos/15.1.1-cuda90
   caliper/2.10.0             (D)    hpctoolkit/2024.01.1            (D)    petsc/3.21.0                (D)    trilinos/15.1.1                (D)
   chai/2024.02.0-cuda90             hpx/1.9.1-cuda90                       phist/1.12.0-openmp                turbine/1.3.0
   chai/2024.02.0             (D)    hpx/1.9.1                       (D)    plumed/2.9.0                       umpire/2024.02.0-cuda90
   conduit/0.9.1                     hypre/2.31.0                           precice/3.1.1                      umpire/2024.02.0               (D)
   cp2k/2024.1-openmp                laghos/3.1                             pruners-ninja/1.0.1                unifyfs/2.0
   darshan-runtime/3.4.4             lammps/20230802.3-cuda90-openmp        pumi/2.2.8                         upcxx/2023.9.0-cuda90
   datatransferkit/3.1.1             lammps/20230802.3-openmp        (D)    py-cinemasci/1.3                   upcxx/2023.9.0                 (D)
   dealii/9.5.1                      lbann/0.104                            py-h5py/3.11.0                     veloc/1.7
   dyninst/13.0.0-openmp             libcatalyst/2.0.0-rc4                  py-libensemble/1.2.2               visit/3.3.3
   ecp-data-vis-sdk/1.0-cuda90       libnrm/0.1.0                           py-petsc4py/3.21.0                 vtk-m/2.0.0-openmp
   ecp-data-vis-sdk/1.0       (D)    libpressio/0.95.1-cuda90-openmp        py-torch/2.2.2-cuda90-openmp       vtk-m/2.1.0-cuda90-openmp      (D)
   exago/1.6.0-cuda80                libpressio/0.95.1-openmp        (D)    py-warpx/23.08                     wannier90/3.1.0
   exago/1.6.0                (D)    libquo/1.4                             quantum-espresso/7.3.1-openmp      xyce/7.8.0
   exaworks/0.1.0                    mercury/2.3.1                          rempi/1.1.0
   faodel/1.2108.1                   metall/0.25                            scr/3.0.1

------------------------------------------------- /spack/share/spack/lmod/linux-ubuntu22.04-x86_64/Core -------------------------------------------------
   aml/0.2.1                 flit/2.1.0                        kokkos/4.3.00-openmp          (D)    nrm/0.1.0                  raja/2024.02.0-cuda90
   argobots/1.2              flux-core/0.61.2-cuda             legion/24.03.0-cuda70                nvhpc/24.3                 raja/2024.02.0        (D)
   bolt/2.0                  flux-core/0.61.2           (D)    legion/24.03.0                (D)    openmpi/5.0.3              superlu/5.3.0
   charliecloud/0.37         fpm/0.10.0-openmp                 libunwind/1.6.2                      papi/7.1.0-cuda            swig/4.0.2-fortran
   cuda/11.8.0               gasnet/2023.9.0                   loki/0.1.7                           papi/7.1.0          (D)    sz3/3.1.7
   cuda/12.2.0        (D)    gmp/6.2.1                         magma/2.8.0-cuda90                   pdt/3.25.2                 umap/2.1.0
   cusz/0.3.1-cuda90         gotcha/1.0.6                      mgard/2023-12-09-cuda90-openmp       plasma/23.8.2              variorum/0.7.0
   darshan-util/3.4.4        kokkos-kernels/4.3.00-cuda90      mgard/2023-12-09-openmp       (D)    py-deephyper/0.6.0         zfp/0.5.5-cuda90
   e4s-alc/1.0.1             kokkos-kernels/4.3.00-openmp (D)  mpark-variant/1.4.0                  py-jupyterhub/1.4.1        zfp/0.5.5             (D)
   e4s-cl/1.0.3              kokkos/4.3.00-cuda90              mpich/4.1.2                   (L)    qthreads/1.18

  Where:
   L:  Module is loaded
```

E4S 24.05 Support for GPUs: AMD

```
$ singularity run e4s-24.05-rocm90a-amd64.sif
Singularity> spack find -x +rocm
-- linux-ubuntu22.04-x86_64 / gcc@11.4.0 ------------------------
amrex@24.04     chai@2024.02.0        ginkgo@1.7.0          hypre@2.31.0    mfem@4.6.0       slate@2023.11.05  superlu-dist@8.2.1  umpire@2024.02.0
arborx@1.6      ecp-data-vis-sdk@1.0  heffte@2.4.0          kokkos@4.3.00   paraview@5.12.0  slepc@3.21.0      tasmanian@8.0       upcxx@2023.9.0
cabana@0.6.0    exago@1.6.0           hpctoolkit@2024.01.1  legion@24.03.0  petsc@3.21.0     strumpack@7.2.0   tau@2.33.2          vtk-m@2.1.0
caliper@2.10.0  gasnet@2023.9.0       hpx@1.9.1             magma@2.8.0     raja@2024.02.0   sundials@7.0.0    trilinos@15.1.1
==> 31 installed packages
Singularity> spack find -x
-- linux-ubuntu22.04-x86_64 / gcc@11.4.0 ------------------------
adios@1.13.1          darshan-runtime@3.4.4  gmp@6.2.1              lbann@0.104              nrm@0.1.0              py-jupyterhub@1.4.1     sz3@3.1.7
adios2@2.7.1          darshan-util@3.4.4     gotcha@1.0.6           legion@24.03.0           nvhpc@24.3             py-libensemble@1.2.2    tasmanian@8.0
alquimia@1.1.0        datatransferkit@3.1.1  gptune@4.0.0           legion@24.03.0           omega-h@9.34.13        py-petsc4py@3.21.0      tasmanian@8.0
aml@0.2.1             dealii@9.5.1           gromacs@2024.1         libcatalyst@2.0.0-rc4    openfoam@2312          py-warpx@23.08          tau@2.33.2
amrex@24.04           dyninst@13.0.0         h5bench@1.4            libnrm@0.1.0             openmpi@5.0.3          qthreads@1.18           tau@2.33.2
amrex@24.04           e4s-alc@1.0.1          hdf5@1.12.3            libpressio@0.95.1        openpmd-api@0.15.2     quantum-espresso@7.3.1  trilinos@13.0.1
arborx@1.6            e4s-cl@1.0.3           hdf5@1.14.3            libquo@1.4               papi@7.1.0             raja@2024.02.0          trilinos@15.1.1
arborx@1.6            ecp-data-vis-sdk@1.0   hdf5-vol-async@1.7     libunwind@1.6.2          papyrus@1.0.2          raja@2024.02.0          trilinos@15.1.1
argobots@1.2          ecp-data-vis-sdk@1.0   hdf5-vol-cache@v1.1    loki@0.1.7               parallel-netcdf@1.12.3 rempi@1.1.0             turbine@1.3.0
ascent@0.9.2          exago@1.6.0            hdf5-vol-log@1.4.0     magma@2.8.0              paraview@5.12.0        scr@3.0.1               umap@2.1.0
axom@0.9.0            exago@1.6.0            hdf5-vol-log@1.4.0     mercury@2.3.1            paraview@5.12.0        slate@2023.11.05        umpire@2024.02.0
bolt@2.0              exaworks@0.1.0         heffte@2.4.0           metall@0.25              parsec@3.0.2209        slate@2023.11.05        umpire@2024.02.0
boost@1.79.0          faodel@1.2108.1        heffte@2.4.0           mfem@4.6.0               pdt@3.25.2             slepc@3.21.0            unifyfs@2.0
bricks@2023.08.25     flecsi@2.2.1           hpctoolkit@2024.01.1   mfem@4.6.0               petsc@3.21.0           slepc@3.21.0            upcxx@2023.9.0
butterflypack@2.4.0   flit@2.1.0             hpctoolkit@2024.01.1   mgard@2023-12-09         petsc@3.21.0           stc@0.9.0               upcxx@2023.9.0
cabana@0.6.0          flux-core@0.61.2       hpx@1.9.1              mpark-variant@1.4.0      phist@1.12.0           strumpack@7.2.0         variorum@0.7.0
cabana@0.6.0          fortrilinos@2.3.0      hpx@1.9.1              mpich@4.1.2              plasma@23.8.2          strumpack@7.2.0         veloc@1.7
caliper@2.10.0        fpm@0.10.0             hypre@2.31.0           mpifileutils@0.11.1      plumed@2.9.0           sundials@7.0.0          visit@3.3.3
caliper@2.10.0        gasnet@2023.9.0        hypre@2.31.0           nccmp@1.9.1.0            precice@3.1.1          sundials@7.0.0          vtk-m@2.0.0
chai@2024.02.0        gasnet@2023.9.0        kokkos@4.3.00          nco@5.1.9                pruners-ninja@1.0.1    superlu@5.3.0           vtk-m@2.1.0
chai@2024.02.0        ginkgo@1.7.0           kokkos@4.3.00          nek5000@19.0             pumi@2.2.8             superlu-dist@8.2.1      wannier90@3.1.0
charliecloud@0.37     ginkgo@1.7.0           kokkos-kernels@4.3.00  nekbone@17.0             py-cinemasci@1.3       superlu-dist@8.2.1      xyce@7.8.0
conduit@0.9.1         globalarrays@5.8.2     laghos@3.1             netcdf-fortran@4.6.1     py-deephyper@0.6.0     swig@4.0.2-fortran      zfp@0.5.5
cp2k@2024.1           glvis@4.2              lammps@20230802.3      netlib-scalapack@2.2.0   py-h5py@3.11.0         sz@2.1.12.5
==> 167 installed packages
Singularity>
```

E4S 24.05 Support for GPUs: AMD (modules)

```
Singularity> module avail

------------------------------------------- /spack/share/spack/lmod/linux-ubuntu22.04-x86_64/mpich/4.1.2-w2qwypv/Core --------------------------
   adios/1.13.1                      fortrilinos/2.3.0                 mfem/4.6.0-gfx90a                 scr/3.0.1
   alquimia/1.1.0                    ginkgo/1.7.0-gfx90a-openmp        mfem/4.6.0                 (D)    slate/2023.11.05-gfx90a-openmp
   amrex/24.04-gfx90a                ginkgo/1.7.0-openmp        (D)    mpifileutils/0.11.1               slate/2023.11.05-openmp        (D)
   amrex/24.04                (D)    globalarrays/5.8.2                nccmp/1.9.1.0                     slepc/3.21.0-gfx90a
   arborx/1.6-gfx90a                 glvis/4.2                         nco/5.1.9                         slepc/3.21.0                   (D)
   arborx/1.6                 (D)    gptune/4.0.0                      nek5000/19.0                      stc/0.9.0
   axom/0.9.0-openmp                 gromacs/2024.1-openmp             nekbone/17.0                      strumpack/7.2.0-gfx90a-openmp
   boost/1.79.0                      h5bench/1.4                       netcdf-fortran/4.6.1              strumpack/7.2.0-openmp         (D)
   bricks/2023.08.25                 hdf5-vol-async/1.7                netlib-scalapack/2.2.0            sundials/7.0.0-gfx90a
   butterflypack/2.4.0-openmp        hdf5-vol-cache/v1.1               omega-h/9.34.13                   sundials/7.0.0                 (D)
   cabana/0.6.0-gfx90a-rocm          hdf5-vol-log/1.4.0                openfoam/2312                     superlu-dist/8.2.1-gfx90a
   cabana/0.6.0               (D)    heffte/2.4.0-gfx90a               openpmd-api/0.15.2                superlu-dist/8.2.1             (D)
   caliper/2.10.0-gfx90a             heffte/2.4.0               (D)    papyrus/1.0.2                     tasmanian/8.0-gfx90a
   caliper/2.10.0             (D)    hpctoolkit/2024.01.1-rocm         parsec/3.0.2209                   tasmanian/8.0                  (D)
   chai/2024.02.0-gfx90a             hpctoolkit/2024.01.1       (D)    petsc/3.21.0-gfx90a               tau/2.33.2-rocm
   chai/2024.02.0             (D)    hpx/1.9.1-gfx90a                  petsc/3.21.0               (D)    tau/2.33.2                     (D)
   conduit/0.9.1                     hpx/1.9.1                  (D)    phist/1.12.0-openmp               trilinos/13.0.1
   cp2k/2024.1-openmp                hypre/2.31.0-gfx90a               plumed/2.9.0                      trilinos/15.1.1-gfx90a
   datatransferkit/3.1.1             hypre/2.31.0               (D)    precice/3.1.1                     trilinos/15.1.1                (D)
   dealii/9.5.1                      laghos/3.1                        pruners-ninja/1.0.1               turbine/1.3.0
   dyninst/13.0.0-openmp             lammps/20230802.3-openmp          pumi/2.2.8                        umpire/2024.02.0-gfx90a
   ecp-data-vis-sdk/1.0-gfx90a       lbann/0.104                       py-h5py/3.11.0                    umpire/2024.02.0               (D)
   ecp-data-vis-sdk/1.0       (D)    libnrm/0.1.0                      py-libensemble/1.2.2              upcxx/2023.9.0-gfx90a
   exago/1.6.0-gfx90a                libpressio/0.95.1-openmp          py-petsc4py/3.21.0                upcxx/2023.9.0                 (D)
   exago/1.6.0                (D)    libquo/1.4                        py-warpx/23.08                    wannier90/3.1.0
   exaworks/0.1.0                    mercury/2.3.1                     quantum-espresso/7.3.1-openmp     xyce/7.8.0
   flecsi/2.2.1                      metall/0.25                       rempi/1.1.0

------------------------------------------------------- /spack/share/spack/lmod/linux-ubuntu22.04-x86_64/Core -------------------------------------
   aml/0.2.1             fpm/0.10.0-openmp                 legion/24.03.0-gfx90a          nrm/0.1.0              qthreads/1.18
   argobots/1.2          gasnet/2023.9.0-gfx90a            legion/24.03.0          (D)    nvhpc/24.3             raja/2024.02.0-gfx90a
   bolt/2.0              gasnet/2023.9.0             (D)   libunwind/1.6.2                openmpi/5.0.3          raja/2024.02.0         (D)
   charliecloud/0.37     gmp/6.2.1                         loki/0.1.7                     papi/7.1.0             superlu/5.3.0
   e4s-alc/1.0.1         gotcha/1.0.6                      magma/2.8.0-gfx90a             pdt/3.25.2             swig/4.0.2-fortran
   e4s-cl/1.0.3          kokkos-kernels/4.3.00-openmp      mgard/2023-12-09-openmp        plasma/23.8.2          sz3/3.1.7
   flit/2.1.0            kokkos/4.3.00-gfx90a              mpark-variant/1.4.0            py-deephyper/0.6.0     umap/2.1.0
   flux-core/0.61.2      kokkos/4.3.00-openmp        (D)   mpich/4.1.2             (L)    py-jupyterhub/1.4.1    variorum/0.7.0

  Where:
   L:  Module is loaded
   D:  Default Module
```

E4S 24.05 Support for GPUs: Intel

```
$ singularity run e4s-24.05-oneapi-amd64.sif
Singularity> H1=$(spack find --format /{hash} +level_zero)
Singularity> H2=$(spack find --format /{hash} +sycl)
Singularity> spack find $H1 $H2
-- linux-ubuntu22.04-x86_64 / oneapi@2024.0.2 --------------------
amrex@24.04  blaspp@2023.11.05  ginkgo@1.7.0  kokkos@4.3.00  lapackpp@2023.11.05  slate@2023.11.05  tau@2.33.2
arborx@1.6   cabana@0.6.0       heffte@2.4.0  kokkos@4.3.00  petsc@3.21.0         sundials@7.0.0    upcxx@2023.9.0
==> 14 installed packages
Singularity> spack find -x
-- linux-ubuntu22.04-x86_64 / gcc@11.4.0 ------------------------
hdf5@1.12.3  papi@7.1.0

-- linux-ubuntu22.04-x86_64 / oneapi@2024.0.2 --------------------
adios@1.13.1           datatransferkit@3.1.1  hdf5-vol-cache@v1.1        mgard@2023-12-09        pruners-ninja@1.0.1  sz3@3.1.7
adios2@2.8.3           dealii@9.5.1           hdf5-vol-log@1.4.0         mpark-variant@1.4.0     pumi@2.2.8           tasmanian@8.0
aml@0.2.1              e4s-alc@1.0.1          heffte@2.4.0               mpifileutils@0.11.1     py-cinemasci@1.7.0   tau@2.33.2
aml@0.2.1              e4s-cl@1.0.3           heffte@2.4.0               nccmp@1.9.1.0           py-h5py@3.11.0       tau@2.33.2
amrex@24.04            ecp-data-vis-sdk@1.0   hpx@1.9.1                  nco@5.1.9               py-jupyterhub@1.4.1  trilinos@13.0.1
amrex@24.04            exago@1.6.0            hypre@2.31.0               nekbone@17.0            py-libensemble@1.2.2 trilinos@15.1.1
arborx@1.6             exaworks@0.1.0         intel-oneapi-mpi@2021.11.0 netcdf-fortran@4.6.1    py-petsc4py@3.21.0   turbine@1.3.0
arborx@1.6             faodel@1.2108.1        kokkos@4.3.00              netlib-scalapack@2.2.0  py-warpx@23.08       umap@2.1.0
argobots@1.2           flecsi@2.2.1           kokkos@4.3.00              nrm@0.1.0               qthreads@1.18        umpire@2024.02.0
ascent@0.8.0           flit@2.1.0             kokkos-kernels@4.3.00      omega-h@9.34.13         raja@2024.02.0       unifyfs@2.0
axom@0.9.0             flux-core@0.61.2       kokkos-kernels@4.3.00      openmpi@5.0.3           rempi@1.1.0          upcxx@2023.9.0
bolt@2.0               fortrilinos@2.3.0      laghos@3.1                 openpmd-api@0.15.2      scr@3.0.1            upcxx@2023.9.0
boost@1.84.0           gasnet@2023.9.0        lammps@20230802.3          papyrus@1.0.2           slate@2023.11.05     variorum@0.7.0
bricks@2023.08.25      ginkgo@1.7.0           lbann@0.104                parallel-netcdf@1.12.3  slate@2023.11.05     veloc@1.7
butterflypack@2.4.0    ginkgo@1.7.0           legion@24.03.0             paraview@5.12.0         slepc@3.21.0         vtk-m@1.7.1
cabana@0.6.0           globalarrays@5.8.2     libcatalyst@2.0.0-rc4      parsec@3.0.2209         stc@0.9.0            wannier90@3.1.0
cabana@0.6.0           glvis@4.2              libnrm@0.1.0               pdt@3.25.2              strumpack@7.2.0      xyce@7.8.0
caliper@2.10.0         gmp@6.2.1              libquo@1.4                 petsc@3.21.0            sundials@7.0.0       zfp@0.5.5
chai@2024.02.0         gotcha@1.0.6           libunwind@1.6.2            petsc@3.21.0            sundials@7.0.0
charliecloud@0.37      gptune@4.0.0           loki@0.1.7                 phist@1.12.0            superlu@5.3.0
conduit@0.9.1          gromacs@2024.1         mercury@2.3.1              plasma@23.8.2           superlu-dist@8.2.1
darshan-runtime@3.4.4  h5bench@1.4            metall@0.25                plumed@2.9.0            swig@4.0.2-fortran
darshan-util@3.4.4     hdf5-vol-async@1.7     mfem@4.6.0                 precice@3.1.1           sz@2.1.12.5
==> 135 installed packages
Singularity> which dpcpp
/opt/intel/oneapi/compiler/2024.0/bin/dpcpp
Singularity>
```

Use of Intel oneAPI BaseKit and HPCToolkit is subject to acceptance of Intel EULA by the user

E4S 24.05 Support for GPUs: Intel (modules)

```
$ singularity run e4s-24.05-oneapi-amd64.sif
Singularity> module avail

------------------------------------ /spack/share/spack/lmod/linux-ubuntu22.04-x86_64/intel-oneapi-mpi/2021.11.0-vmuf6bv/Core -------------------------------
   adios/1.13.1                       ginkgo/1.7.0-sycl-openmp (D)    nccmp/1.9.1.0                slate/2023.11.05-openmp
   amrex/24.04-sycl                   globalarrays/5.8.2              nco/5.1.9                    slate/2023.11.05-sycl-openmp (D)
   amrex/24.04                (D)     glvis/4.2                       nekbone/17.0                 slepc/3.21.0
   arborx/1.6-sycl                    gptune/4.0.0                    netcdf-fortran/4.6.1         stc/0.9.0
   arborx/1.6                 (D)     gromacs/2024.1-openmp           netlib-scalapack/2.2.0       strumpack/7.2.0-openmp
   axom/0.9.0-openmp                  h5bench/1.4                     omega-h/9.34.13              sundials/7.0.0-sycl
   boost/1.84.0                       hdf5-vol-async/1.7              openpmd-api/0.15.2           sundials/7.0.0               (D)
   bricks/2023.08.25                  hdf5-vol-cache/v1.1             papyrus/1.0.2                superlu-dist/8.2.1
   butterflypack/2.4.0-openmp         hdf5-vol-log/1.4.0              parsec/3.0.2209              tasmanian/8.0
   cabana/0.6.0-sycl                  heffte/2.4.0-sycl               petsc/3.21.0-sycl            tau/2.33.2-level-zero
   cabana/0.6.0               (D)     heffte/2.4.0             (D)    petsc/3.21.0          (D)    tau/2.33.2                   (D)
   caliper/2.10.0                     hpx/1.9.1                       phist/1.12.0-openmp          trilinos/13.0.1
   chai/2024.02.0                     hypre/2.31.0                    plumed/2.9.0                 trilinos/15.1.1              (D)
   conduit/0.9.1                      laghos/3.1                      precice/3.1.1                turbine/1.3.0
   datatransferkit/3.1.1              lammps/20230802.3-openmp        pruners-ninja/1.0.1          umpire/2024.02.0
   dealii/9.5.1                       lbann/0.104                     pumi/2.2.8                   upcxx/2023.9.0-level-zero
   ecp-data-vis-sdk/1.0               libnrm/0.1.0                    py-h5py/3.11.0               upcxx/2023.9.0               (D)
   exago/1.6.0                        libquo/1.4                      py-libensemble/1.2.2         wannier90/3.1.0
   exaworks/0.1.0                     mercury/2.3.1                   py-petsc4py/3.21.0           xyce/7.8.0
   flecsi/2.2.1                       metall/0.25                     py-warpx/23.08
   fortrilinos/2.3.0                  mfem/4.6.0                      rempi/1.1.0
   ginkgo/1.7.0-openmp                mpifileutils/0.11.1             scr/3.0.1

------------------------------------------------------- /spack/share/spack/lmod/linux-ubuntu22.04-x86_64/Core -------------------------------------------------------
   aml/0.2.1-level-zero       e4s-cl/1.0.3       intel-oneapi-mpi/2021.11.0   (L)    libunwind/1.6.2           papi/7.1.0             superlu/5.3.0
   aml/0.2.1           (D)    flit/2.1.0         kokkos-kernels/4.3.00-openmp        loki/0.1.7                pdt/3.25.2             swig/4.0.2-fortran
   argobots/1.2               flux-core/0.61.2   kokkos-kernels/4.3.00-sycl   (D)    mgard/2023-12-09-openmp   plasma/23.8.2          sz3/3.1.7
   bolt/2.0                   gasnet/2023.9.0    kokkos/4.3.00-openmp                mpark-variant/1.4.0       py-jupyterhub/1.4.1    umap/2.1.0
   charliecloud/0.37          gmp/6.2.1          kokkos/4.3.00-sycl-openmp    (D)    nrm/0.1.0                 qthreads/1.18          variorum/0.7.0
   e4s-alc/1.0.1              gotcha/1.0.6       legion/24.03.0                      openmpi/5.0.3             raja/2024.02.0

------------------------------------------------------------------ /opt/intel/oneapi/modulefiles -------------------------------------------------------------------
   advisor/latest                compiler32/latest             dpct/latest             intel_ipp_intel64/latest          mpi/latest
   advisor/2024.0         (D)    compiler32/2024.0.2    (D)    dpct/2024.0.0    (D)    intel_ipp_intel64/2021.10  (D)    mpi/2021.11      (L,D)
   ccl/latest                    dal/latest                    dpl/latest              intel_ippcp_intel64/latest        oclfpga/latest
   ccl/2021.11.2          (D)    dal/2024.0.0           (D)    dpl/2022.3       (D)    intel_ippcp_intel64/2021.9 (D)    oclfpga/2024.0.0 (D)
   compiler-rt/latest            debugger/latest               ifort/latest            itac/latest                       tbb/latest
   compiler-rt/2024.0.2   (D)    debugger/2024.0.0      (D)    ifort/2024.0.2   (D)    itac/2022.0               (D)     tbb/2021.11      (D)
   compiler-rt32/latest          dev-utilities/latest          ifort32/latest          mkl/latest                        vtune/latest
   compiler-rt32/2024.0.2 (D)    dev-utilities/2024.0.0 (D)    ifort32/2024.0.2 (D)    mkl/2024.0                (D)     vtune/2024.0     (D)
   compiler/latest               dnnl/latest                   inspector/latest        mkl32/latest
   compiler/2024.0.2      (D)    dnnl/3.3.0             (D)    inspector/2024.0 (D)    mkl32/2024.0              (D)

  Where:
   L:  Module is loaded
   D:  Default Module
```

Use of Intel oneAPI BaseKit and HPCToolkit is subject to acceptance of Intel EULA by the user

E4S 24.05 Support for GPUs: Intel Data Center GPU Max (aka PVC)

```
$ singularity run e4s-24.05-oneapi-amd64.sif
Singularity> clinfo -l
Platform #0: Intel(R) FPGA Emulation Platform for OpenCL(TM)
 `-- Device #0: Intel(R) FPGA Emulation Device
Platform #1: Intel(R) OpenCL
 `-- Device #0: Intel(R) Xeon(R) Silver 4410T
Platform #2: Intel(R) OpenCL Graphics
 `-- Device #0: Intel(R) Data Center GPU Max 1100
Singularity> spack find -dl heffte+sycl
-- linux-ubuntu22.04-x86_64 / oneapi@2024.0.2 --------------------
dkawent heffte@2.4.0
biswww4     cmake@3.27.9
r4maiir         curl@8.6.0
je4uymd             nghttp2@1.57.0
tjfjf56             openssl@3.2.1
3sifbb5                 ca-certificates-mozilla@2023-05-30
6xkucfz                 perl@5.38.0
x7anufu                     berkeley-db@18.1.40
uqtwnme                     bzip2@1.0.8
7akrhou                         diffutils@3.10
bg6qww5                     gdbm@1.23
5bu3onp                         readline@8.2
ua57skc             pkgconf@1.9.5
s45qlot         ncurses@6.4
ypemcku         zlib-ng@2.1.6
d6bcnaw     gmake@4.4.1
rzaojfz     intel-oneapi-mkl@2024.0.0
rfpr243         intel-tbb@2021.9.0
6ii2fwq             hwloc@2.9.1
zxupvhj                 libpciaccess@0.17
5a7ydse                     libtool@2.4.7
s4zav25                         findutils@4.9.0
wdc4qnd                         m4@1.4.19
fcw37kn                             libsigsegv@2.14
if4y4n2                     util-macros@1.19.3
tgjrkey                 libxml2@2.10.3
khmhytm                     libiconv@1.17
36cbr64                     xz@5.4.6
vmuf6bv     intel-oneapi-mpi@2021.11.0
flx6gxx     intel-oneapi-runtime@2024.0.2
6cqtdnc         gcc-runtime@11.4.0

==> 1 installed package
Singularity>
```

E4S 24.05 packages in oneAPI containers are now built with Intel compilers with Intel MPI

24.05 Release: 129+ Official Products + dependencies (gcc, ppc64le)

```
 1:  adios2              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/adios2-2.10.0-4mywyu6vlmtzbxbcwgv3nujuigmjb3tq
 2:  alquimia            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/alquimia-1.1.0-yrlpkjk3duxcvdjpks7kat3u35dsnqsg
 3:  aml                 /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/aml-0.2.1-edhdhhxpsn72i7ofsm2pbqjimmrorsbp
 4:  amrex               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/amrex-24.04-bwleaeu5zpcnzyrfviphfmopmvax5rmv
 5:  arborx              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/arborx-1.6-5b36lowtoilu2ybfwtcgzro5eyd3rnzg
 6:  argobots            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/argobots-1.2-cjgy6obofkgafnwsip76yfbbpeay6q6q
 7:  ascent              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/ascent-0.9.2-wj5omuuqmprkb7dpsnlvgnactjq57jbk
 8:  axom                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/axom-0.9.0-bhmt6aumzlkhtn4bbpng3dlpaam454am
 9:  bolt                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/bolt-2.0-hicd2qb5hhsd6hj3tmkkzkobtkmeuh2p
10:  blaspp              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/blaspp-2023.11.05-6qt76nm5das63yqzvw4gwqpkwvojw62j
11:  bricks              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/bricks-2023.08.25-rr4l3jiaiywhpb6hyzcp2bbqgnxns243
12:  butterflypack       /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/butterflypack-2.4.0-m2xskltwx6ozcuh5gzdvt5fbpiskmq5h
13:  cabana              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/cabana-0.6.0-t4o4rifcz6vg7l4o64wix2u4criezvtx
14:  caliper             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/caliper-2.10.0-tcwrtpxnfvmlcatmukmlj2qgswgis2yj
15:  camp                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/camp-2024.02.0-hizqxenz3rfcba7ban53nxhtl3xtf3eb
16:  chai                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/chai-2024.02.0-gca7wviucemmenptd2tlhpw3f2m5h6sf
17:  charliecloud        /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/charliecloud-0.37-ciit4l5dfobqxsmwdxsrjqvsuego77fw
18:  conduit             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/conduit-0.9.1-jyq2cfw6yubjd4epfm2rjz75gluvlt2g
19:  cp2k                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/cp2k-2024.1-bpgb2kq3xinl25pj7dz4hv4vyprjj7nf
20:  cusz                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/cusz-0.3.1-lav7dlxpjkm7ghhunwm3j3ttdvghgm7l
21:  darshan-runtime     /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/darshan-runtime-3.4.4-icj7mpijxjr6bb3jodjggxm4b26p3zgi
22:  datatransferkit     /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/datatransferkit-3.1.1-kyyx2fqideedc2xcnl4q2gkol2gdfobw
23:  dyninst             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/dyninst-13.0.0-ir3mzxecf5oy6cax73eguc3wakru5rwn
24:  e4s-alc             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/e4s-alc-1.0.1-sr7ms5he5qskkk5d4di5w5catg5vdr3q
25:  e4s-cl              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/e4s-cl-1.0.3-axwr3nbv6fqpynq2m27gua3wnmkf47fr
26:  ecp-data-vis-sdk    /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/ecp-data-vis-sdk-1.0-hw5q2rqqtdyxw467jlrgx6wsdj7hcwrc
27:  exago               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/exago-1.6.0-yjrebei5otf7a6tpohjycr7t3a5vrokw
28:  exaworks            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/exaworks-0.1.0-cnjtbt4fvscmgus5nnhh6wirdq2lxq7r
29:  faodel              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/faodel-1.2108.1-ur7lcltn3od3ujnx5gjdfhtd7fjaflfg
30:  flecsi              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/flecsi-2.2.1-jkqf4nklyeb5pyxjfwr4msgqqhhcg62u
31:  flit                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/flit-2.1.0-pgpjuv4xcuudo4b72en7dknnvdkjnusy
32:  flux-core           /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/flux-core-0.61.2-uqggildy4da6acaohij4jybgj6zuaico
33:  flux-sched          /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/flux-sched-0.33.1-q6nr6hh453qwgba3qidr37vkt7gk2ace
34:  fortrilinos         /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/fortrilinos-2.3.0-lkg57u7lflggx2umgw4g3vbz7edogl6m
35:  gasnet              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/gasnet-2023.9.0-vlx5a2s453ll5isj3w3yen6e6b2djd4y
36:  ginkgo              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/ginkgo-1.7.0-u5cyewkyz26l7gz6vxp7jy2g25q4gtel
37:  globalarrays        /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/globalarrays-5.8.2-yhfh7qpapucntwvtvyrlmz2puznfbwxu
38:  gotcha              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/gotcha-1.0.6-p5u2dmwm77x4ahrdbnpaviudu2znsixn
39:  gptune              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/gptune-4.0.0-qktwtnxi33adkuilcjphwqu46245f2yg
40:  gromacs             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/gromacs-2024.1-u4evhzqw7vvdw5h4lee57ixdmdnw3f64
41:  h5bench             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/h5bench-1.4-psbgg5epibb63bub6tdlqpmzxulyjrwa
42:  hdf5                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hdf5-1.14.3-uj64b2jsywkmojwgildwyhzuz7qsr2uj
43:  hdf5-vol-cache      /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hdf5-vol-cache-v1.1-kkqkpxxwwql2wlhkkdwewone6i6j3ob6
```

GPU runtimes for IBM Power
- CUDA 12.3
- NVHPC 24.3

Languages
- Julia with MPI and CUDA
- Python
- Rust

EDA Tools
- Xyce

CFD Tools
- OpenFOAM
- Nek5000

AI packages for NVIDIA GPU
- TensorFlow
- PyTorch
- LBANN

PESO

24.05 Release: 129+ Official Products + dependencies (gcc, ppc64le)

```
44:  hdf5-vol-async   /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hdf5-vol-async-1.7-rphrjjaaimhkkq3exdlijxzev5lzjqrc
45:  hdf5-vol-log     /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hdf5-vol-log-1.4.0-vzznu6hwc23psnw6ou5outp4hot3ji2p
46:  heffte           /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/heffte-2.4.0-rhu5c2refev3kvurytrvhaino7x7imej
47:  hiop             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hiop-1.0.0-ih4gsmzzsqm64tignzp4fhvcvarpqpkx
48:  hpctoolkit       /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hpctoolkit-2024.01.1-g35avbvbj3jgbvillhs4mg5x7wdf5x26
49:  hpx              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hpx-1.9.1-erambaukxm2hteguyetd5yzxtkppbhn
50:  hypre            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hypre-2.31.0-ezvr6ifagf3g7ufweqc5c2vlyzkga63b
51:  kokkos           /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/kokkos-4.3.00-uu37sanqg7d2cyfssrelv4bgttk6d7tq
52:  kokkos-kernels   /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/kokkos-kernels-4.3.00-5dyqjybokzb7wiazn2s3g52hvv7365kj
53:  laghos           /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/laghos-3.1-sfyrigwy5536gm52y2kk5gcwmflitfon
54:  lammps           /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/lammps-20230802.3-z4yryzdnkbxpp7ytfb3zvffhz6c3qron
55:  lapackpp         /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/lapackpp-2023.11.05-xpwxq6rkmlqvzgroria4vpjblv5myjzj
56:  lbann            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/lbann-0.104-l2pryljak27256xnnihbd3wnhta6yk7y
57:  legion           /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/legion-24.03.0-pot5up5muaf3y3e7j4uayp4v3vo7h6e6
58:  libcatalyst      /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/libcatalyst-2.0.0-rc4-wg3z6wnrtwh47hnmlva6duj5hbac3zpe
59:  libnrm           /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/libnrm-0.1.0-47xh46x5ml2v4vp55mdi67qcbl3nj3xr
60:  libpressio       /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/libpressio-0.95.1-hjgiot6whwkawchjktfeq43dzi3ghsca
61:  libquo           /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/libquo-1.4-cdeiq3wetcnanqlmok7duteln6wp4kqa
62:  loki             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/loki-0.1.7-dwwe6amjkamkklltgsa5r55gbvei3fsnm
63:  magma            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/magma-2.8.0-o5u5szok4n7n7gdn4n54tf36u76x5bgj
64:  mercury          /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mercury-2.3.1-xvsbytg7t367b3tb7gjq7tnlm3otsedy
65:  metall           /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/metall-0.25-5iivbjyqjpvowr6l7sx73xnbth3dphuo
66:  mfem             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mfem-4.6.0-t6jbf3uw36tllgeqbcx2xtphukdv2nw2
67:  mgard            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mgard-2023-12-09-4ee5l7b2ncfkqrftdeeg45wp4qadwi53
68:  mpark-variant    /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mpark-variant-1.4.0-sei3mwwvskd4lfbywt42uif3gg37rhzw
69:  mpich            /usr/local/mpich/install/mpich
70:  mpifileutils     /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mpifileutils-0.11.1-tcraj652kgyjsfch7ungznxan5ygyvpx
71:  nccmp            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/nccmp-1.9.1.0-5yevvifo4f5jusyabvbqb4joei3oplqx
72:  nco              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/nco-5.1.9-5oolyi3l7uvrno6oq2dznbpx6rqidkz7
73:  netcdf-c         /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/netcdf-c-4.9.2-q2ccrgfelps5slzjjto2l5lglguk2hhl
74:  nek5000          /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/nek5000-19.0-ps5q5hqavhycikq5sroqdjcvulhcd5vh
75:  nekbone          /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/nekbone-17.0-4vmrblchieq46b7dousyuwhb4nig24c5
76:  netcdf-fortran   /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/netcdf-fortran-4.6.1-qejpcvcjjvdtmwreqyjuhnxwy524cfvv
77:  netlib-scalapack /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/netlib-scalapack-2.2.0-cicbt5pm7gnnpkqff6p443msaljvzv35
78:  nrm              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/nrm-0.1.0-nzpf55v4ueubh32edllbjd5qvfpsz5by
79:  omega-h          /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/omega-h-9.34.13-5zcdzuo3rqummrto56ee572dygn6incn
80:  openfoam         /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/openfoam-2312-g46ccuoauusyfllgjafiqkp7n5xcuuir
81:  openmpi          /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/openmpi-5.0.3-h5hjbaickcuuhqtd2uyxnhzhtg3nhiac
82:  openpmd-api      /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/openpmd-api-0.15.2-r4qx34xrjkev72aj25ffiejndfztaanv
83:  papi             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/papi-7.1.0-6hakrvhuqhrytlrtecv7f2xrjuc4p5qh
84:  papyrus          /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/papyrus-1.0.2-grgwkvgyt5fdj4hne6if3atmerrgrqbk
85:  parallel-netcdf  /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/parallel-netcdf-1.12.3-653gdk6izl5edfk4ysp4sjz2qhyfd7zs
86:  paraview         /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/paraview-5.12.0-vr5g7q2jlwo55nsjoh7rrijexynng74p
```

PESO

24.05 Release: 129+ Official Products + dependencies (gcc, ppc64le)

```
  87:  parsec              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/parsec-3.0.2209-twturaln4d77hdqf64ofunuu56piwibk
  88:  pdt                 /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/pdt-3.25.2-2n2lhyvn3nm2y2vowqmlj2673dutwctw
  89:  petsc               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/petsc-3.21.0-qxn7tpehgwooi522petq5wxzdxaufhfg
  90:  plasma              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/plasma-23.8.2-cao4i4s5672kifhbpup6xwgi52mis7ob
  91:  plumed              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/plumed-2.9.0-qxcydzenow7kbomzxj5fxyk3b2xwrqai
  92:  precice             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/precice-3.1.1-bfrw5vq7a3kqb35gzxvlzoptbwqzoc2z
  93:  pruners-ninja       /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/pruners-ninja-1.0.1-dxhdaubpsx2d5mmmccq65b2d3c6puudi
  94:  pumi                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/pumi-2.2.8-udnmla2lqh42zbdn6qghou6cemkh4n4i
  95:  py-cinemasci        /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-cinemasci-1.3-bf32tfxe2noymbryi75la2ucji3mlgnj
  96:  py-deephyper        /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-deephyper-0.6.0-lfitvur3t3w6xvdw7nxjlusubj7zefuj
  97:  py-jupyterhub       /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-jupyterhub-1.4.1-2umgloyedcacxbxqrzajrvrkk2yb7vrr
  98:  py-libensemble      /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-libensemble-1.2.2-stqjpms2zjbrc3kr6du3u3qobnvlxvbs
  99:  py-parsl            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-parsl-2023.08.21-vvrbwbgthdhxlziwmw75uwjs4vmf2zo7
 100:  py-radical-saga     /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-radical-saga-1.47.0-gdf2x57uw6d6ed3g4limwuwvtmfu2sg6
 101:  qthreads            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/qthreads-1.18-5vyo4usqqs4xchanya53x35bkbjn432i
 102:  quantum-espresso    /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/quantum-espresso-7.3.1-tr5u7ypte5wvmv3quttqoxqhrn4kdhej
 103:  raja                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/raja-2024.02.0-emku4lhtf7kmwkuv4h3nqu67f5bwvnh2
 104:  rempi               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/rempi-1.1.0-g7khmsbho6hgcskvekirusznufbykovd
 105:  scr                 /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/scr-3.0.1-ck7ty6dfpfegyfac34o2mjqfv4x23bid
 106:  slate               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/slate-2023.11.05-o5amlujl2hflttmmewz5nvxif3oe74wj
 107:  slepc               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/slepc-3.21.0-hpxryrwxb2bkdkrawcm4h6ke5mpdwqtr
 108:  stc                 /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/stc-0.9.0-rksccd5aak46xbou3uznfwwlxx2wgcjq
 109:  strumpack           /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/strumpack-7.2.0-7timxa4warrhedcyfkq2bta2gnyf4lym
 110:  sundials            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/sundials-7.0.0-fayjxrppzaz2moyvakwmioimjrupyxzs
 111:  superlu-dist        /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/superlu-dist-8.2.1-y7idnksf47vqgyolauq6o4s44zqbslbq
 112:  swig                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/swig-4.1.1-j5tfvxplktjzzrm2kthhvhm3f7uibiu7
 113:  sz                  /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/sz-2.1.12.5-2xyh5o7acpyqyixkwlpula6pyri3vno5
 114:  sz3                 /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/sz3-3.1.7-wvgazrocefekek7rfureaw7wydxkkjd7
 115:  tasmanian           /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/tasmanian-8.0-35x3bervcakfor3qk53rd3v2b3bolsyq
 116:  tau                 /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/tau-2.33.2-egc365hvetw246c7a2gv5qr2nfg4vdkr
 117:  trilinos            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/trilinos-15.1.1-ta5ituxhngh3t34ucn5m3gqcnho67k5v
 118:  turbine             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/turbine-1.3.0-jmwoarv4odjqymvmmvuowg3szhay6fdx
 119:  umap                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/umap-2.1.0-tc6dxxesbekx4ma7qatziycgku2flziu
 120:  umpire              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/umpire-2024.02.0-5pcmc3ktm2anz52qdvkhuhqcxmfrx5i2
 121:  unifyfs             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/unifyfs-2.0-3uqqozjnt4xekmnmj5vzmvfom74y6gbc
 122:  upcxx               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/upcxx-2023.9.0-gnr7mpf4fvhe5e3pkgn4eibf2lxsbrwd
 123:  veloc               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/veloc-1.7-vpu5p6qwmkkd2ooofmked65a65ewnbcp
 124:  visit               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/visit-3.3.3-jctbqnhkzclzehwnubcz6fomaxfnv7xa
 125:  vtk-m               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/vtk-m-2.1.0-nubx22k6jgf2tsv75csote3unig6khzb
 126:  wannier90           /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/wannier90-3.1.0-5rdgw6ole66arwuzzaxsnxg4qppyxtaj
 127:  warpx               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/warpx-23.08-bn5c5ovcjddfa6smplo6wikxmng5grcj
 128:  xyce                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/xyce-7.8.0-gm35vkgbdciou2cpv6tp5etraprqq7vm
 129:  zfp                 /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/zfp-1.0.0-jvxcpqnzitfatcsu4rf25sgqcelzma73
```

Supports
IBM Power10 and
Power 9 processors

PESO

E4S 24.05 Support for GPUs: NVIDIA CUDA on IBM ppc64le

```
$ singularity run --nv e4s-24.05-cuda70-ppc64.sif
Singularity> spack find -x +cuda
-- linux-ubuntu20.04-ppc64le / gcc@9.4.0 ------------------------
adios2@2.10.0      caliper@2.10.0      flux-core@0.61.2      hypre@2.31.0          magma@2.8.0       parsec@3.0.2209   sundials@7.0.0      vtk-m@2.1.0
amrex@24.04        chai@2024.02.0      ginkgo@1.7.0          kokkos@4.3.00         mfem@4.6.0        petsc@3.21.0      superlu-dist@8.2.1  zfp@0.5.5
arborx@1.6         cusz@0.3.1          gromacs@2024.1        kokkos-kernels@4.3.00 mgard@2023-12-09  raja@2024.02.0    tasmanian@8.0
axom@0.9.0         ecp-data-vis-sdk@1.0 heffte@2.4.0         lammps@20230802.3     omega-h@9.34.13   slate@2023.11.05  tau@2.33.2
bricks@2023.08.25  exago@1.6.0          hpctoolkit@2024.01.1  lbann@0.104           papi@7.1.0        slepc@3.21.0      umpire@2024.02.0
cabana@0.6.0       flecsi@2.2.1        hpx@1.9.1             legion@24.03.0        paraview@5.12.0   strumpack@7.2.0   upcxx@2023.9.0
==> 44 installed packages
Singularity> spack find -x
-- linux-ubuntu20.04-ppc64le / gcc@9.4.0 ------------------------
adios@1.13.1          cp2k@2024.1             glvis@4.2              lammps@20230802.3      netcdf-fortran@4.6.1   py-deephyper@0.6.0      sz3@3.1.7
adios2@2.7.1          cuda@11.4.4             gmp@6.2.1              lammps@20230802.3      netlib-scalapack@2.2.0 py-h5py@3.11.0          tasmanian@8.0
adios2@2.10.0         cusz@0.3.1              gotcha@1.0.6           lbann@0.104            nrm@0.1.0              py-jupyterhub@1.4.1     tasmanian@8.0
alquimia@1.1.0        darshan-runtime@3.4.4   gptune@4.0.0           lbann@0.104            nvhpc@24.1             py-libensemble@1.2.2    tau@2.33.2
aml@0.2.1             darshan-util@3.4.4      gromacs@2024.1         legion@24.03.0         omega-h@9.34.13        py-petsc4py@3.21.0      tau@2.33.2
amrex@24.04           datatransferkit@3.1.1   gromacs@2024.1         legion@24.03.0         omega-h@9.34.13        py-warpx@23.08          trilinos@13.0.1
amrex@24.04           dyninst@13.0.0          h5bench@1.4            libcatalyst@2.0.0-rc4  openfoam@2312          qthreads@1.18           trilinos@15.1.1
arborx@1.6            e4s-alc@1.0.1           hdf5@1.12.3            libnrm@0.1.0           openmpi@5.0.3          quantum-espresso@7.3.1  turbine@1.3.0
arborx@1.6            e4s-cl@1.0.3            hdf5@1.14.3            libpressio@0.95.1      openpmd-api@0.15.2     raja@2024.02.0          umap@2.1.0
argobots@1.2          ecp-data-vis-sdk@1.0    hdf5-vol-async@1.7     libquo@1.4             papi@7.1.0             raja@2024.02.0          umpire@2024.02.0
ascent@0.9.2          ecp-data-vis-sdk@1.0    hdf5-vol-cache@v1.1    libunwind@1.6.2        papi@7.1.0             rempi@1.1.0             umpire@2024.02.0
axom@0.9.0            exago@1.6.0             hdf5-vol-log@1.4.0     loki@0.1.7             papyrus@1.0.2          scr@3.0.1               unifyfs@2.0
axom@0.9.0            exago@1.6.0             hdf5-vol-log@1.4.0     magma@2.8.0            parallel-netcdf@1.12.3 slate@2023.11.05        upcxx@2023.9.0
bolt@2.0              exaworks@0.1.0          heffte@2.4.0           mercury@2.3.1          paraview@5.12.0        slate@2023.11.05        upcxx@2023.9.0
boost@1.84.0          faodel@1.2108.1         heffte@2.4.0           metall@0.25            paraview@5.12.0        slepc@3.21.0            veloc@1.7
bricks@2023.08.25     flecsi@2.2.1            hpctoolkit@2024.01.1   mfem@4.6.0             parsec@3.0.2209        slepc@3.21.0            visit@3.3.3
bricks@2023.08.25     flecsi@2.2.1            hpctoolkit@2024.01.1   mfem@4.6.0             parsec@3.0.2209        stc@0.9.0               vtk-m@2.0.0
butterflypack@2.4.0   flit@2.1.0              hpx@1.9.1              mgard@2023-12-09       pdt@3.25.2             strumpack@7.2.0         vtk-m@2.1.0
cabana@0.6.0          flux-core@0.61.2        hpx@1.9.1              mgard@2023-12-09       petsc@3.21.0           strumpack@7.2.0         wannier90@3.1.0
cabana@0.6.0          flux-core@0.61.2        hypre@2.31.0           mpark-variant@1.4.0    petsc@3.21.0           sundials@7.0.0          xyce@7.8.0
caliper@2.10.0        fortrilinos@2.3.0       hypre@2.31.0           mpich@4.1.2            plasma@23.8.2          sundials@7.0.0          zfp@0.5.5
caliper@2.10.0        fpm@0.10.0              kokkos@4.3.00          mpifileutils@0.11.1    plumed@2.9.0           superlu@5.3.0           zfp@0.5.5
chai@2024.02.0        gasnet@2023.9.0         kokkos@4.3.00          nccmp@1.9.1.0          precice@3.1.1          superlu-dist@8.2.1
chai@2024.02.0        ginkgo@1.7.0            kokkos-kernels@4.3.00  nco@5.1.9              pruners-ninja@1.0.1    superlu-dist@8.2.1
charliecloud@0.37     ginkgo@1.7.0            kokkos-kernels@4.3.00  nek5000@19.0           pumi@2.2.8             swig@4.0.2-fortran
conduit@0.9.1         globalarrays@5.8.2      laghos@3.1             nekbone@17.0           py-cinemasci@1.3       sz@2.1.12.5
==> 178 installed packages
Singularity>
```

E4S 24.05 Support for GPUs: NVIDIA CUDA on ppc64le (modules)

```
$ singularity run --nv e4s-24.05-cuda70-ppc64.sif
Singularity> module avail

------------------------------------------ /spack/share/spack/lmod/linux-ubuntu20.04-ppc64le/mpich/4.1.2-nysjgwr/Core ------------------------------------
   adios/1.13.1                       flecsi/2.2.1                    (D)    mercury/2.3.1                      rempi/1.1.0
   adios2/2.7.1                       fortrilinos/2.3.0                      metall/0.25                        scr/3.0.1
   adios2/2.10.0-cuda70        (D)    ginkgo/1.7.0-cuda70-openmp             mfem/4.6.0-cuda70                  slate/2023.11.05-cuda70-openmp
   alquimia/1.1.0                     ginkgo/1.7.0-openmp             (D)    mfem/4.6.0                 (D)     slate/2023.11.05-openmp     (D)
   amrex/24.04-cuda70                 globalarrays/5.8.2                     mpifileutils/0.11.1                slepc/3.21.0-cuda70
   amrex/24.04                 (D)    glvis/4.2                              nccmp/1.9.1.0                      slepc/3.21.0                (D)
   arborx/1.6-cuda70                  gptune/4.0.0                           nco/5.1.9                          stc/0.9.0
   arborx/1.6                  (D)    gromacs/2024.1-cuda70-openmp           nek5000/19.0                       strumpack/7.2.0-cuda70-openmp
   ascent/0.9.2-openmp                gromacs/2024.1-openmp           (D)    nekbone/17.0                       strumpack/7.2.0-openmp      (D)
   axom/0.9.0-cuda70-openmp           h5bench/1.4                            netcdf-fortran/4.6.1               sundials/7.0.0-cuda70
   axom/0.9.0-openmp           (D)    hdf5-vol-async/1.7                     netlib-scalapack/2.2.0             sundials/7.0.0              (D)
   boost/1.84.0                       hdf5-vol-cache/v1.1                    omega-h/9.34.13-cuda70             superlu-dist/8.2.1-cuda70
   bricks/2023.08.25-cuda             hdf5-vol-log/1.4.0-threadsafe          omega-h/9.34.13             (D)    superlu-dist/8.2.1          (D)
   bricks/2023.08.25           (D)    hdf5-vol-log/1.4.0              (D)    openfoam/2312                      sz/2.1.12.5
   butterflypack/2.4.0-openmp         hdf5/1.12.3                            openpmd-api/0.15.2                 tasmanian/8.0-cuda70
   cabana/0.6.0-cuda70                hdf5/1.14.3                     (D)    papyrus/1.0.2                      tasmanian/8.0               (D)
   cabana/0.6.0                (D)    heffte/2.4.0-cuda70                    parallel-netcdf/1.12.3             tau/2.33.2-cuda
   caliper/2.10.0-cuda70              heffte/2.4.0                    (D)    paraview/5.12.0-cuda70             tau/2.33.2                  (D)
   caliper/2.10.0              (D)    hpctoolkit/2024.01.1-cuda              paraview/5.12.0             (D)    trilinos/13.0.1
   chai/2024.02.0-cuda70              hpctoolkit/2024.01.1            (D)    parsec/3.0.2209-cuda70             trilinos/15.1.1             (D)
   chai/2024.02.0              (D)    hpx/1.9.1-cuda70                       parsec/3.0.2209             (D)    turbine/1.3.0
   conduit/0.9.1                      hpx/1.9.1                       (D)    petsc/3.21.0-cuda70                umpire/2024.02.0-cuda70
   cp2k/2024.1-openmp                 hypre/2.31.0-cuda70                    petsc/3.21.0                (D)    umpire/2024.02.0            (D)
   darshan-runtime/3.4.4              hypre/2.31.0                    (D)    plumed/2.9.0                       unifyfs/2.0
   datatransferkit/3.1.1              laghos/3.1                             precice/3.1.1                      upcxx/2023.9.0-cuda70
   dyninst/13.0.0-openmp              lammps/20230802.3-cuda70-openmp        pruners-ninja/1.0.1                upcxx/2023.9.0              (D)
   ecp-data-vis-sdk/1.0-cuda70        lammps/20230802.3-openmp        (D)    pumi/2.2.8                         veloc/1.7
   ecp-data-vis-sdk/1.0        (D)    lbann/0.104-cuda70                     py-cinemasci/1.3                   visit/3.3.3
   exago/1.6.0-cuda70                 lbann/0.104                     (D)    py-h5py/3.11.0                     vtk-m/2.0.0-openmp
   exago/1.6.0                 (D)    libcatalyst/2.0.0-rc4                  py-libensemble/1.2.2               vtk-m/2.1.0-cuda70-openmp   (D)
   exaworks/0.1.0                     libnrm/0.1.0                           py-petsc4py/3.21.0                 wannier90/3.1.0
   faodel/1.2108.1                    libpressio/0.95.1-openmp               py-warpx/23.08                     xyce/7.8.0
   flecsi/2.2.1-cuda70                libquo/1.4                             quantum-espresso/7.3.1-openmp

------------------------------------------------------ /spack/share/spack/lmod/linux-ubuntu20.04-ppc64le/Core -------------------------------------------
   aml/0.2.1              flux-core/0.61.2-cuda                legion/24.03.0-cuda70                nvhpc/24.1                   raja/2024.02.0     (D)
   argobots/1.2           flux-core/0.61.2             (D)     legion/24.03.0               (D)     openmpi/5.0.3                superlu/5.3.0
   bolt/2.0               fpm/0.10.0-openmp                    libunwind/1.6.2                      papi/7.1.0-cuda              swig/4.0.2-fortran
   charliecloud/0.37      gasnet/2023.9.0                      loki/0.1.7                           papi/7.1.0            (D)    sz3/3.1.7
   cuda/11.4.4            gmp/6.2.1                            magma/2.8.0-cuda70                   pdt/3.25.2                   umap/2.1.0
   cusz/0.3.1-cuda70      gotcha/1.0.6                         mgard/2023-12-09-cuda70-openmp       plasma/23.8.2                zfp/0.5.5-cuda70
   darshan-util/3.4.4     kokkos-kernels/4.3.00-cuda70         mgard/2023-12-09-openmp      (D)     py-deephyper/0.6.0           zfp/0.5.5          (D)
   e4s-alc/1.0.1          kokkos-kernels/4.3.00-openmp (D)     mpark-variant/1.4.0                  py-jupyterhub/1.4.1
   e4s-cl/1.0.3           kokkos/4.3.00-cuda70                 mpich/4.1.2                  (L)     qthreads/1.18
   flit/2.1.0             kokkos/4.3.00-openmp         (D)     nrm/0.1.0                            raja/2024.02.0-cuda70

  Where:
   L:  Module is loaded
```

24.05 Release: 129+ Official Products + dependencies (gcc, aarch64)

1:	adios2	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/adios2-2.10.0-6ghcc63h22rquuf4nx6tt54mauu2ixro
2:	alquimia	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/alquimia-1.1.0-gvg6hbzzzvjf3av2ojirvcs4l2gnvmz5
3:	aml	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/aml-0.2.1-5ikenqjgopmm57bwbhdupm66dbh6rf47
4:	amrex	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/amrex-24.04-mvddhhwf7trh4tfcb5moh563egz3e5cs
5:	arborx	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/arborx-1.6-caj5jdiw62ozuuc4e3syxhaqnw4mk4je
6:	argobots	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/argobots-1.2-vbc2lyssji6a2visay3rldt2bkkimasc
7:	ascent	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/ascent-0.9.2-gpofjh6z42zehtzhx4ynunsn6xg2tpwd
8:	axom	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/axom-0.9.0-uuleud4nc3lvlbystoa7o5wv7beomk75
9:	bolt	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/bolt-2.0-2r42gybfzpola3w6ovuuao7soy67kp4q
10:	blaspp	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/blaspp-2023.11.05-f55qetuxxzixfobftmrmhb3hq6dhr5mt
11:	butterflypack	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/butterflypack-2.4.0-d7ab5yd3xengbeybs5tash3xgef22zdq
12:	cabana	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/cabana-0.6.0-gjppai6hg2ff3cxbwwp6m6vodwhvgcz3
13:	caliper	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/caliper-2.10.0-sdiesyq2qbvogxeus5y4fuu3vvxvyur3
14:	camp	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/camp-2024.02.0-3mtlbtdjlfbg67sbtx4o3ortd5r6f627
15:	chai	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/chai-2024.02.0-u2yq6ypb7unkdine2ezukiqvnlzbbtif
16:	charliecloud	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/charliecloud-0.37-mciysr4it6aopbfctf3at672do4fjn53
17:	conduit	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/conduit-0.9.1-ym22iakg77tiysk4rnkpt3bp2ak7m6k4
18:	cp2k	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/cp2k-2024.1-jmtia5cqi6wzxyoivyyummzarcaty5yv
19:	cusz	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/cusz-0.3.1-tlld3auwun5dpbtphovlfnmhk5iqmhug
20:	darshan-runtime	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/darshan-runtime-3.4.4-emr4ohzzm5x6z4tetcijtyqgtgbrtbb4
21:	datatransferkit	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/datatransferkit-3.1.1-qvezooq4jdrvpwlrbdhxobeirbmzcm6u
22:	dealii	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/dealii-9.5.1-eiohdqkvildybne5wmla67qrmlhwgkty
23:	dyninst	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/dyninst-13.0.0-4z3n5gysh3tmx2alhpyucjdx7wfh2gzl
24:	e4s-alc	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/e4s-alc-1.0.1-3ev7dh6ka3hypewqrlkdcke2i5e3pqyn
25:	e4s-cl	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/e4s-cl-1.0.3-3etccdyighe7id7plgxan4xojlygg4mi
26:	ecp-data-vis-sdk	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/ecp-data-vis-sdk-1.0-dhbsnnadpsk42ryapqfjgazqkywzfmux
27:	exago	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/exago-1.6.0-2ml5o6mw6bwbnlruo467sx6ddctu3jex
28:	exaworks	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/exaworks-0.1.0-besrojhvmzazyw5dovrazwbj6dv7o2wm
29:	faodel	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/faodel-1.2108.1-fkp5y563leot4bhysuavl7d53amu6il4
30:	flecsi	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/flecsi-2.2.1-j4q3br4qfpld4hs3tsxiw2li4k2knivz
31:	flit	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/flit-2.1.0-2lv57j4ld4obabdo4hullhvws4ytjjhu
32:	flux-core	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/flux-core-0.61.2-ajft6dpvm33obtng6lejkyjayl74nvvv
33:	flux-sched	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/flux-sched-0.33.1-4iw6tf53o2dr6zqhwc46mtfmsqnmkxc6
34:	fortrilinos	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/fortrilinos-2.3.0-q4ymfaepxmumkbaehnsew4xs276u63g5
35:	gasnet	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/gasnet-2023.9.0-xiwypzsal5d2tpad35qepd7mp4muqlns
36:	ginkgo	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/ginkgo-1.7.0-ci6owbjpwvlotsi2zvdufy2whedakh4g
37:	globalarrays	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/globalarrays-5.8.2-6ir4fzlkkavggncstkdj4yq6idi4hfps
38:	gotcha	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/gotcha-1.0.6-vfxjvwkfrb3kht356vyzqkcjhqoimoit
39:	gptune	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/gptune-4.0.0-qno43tcmumpsinjydqpjkddpqfdp725g
40:	gromacs	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/gromacs-2024.1-sejgfwcsj5w2wkrj6mppgnwh47dh47my
41:	h5bench	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/h5bench-1.4-a5rulvpvng2x4hsvvg7afapsq6scc7l4
42:	hdf5	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/hdf5-1.14.3-a5jhlbotlwlok7emxegh2n3rlo5bbi2u
43:	hdf5-vol-cache	/spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/hdf5-vol-cache-v1.1-aojtklybnn7brnrcpu53bkpvbm7aem5b

GPU runtimes for aarch64
- CUDA 12.3
- NVHPC 24.3

Languages
- Julia with MPI and CUDA
- Rust
- Python

EDA
- Xyce

AI packages for NVIDIA GPU
- TensorFlow
- Torchbraid
- PyTorch
- JAX
- Horovod
- LBANN

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24.05 Release: 129+ Official Products + dependencies (gcc, aarch64)

```
44:  hdf5-vol-async     /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/hdf5-vol-async-1.7-j3f4uaydqckpj5hdg6i2b44t5s3yufdo
45:  hdf5-vol-log       /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/hdf5-vol-log-1.4.0-eizpsgpmueskeqbl25a2slmu5sq2deqe
46:  heffte             /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/heffte-2.4.0-wgtw2comz7mqhjbop5wrbnqdhl7zxbok
47:  hiop               /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/hiop-1.0.0-hz42rs5mgagel46dnqkmrukwcs25msyq
48:  hpctoolkit         /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/hpctoolkit-2024.01.1-jowellvzehjlubxlh6qmknp6xluffpul
49:  hpx                /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/hpx-1.9.1-uszuanwdmr7ow3xzgz6dnva3xonsocph
50:  hypre              /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/hypre-2.31.0-2f4bdwlvqz2muy47b2z4v6n3pu4ysr4s
51:  kokkos             /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/kokkos-4.3.00-27nigksrtxrz32ryotzjcrz24xfiuy5t
52:  kokkos-kernels     /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/kokkos-kernels-4.3.00-afyzbhfh6phlg4rslkksne4todflpcuy
53:  laghos             /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/laghos-3.1-uycaf35oe2qp2ckzfiba6pazttrjyxfs
54:  lammps             /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/lammps-20230802.3-bhu4p32awwnr6efdeiusk27en2e5yclv
55:  lapackpp           /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/lapackpp-2023.11.05-y2qponsen5xua24bolyqctquutdkv3u4
56:  lbann              /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/lbann-0.104-qzuhlqxtcf7gwysxdu4wvmfjaziaxqns
57:  legion             /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/legion-24.03.0-7ehhdi2gids5hipahw5bbn624gvzaefj
58:  libcatalyst        /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/libcatalyst-2.0.0-rc4-t2rlrfpuxhpvpes2tpjlch3txsvuyoa6
59:  libnrm             /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/libnrm-0.1.0-erwut7zi7gydlufvowk5de6o6zgg3bp3
60:  libpressio         /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/libpressio-0.95.1-mukxihp4kralpiivi3ddryb3m5dbuodv
61:  libquo             /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/libquo-1.4-smoqjhw2akp2v3jobdfg3pg4bnqrkdtg
62:  loki               /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/loki-0.1.7-fx626uppfiudalsnwrrwxghf7ybtzcly
63:  magma              /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/magma-2.8.0-wynpg43h3q6br6jphkix4nygpsrdeb57
64:  mercury            /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/mercury-2.3.1-ze3twrh5lfjwxan233kgk7xzdeohi2zs
65:  metall             /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/metall-0.25-lktiuohcugndo3iycl3yzoqzatla7aqf
66:  mfem               /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/mfem-4.6.0-3lakzmxzbizkr7zk32tmz6vjvaezqqwy
67:  mgard              /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/mgard-2023-12-09-6w3hnrowm6ws3nsqh7haaz2izxpiifbw
68:  mpark-variant      /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/mpark-variant-1.4.0-zhfe553bd6vqjbpwqzv4tz2nccotjhca
69:  mpich              /usr/local/mpich/install/mpich
70:  mpifileutils       /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/mpifileutils-0.11.1-dlexlldenlg3l2epfepgsqrfjyz3o2fz
71:  nccmp              /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/nccmp-1.9.1.0-jta4ps6vueurjrlz4z5ojh65g4k7ruuj
72:  nco                /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/nco-5.1.9-4datcziexpr6okv37t7ecrsjcdx5hibq
73:  netcdf-c           /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/netcdf-c-4.9.2-ldjfltzldbtx3g7h7ukgsmu6x5r7ehsk
74:  nek5000            /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/nek5000-19.0-u422ljvomqzo3ccxr7df5ceicpofiskx
75:  nekbone            /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/nekbone-17.0-eeyqxieob5a7b34kehnlunpzjincj4qc
76:  netcdf-fortran     /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/netcdf-fortran-4.6.1-2m3i5jiejanjrlefajm7suup26pn743m
77:  netlib-scalapack   /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/netlib-scalapack-2.2.0-4cfnvsqedcqexvuemttducrvmpdv2ba3
78:  nrm                /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/nrm-0.1.0-a4vpyi7molfeplaphkhmgxj2jravonza
79:  omega-h            /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/omega-h-9.34.13-iwis47irwmamthl6yrn7bhi2xmp3lnt5
80:  openfoam           /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/openfoam-2312-ueiiuvm4p6i4fdkevrskt5wyamrjyxa7
81:  openmpi            /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/openmpi-5.0.3-e7lfno4p6apwr2j2bsxqufo6cm6lqt26
82:  openpmd-api        /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/openpmd-api-0.15.2-2bhzfplnrw5eyggnlky5cra6uwpuuefp
83:  papi               /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/papi-7.1.0-3cjyy3sglpak3ezodxnrnosjqheojye3
84:  papyrus            /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/papyrus-1.0.2-fce6d26ux5h3372pbnkjcrwuwasijixt
85:  parallel-netcdf    /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/parallel-netcdf-1.12.3-7rsvz6skyl26tth22fw6mzay5fyb5get
86:  paraview           /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/paraview-5.12.0-knxiqkqipkw5nlm3ojuztwaoqizfunmh
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```
  87:  parsec              /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/parsec-3.0.2209-r4xhui5xwc4rdeczyprxifzxehg2sr43
  88:  pdt                 /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/pdt-3.25.2-ivmoilfn62eljhxlcxm23uigwcyqlwxe
  89:  petsc               /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/petsc-3.21.0-xcy6yvpkfrgucibu4mau5lduono5bp6o
  90:  phist               /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/phist-1.12.0-h3i3r6ow6qtorbvzwsfaeyuzuxelnusj
  91:  plasma              /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/plasma-23.8.2-fqak2syszks6mgtghogxiqfgk4yd5hfo
  92:  plumed              /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/plumed-2.9.0-hlz37jxoumfbhcrbd3mtdaaoe2tq57nx
  93:  precice             /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/precice-3.1.1-bdig3zhdpcq7od6j3oxdvoohqzmuauqz
  94:  pruners-ninja       /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/pruners-ninja-1.0.1-63u64he2lmhxolao2mss4f24qmjf47w4
  95:  pumi                /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/pumi-2.2.8-ml6oezslqss2hqznxafg6psatgtsjspv
  96:  py-cinemasci        /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/py-cinemasci-1.3-wdqx64i7vkpcwghhawtkhyw52gytc6al
  97:  py-deephyper        /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/py-deephyper-0.6.0-ix47mwjembqihtziysmi4s35cbbuxgxm
  98:  py-jupyterhub       /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/py-jupyterhub-1.4.1-wcwqckcsivk3tsvhein2ws3w5pphmvpn
  99:  py-libensemble      /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/py-libensemble-1.2.2-zkccbmouf2d46bujwfaryydmok3xkyrr
 100:  py-parsl            /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/py-parsl-2023.08.21-ms77xmllidr5hs3vlohh3o7ns3d4kzuc
 101:  py-radical-saga     /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/py-radical-saga-1.47.0-4qmdkvnbvinfvcleyjcefb5mtzvnaolx
 102:  qthreads            /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/qthreads-1.18-bm57wjgdsozxyvnqupeinx3pwo6zxfd5
 103:  quantum-espresso    /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/quantum-espresso-7.3.1-z7ea4yjnw2ro2f5ddl44dvgwcc7c2zkh
 104:  raja                /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/raja-2024.02.0-obhlpg6mjbtdo3z4b3bhiucrlz2eak63
 105:  rempi               /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/rempi-1.1.0-hpwq3dpeeb7sp6oq4soaffimjod4hs67
 106:  scr                 /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/scr-3.0.1-btrzdhg722likiqsjmx7wcxcenshf26t
 107:  slate               /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/slate-2023.11.05-4hioqk2r253sdlnumfvo7weenousvnab
 108:  slepc               /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/slepc-3.21.0-oy3tpt5xldfjr4ja3fw2bvmzhbjm3qmi
 109:  stc                 /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/stc-0.9.0-w26jykjhy7jplcboerywxwz7c6kano2z
 110:  strumpack           /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/strumpack-7.2.0-4gwaf4ct7ismtpcm6bmyv55lfdjw7io6
 111:  sundials            /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/sundials-7.0.0-6x2hik7kisjvmcgglhsmw54r7n4y32sl
 112:  superlu-dist        /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/superlu-dist-8.2.1-kotxw7gvg5255p7kjs6ppf545pkc7rkm
 113:  swig                /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/swig-4.1.1-lvzc2pxnxmbqijfsxmtwcmzoowueok5r
 114:  sz3                 /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/sz3-3.1.7-xnapk3uhx7o5qaidg662cbopv7qorifz
 115:  tasmanian           /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/tasmanian-8.0-4b5qz6ncn54upq2n3wh5hlj5vp56hcpx
 116:  tau                 /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/tau-2.33.2-2shla7xbcuheaa47u2tbh3tyuej6no3c
 117:  trilinos            /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/trilinos-15.1.1-ysnqypzikooecocdn4jf52qhxupwg26l
 118:  turbine             /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/turbine-1.3.0-c32cj7t4ko2hhheyq2amy4d5rx547jd2
 119:  umap                /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/umap-2.1.0-4b6ddoyw2hyvprqaj4ipqz6nbdbitecp
 120:  umpire              /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/umpire-2024.02.0-7ailt32jsqiqwpabqc7qmzqvmwkvi6va
 121:  unifyfs             /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/unifyfs-2.0-gygei64redfwz2aaegopvsg3ww2645od
 122:  upcxx               /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/upcxx-2023.9.0-5havylu2zjpv2xlwsc45xongicem4r43
 123:  veloc               /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/veloc-1.7-dnkgys2zc3zakdawnc7pjupu37fs4ndm
 124:  visit               /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/visit-3.3.3-gbqv6cz4yvv2tjok2wgxy73uebyu6frv
 125:  vtk-m               /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/vtk-m-2.1.0-acc67nis57rynnrnhmygedk6mbd4n5nu
 126:  wannier90           /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/wannier90-3.1.0-awlltjw4gylq4ll2v2n6ygz5if5ddl7d
 127:  warpx               /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/warpx-23.08-dsdppgi4n6h4qcienokmexwbe67eahbd
 128:  xyce                /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/xyce-7.8.0-7xl4glfi4r4envhkcuj47ahuylniswpb
 129:  zfp                 /spack/opt/spack/linux-ubuntu22.04-aarch64/gcc-11.4.0/zfp-1.0.0-mwlsmj2iommgwycsdk3hw4rcuygehk5w
```

PESO

E4S Support for GPUs: CUDA on aarch64

```
$ singularity run --nv e4s-24.05-cuda90-arm64.sif
Singularity> spack find -x +cuda
-- linux-ubuntu22.04-aarch64 / gcc@11.4.0 ------------------------
adios2@2.10.0   chai@2024.02.0        gromacs@2024.1        kokkos-kernels@4.3.00  mgard@2023-12-09  slepc@3.21.0        trilinos@15.1.1
amrex@24.04     cusz@0.3.1            heffte@2.4.0          lammps@20230802.3      papi@7.1.0        strumpack@7.2.0     umpire@2024.02.0
arborx@1.6      ecp-data-vis-sdk@1.0  hpctoolkit@2024.01.1  legion@24.03.0         parsec@3.0.2209   sundials@7.0.0      upcxx@2023.9.0
axom@0.9.0      flecsi@2.2.1          hpx@1.9.1             libpressio@0.95.1      petsc@3.21.0      superlu-dist@8.2.1  vtk-m@2.1.0
cabana@0.6.0    flux-core@0.61.2      hypre@2.31.0          magma@2.8.0            raja@2024.02.0    tasmanian@8.0       zfp@0.5.5
caliper@2.10.0  ginkgo@1.7.0          kokkos@4.3.00         mfem@4.6.0             slate@2023.11.05  tau@2.33.2
==> 41 installed packages
Singularity> spack find -x
-- linux-ubuntu22.04-aarch64 / gcc@11.4.0 ------------------------
adios@1.13.1           datatransferkit@3.1.1  hdf5-vol-async@1.7     mercury@2.3.1          petsc@3.21.0           sundials@7.0.0
adios2@2.7.1           dealii@9.5.1           hdf5-vol-cache@v1.1    metall@0.25            petsc@3.21.0           superlu@5.3.0
adios2@2.10.0          dyninst@13.0.0         hdf5-vol-log@1.4.0     mfem@4.6.0             phist@1.12.0           superlu-dist@8.2.1
alquimia@1.1.0         e4s-alc@1.0.1          heffte@2.4.0           mfem@4.6.0             plasma@23.8.2          superlu-dist@8.2.1
aml@0.2.1              e4s-cl@1.0.3           heffte@2.4.0           mgard@2023-12-09       plumed@2.9.0           swig@4.0.2-fortran
amrex@24.04            ecp-data-vis-sdk@1.0   hpctoolkit@2024.01.1   mgard@2023-12-09       precice@3.1.1          sz@2.1.12.5
amrex@24.04            ecp-data-vis-sdk@1.0   hpctoolkit@2024.01.1   mpark-variant@1.4.0    pruners-ninja@1.0.1    sz3@3.1.7
arborx@1.6             exago@1.6.0            hpx@1.9.1              mpich@4.1.2            pumi@2.2.8             tasmanian@8.0
arborx@1.6             exaworks@0.1.0         hpx@1.9.1              mpifileutils@0.11.1    py-cinemasci@1.3       tasmanian@8.0
argobots@1.2           faodel@1.2108.1        hypre@2.31.0           nccmp@1.9.1.0          py-deephyper@0.6.0     tau@2.33.2
ascent@0.9.2           flecsi@2.2.1           hypre@2.31.0           nco@5.1.9              py-h5py@3.11.0         tau@2.33.2
axom@0.9.0             flecsi@2.2.1           kokkos@4.3.00          nek5000@19.0           py-jupyterhub@1.4.1    trilinos@13.0.1
axom@0.9.0             flit@2.1.0             kokkos@4.3.00          nekbone@17.0           py-libensemble@1.2.2   trilinos@15.1.1
bolt@2.0               flux-core@0.61.2       kokkos-kernels@4.3.00  netcdf-fortran@4.6.1   py-petsc4py@3.21.0     trilinos@15.1.1
boost@1.79.0           flux-core@0.61.2       kokkos-kernels@4.3.00  netlib-scalapack@2.2.0 py-warpx@23.08         turbine@1.3.0
butterflypack@2.4.0    fortrilinos@2.3.0      laghos@3.1             nrm@0.1.0              qthreads@1.18          umap@2.1.0
cabana@0.6.0           fpm@0.10.0             lammps@20230802.3      nvhpc@24.3             quantum-espresso@7.3.1 umpire@2024.02.0
cabana@0.6.0           gasnet@2023.9.0        lammps@20230802.3      omega-h@9.34.13        raja@2024.02.0         umpire@2024.02.0
caliper@2.10.0         ginkgo@1.7.0           lbann@0.104            openfoam@2312          raja@2024.02.0         unifyfs@2.0
caliper@2.10.0         ginkgo@1.7.0           legion@24.03.0         openmpi@5.0.3          rempi@1.1.0            upcxx@2023.9.0
chai@2024.02.0         globalarrays@5.8.2     legion@24.03.0         openpmd-api@0.15.2     scr@3.0.1              upcxx@2023.9.0
chai@2024.02.0         glvis@4.2              libcatalyst@2.0.0-rc4  papi@7.1.0             slate@2023.11.05       veloc@1.7
charliecloud@0.37      gmp@6.2.1              libnrm@0.1.0           papi@7.1.0             slate@2023.11.05       visit@3.3.3
conduit@0.9.1          gotcha@1.0.6           libpressio@0.95.1      papyrus@1.0.2          slepc@3.21.0           vtk-m@2.0.0
cp2k@2024.1            gptune@4.0.0           libpressio@0.95.1      parallel-netcdf@1.12.3 slepc@3.21.0           vtk-m@2.1.0
cuda@12.2.0            gromacs@2024.1         libquo@1.4             paraview@5.12.0        stc@0.9.0              wannier90@3.1.0
cusz@0.3.1             gromacs@2024.1         libunwind@1.6.2        parsec@3.0.2209        strumpack@7.2.0        xyce@7.8.0
darshan-runtime@3.4.4  h5bench@1.4            loki@0.1.7             parsec@3.0.2209        strumpack@7.2.0        zfp@0.5.5
darshan-util@3.4.4     hdf5@1.12.3            magma@2.8.0            pdt@3.25.2             sundials@7.0.0         zfp@0.5.5
==> 174 installed packages
Singularity>
```

E4S 24.05 supports CUDA architectures 75 (T4), 80 (A100), as well as 90 (H100/GH200)

E4S Support for GPUs: CUDA on aarch64 (modules)

```
------------------------------------ /spack/share/spack/lmod/linux-ubuntu22.04-aarch64/mpich/4.1.2-jbngz7b/Core ------------------------------------
   adios/1.13.1                       ginkgo/1.7.0-cuda90-openmp             metall/0.25                        rempi/1.1.0
   alquimia/1.1.0                     ginkgo/1.7.0-openmp             (D)    mfem/4.6.0-cuda90                  scr/3.0.1
   amrex/24.04-cuda90                 globalarrays/5.8.2                     mfem/4.6.0                  (D)    slate/2023.11.05-cuda90-openmp
   amrex/24.04                 (D)    glvis/4.2                              mpifileutils/0.11.1                slate/2023.11.05-openmp         (D)
   arborx/1.6-cuda90                  gptune/4.0.0                           nccmp/1.9.1.0                      slepc/3.21.0-cuda90
   arborx/1.6                  (D)    gromacs/2024.1-cuda90-openmp           nco/5.1.9                          slepc/3.21.0                    (D)
   axom/0.9.0-cuda90-openmp           gromacs/2024.1-openmp           (D)    nek5000/19.0                       stc/0.9.0
   axom/0.9.0-openmp           (D)    h5bench/1.4                            nekbone/17.0                       strumpack/7.2.0-cuda90-openmp
   boost/1.79.0                       hdf5-vol-async/1.7                     netcdf-fortran/4.6.1               strumpack/7.2.0-openmp          (D)
   butterflypack/2.4.0-openmp         hdf5-vol-cache/v1.1                    netlib-scalapack/2.2.0             sundials/7.0.0-cuda90
   cabana/0.6.0-cuda90                hdf5-vol-log/1.4.0                     omega-h/9.34.13                    sundials/7.0.0                  (D)
   cabana/0.6.0                (D)    heffte/2.4.0-cuda90                    openfoam/2312                      superlu-dist/8.2.1-cuda90
   caliper/2.10.0-cuda90              heffte/2.4.0                    (D)    openpmd-api/0.15.2                 superlu-dist/8.2.1              (D)
   caliper/2.10.0              (D)    hpctoolkit/2024.01.1-cuda              papyrus/1.0.2                      tasmanian/8.0-cuda90
   chai/2024.02.0-cuda90              hpctoolkit/2024.01.1            (D)    parsec/3.0.2209-cuda90             tasmanian/8.0                   (D)
   chai/2024.02.0              (D)    hpx/1.9.1-cuda90                       parsec/3.0.2209             (D)    tau/2.33.2-cuda
   conduit/0.9.1                      hpx/1.9.1                       (D)    petsc/3.21.0-cuda90                tau/2.33.2                      (D)
   cp2k/2024.1-openmp                 hypre/2.31.0-cuda90                    petsc/3.21.0                (D)    trilinos/13.0.1
   datatransferkit/3.1.1              hypre/2.31.0                    (D)    phist/1.12.0-openmp                trilinos/15.1.1-cuda90
   dealii/9.5.1                       laghos/3.1                             plumed/2.9.0                       trilinos/15.1.1                 (D)
   dyninst/13.0.0-openmp              lammps/20230802.3-cuda90-openmp        precice/3.1.1                      turbine/1.3.0
   ecp-data-vis-sdk/1.0-cuda90        lammps/20230802.3-openmp        (D)    pruners-ninja/1.0.1                umpire/2024.02.0-cuda90
   ecp-data-vis-sdk/1.0        (D)    lbann/0.104                            pumi/2.2.8                         umpire/2024.02.0                (D)
   exago/1.6.0                        libnrm/0.1.0                           py-h5py/3.11.0                     upcxx/2023.9.0-cuda90
   exaworks/0.1.0                     libpressio/0.95.1-cuda90-openmp        py-libensemble/1.2.2               upcxx/2023.9.0                  (D)
   flecsi/2.2.1-cuda90                libpressio/0.95.1-openmp        (D)    py-petsc4py/3.21.0                 wannier90/3.1.0
   flecsi/2.2.1                (D)    libquo/1.4                             py-warpx/23.08                     xyce/7.8.0
   fortrilinos/2.3.0                  mercury/2.3.1                          quantum-espresso/7.3.1-openmp

------------------------------------------------ /spack/share/spack/lmod/linux-ubuntu22.04-aarch64/Core ------------------------------------------------
   aml/0.2.1                   fpm/0.10.0-openmp                  loki/0.1.7                         pdt/3.25.2
   argobots/1.2                gasnet/2023.9.0                    magma/2.8.0-cuda90                 plasma/23.8.2
   bolt/2.0                    gmp/6.2.1                          mgard/2023-12-09-cuda90-openmp     py-deephyper/0.6.0
   charliecloud/0.37           gotcha/1.0.6                       mgard/2023-12-09-openmp     (D)    py-jupyterhub/1.4.1
   cuda/12.2.0                 kokkos-kernels/4.3.00-cuda90       mpark-variant/1.4.0                qthreads/1.18
   cusz/0.3.1-cuda90           kokkos-kernels/4.3.00-openmp (D)   mpich/4.1.2                 (L)    raja/2024.02.0-cuda90
   e4s-alc/1.0.1               kokkos/4.3.00-cuda90               nrm/0.1.0                          raja/2024.02.0           (D)
   e4s-cl/1.0.3                kokkos/4.3.00-openmp        (D)    nvhpc/24.3                         superlu/5.3.0
   flit/2.1.0                  legion/24.03.0-cuda70              openmpi/5.0.3                      swig/4.0.2-fortran
   flux-core/0.61.2-cuda       legion/24.03.0              (D)    papi/7.1.0-cuda                    sz3/3.1.7
   flux-core/0.61.2      (D)   libunwind/1.6.2                    papi/7.1.0                  (D)    umap/2.1.0
```

E4S 24.05 supports CUDA architectures 75 (T4), 80 (A100), as well as 90 (H100/GH200)

E4S DOE LLVM Release: x86_64, ppc64le, and aarch64

```
Singularity> spack find -x
-- linux-ubuntu20.04-x86_64 / clang@16.0.2 ----------------------
adios@1.13.1  cabana@0.5.0       globalarrays@5.8.2  heffte@2.3.0     mfem@4.5.2           parsec@3.0.2209  sundials@6.5.1      umpire@2022.03.1
aml@0.2.0     chai@2022.03.0     gmp@6.2.1           hypre@2.28.0     mpark-variant@1.4.0  pdt@3.25.1       superlu@5.3.0       upcxx@2023.3.0
amrex@23.05   charliecloud@0.32  gotcha@1.0.4        legion@23.03.0   mpich@4.1.1          plumed@2.8.2     swig@4.0.2-fortran
arborx@1.3    flit@2.1.0         h5bench@1.3         libnrm@0.1.0     nccmp@1.9.0.1        pumi@2.2.7       tasmanian@7.9
argobots@1.1  flux-core@0.49.0   hdf5-vol-async@1.5  libquo@1.3.1     nco@5.1.5            qthreads@1.16    turbine@1.3.0
bolt@2.0      gasnet@2023.3.0    hdf5-vol-log@1.4.0  libunwind@1.6.2  papyrus@1.0.2        stc@0.9.0        umap@2.1.0

-- linux-ubuntu20.04-x86_64 / gcc@11.1.0 ------------------------
cmake@3.26.3  llvm-doe@16.0.2

Singularity> spack find -x
-- linux-ubuntu20.04-ppc64le / clang@16.0.2 ---------------------
adios@1.13.1  cabana@0.5.0       globalarrays@5.8.2  heffte@2.3.0     mfem@4.5.2           parsec@3.0.2209  sundials@6.5.1      umpire@2022.03.1
aml@0.2.0     chai@2022.03.0     gmp@6.2.1           hypre@2.28.0     mpark-variant@1.4.0  pdt@3.25.1       superlu@5.3.0       upcxx@2023.3.0
amrex@23.05   charliecloud@0.32  gotcha@1.0.4        legion@23.03.0   mpich@4.1.1          plumed@2.8.2     swig@4.0.2-fortran
arborx@1.3    flit@2.1.0         h5bench@1.3         libnrm@0.1.0     nccmp@1.9.0.1        pumi@2.2.7       tasmanian@7.9
argobots@1.1  flux-core@0.49.0   hdf5-vol-async@1.5  libquo@1.3.1     nco@5.1.5            qthreads@1.16    turbine@1.3.0
bolt@2.0      gasnet@2023.3.0    hdf5-vol-log@1.4.0  libunwind@1.6.2  papyrus@1.0.2        stc@0.9.0        umap@2.1.0

-- linux-ubuntu20.04-ppc64le / gcc@11.1.0 -----------------------
cmake@3.26.3  llvm-doe@16.0.2

Singularity> spack find -x
-- linux-ubuntu20.04-aarch64 / clang@16.0.2 ---------------------
adios@1.13.1  cabana@0.5.0       globalarrays@5.8.2  heffte@2.3.0     mfem@4.5.2           parsec@3.0.2209  sundials@6.5.1      umpire@2022.03.1
aml@0.2.0     chai@2022.03.0     gmp@6.2.1           hypre@2.28.0     mpark-variant@1.4.0  pdt@3.25.1       superlu@5.3.0       upcxx@2023.3.0
amrex@23.05   charliecloud@0.32  gotcha@1.0.4        legion@23.03.0   mpich@4.1.1          plumed@2.8.2     swig@4.0.2-fortran
arborx@1.3    flit@2.1.0         h5bench@1.3         libnrm@0.1.0     nccmp@1.9.0.1        pumi@2.2.7       tasmanian@7.9
argobots@1.1  flux-core@0.49.0   hdf5-vol-async@1.5  libquo@1.3.1     nco@5.1.5            qthreads@1.16    turbine@1.3.0
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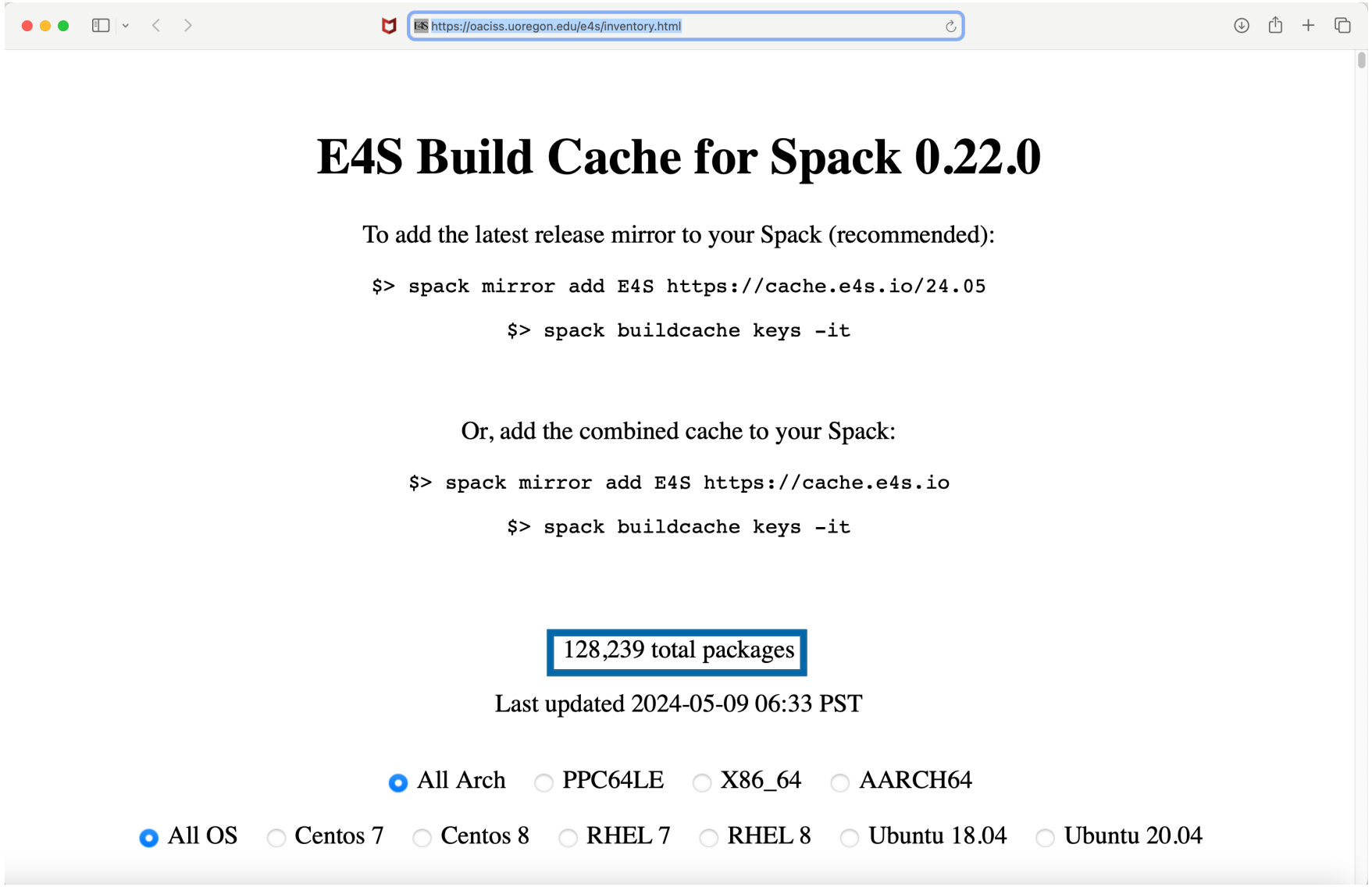
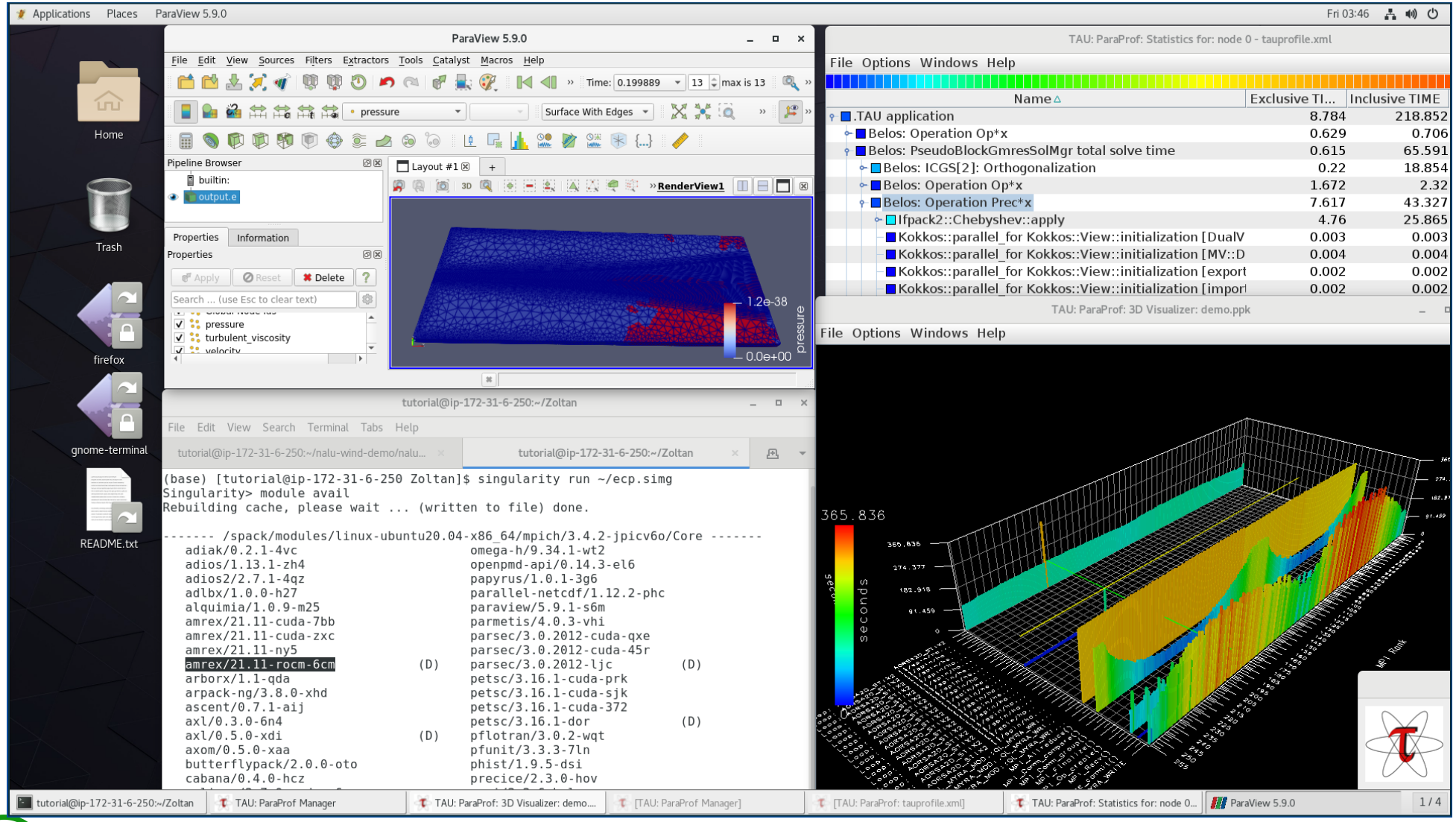
-- linux-ubuntu20.04-aarch64 / gcc@11.1.0 -----------------------
cmake@3.26.3  llvm-doe@16.0.2
```

E4S Build Cache for Spack 0.22.0 hosted at U. Oregon



- Over 125K binaries!
- No need to recompile from source code

E4S 24.05 AWS image: ami-0e752117cfa13cb9b in US-West-2 (OR)

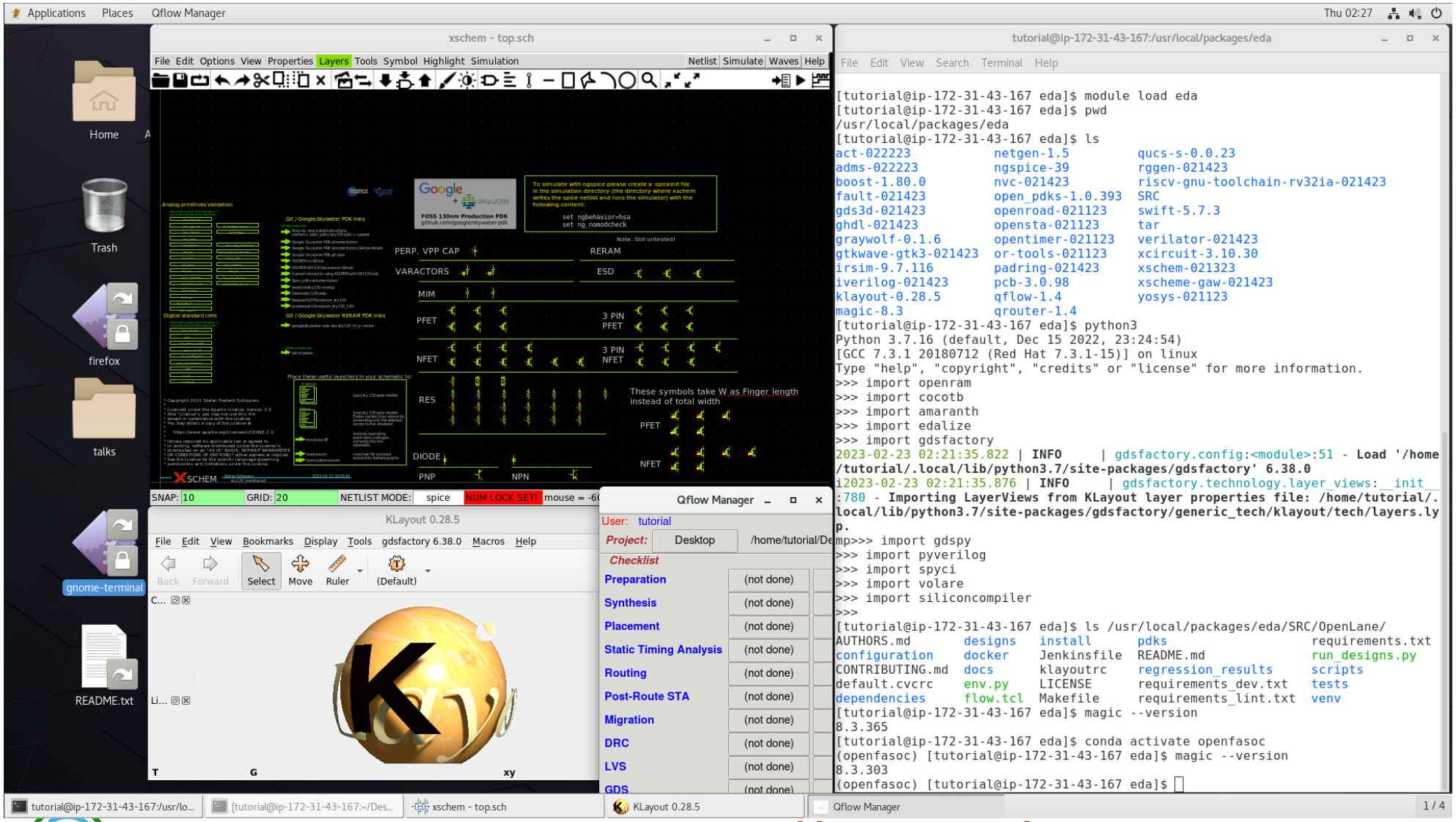


E4S AWS

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

E4S for Commercial Cloud Platforms for EDA on AWS

- E4S: HPC Software Ecosystem – a curated software portfolio for Electronic Design Automation



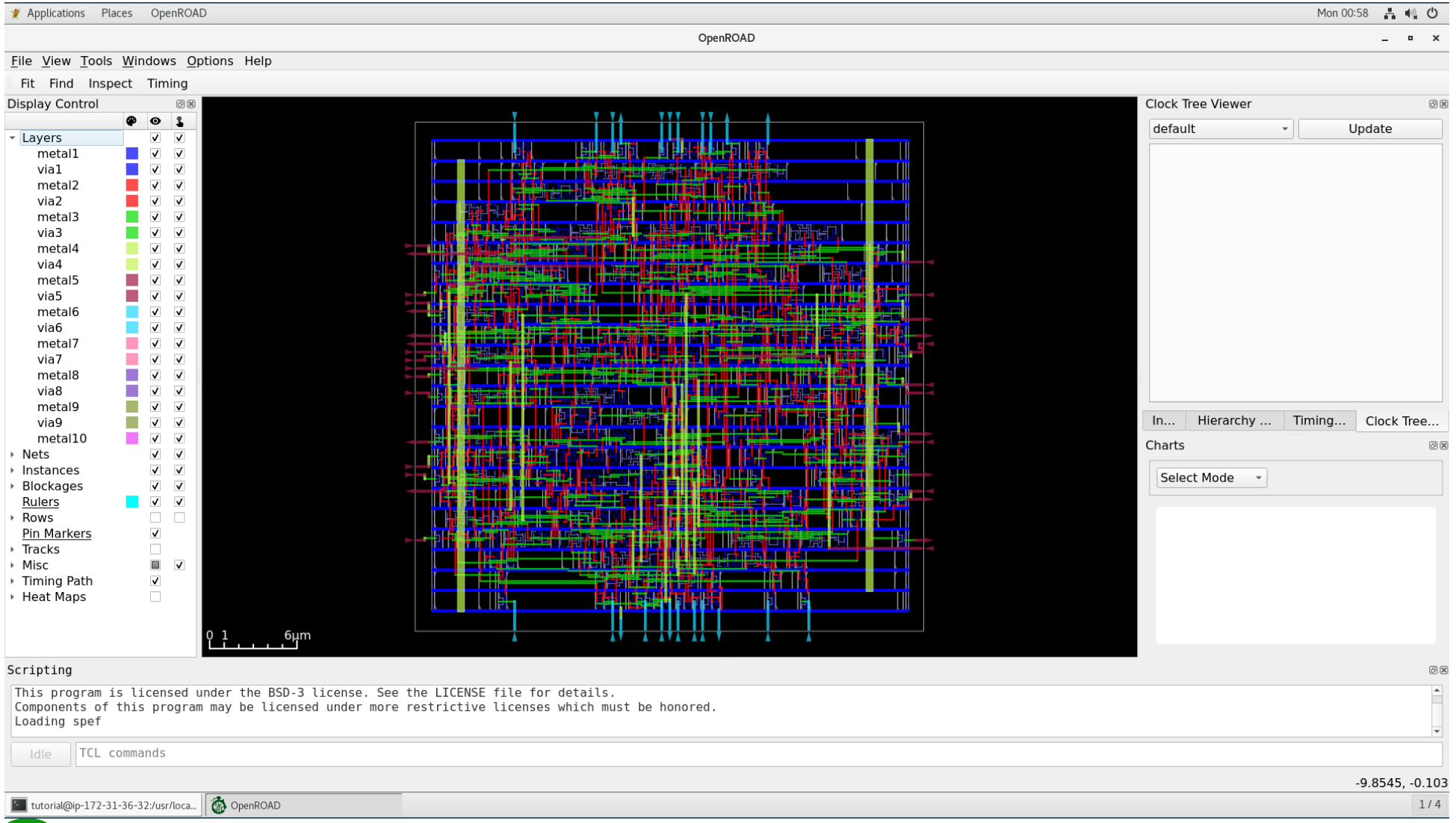
https://e4s.io/eda

E4S EDA on AWS

- Magic
- ACT
- Klayout
- Qflow
- Xschem
- Xcircuit
- Yosys
- Volator
- OpenROAD
- OpenLane
- iVerilog
- Gtkwave
- Irsim
- Qrouter
- Fault
- GDS3D
- Rggen
- Python tools
  - Cocotb
  - Amaranth
  - Edalize
  - Gdsfactory
  - Gdspy
  - OpenRAM
  - Gdstk
  - Silicon compiler
  - Volare …
- PDKs
  - GF
  - Skywater

E4S for Commercial Cloud Platforms for EDA on AWS

- E4S: HPC Software Ecosystem – a curated software portfolio for Electronic Design Automation. Microwatt CPU (IBM) in OpenROAD.



OpenROAD GUI

E4S EDA on AWS

- Magic
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- Klayout
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  - Skywater

E4S for Commercial Cloud Platforms for EDA on AWS

- E4S: HPC Software Ecosystem – a curated software portfolio for Electronic Design Automation

#	Packages currently in E4S	URL
1	Magic	http://opencircuitdesign.com/magic/
2	Xyce	https://xyce.sandia.gov
3	NGSPICE	https://ngspice.sourceforge.io
4	KLayout	https://www.klayout.de
5	Qflow	http://opencircuitdesign.com/qflow
6	OR-Tools	https://developers.google.com/optimization
7	IRSIM	http://opencircuitdesign.com/irsim/
8	OpenROAD	https://github.com/The-OpenROAD-Project/OpenROAD
9	OpenLane	https://openlane.readthedocs.io/
10	OpenFASOC	https://openfasoc.readthedocs.io/
11	Open_PDKs	http://opencircuitdesign.com/open_pdks/
12	Netgen	http://opencircuitdesign.com/netgen/

#	Packages currently in E4S	URL
13	Yosys	https://github.com/YosysHQ/yosys
14	Xcircuit	http://opencircuitdesign.com/xcircuit/
15	Graywolf	https://github.com/rubund/graywolf
16	OpenSTA	https://github.com/The-OpenROAD-Project/OpenSTA
17	OpenTimer	https://github.com/OpenTimer/OpenTimer
18	Qrouter	http://opencircuitdesign.com/qrouter/
19	Xschem	https://github.com/silicon-vlsi-org/eda-xschem
20	RISC-V GNU Toolchain	https://github.com/riscv-collab/riscv-gnu-toolchain
21	Fault: Design for Test	https://github.com/AUCOHL/Fault
22	NVC	https://github.com/nickg/nvc
23	Amaranth	https://github.com/amaranth-lang/amaranth
24	Cocotb	https://github.com/cocotb/cocotb

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https://e4s.io/eda

E4S for Commercial Cloud Platforms for EDA on AWS

- E4S: HPC Software Ecosystem – a curated software portfolio for Electronic Design Automation

#	Packages currently in E4S	URL
25	Covered	https://github.com/hpretl/verilog-covered
26	Edalize	https://github.com/olofk/edalize
27	Gaw3-xschem	https://github.com/StefanSchippers/xschem-gaw.git
28	GDSFactory	https://github.com/gdsfactory/gdsfactory
29	GDSPy	https://github.com/heitzmann/gdspy
30	GDS3D	https://github.com/trilomix/GDS3D
31	Ghdl	https://github.com/ghdl/ghdl
32	Gtkwave	https://github.com/gtkwave/gtkwave
33	iic-osic	https://github.com/hpretl/iic-osic.git
34	Iverilog	https://github.com/steveicarus/iverilog.git
35	Netlistsvg	https://github.com/nturley/netlistsvg
36	Ngspyce	https://github.com/ignamv/ngspyce

#	Packages currently in E4S	URL
37	Padring	https://github.com/donn/padring
38	Pyverilog	https://github.com/PyHDI/Pyverilog
39	OpenRAM	https://github.com/VLSIDA/OpenRAM
40	Rggen	https://github.com/rggen/rggen
41	Spyci	https://github.com/gmagno/spyci
42	Volare	https://github.com/efabless/volare
43	Siliconcompiler	https://github.com/siliconcompiler/siliconcompiler
44	Verilator	https://github.com/verilator/verilator
45	Sky130	SkyWater Technologies 130nm CMOS PDK
46	Actflow	https://github.com/asyncvlsi/actflow.git
47	Qucs-s	https://github.com/Qucs
48	ADMS	https://github.com/Qucs/ADMS.git
49	Gdstk	https://heitzmann.github.io/gdstk/
50	xcell	https://github.com/asyncvlsi/xcell.git

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https://e4s.io/eda

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|docker] --image <file> --source <startup_cmds.sh>
  - e4s-cl mpirun -np <N> <command>
- Usage:

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

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

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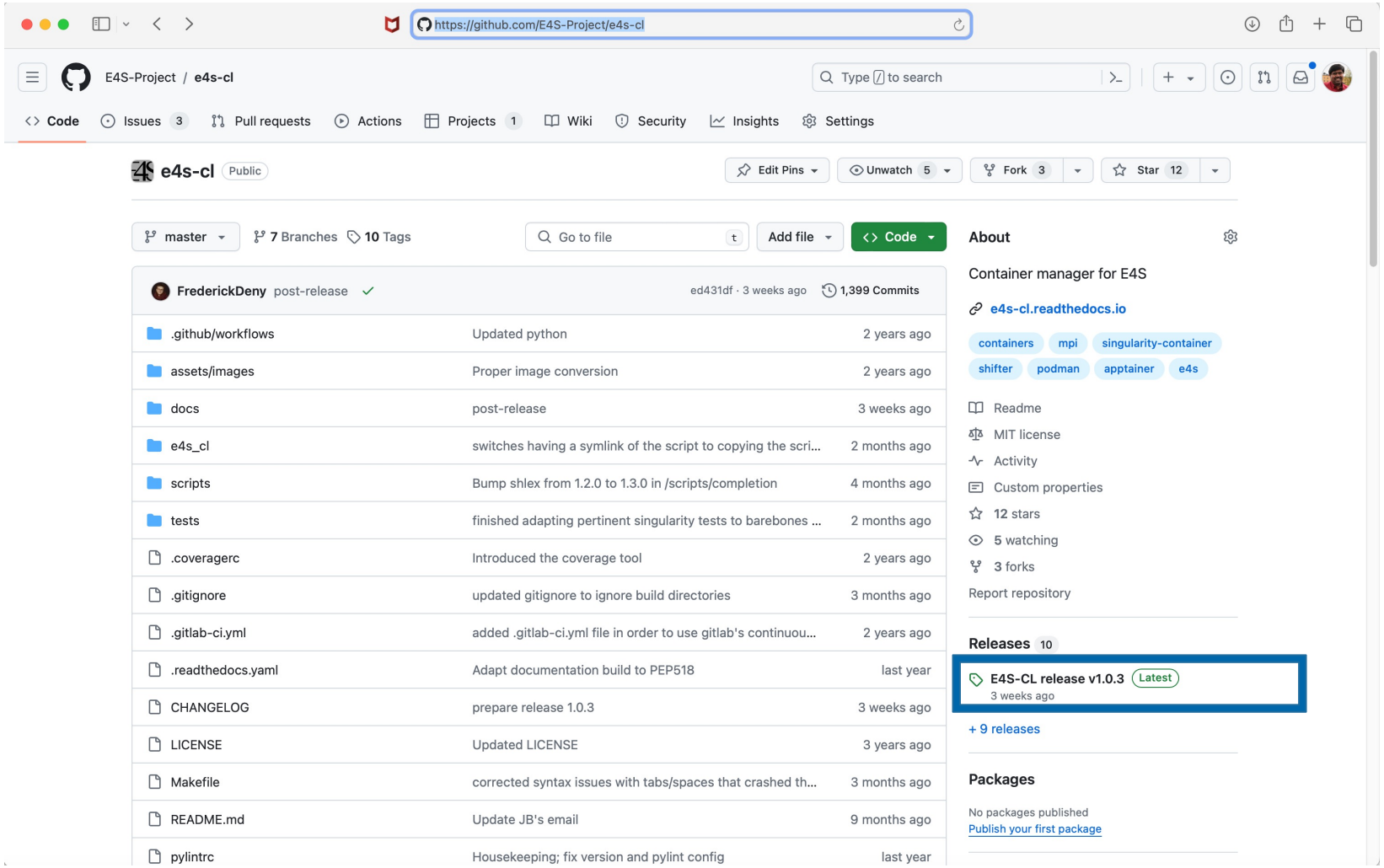
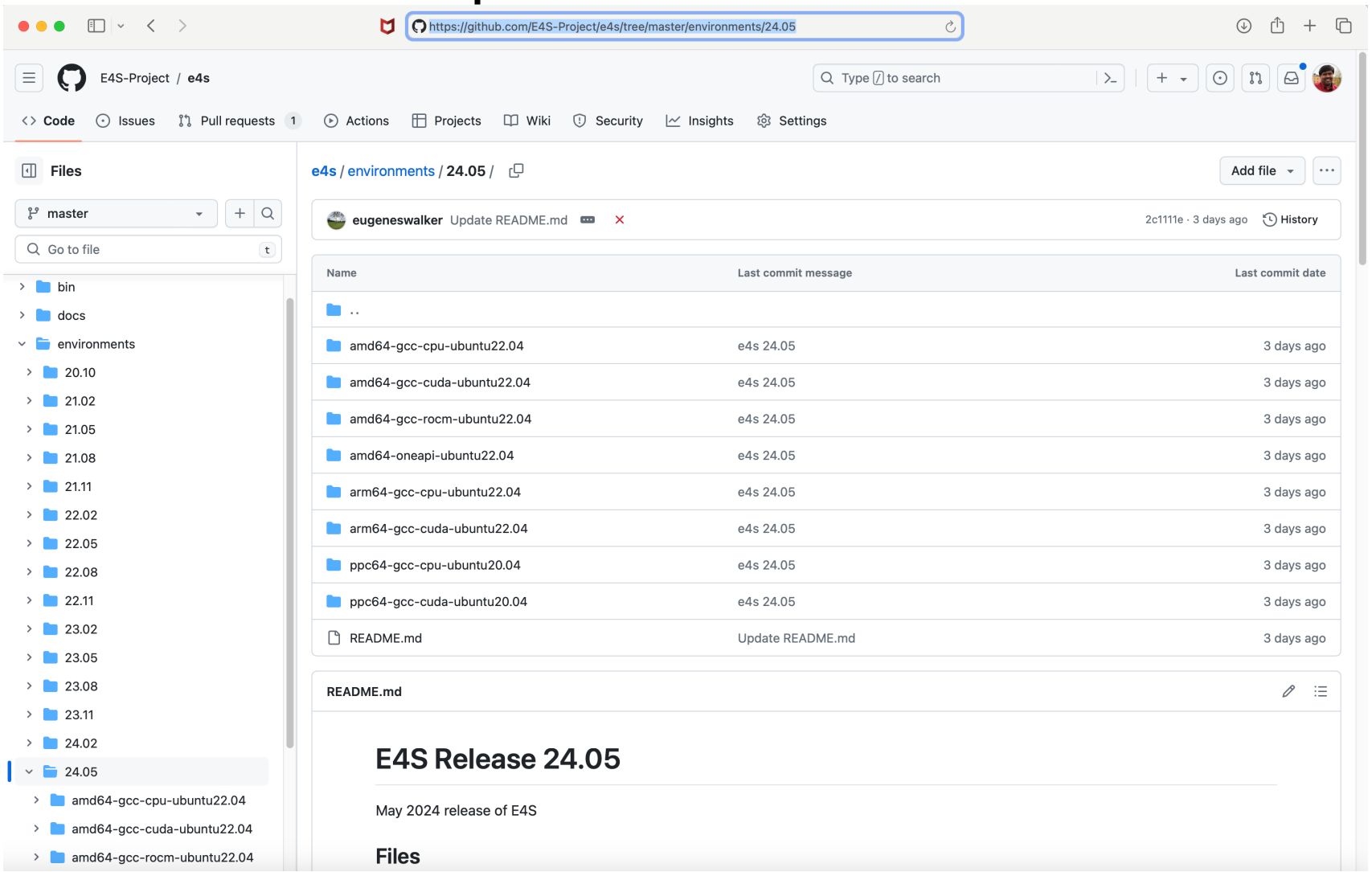
New release of e4s-cl on GitHub



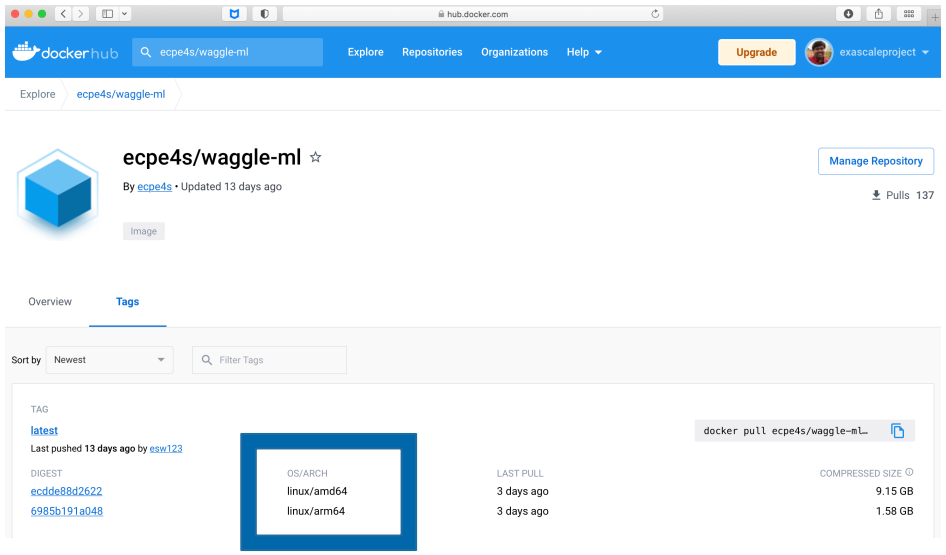
https://github.com/E4S-Project/e4s-cl

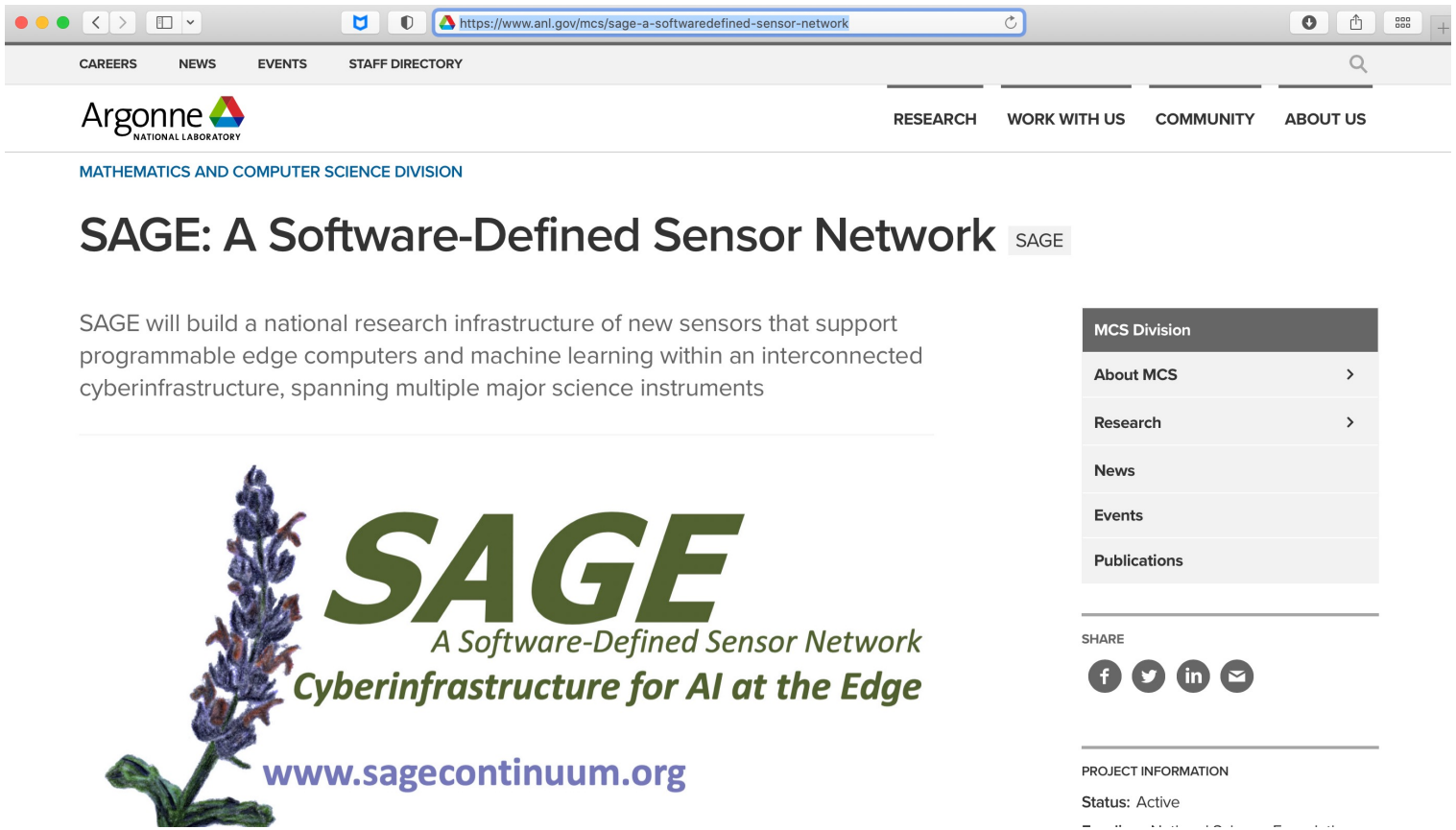
E4S: Open Source Development on GitHub



https://github.com/E4S-Project

Release of custom E4S images: Waggle and SAGE projects





% docker pull ecpe4s/waggle-ml

Thank you

https://www.exascaleproject.org

This research was supported by the Exascale Computing Project (17-SC-20-SC), a joint project of the U.S. Department of Energy's Office of Science and National Nuclear Security Administration, responsible for delivering a capable exascale ecosystem, including software, applications, and hardware technology, to support the nation's exascale computing imperative.

Thank you to all collaborators in the ECP and broader computational science communities. The work discussed in this presentation represents creative contributions of many people who are passionately working toward next-generation computational science.

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- https://science.osti.gov/ascr
- https://www.pesoproject.org

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