E4S: The Extreme-scale Scientific Software Stack Release 24.11

Release 24.11 notes

November 15, 2024

E4S 24.11: What's New?

- E4S includes 132+ HPC packages on ARM, x86_64, and ppc64le platforms, 132K+ binaries in E4S build Cache.
- E4S improves support for a cross-platform AI/ML software stack including packages like NVIDIA NeMo™, Huggingface_hub, DeepHyper, Google.generativeai (Gemini API), OpenAI (API), TorchBraid, Pandas, Scikit-Learn, JAX, PyTorch, TensorFlow, Horovod, OpenCV, and LBANN with support for GPUs.
- Support for new architecture: AMD MI300A/MI300X (gfx942).
- New language and runtime: Chapel
- New applications: NWChem, WRF, FFTX
- E4S DocPortal updated with AI/ML tools.
- CUDA upgraded from to 12.6 (aarch64), ROCm upgraded to 6.2.1, oneAPI upgraded to 2024.2.0.
- 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, Azure, and Google Cloud Marketplace with NVIDIA GPUs with VNC based remote desktop and Torque (qsub) and SLURM (sbatch) for multi-node execution:
  - https://adaptivecomputing.com/
  - https://paratoolspro.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 132+ HPC, EDA (e.g., Xyce), and AI/ML packages (e.g., NVIDIA NeMo™, 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.
- 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.
- E4S 24.11 released on November 15, 2024: https://e4s.io/talks/E4S_24.11.pdf

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 24.11 – 125 full release products
- Nov 15, 2024: E4S 24.11 – 132 full release products

https://e4s.io

Lead: Sameer Shende (U Oregon)

Also include other products .e.g.,
AI: NVIDIA NeMo™, 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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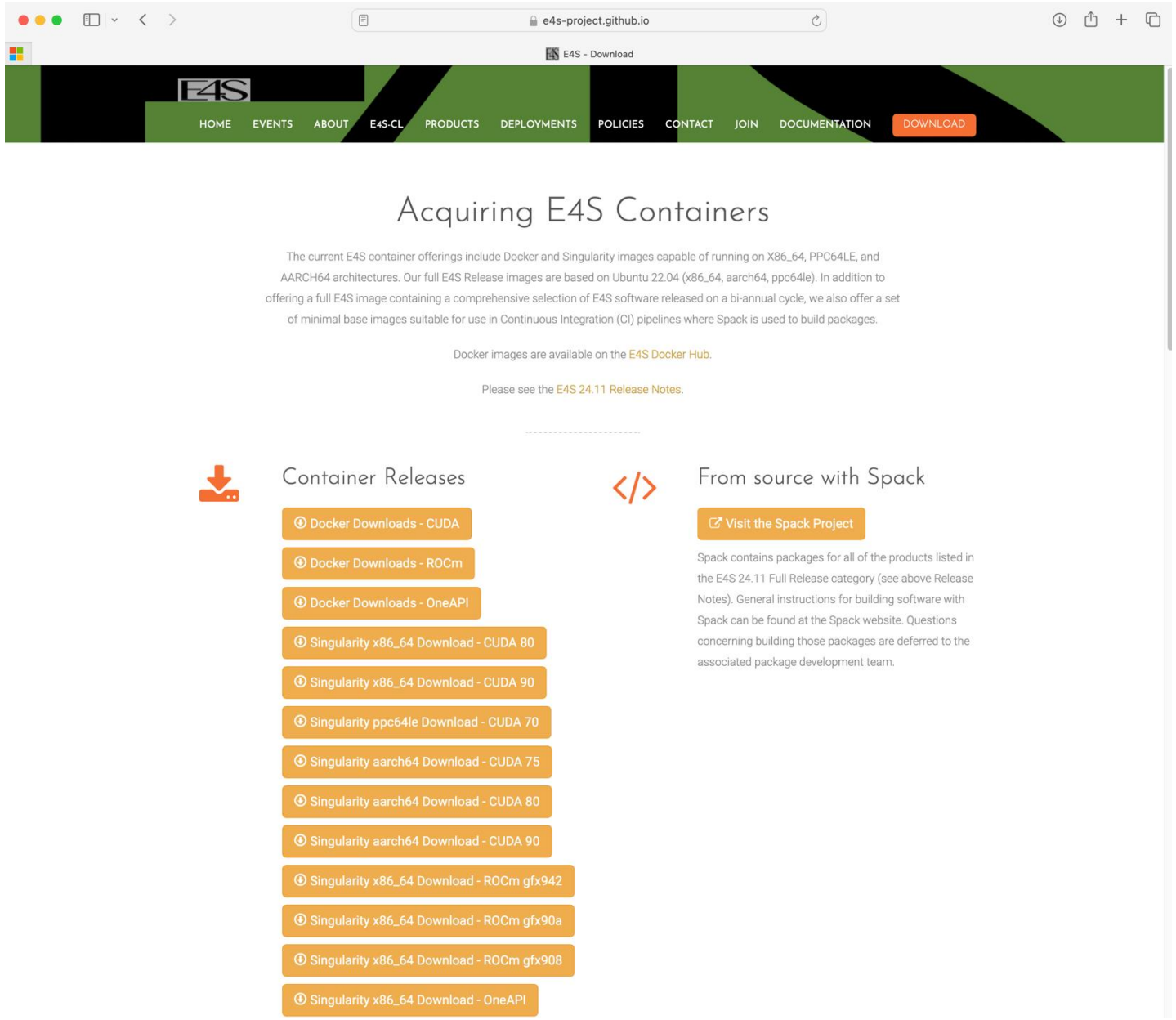
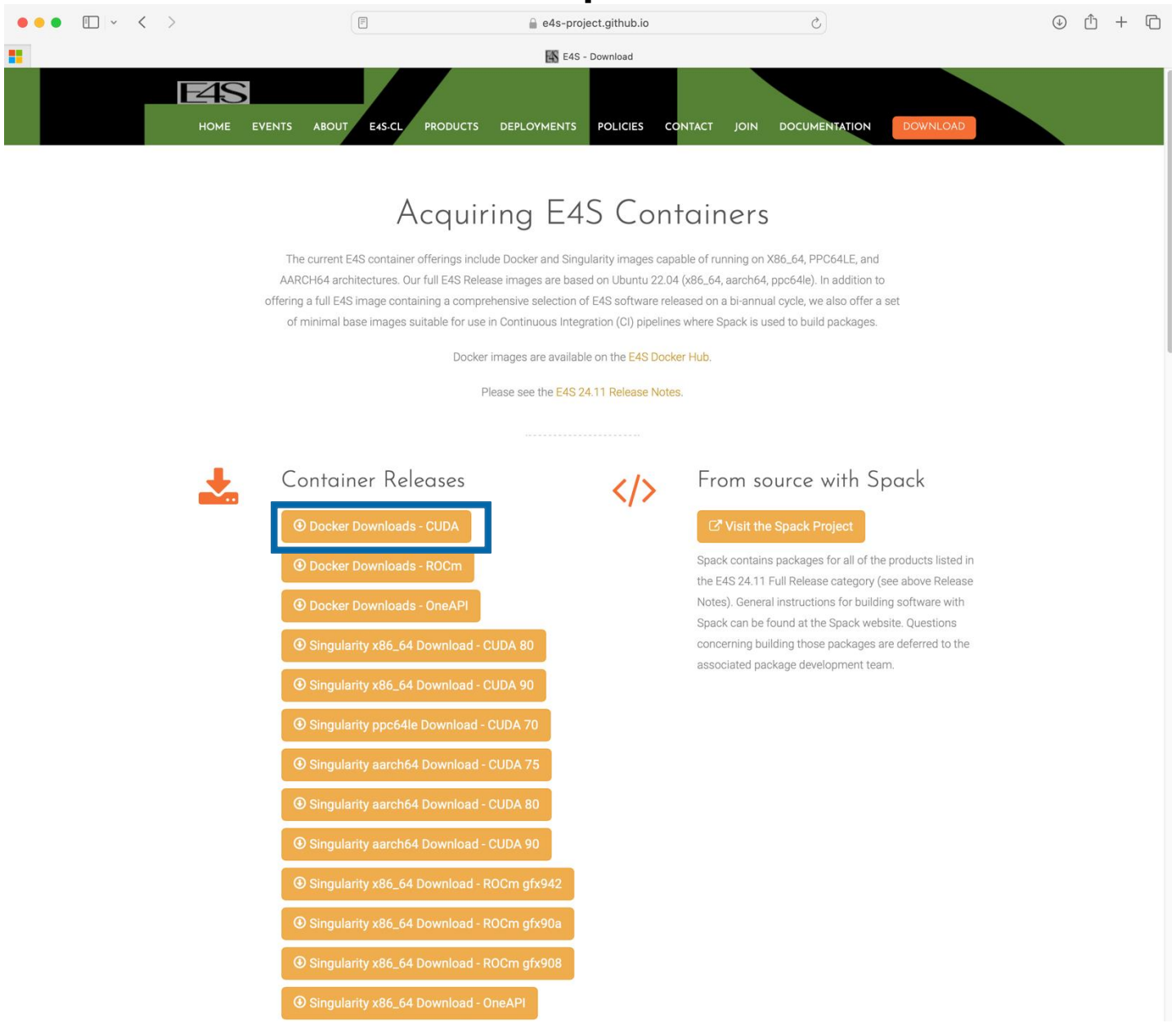
E4S Container Download from https://e4s.io

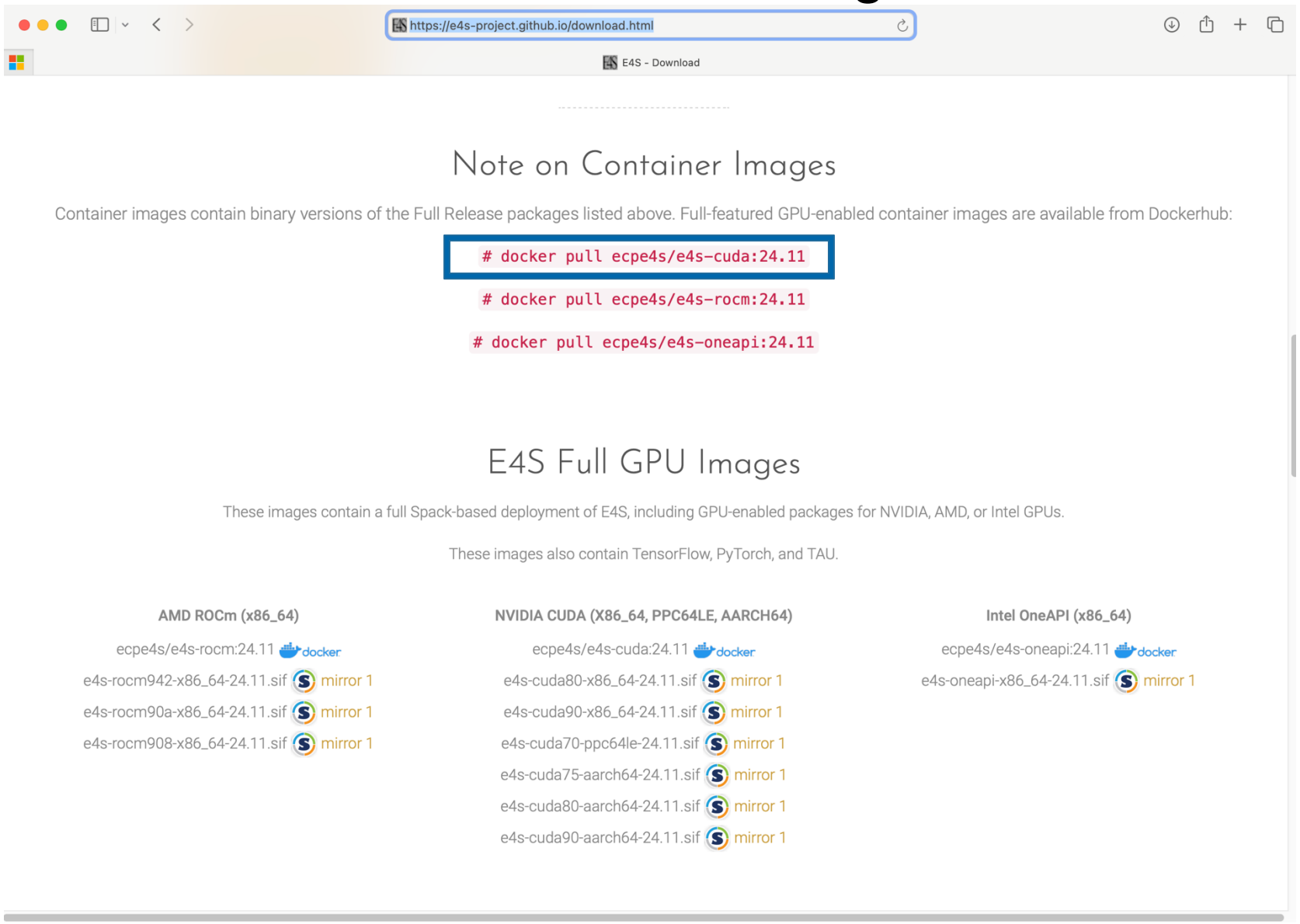


E4S Container Download from https://e4s.io



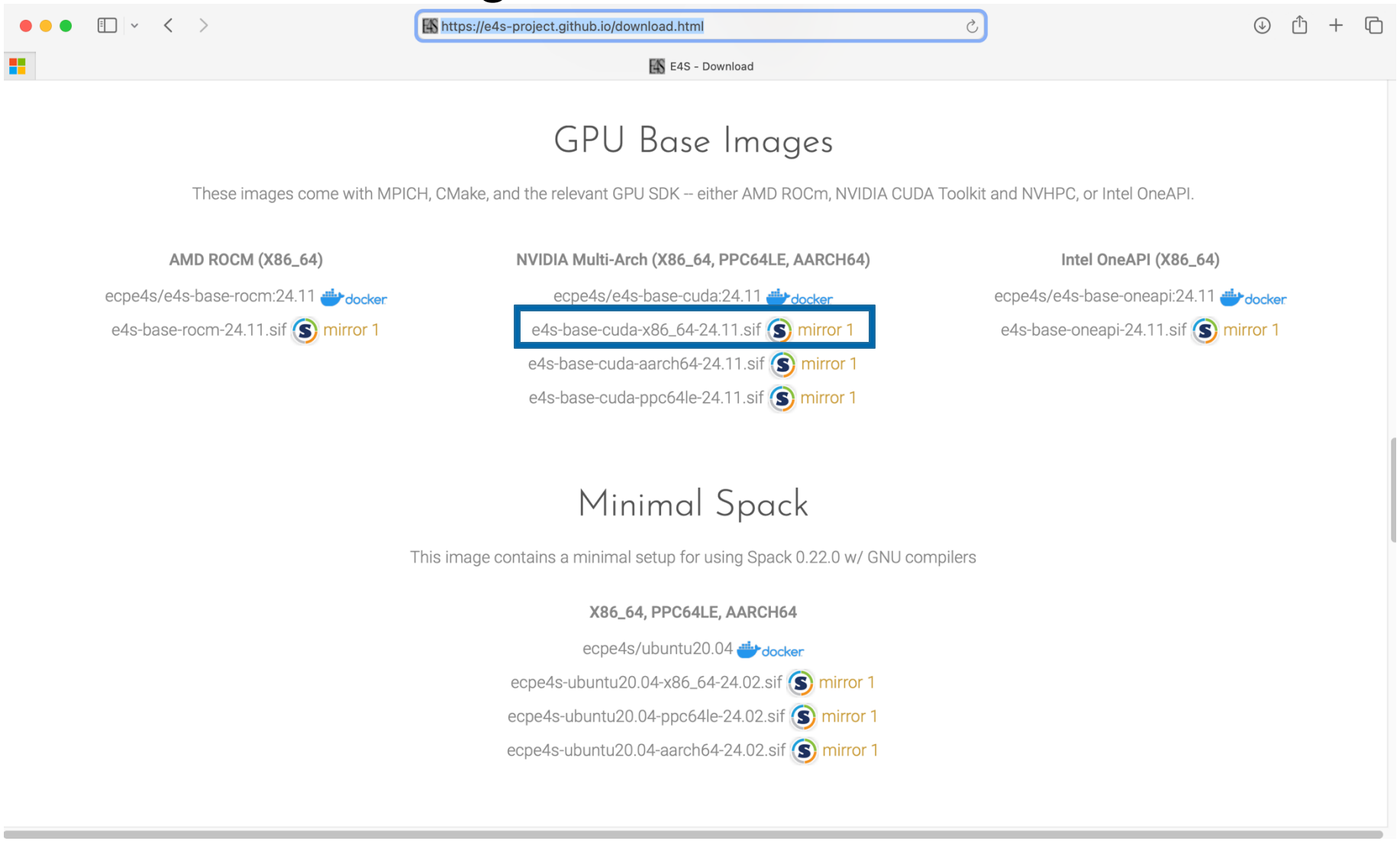
- Separate full featured Singularity images for 3 GPU architectures
- GPU full featured images for
  - x86_64 (Intel, AMD, NVIDIA)
  - ppc64le (NVIDIA)
  - aarch64 (NVIDIA)
- Full featured images available on Dockerhub
- 132+ products on 3 architectures

Download E4S 24.11 GPU Container Images: AMD, Intel, and NVIDIA



https://e4s.io

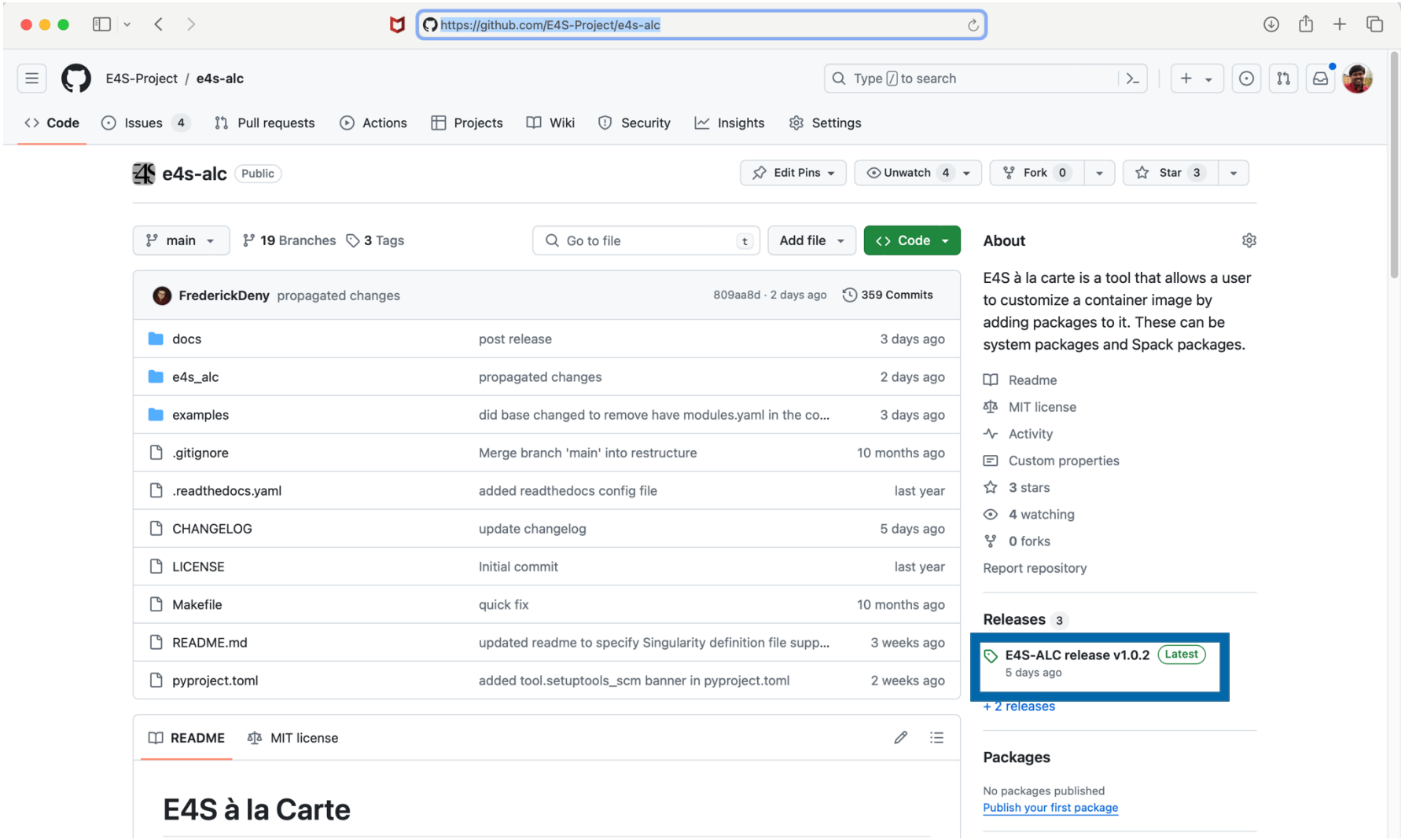
E4S base container images allow users to customize their containers



- Intel oneAPI
- AMD ROCm
- NVIDIA NVHPC and CUDA

https://e4s.io

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

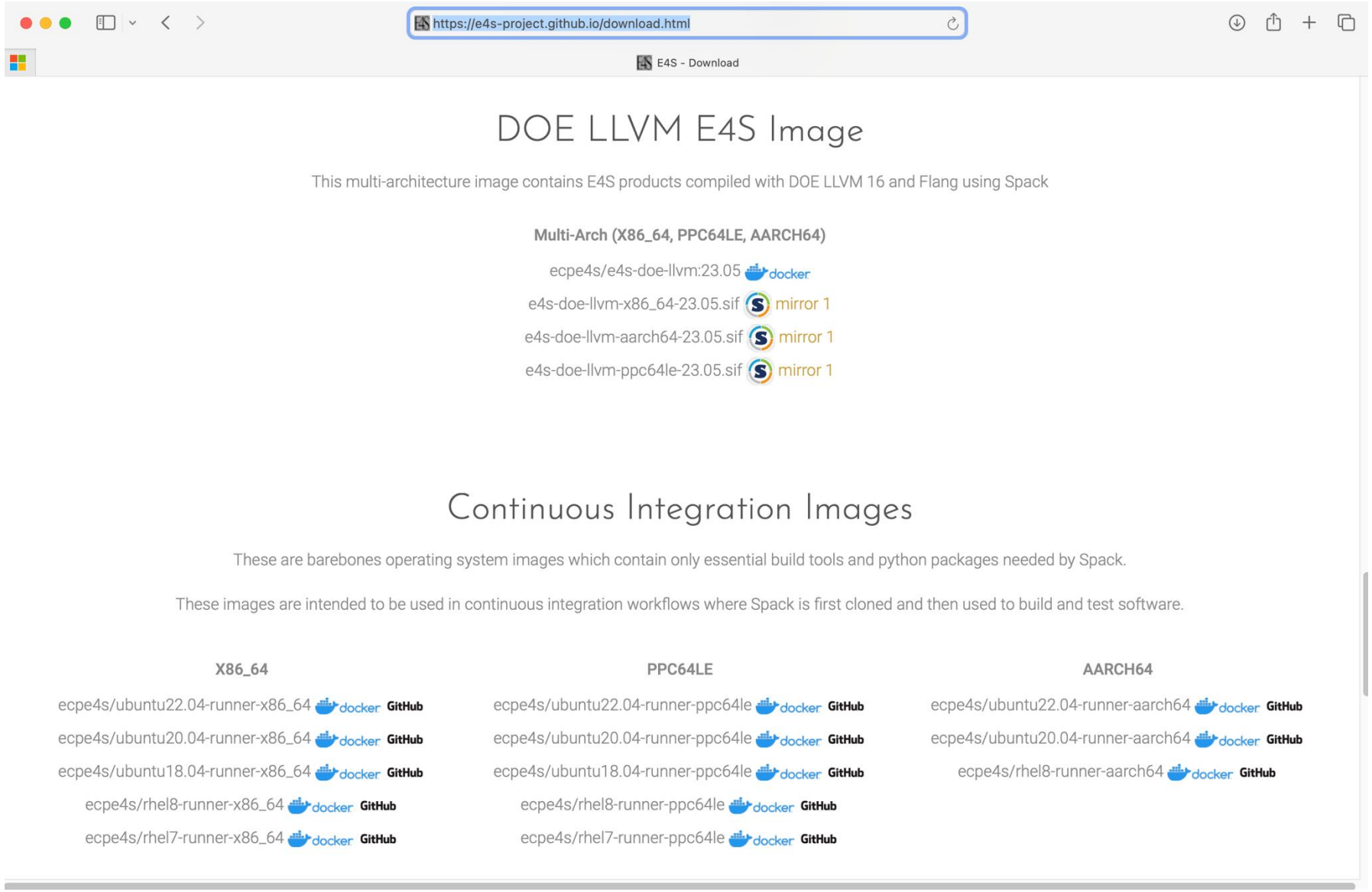


Add to a base image:

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

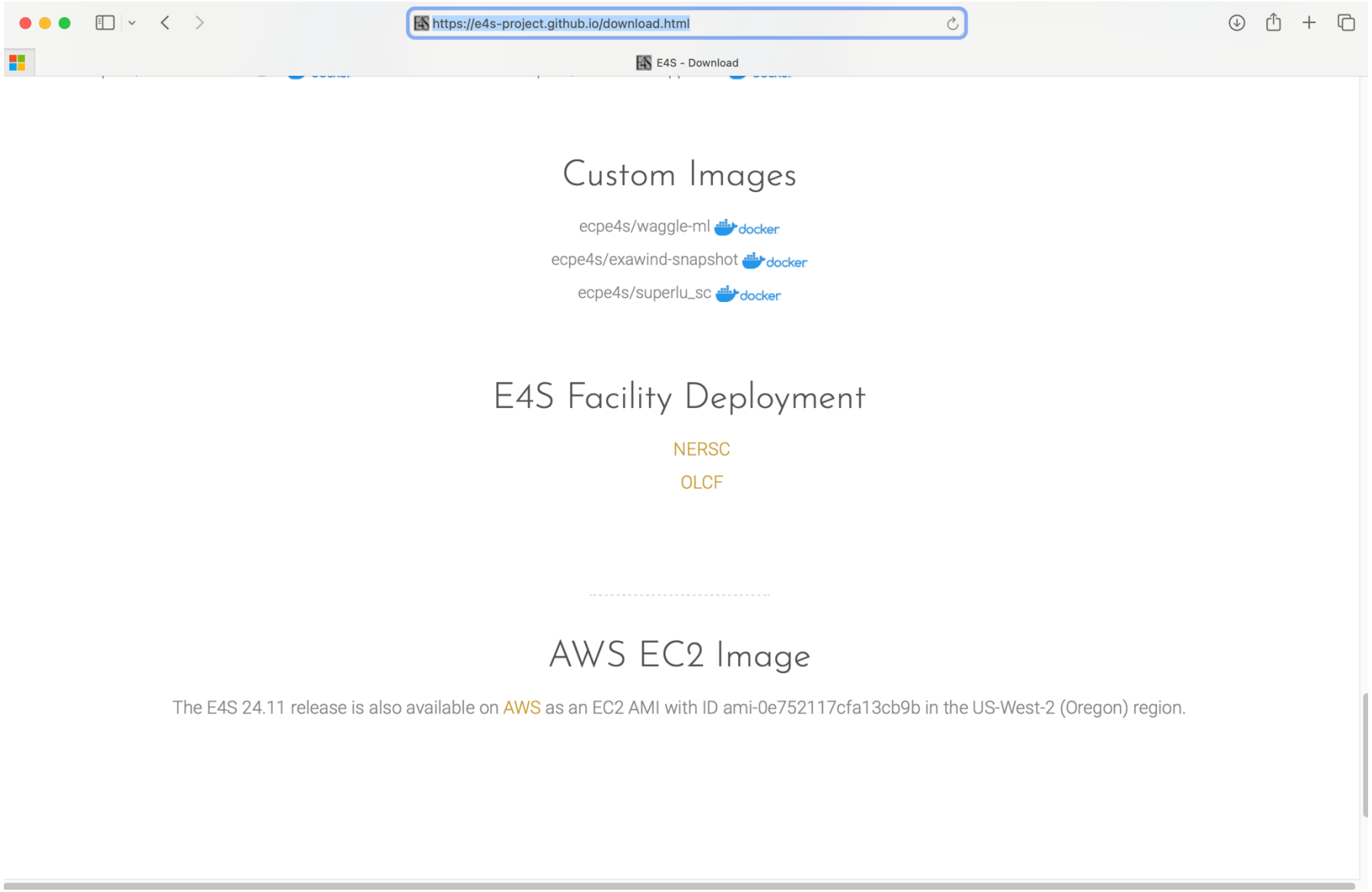
https://github.com/E4S-Project/e4s-alc

E4S DOE LLVM and CI images



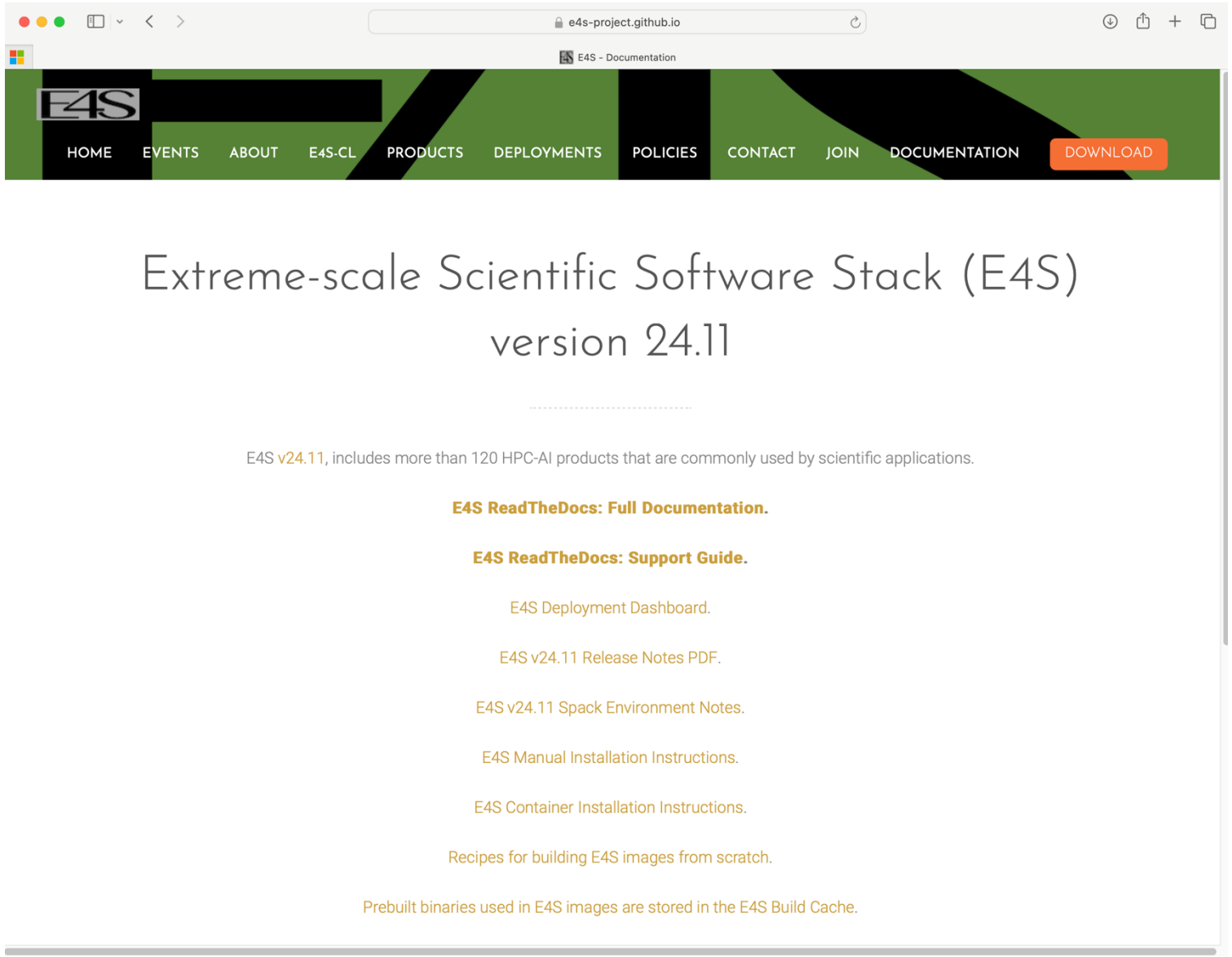
https://e4s.io

E4S Facility Deployment and AWS EC2 Image



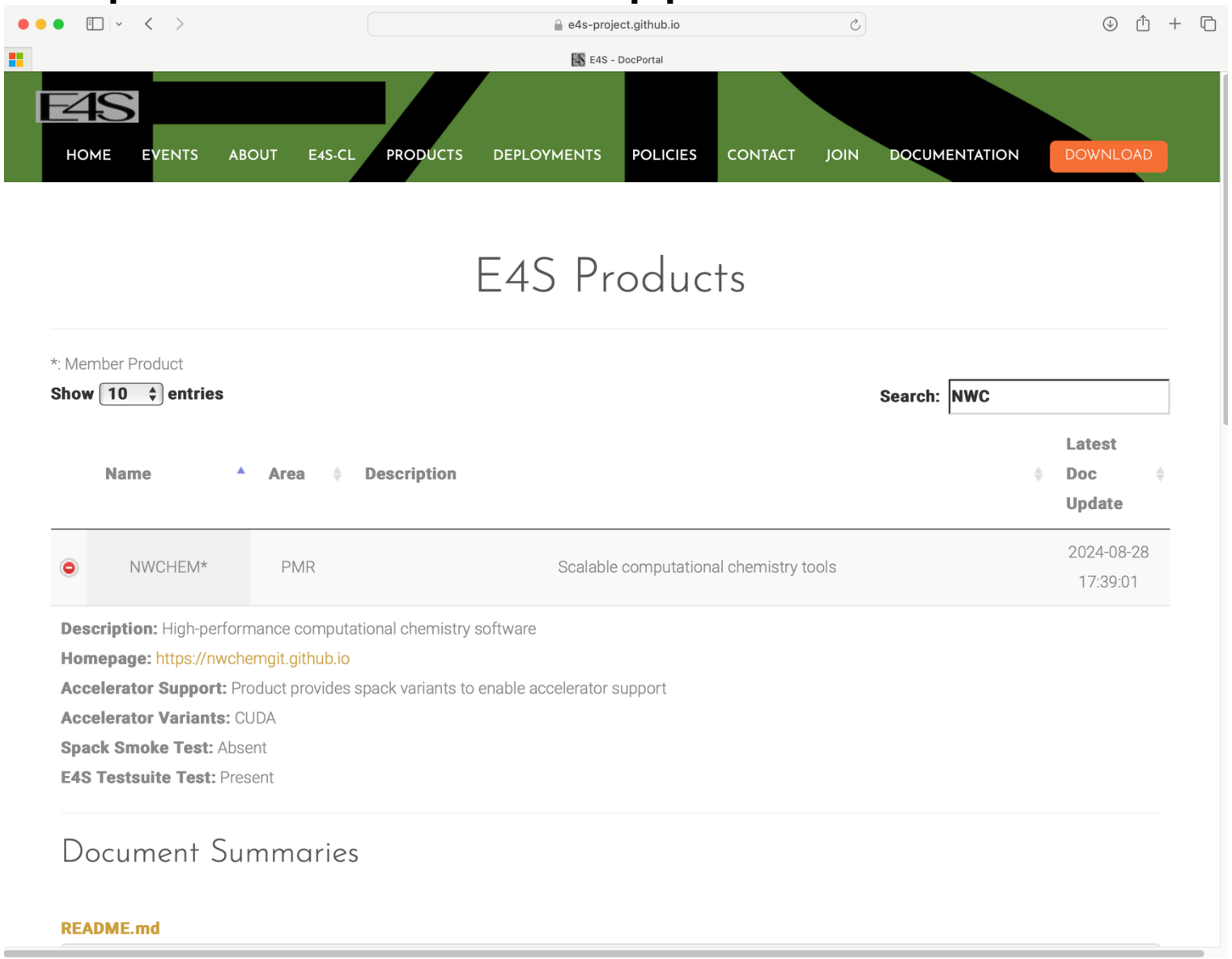
DOE Facility Deployment Dashboard: https://dashboard.e4s.io

E4S 24.11 Detailed Documentation for Bare-metal Installation



https://e4s.io

E4S DocPortal updated with new applications and AI/ML tools



https://e4s.io

24.11 Release: 132+ Official Products + dependencies (gcc, x86_64)

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 3:  aml                 /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/aml-0.2.1-um7i2rjzcwvuuvdcv2b65glixxtigwgp
 4:  amrex               /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/amrex-24.10-qj6rcrnpr25y2cgjwdoj2epxqjzl5aue
 5:  arborx              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/arborx-1.7-niomjhe5p4a4hh325j6chbth7l7ayqkt
 6:  argobots            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/argobots-1.2-y42c2tjyqheivojca5r4gtwav2frhxfq
 7:  ascent              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/ascent-0.9.3-howf7taucprs2x6gjytrzb7i27qyk2di
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 9:  bolt                /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/bolt-2.0-lbkmf6wfvfwy6bwvjgwqembrym2rsj3r
10:  blaspp              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/blaspp-2024.05.31-lighi4eqakal3xrpvvrohprkct6z5cbq
11:  bricks              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/bricks-2023.08.25-xaeozuhghlsrop5dvdv4kg7xsjazwiyt
12:  butterflypack       /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/butterflypack-2.4.0-fxwv7xee5hakm2x5ahyqkdzfaot4ds6m
13:  cabana              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/cabana-0.7.0-3tmy6mngjng347yg6nobbcqj4ypiz6aw
14:  caliper             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/caliper-2.11.0-w3e26s2efd5mccldzy4snlr7jhycdbw6
15:  camp                /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/camp-2024.07.0-igtbsjmqxaf75vksiskskv3cxlois5d4
16:  chai                /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/chai-2024.07.0-7i44tof2afbfy7hgbqqwl6chvge3n2oj
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18:  charliecloud        /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/charliecloud-0.38-axau5dagasekbzortmqohz3sbd2drxwc
19:  conduit             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/conduit-0.9.2-4lop2wk6c7cgt4n3pen6ixgotuxebvfd
20:  cp2k                /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/cp2k-2024.3-rpajcg3ekrpzceaqdddluoaf56rjjf63
21:  cusz                /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/cusz-0.6.0-ua6535ctrntpiu4w6tv7vois3vtaksn2
22:  darshan-runtime     /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/darshan-runtime-3.4.5-h23riorxiw6hh5w6b6b2ctadf46vbbsn
23:  datatransferkit     /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/datatransferkit-3.1.1-fijc2te2pqwsoz42367zu6ocipcosl4x
24:  dealii              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/dealii-9.5.1-7gooirgib4zmobwddrrrtzzbvs3quggi
25:  dyninst             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/dyninst-13.0.0-dhrv3i7ne73qsx4zncdbiwu67sojttha
26:  e4s-alc             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/e4s-alc-1.0.2-7nffclyxawkf3rihrvnyjj3n7blf6vpx
27:  e4s-cl              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/e4s-cl-1.0.4-kqi6dddd5n5lx3qaamfubqdqcz7zbjss
28:  ecp-data-vis-sdk    /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/ecp-data-vis-sdk-1.0-kv6y4i5hwnnu46xond4axik4acyu2rzx
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38:  gasnet              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/gasnet-2024.5.0-a6mvbkjs4m7fdxdcqv5o423sktdgtmmb
39:  ginkgo              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/ginkgo-1.8.0-qpn6kl7mlbesvmkzct46raa7hmzdhd6y
40:  globalarrays        /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/globalarrays-5.8.2-5byrunc5uqpdvstblfkuo62v7li6iktm
41:  gotcha              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/gotcha-1.0.7-azqu52zgl7yhkw2gerth77d2o4vr6ueo
42:  gptune              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/gptune-4.0.0-yzr7cb2u343pzmfi4salvtbqn34pqxys
43:  gromacs             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/gromacs-2024.3-bvmfbqkhii4mnj5eok6o6xwo3ekzsegl
44:  h5bench             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/h5bench-1.4-pvq4cwhbezgrp4kt4jt4zwnbdbgupfrr
```

GPU runtimes

- AMD (ROCm)
  - 6.2.1
- NVIDIA (CUDA)
  - 12.2
- NVHPC
  - 24.9
- Intel oneAPI 2024.2.0

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24.11 Release: 132+ Official Products + dependencies (gcc, x86_64)

45:	hdf5	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/hdf5-1.14.5-6gftpz5y6pewmq4htrv4pvyusx2ucb5m
46:	hdf5-vol-cache	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/hdf5-vol-cache-v1.1-mdjhbwzgeuu4oael5776dg2rdnstztow
47:	hdf5-vol-async	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/hdf5-vol-async-1.7-ysvyfanlwo22pwxmnpfg4uc3v5g7q734
48:	hdf5-vol-log	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/hdf5-vol-log-1.4.0-cmdphf2yvco7muxsie74vresudtoka6k
49:	heffte	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/heffte-2.4.0-n4cczmu374zwvbgtq6ivj7tftgkbes7w
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60:	libcatalyst	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/libcatalyst-2.0.0-wmryn2xoazqxcliwr5zsuptya6t7c3r7
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62:	libpressio	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/libpressio-0.99.4-hnscophslfa7qceldjh5otilcnkomth3
63:	libquo	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/libquo-1.4-b23b2c2gxo2k6gbd3b3sbqlhjwfapxef
64:	loki	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/loki-0.1.7-h5fwksmknmf4xcprze3w6nximk35qdmr
65:	magma	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/magma-2.8.0-hcbbkvi56bmvkhoalgh6fiznvymbgp46
66:	mercury	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/mercury-2.3.1-tpdwawhejfgph3c3r6ljrtf3y6zstfg4
67:	metall	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/metall-0.28-nsase6ghkowatq2qps2hin7x2mqcgwvi
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69:	mgard	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/mgard-2023-12-09-fxzwqezvoxiasi5gz4acduvr3ytquxbx
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71:	mpich	/usr/local/mpich/install/mpich
72:	mpifileutils	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/mpifileutils-0.11.1-nwd2qjjxnm4cbnwkhuitzjvks5kunt7q
73:	nccmp	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/nccmp-1.9.1.0-wxmr6dvro3sa4w63ssc6emnaqyucz3af
74:	nco	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/nco-5.2.4-zjl5pldmbwkkodhnuledgvoue55ek4uh
75:	nek5000	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/nek5000-19.0-dnczzmmqys75oxvb67g2cdyeyo5hkhdg
76:	nekbone	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/nekbone-17.0-4otvcgwld4x726c4izqjz4juavv2gn5n
77:	netcdf-fortran	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/netcdf-fortran-4.6.1-46yy72aftgzzgn6il4tl75lsfhvrx7wt
78:	netlib-scalapack	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/netlib-scalapack-2.2.0-zdskhgrbnit2p66ocwworxyr3yny64am
79:	nrm	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/nrm-0.1.0-22bucvue7afoqopfei7mjbtniztokob2
80:	nwchem	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/nwchem-7.2.3-bhf6p5dpfhceizb455b7yzecnehchyw6
81:	omega-h	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/omega-h-9.34.13-dse3dlpweicswst4gqro6tj2ykvdkqqv
82:	openfoam	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/openfoam-2312-rneedoueqezu7degtjhhe7wgxzh5r6tm
83:	openmpi	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/openmpi-5.0.5-y2n6rgve4vtb5tn2ja2fkpdoika5na7t
84:	openpmd-api	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/openpmd-api-0.16.0-3wdhvkspqg3zyruqr6yxo2ymfcojpbzl
85:	papi	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/papi-7.1.0-y2r2j4wpyzxl6bswtoujx5vlkmvzsui4
86:	papyrus	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/papyrus-1.0.2-3kc4d5gkeffjb4ynssjdcjt3263q54ab
87:	parallel-netcdf	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/parallel-netcdf-1.12.3-yhvlrjtdpkfsz2ks6l4mrrmi7fcn4hv4
88:	paraview	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/paraview-5.13.1-57dbd2bnczh6boehiho55cyjzecbt2zv

PESO

24.11 Release: 132+ Official Products + dependencies (gcc, x86_64)

```
 89:  parsec            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/parsec-3.0.2209-hkyu7eadk3ompvl26qbks43ig7ubbkr5
 90:  pdt               /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/pdt-3.25.2-njatamqvcyoenbaqcfykut236pgpzmg5
 91:  petsc             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/petsc-3.22.0-xqaokru57p65fnujzhe46oibuz2cj6iy
 92:  phist             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/phist-1.12.1-ttvy5sxtyz6o23wuvhbpdr4o4slynjwm
 93:  plasma            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/plasma-24.8.7-boidkyf2g3ivpgz2pfeatq6jm7zaatvs
 94:  plumed            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/plumed-2.9.2-6j47srexguggofkmjrpihytexgakdfhw
 95:  precice           /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/precice-3.1.2-o7prc6wqlx46tvwkb27ewr7ggxktetiu
 96:  pruners-ninja     /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/pruners-ninja-1.0.1-bxhxm47tfeamn32hcgqtubqosia3arjw
 97:  pumi              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/pumi-2.2.8-obecbm7tgul54yydoefxvl4bk3p6wo6p
 98:  py-cinemasci      /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/py-cinemasci-1.3-juxfpomndnt7nxagyqoikzwzmi2lqhdz
 99:  py-deephyper      /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/py-deephyper-0.6.0-l7wuzhvl3rbdao7aqxggcckfpfcmle5f
100:  py-jupyterhub     /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/py-jupyterhub-1.4.1-q6v3kng5b2uv7my6b2jwolbx5hjqoaju
101:  py-libensemble    /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/py-libensemble-1.4.2-dwn4j3guwwg7gf4scgikrsi4xf34lreu
102:  py-parsl          /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/py-parsl-2023.08.21-6qv2sz36iww2iqcbizmgbvvkrq4wctyf
103:  py-radical-saga   /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/py-radical-saga-1.47.0-h6ilsdskhrcwswaubyhqlgmvuakz2rmx
104:  qthreads          /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/qthreads-1.18-47igdbozrdzpb3d7ugl7rtlivip43zzb
105:  quantum-espresso  /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/quantum-espresso-7.3.1-gxjb4l6ebquee4cd3s6wtblday5hkrek
106:  raja              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/raja-2024.07.0-x5umeq7y6dkbg24gvynfynuhthbrstgk
107:  rempi             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/rempi-1.1.0-wc7zoqyhjpwooti6w3tfhakfvzfin6j7
108:  scr               /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/scr-3.0.1-orihokmj337do4g3fxwni3flzbuoy4ve
109:  slate             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/slate-2024.05.31-2ecdyrkid477yd3n2bp2m2mp2jxeqplq
110:  slepc             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/slepc-3.22.0-czym6tt5cma6iwuuffgx3ps5lt7hytcz
111:  stc               /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/stc-0.9.0-ybrlcxfyjtziof2umiea6bpw4ashzjcr
112:  strumpack         /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/strumpack-7.2.0-fsg63gooztalx7gyjjwzvlyfvryrorgb
113:  sundials          /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/sundials-7.1.1-vyp5hzc2igldtpii3qrkdeyasuggl5um
114:  superlu-dist      /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/superlu-dist-8.2.1-jcccuenwobtjuovmu4fry2trf6zdpwue
115:  swig              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/swig-4.1.1-gnw7j6q5wdctjirbqwcdm62rtrjfigfn
116:  sz3               /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/sz3-3.2.0-jkh6xikf24u7twxqtormgcrv2ephey3j
117:  tasmanian         /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/tasmanian-8.0-g7c3luju2qnluvul5vgxjrhczqlqsymg
118:  tau               /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/tau-2.34-77jqzzvfxwge47jxgh3dctiikh4ihhni
119:  trilinos          /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/trilinos-16.0.0-pi4g4hlvonmkxehtczq5irbhp2towxfs
120:  turbine           /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/turbine-1.3.0-ul2nrms5k2dhs3e55tw3io5bmbb2fh7i
121:  umap              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/umap-2.1.1-s5vkw5g44qmltngwpo7rr3pgiy55ed4d
122:  umpire            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/umpire-2024.07.0-76aq7phrhfeh5t3rkc6qq3pzytfmtcpn
123:  unifyfs           /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/unifyfs-2.0-oa6yjltv2nkfti5mf6dvi5etbh45fwv4
124:  upcxx             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/upcxx-2023.9.0-6ujtk32su3pd4fptu5rv5aywtevg7wpm
125:  variorum          /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/variorum-0.8.0-ryt7oqpkh2yhnznoc33esdcxnnztcoqp
126:  veloc             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/veloc-1.7-6yqgctazcu3tzazt6iiyr62bj3rtyenj
127:  visit             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/visit-3.3.3-xeoojeuxgi3o4dl5iyxudwv6bbvkvagv
128:  vtk-m             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/vtk-m-2.2.0-z4p7ayhzobpfkqkooxptmmmhx7wlh7yl
129:  wannier90         /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/wannier90-3.1.0-xdvmgbczsrgdpacfmals75rru2vksoyb
130:  wrf               /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/wrf-4.5.2-jw3bykeqmnqxjsfjhc4vb3pmijqcofrt
131:  xyce              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/xyce-7.8.0-ssv6luer2sm3hpjs4canpwo74rrgrnrb
132:  zfp               /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/zfp-1.0.0-vgp33oumk4xnqzbnwnxosrisvofqxja2
```

Languages:

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

AI products

- NVIDIA NeMo™
- TensorBraid
- DeepHyper
- OpenAI
- Tensorflow
- Pytorch
- JAX
- Horovod
- LBANN

EDA Tools:

- Xyce

3D Visualization

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

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-24.11-cuda90-arm64.sif
Singularity> nvidia-smi
Fri Nov 15 20:18:04 2024
+-----------------------------------------------------------------------------------------+
| NVIDIA-SMI 550.54.15              Driver Version: 550.54.15      CUDA Version: 12.4     |
|-----------------------------------------+------------------------+----------------------+
| 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   24C    P0             84W /  700W |     139MiB /  97871MiB |      0%      Default |
|                                         |                        |             Disabled |
+-----------------------------------------+------------------------+----------------------+

+-----------------------------------------------------------------------------------------+
| Processes:                                                                              |
|  GPU   GI   CI        PID   Type   Process name                              GPU Memory |
|        ID   ID                                                               Usage      |
|=========================================================================================|
|    0   N/A  N/A      3666      G   /usr/libexec/Xorg                              4MiB |
+-----------------------------------------------------------------------------------------+
Singularity> python
Python 3.10.15 (main, Sep  7 2024, 18:35:38) [GCC 13.2.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import torch
>>> torch.__version__
'2.5.0'
>>> torch.cuda.get_arch_list()
['sm_75', 'sm_80', 'sm_90']
>>> torch.cuda.get_device_name(0)
'NVIDIA GH200 480GB'
>>>
Singularity> grep _NAME /etc/os-release
PRETTY_NAME="Ubuntu 24.04.1 LTS"
```

Updated:
PyTorch: 2.5.0

E4S 24.11 supports NVIDIA Grace-Hopper GH200 GPUs with TensorFlow and PyTorch

E4S Support for AI/ML and Python tools

```
$ singularity run --nv e4s-24.11-cuda90-amd64.sif
Singularity> python
Python 3.10.12 (main, Sep 11 2024, 15:47:36) [GCC 11.4.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import nemo
>>> import openai
>>> import google.generativeai
>>> import tensorflow
>>> import torch
>>> import huggingface_hub
>>> import jax
>>> import deephyper
>>> import pandas
>>> import cv2
>>> import sklearn
>>> import open3d
>>> import numpy
>>> import scipy
>>> import matplotlib
>>> import seaborn
>>> import plotly
>>> import mpi4py
>>> nemo.__version__
'2.0.0rc1'
>>> tensorflow.__version__
'2.16.1'
>>> torch.__version__
'2.3.0+cu121'
>>> torch.cuda.get_arch_list()
['sm_50', 'sm_60', 'sm_70', 'sm_75', 'sm_80', 'sm_86', 'sm_90']
>>>
Singularity>
```

Updated:
Tensorflow: 2.16.1
NVIDIA NeMo™: 2.0.0rc1

E4S 24.11 Support for GPUs: NVIDIA

```
$ singularity run --nv e4s-24.11-cuda90-arm64.sif
Singularity> spack find -x +cuda
-- linux-ubuntu24.04-aarch64 / gcc@13.2.0 ------------------------
adios2@2.10.1  caliper@2.11.0       flecsi@2.3.0      hpctoolkit@2024.01.1  legion@24.09.0     petsc@3.22.0      sundials@7.1.1      umpire@2024.07.0
amrex@24.10    chai@2024.07.0       flux-core@0.66.0  hpx@1.10.0            libpressio@0.99.4  raja@2024.07.0    superlu-dist@8.2.1  vtk-m@2.2.0
arborx@1.7     cusz@0.6.0           ginkgo@1.8.0      hypre@2.32.0          mfem@4.7.0         slate@2024.05.31  tasmanian@8.0       zfp@0.5.5
axom@0.9.0     ecp-data-vis-sdk@1.0 gromacs@2024.3    kokkos@4.4.01         mgard@2023-12-09   slepc@3.22.0      tau@2.34
cabana@0.7.0   fftx@1.2.0           heffte@2.4.0      kokkos-kernels@4.4.01 parsec@3.0.2209    strumpack@7.2.0   trilinos@16.0.0
==> 38 installed packages
Singularity> spack find -x
-- linux-ubuntu24.04-aarch64 / gcc@13.2.0 ------------------------
adios@1.13.1         cusz@0.6.0             gmp@6.3.0            lbann@0.104          nrm@0.1.0          py-jupyterhub@1.4.1     tasmanian@8.0
adios2@2.10.1        darshan-runtime@3.4.5  gotcha@1.0.7         legion@24.09.0       nvhpc@24.9         py-libensemble@1.4.2    tau@2.34
adios2@2.10.1        darshan-util@3.4.5     gptune@4.0.0         legion@24.09.0       nwchem@7.2.3       py-petsc4py@3.22.0      tau@2.34
alquimia@1.1.0       datatransferkit@3.1.1  gromacs@2024.3       libcatalyst@2.0.0    omega-h@9.34.13    qthreads@1.18           trilinos@16.0.0
aml@0.2.1            dealii@9.5.1           gromacs@2024.3       libnrm@0.1.0         openfoam@2312      quantum-espresso@7.3.1  trilinos@16.0.0
amrex@24.10          dyninst@13.0.0         h5bench@1.4          libpressio@0.99.4    openmpi@5.0.5      raja@2024.07.0          turbine@1.3.0
amrex@24.10          e4s-alc@1.0.2          hdf5@1.12.3          libpressio@0.99.4    openpmd-api@0.16.0 raja@2024.07.0          umap@2.1.1
arborx@1.7           e4s-cl@1.0.4           hdf5@1.14.5          libquo@1.4           papi@7.1.0         rempi@1.1.0             umpire@2024.07.0
arborx@1.7           ecp-data-vis-sdk@1.0   hdf5-vol-async@1.7   libunwind@1.6.2      papyrus@1.0.2      scr@3.0.1               umpire@2024.07.0
argobots@1.2         exago@1.6.0            hdf5-vol-cache@v1.1  loki@0.1.7           parallel-netcdf@1.12.3 slate@2024.05.31    upcxx@2023.9.0
ascent@0.9.3         exaworks@0.1.0         hdf5-vol-log@1.4.0   mercury@2.3.1        paraview@5.13.1    slate@2024.05.31        veloc@1.7
axom@0.9.0           faodel@1.2108.1        heffte@2.4.0         metall@0.28          parsec@3.0.2209    slepc@3.22.0            vtk-m@2.2.0
axom@0.9.0           fftx@1.2.0             heffte@2.4.0         mfem@4.7.0           parsec@3.0.2209    slepc@3.22.0            vtk-m@2.2.0
boost@1.79.0         fftx@1.2.0             hpctoolkit@2024.01.1 mfem@4.7.0           pdt@3.25.2         stc@0.9.0               wannier90@3.1.0
butterflypack@2.4.0  flecsi@2.3.0           hpctoolkit@2024.01.1 mgard@2023-12-09     petsc@3.22.0       strumpack@7.2.0         warpx@24.10
cabana@0.7.0         flecsi@2.3.0           hpx@1.10.0           mgard@2023-12-09     petsc@3.22.0       strumpack@7.2.0         wps@4.5
cabana@0.7.0         flit@2.1.0             hpx@1.10.0           mpark-variant@1.4.0  phist@1.12.1       sundials@7.1.1          wrf@4.5.2
caliper@2.11.0       flux-core@0.66.0       hypre@2.32.0         mpich@4.2.3          plasma@24.8.7      sundials@7.1.1          xyce@7.8.0
caliper@2.11.0       flux-core@0.66.0       hypre@2.32.0         mpifileutils@0.11.1  plumed@2.9.2       superlu@5.3.0           zfp@0.5.5
chai@2024.07.0       fpm@0.10.0             kokkos@4.4.01        nccmp@1.9.1.0        precice@3.1.2      superlu-dist@8.2.1      zfp@1.0.0
chai@2024.07.0       gasnet@2024.5.0        kokkos@4.4.01        nco@5.2.4            pruners-ninja@1.0.1 superlu-dist@8.2.1
chapel@2.2.0         ginkgo@1.8.0           kokkos-kernels@4.4.01 nek5000@19.0        pumi@2.2.8         swig@4.0.2-fortran
charliecloud@0.38    ginkgo@1.8.0           kokkos-kernels@4.4.01 nekbone@17.0        py-cinemasci@1.7.0 sz@2.1.12.5
conduit@0.9.2        globalarrays@5.8.2     laghos@3.1           netcdf-fortran@4.6.1 py-deephyper@0.6.0 sz3@3.2.0
cuda@12.6.2          glvis@4.2              lammps@20240829      netlib-scalapack@2.2.0 py-h5py@3.11.0   tasmanian@8.0
==> 170 installed packages
```

E4S 24.11 Support for GPUs: NVIDIA (modules)

```
$ singularity run --nv e4s-24.11-cuda90-amd64.sif
Singularity> module avail

------------------------------------------------ /spack/share/spack/lmod/linux-ubuntu22.04-x86_64/mpich/4.2.3-5o2ypwn/Core ------------------------------------------------
   adios/1.13.1                      flecsi/2.3.0                  (D)    mfem/4.7.0                    (D)    slepc/3.22.0-cuda90
   adios2/2.7.1                      fortrilinos/2.3.0                    mpifileutils/0.11.1                  slepc/3.22.0                  (D)
   adios2/2.10.1-cuda90       (D)    ginkgo/1.8.0-cuda90-openmp           nccmp/1.9.1.0                        stc/0.9.0
   alquimia/1.1.0                    ginkgo/1.8.0-openmp           (D)    nco/5.2.4                            strumpack/7.2.0-cuda90-openmp
   amrex/24.10-cuda90                globalarrays/5.8.2                   nek5000/19.0                         strumpack/7.2.0-openmp        (D)
   amrex/24.10                (D)    glvis/4.2                            nekbone/17.0                         sundials/7.1.1-cuda90
   arborx/1.7-cuda90                 gptune/4.0.0                         netcdf-fortran/4.6.1                 sundials/7.1.1                (D)
   arborx/1.7                 (D)    gromacs/2024.3-cuda90-openmp         netlib-scalapack/2.2.0               superlu-dist/8.2.1-cuda90
   ascent/0.9.3-openmp               gromacs/2024.3-openmp         (D)    nwchem/7.2.3                         superlu-dist/8.2.1            (D)
   axom/0.9.0-cuda90-openmp          h5bench/1.4                          omega-h/9.34.13                      sz/2.1.12.5
   axom/0.9.0-openmp          (D)    hdf5-vol-async/1.7                   openfoam/2312                        tasmanian/8.0-cuda90
   boost/1.79.0                      hdf5-vol-cache/v1.1                  openpmd-api/0.16.0                   tasmanian/8.0                 (D)
   bricks/2023.08.25-cuda            hdf5-vol-log/1.4.0                   papyrus/1.0.2                        tau/2.34-cuda
   bricks/2023.08.25          (D)    hdf5/1.12.3                          parallel-netcdf/1.12.3               tau/2.34                      (D)
   butterflypack/2.4.0-openmp        heffte/2.4.0-cuda90                  paraview/5.13.1-cuda90               trilinos/13.0.1
   cabana/0.7.0-cuda90               heffte/2.4.0                  (D)    paraview/5.13.1               (D)    trilinos/16.0.0-cuda90
   cabana/0.7.0               (D)    hpctoolkit/2024.01.1-cuda            parsec/3.0.2209-cuda90               trilinos/16.0.0               (D)
   caliper/2.11.0-cuda90             hpctoolkit/2024.01.1          (D)    parsec/3.0.2209               (D)    turbine/1.3.0
   caliper/2.11.0             (D)    hpx/1.10.0-cuda90                    petsc/3.22.0-cuda90                  umpire/2024.07.0-cuda90
   chai/2024.07.0-cuda90             hpx/1.10.0                    (D)    petsc/3.22.0                  (D)    umpire/2024.07.0              (D)
   chai/2024.07.0             (D)    hypre/2.32.0-cuda90                  phist/1.12.1-openmp                  unifyfs/2.0
   conduit/0.9.2                     hypre/2.32.0                  (D)    plumed/2.9.2                         upcxx/2023.9.0-cuda90
   cp2k/2024.3-openmp                laghos/3.1                           precice/3.1.2                        upcxx/2023.9.0                (D)
   darshan-runtime/3.4.5             lammps/20240829-cuda90-openmp        pruners-ninja/1.0.1                  veloc/1.7
   datatransferkit/3.1.1             lammps/20240829-openmp        (D)    pumi/2.2.8                           visit/3.3.3
   dealii/9.5.1                      lbann/0.104                          py-cinemasci/1.3                     vtk-m/2.2.0-cuda90-openmp
   dyninst/13.0.0-openmp             libcatalyst/2.0.0                    py-h5py/3.11.0                       vtk-m/2.2.0-openmp            (D)
   ecp-data-vis-sdk/1.0-cuda90       libnrm/0.1.0                         py-libensemble/1.4.2                 wannier90/3.1.0
   ecp-data-vis-sdk/1.0       (D)    libpressio/0.99.4-cuda90-openmp      py-petsc4py/3.22.0                   wps/4.5
   exago/1.6.0-cuda80                libpressio/0.99.4-openmp      (D)    quantum-espresso/7.3.1-openmp        wrf/4.5.2
   exago/1.6.0                (D)    libquo/1.4                           rempi/1.1.0                          xyce/7.8.0
   exaworks/0.1.0                    mercury/2.3.1                        scr/3.0.1
   faodel/1.2108.1                   metall/0.28                          slate/2.024.05.31-cuda90-openmp
   flecsi/2.3.0-cuda90               mfem/4.7.0-cuda90                    slate/2.024.05.31-openmp      (D)

------------------------------------------------------------ /spack/share/spack/lmod/linux-ubuntu22.04-x86_64/Core ------------------------------------------------------------
   aml/0.2.1                 fftx/1.2.0                  (D)    kokkos/4.4.01-openmp          (D)    nvhpc/24.9                 superlu/5.3.0
   argobots/1.2              flit/2.1.0                         legion/24.09.0-cuda70                nvhpc/25.5                 swig/4.0.2-fortran
   bolt/2.0                  flux-core/0.66.0-cuda              legion/24.09.0                (D)    papi/7.1.0-cuda            sz3/3.2.0
   chapel/2.2.0-cuda90       flux-core/0.66.0            (D)    libunwind/1.6.2                      papi/7.1.0           (D)    umap/2.1.1
   chapel/2.2.0       (D)    fpm/0.10.0-openmp                  loki/0.1.7                           pdt/3.25.2                 variorum/0.8.0
   charliecloud/0.38         gasnet/2024.5.0                    magma/2.8.0-cuda90                   plasma/24.8.7              zfp/0.5.5-cuda90
   cusz/0.6.0-cuda90         gmp/6.3.0                          mgard/2023-12-09-cuda90-openmp       py-deephyper/0.6.0         zfp/0.5.5          (D)
   darshan-util/3.4.5        gotcha/1.0.7                       mgard/2023-12-09-openmp       (D)    py-jupyterhub/1.4.1
   e4s-alc/1.0.2             kokkos-kernels/4.4.01-cuda90       mpark-variant/1.4.0                  qthreads/1.18
   e4s-cl/1.0.4              kokkos-kernels/4.4.01-openmp (D)   mpich/4.2.3                   (L)    raja/2024.07.0-cuda90
```

E4S 24.11 Support for GPUs: AMD MI300A/MI300X (gfx942)

```
$ singularity run e4s-24.11-rocm942-amd64.sif
Singularity> spack find -x +rocm
-- linux-ubuntu22.04-x86_64 / gcc@11.4.0 ------------------------
amrex@24.10    caliper@2.11.0  gasnet@2024.5.0  hpctoolkit@2024.01.1  kokkos@4.4.01   mfem@4.7.0      slate@2024.05.31  sundials@7.1.1      tau@2.34          upcxx@2023.9.0
arborx@1.7     chai@2024.07.0  ginkgo@1.8.0     hpx@1.10.0            legion@24.09.0  petsc@3.22.0    slepc@3.22.0      superlu-dist@8.2.1  trilinos@16.0.0   vtk-m@2.2.0
cabana@0.7.0   fftx@1.2.0      heffte@2.4.0     hypre@2.32.0          magma@2.8.0     raja@2024.07.0  strumpack@7.2.0   tasmanian@8.0       umpire@2024.07.0
==> 29 installed packages
Singularity> spack find -x
-- linux-ubuntu22.04-x86_64 / gcc@11.4.0 ------------------------
adios@1.13.1          cp2k@2024.3            glvis@4.2              legion@24.09.0          omega-h@9.34.13         qthreads@1.18           tau@2.34
adios2@2.7.1          darshan-runtime@3.4.5  gmp@6.3.0              libcatalyst@2.0.0       openfoam@2312           quantum-espresso@7.3.1  trilinos@13.0.1
alquimia@1.1.0        darshan-util@3.4.5     gotcha@1.0.7           libnrm@0.1.0            openmpi@5.0.5           raja@2024.07.0          trilinos@16.0.0
aml@0.2.1             datatransferkit@3.1.1  gptune@4.0.0           libpressio@0.99.4       openpmd-api@0.16.0      raja@2024.07.0          trilinos@16.0.0
amrex@24.10           dealii@9.5.1           gromacs@2024.3         libquo@1.4              papi@7.1.0              rempi@1.1.0             turbine@1.3.0
amrex@24.10           dyninst@13.0.0         h5bench@1.4            libunwind@1.6.2         papyrus@1.0.2           scr@3.0.1               umap@2.1.1
arborx@1.7            e4s-alc@1.0.2          hdf5@1.12.3            loki@0.1.7              parallel-netcdf@1.12.3  slate@2024.05.31        umpire@2024.07.0
arborx@1.7            e4s-cl@1.0.4           hdf5-vol-async@1.7     magma@2.8.0             paraview@5.13.1         slate@2024.05.31        umpire@2024.07.0
argobots@1.2          ecp-data-vis-sdk@1.0   hdf5-vol-cache@v1.1    mercury@2.3.1           parsec@3.0.2209         slepc@3.22.0            unifyfs@2.0
ascent@0.9.3          exago@1.6.0            heffte@2.4.0           metall@0.28             pdt@3.25.2              slepc@3.22.0            upcxx@2023.9.0
axom@0.9.0            exaworks@0.1.0         heffte@2.4.0           mfem@4.7.0              petsc@3.22.0            stc@0.9.0               upcxx@2023.9.0
bolt@2.0              faodel@1.2108.1        hpctoolkit@2024.01.1   mfem@4.7.0              petsc@3.22.0            strumpack@7.2.0         variorum@0.8.0
boost@1.79.0          fftx@1.2.0             hpctoolkit@2024.01.1   mgard@2023-12-09        phist@1.12.1            strumpack@7.2.0         veloc@1.7
bricks@2023.08.25     fftx@1.2.0             hpx@1.10.0             mpark-variant@1.4.0     plasma@24.8.7           sundials@7.1.1          visit@3.3.3
butterflypack@2.4.0   flecsi@2.3.0           hpx@1.10.0             mpich@4.2.3             plumed@2.9.2            sundials@7.1.1          vtk-m@2.2.0
cabana@0.7.0          flit@2.1.0             hypre@2.32.0           mpifileutils@0.11.1     precice@3.1.2           superlu@5.3.0           vtk-m@2.2.0
cabana@0.7.0          flux-core@0.66.0       hypre@2.32.0           nccmp@1.9.1.0           pruners-ninja@1.0.1     superlu-dist@8.2.1      wannier90@3.1.0
caliper@2.11.0        fortrilinos@2.3.0      kokkos@4.4.01          nco@5.2.4               pumi@2.2.8              superlu-dist@8.2.1      wps@4.5
caliper@2.11.0        fpm@0.10.0             kokkos@4.4.01          nek5000@19.0            py-cinemasci@1.3        swig@4.0.2-fortran      wrf@4.5.2
chai@2024.07.0        gasnet@2024.5.0        kokkos-kernels@4.4.01  nekbone@17.0            py-deephyper@0.6.0      sz@2.1.12.5             xyce@7.8.0
chai@2024.07.0        gasnet@2024.5.0        laghos@3.1             netcdf-fortran@4.6.1    py-h5py@3.11.0          sz3@3.2.0               zfp@0.5.5
chapel@2.2.0          ginkgo@1.8.0           lammps@20240829        netlib-scalapack@2.2.0  py-jupyterhub@1.4.1     tasmanian@8.0
charliecloud@0.38     ginkgo@1.8.0           lbann@0.104            nrm@0.1.0               py-libensemble@1.4.2    tasmanian@8.0
conduit@0.9.2         globalarrays@5.8.2     legion@24.09.0         nwchem@7.2.3            py-petsc4py@3.22.0      tau@2.34
==> 165 installed packages
Singularity>
```

E4S 24.11 Support for GPUs: AMD (modules for gfx942)

```
Singularity> module avail

---------------------------------------------- /spack/share/spack/lmod/linux-ubuntu22.04-x86_64/mpich/4.2.3-5o2ypwn/Core ----------------------------------------------
   adios/1.13.1                      exago/1.6.0                      lbann/0.104                      petsc/3.22.0                  (D)    tasmanian/8.0-gfx942
   adios2/2.7.1                      exaworks/0.1.0                   libcatalyst/2.0.0                phist/1.12.1-openmp                 tasmanian/8.0          (D)
   alquimia/1.1.0                    faodel/1.2108.1                  libnrm/0.1.0                     plumed/2.9.2                        tau/2.34-rocm
   amrex/24.10-gfx942                flecsi/2.3.0                     libpressio/0.99.4-openmp         precice/3.1.2                       tau/2.34               (D)
   amrex/24.10               (D)     fortrilinos/2.3.0                libquo/1.4                       pruners-ninja/1.0.1                 trilinos/13.0.1
   arborx/1.7-gfx942                 ginkgo/1.8.0-gfx942-openmp       mercury/2.3.1                    pumi/2.2.8                          trilinos/16.0.0-gfx942
   arborx/1.7                (D)     ginkgo/1.8.0-openmp       (D)    metall/0.28                      py-cinemasci/1.3                    trilinos/16.0.0        (D)
   ascent/0.9.3-openmp               globalarrays/5.8.2               mfem/4.7.0-gfx942                py-h5py/3.11.0                      turbine/1.3.0
   axom/0.9.0-openmp                 glvis/4.2                        mfem/4.7.0                (D)    py-libensemble/1.4.2                umpire/2024.07.0-gfx942
   boost/1.79.0                      gptune/4.0.0                     mpifileutils/0.11.1              py-petsc4py/3.22.0                  umpire/2024.07.0       (D)
   bricks/2023.08.25                 gromacs/2024.3-openmp            nccmp/1.9.1.0                    quantum-espresso/7.3.1-openmp       unifyfs/2.0
   butterflypack/2.4.0-openmp        h5bench/1.4                      nco/5.2.4                        rempi/1.1.0                         upcxx/2023.9.0-gfx942
   cabana/0.7.0-gfx942-rocm          hdf5-vol-async/1.7               nek5000/19.0                     scr/3.0.1                           upcxx/2023.9.0         (D)
   cabana/0.7.0              (D)     hdf5-vol-cache/v1.1              nekbone/17.0                     slate/2024.05.31-gfx942-openmp      veloc/1.7
   caliper/2.11.0-gfx942             hdf5/1.12.3                      netcdf-fortran/4.6.1             slate/2024.05.31-openmp       (D)   visit/3.3.3
   caliper/2.11.0            (D)     heffte/2.4.0-gfx942              netlib-scalapack/2.2.0           slepc/3.22.0-gfx942                 vtk-m/2.2.0-gfx942
   chai/2024.07.0-gfx942             heffte/2.4.0              (D)    nwchem/7.2.3                     slepc/3.22.0                  (D)   vtk-m/2.2.0-openmp     (D)
   chai/2024.07.0            (D)     hpctoolkit/2024.01.1-rocm        omega-h/9.34.13                  stc/0.9.0                           wannier90/3.1.0
   conduit/0.9.2                     hpctoolkit/2024.01.1      (D)    openfoam/2312                    strumpack/7.2.0-gfx942-openmp       wps/4.5
   cp2k/2024.3-openmp                hpx/1.10.0-gfx942                openpmd-api/0.16.0               strumpack/7.2.0-openmp        (D)   wrf/4.5.2
   darshan-runtime/3.4.5             hpx/1.10.0                (D)    papyrus/1.0.2                    sundials/7.1.1-gfx942               xyce/7.8.0
   datatransferkit/3.1.1             hypre/2.32.0-gfx942              parallel-netcdf/1.12.3           sundials/7.1.1                (D)
   dealii/9.5.1                      hypre/2.32.0              (D)    paraview/5.13.1                  superlu-dist/8.2.1-gfx942
   dyninst/13.0.0-openmp             laghos/3.1                       parsec/3.0.2209                  superlu-dist/8.2.1            (D)
   ecp-data-vis-sdk/1.0              lammps/20240829-openmp           petsc/3.22.0-gfx942              sz/2.1.12.5

------------------------------------------------------------ /spack/share/spack/lmod/linux-ubuntu22.04-x86_64/Core -------------------------------------------------------------
   aml/0.2.1             fftx/1.2.0-gfx942             gotcha/1.0.7                      magma/2.8.0-gfx942            plasma/24.8.7                 sz3/3.2.0
   argobots/1.2          fftx/1.2.0             (D)    kokkos-kernels/4.4.01-openmp      mgard/2023-12-09-openmp       py-deephyper/0.6.0            umap/2.1.1
   bolt/2.0              flit/2.1.0                    kokkos/4.4.01-gfx942              mpark-variant/1.4.0           py-jupyterhub/1.4.1           variorum/0.8.0
   chapel/2.2.0          flux-core/0.66.0              kokkos/4.4.01-openmp       (D)    mpich/4.2.3            (L)    qthreads/1.18                 zfp/0.5.5
   charliecloud/0.38     fpm/0.10.0-openmp             legion/24.09.0-gfx942             nrm/0.1.0                     raja/2024.07.0-gfx942
   darshan-util/3.4.5    gasnet/2024.5.0-gfx942        legion/24.09.0             (D)    openmpi/5.0.5                 raja/2024.07.0         (D)
   e4s-alc/1.0.2         gasnet/2024.5.0        (D)    libunwind/1.6.2                   papi/7.1.0                    superlu/5.3.0
   e4s-cl/1.0.4          gmp/6.3.0                     loki/0.1.7                        pdt/3.25.2                    swig/4.0.2-fortran

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

E4S 24.11 Support for GPUs: Intel

```
$ singularity run e4s-24.11-oneapi-amd64.sif
Singularity> which dpcpp
/opt/intel/oneapi/compiler/2024.2/bin/dpcpp
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@2024.2.1 ------------------
amrex@24.10  arborx@1.7  cabana@0.7.0  ginkgo@1.8.0  heffte@2.4.0  kokkos@4.4.01  kokkos@4.4.01  kokkos@4.4.01  petsc@3.22.0  sundials@7.1.1  tau@2.34  upcxx@2023.9.0
==> 12 installed packages
Singularity> spack find -x
-- linux-ubuntu22.04-x86_64 / gcc@11.4.0 -----------------------
papi@7.1.0

-- linux-ubuntu22.04-x86_64 / oneapi@2024.2.1 ------------------
adios@1.13.1          charliecloud@0.38      globalarrays@5.8.2          kokkos-kernels@4.4.01  netlib-scalapack@2.2.0  py-h5py@3.11.0         tasmanian@8.0
adios2@2.8.3          conduit@0.9.2          glvis@4.2                   laghos@3.1             nrm@0.1.0               py-jupyterhub@1.4.1    tau@2.34
aml@0.2.1             darshan-runtime@3.4.5  gmp@6.3.0                   lammps@20240829        nwchem@7.2.3            py-libensemble@1.4.2   tau@2.34
aml@0.2.1             darshan-util@3.4.5     gotcha@1.0.7                legion@24.09.0         omega-h@9.34.13         py-petsc4py@3.22.0     trilinos@13.0.1
amrex@24.10           datatransferkit@3.1.1  gptune@4.0.0                libcatalyst@2.0.0      openmpi@5.0.5           qthreads@1.18          trilinos@16.0.0
amrex@24.10           dealii@9.5.1           gromacs@2024.3              libnrm@0.1.0           openpmd-api@0.16.0      raja@2024.07.0         turbine@1.3.0
arborx@1.7            e4s-alc@1.0.2          h5bench@1.4                 libquo@1.4             papyrus@1.0.2           rempi@1.1.0            umap@2.1.1
arborx@1.7            e4s-cl@1.0.4           hdf5@1.12.3                 libunwind@1.6.2        parallel-netcdf@1.12.3  scr@3.0.1              umpire@2024.07.0
argobots@1.2          ecp-data-vis-sdk@1.0   hdf5-vol-async@1.7          loki@0.1.7             paraview@5.13.1         slate@2024.05.31       unifyfs@2.0
ascent@0.9.3          exago@1.6.0            hdf5-vol-cache@v1.1         mercury@2.3.1          parsec@3.0.2209         slepc@3.22.0           upcxx@2023.9.0
axom@0.9.0            exaworks@0.1.0         hdf5-vol-log@1.4.0          metall@0.28            pdt@3.25.2              stc@0.9.0              upcxx@2023.9.0
bolt@2.0              faodel@1.2108.1        heffte@2.4.0                mfem@4.7.0             petsc@3.22.0            strumpack@7.2.0        variorum@0.8.0
boost@1.86.0          flecsi@2.3.0           heffte@2.4.0                mgard@2023-12-09       petsc@3.22.0            sundials@7.1.1         veloc@1.7
bricks@2023.08.25     flit@2.1.0             hpx@1.10.0                  mpark-variant@1.4.0    phist@1.12.1            sundials@7.1.1         vtk-m@2.2.0
butterflypack@2.4.0   flux-core@0.66.0       hypre@2.32.0                mpifileutils@0.11.1    plumed@2.9.2            superlu@5.3.0          wannier90@3.1.0
cabana@0.7.0          fortrilinos@2.3.0      intel-oneapi-mpi@2021.13.1  nccmp@1.9.1.0          precice@3.1.2           superlu-dist@8.2.1     warpx@24.10
cabana@0.7.0          gasnet@2024.5.0        kokkos@4.4.01               nco@5.2.4              pruners-ninja@1.0.1     swig@4.0.2-fortran     wrf@4.5.2
caliper@2.11.0        ginkgo@1.8.0           kokkos@4.4.01               nekbone@17.0           pumi@2.2.8              sz@2.1.12.5            xyce@7.8.0
chai@2024.07.0        ginkgo@1.8.0           kokkos-kernels@4.4.01       netcdf-fortran@4.6.1   py-cinemasci@1.7.0      sz3@3.2.0              zfp@0.5.5
==> 134 installed packages
Singularity>
```

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

E4S 24.11 Support for GPUs: Intel (modules)

```
$ singularity run e4s-24.11-oneapi-amd64.sif
Singularity> module avail

------------------------------------------ /spack/share/spack/lmod/linux-ubuntu22.04-x86_64/intel-oneapi-mpi/2021.13.1-4rnwxwm/Core ------------------------------------------
   adios/1.13.1                     exago/1.6.0                    laghos/3.1                parsec/3.0.2209               superlu-dist/8.2.1
   adios2/2.8.3                     exaworks/0.1.0                 lammps/20240829-openmp    petsc/3.22.0-sycl             sz/2.1.12.5
   amrex/24.10-sycl                 faodel/1.2108.1                libcatalyst/2.0.0         petsc/3.22.0           (D)    tasmanian/8.0
   amrex/24.10               (D)    flecsi/2.3.0                   libnrm/0.1.0              phist/1.12.1-openmp           tau/2.34-level-zero
   arborx/1.7-sycl                  fortrilinos/2.3.0              libquo/1.4                plumed/2.9.2                  tau/2.34                  (D)
   arborx/1.7                (D)    ginkgo/1.8.0-openmp            mercury/2.3.1             precice/3.1.2                 trilinos/13.0.1
   ascent/0.9.3-openmp              ginkgo/1.8.0-sycl-openmp (D)   metall/0.28               pruners-ninja/1.0.1           trilinos/16.0.0           (D)
   axom/0.9.0-openmp                globalarrays/5.8.2             mfem/4.7.0                pumi/2.2.8                    turbine/1.3.0
   boost/1.86.0                     glvis/4.2                      mpifileutils/0.11.1       py-cinemasci/1.7.0            umpire/2024.07.0
   bricks/2023.08.25                gptune/4.0.0                   nccmp/1.9.1.0             py-h5py/3.11.0                unifyfs/2.0
   butterflypack/2.4.0-openmp       gromacs/2024.3-openmp          nco/5.2.4                 py-libensemble/1.4.2          upcxx/2023.9.0-level-zero
   cabana/0.7.0-sycl                h5bench/1.4                    nekbone/17.0              py-petsc4py/3.22.0            upcxx/2023.9.0            (D)
   cabana/0.7.0              (D)    hdf5-vol-async/1.7             netcdf-fortran/4.6.1      rempi/1.1.0                   veloc/1.7
   caliper/2.11.0                   hdf5-vol-cache/v1.1            netlib-scalapack/2.2.0    scr/3.0.1                     vtk-m/2.2.0-openmp
   chai/2024.07.0                   hdf5-vol-log/1.4.0             nwchem/7.2.3              slate/2024.05.31-openmp       wannier90/3.1.0
   conduit/0.9.2                    hdf5/1.12.3                    omega-h/9.34.13           slepc/3.22.0                  warpx/24.10
   darshan-runtime/3.4.5            heffte/2.4.0-sycl              openpmd-api/0.16.0        stc/0.9.0                     wrf/4.5.2
   datatransferkit/3.1.1            heffte/2.4.0           (D)     papyrus/1.0.2             strumpack/7.2.0-openmp        xyce/7.8.0
   dealii/9.5.1                     hpx/1.10.0                     parallel-netcdf/1.12.3    sundials/7.1.1-sycl
   ecp-data-vis-sdk/1.0             hypre/2.32.0                   paraview/5.13.1           sundials/7.1.1         (D)

---------------------------------------------------------- /spack/share/spack/lmod/linux-ubuntu22.04-x86_64/Core ----------------------------------------------------------
   aml/0.2.1-level-zero       e4s-alc/1.0.2       gotcha/1.0.7                      legion/24.09.0            openmpi/5.0.5          superlu/5.3.0
   aml/0.2.1           (D)    e4s-cl/1.0.4        intel-oneapi-mpi/2021.13.1  (L)   libunwind/1.6.2           papi/7.1.0             swig/4.0.2-fortran
   argobots/1.2               flit/2.1.0          kokkos-kernels/4.4.01-openmp      loki/0.1.7                pdt/3.25.2             sz3/3.2.0
   bolt/2.0                   flux-core/0.66.0    kokkos-kernels/4.4.01-sycl  (D)   mgard/2023-12-09-openmp   py-jupyterhub/1.4.1    umap/2.1.1
   charliecloud/0.38          gasnet/2024.5.0     kokkos/4.4.01-openmp              mpark-variant/1.4.0       qthreads/1.18          variorum/0.8.0
   darshan-util/3.4.5         gmp/6.3.0           kokkos/4.4.01-sycl-openmp   (D)   nrm/0.1.0                 raja/2024.07.0         zfp/0.5.5

------------------------------------------------------------------------ /opt/intel/oneapi/modulefiles ------------------------------------------------------------------------
   compiler-intel-llvm/latest           compiler-rt/2024.2.1   (D)    compiler32/latest           dev-utilities/2024.2.0 (D)    ifort32/latest          mkl32/2024.2 (D)
   compiler-intel-llvm/2024.2.1   (D)    compiler-rt32/latest          compiler32/2024.2.1  (D)    dpl/latest                    ifort32/2024.2.1 (D)    mpi/latest
   compiler-intel-llvm32/latest         compiler-rt32/2024.2.1 (D)    debugger/latest             dpl/2022.6             (D)    mkl/latest              mpi/2021.13  (L,D)
   compiler-intel-llvm32/2024.2.1 (D)   compiler/latest               debugger/2024.2.1    (D)    ifort/latest                  mkl/2024.2       (D)    tbb/latest
   compiler-rt/latest                   compiler/2024.2.1      (D)    dev-utilities/latest        ifort/2024.2.1         (D)    mkl32/latest            tbb/2021.13  (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 24.11 Support for GPUs: Intel Data Center GPU Max (aka PVC)

```
$ singularity run e4s-24.11-oneapi-amd64.sif
Singularity> clinfo -l
Platform #0: 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@2024.2.1 --------------------
bgzjzfi heffte@2.4.0
hqtw4rg     cmake@3.30.5
oc76dql         curl@8.10.1
kd2d6sa             nghttp2@1.63.0
rp7hivc                 diffutils@3.10
qd3kp7f                     libiconv@1.17
3o4lhcu             openssl@3.3.1
dvytffa                 ca-certificates-mozilla@2023-05-30
r2azcny                 perl@5.40.0
to7g4ls                     berkeley-db@18.1.40
oetqqtm                     bzip2@1.0.8
pzkmhkl                     gdbm@1.23
ktlnsdu                         readline@8.2
z2xre3x             pkgconf@2.2.0
ki4aqx3         ncurses@6.5
fxinqb2         zlib-ng@2.2.1
yyo2lhg     glibc@2.35
6ducv27     gmake@4.4.1
mbify66     intel-oneapi-mkl@2024.2.1
4rnwxwm     intel-oneapi-mpi@2021.13.1
huznav2     intel-oneapi-runtime@2024.2.1
d2rzyjn         gcc-runtime@11.4.0

==> 1 installed package
Singularity>
```

E4S 24.11 packages in oneAPI containers are built with Intel compilers and Intel MPI

24.11 Release: 132+ Official Products + dependencies (gcc, aarch64)

1:	adios2	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/adios2-2.10.1-wcrbm5ehsvswacphnafskozpn53qg6z6
2:	alquimia	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/alquimia-1.1.0-24s63jo2vwzs7srkch56z2c67kbfxl73
3:	aml	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/aml-0.2.1-vatn7j5r6vox3ysmxy32jmprfz77va3n
4:	amrex	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/amrex-24.10-v7onxbbvkcfvudu3x6g2sgke7dcvpkm7
5:	arborx	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/arborx-1.7-6lrwjfuno5x2wgssu7uvv6polkweox2s
6:	argobots	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/argobots-1.2-iebz4danattybc7m25wbpiq5q5uflgbt
7:	ascent	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/ascent-0.9.3-x4is6fc34aywkzpqv2sn6mtcv3b47635
8:	axom	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/axom-0.9.0-gchnsew3vr46ucxpz7njof3zrla2a2ib
9:	blaspp	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/blaspp-2024.05.31-aesxpcp6g2uympe365ureag6ehevk4ag
10:	butterflypack	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/butterflypack-2.4.0-dfmptp5plmh2h4c4rckx77il2hlzkj5s
11:	cabana	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/cabana-0.7.0-vyrbrpdyt4mkwvcrs3wbohnxdgyyb63e
12:	caliper	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/caliper-2.11.0-qkniswj56tv3jyuukabtghsolpr4wwye
13:	camp	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/camp-2024.07.0-f3vyohc3lioug363tfhvlc6zaxbx6fmz
14:	chai	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/chai-2024.07.0-3o2v7o5jccjnz3i27v6ijji7r7ss654a
15:	chapel	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/chapel-2.2.0-o4xsgrmcuj3t33kx3uba76fpey667hps
16:	charliecloud	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/charliecloud-0.38-vsr2fzrxqh5mqywwzrc4jsgqepq7kurx
17:	conduit	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/conduit-0.9.2-zyyluorhyw5frwa4lf6yfdth6guqofj7
18:	cusz	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/cusz-0.6.0-cm7ov2glcdjbyfhkpcq6f2oy5dpzjw3r
19:	darshan-runtime	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/darshan-runtime-3.4.5-3yu7betyrjfsruucmhaobf4yhacnoy35
20:	datatransferkit	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/datatransferkit-3.1.1-47zlliw4bym5lzdsgpywejxc3jf4bulq
21:	dealii	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/dealii-9.5.1-4v7thkpfddz7z2zsuoljr4j3nt5nzzft
22:	dyninst	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/dyninst-13.0.0-vdumbeagatbwvxyoyvhqm4o4zmv4z3pt
23:	e4s-alc	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/e4s-alc-1.0.2-avzom6k7u7tvnyzgzogklynfu3oulcmd
24:	e4s-cl	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/e4s-cl-1.0.4-yacccy2bpch2spvh6jzxcssevfxq3246
25:	ecp-data-vis-sdk	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/ecp-data-vis-sdk-1.0-6ohpbzgcaearuevpteuqmjgixgi5rkd7
26:	exago	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/exago-1.6.0-qpo52m4tii3gfx7g2sarf3ekuznxihpx
27:	exaworks	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/exaworks-0.1.0-7cgmpf3ii4ukxtmh2wa4xqj7piscbmbb
28:	faodel	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/faodel-1.2108.1-skiymhqr7zeu77sp5tti4v5pkzfalz63
29:	fftx	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/fftx-1.2.0-2qkmx5gtooncl3h2nuevdozg2afvvoz5
30:	flecsi	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/flecsi-2.3.0-ubr2dnhfqmcyztjtabdsqjptjk2e445u
31:	flit	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/flit-2.1.0-hzym42hzdt7j6tndqg7hhkxgk57tykmp
32:	flux-core	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/flux-core-0.66.0-boyiylyfxyxlmgflkun7e733maa3xc4r
33:	flux-sched	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/flux-sched-0.38.0-w4l5346tgupkprju5g6gfcr7h5lfnqof
34:	gasnet	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/gasnet-2024.5.0-imijnv7k5s77pr3hdfzd6wvbaarkmu2i
35:	ginkgo	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/ginkgo-1.8.0-xry7pyyykxbejuhsql7lo4adcyapwqrc
36:	globalarrays	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/globalarrays-5.8.2-juubbubwy73p4xocypjwaq7ggl3lw23i
37:	glvis	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/glvis-4.2-6tgdrhbw4w7xcumyrngl73xorc6bl4pv
38:	gotcha	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/gotcha-1.0.7-yvgfxup2rjrisikm7vmm44kkjixsldak
39:	gptune	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/gptune-4.0.0-n7mabd2bdronrv6mxzj2rfxwin333pok
40:	gromacs	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/gromacs-2024.3-n3cfbtvnqo62ffmhinavwtqvwhxhvbfu
41:	h5bench	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/h5bench-1.4-pk4gzolyywksyo2usmxusmnhzrdsmdz4
42:	hdf5	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/hdf5-1.14.5-y4o537dotpnsj6mudycfldjk4gwg737k
43:	hdf5-vol-cache	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/hdf5-vol-cache-v1.1-vrrebjdz5nmymo6by2id5m4d2id4mh7k
44:	hdf5-vol-async	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/hdf5-vol-async-1.7-sksycdh3ljejtzyhjimw47qucqgczhxu

GPU runtimes for aarch64
- CUDA 12.3
- NVHPC 24.3

Languages
- Chapel
- Julia with MPI and CUDA
- Rust
- Python

EDA
- Xyce

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

PESO

24.11 Release: 132+ Official Products + dependencies (gcc, aarch64)

45:	hdf5-vol-log	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/hdf5-vol-log-1.4.0-jhbv2mh5rgcou4njhrttkphlcyb7qbuu
46:	heffte	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/heffte-2.4.0-dnmp7wt7mnv2oa2hvbyz3m6zupjelb36
47:	hiop	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/hiop-1.0.0-kkt2qeoi5vwbbg65tqbrvbn3xloiylzw
48:	hpctoolkit	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/hpctoolkit-2024.01.1-qibfw3pmca7mpf4vcpljy7wxumtmsjk4
49:	hpx	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/hpx-1.10.0-exp37p4blignhnhtshdbmxsfhzy5t4qy
50:	hypre	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/hypre-2.32.0-62bftaqwaxfricf3nmi67mlzowodnxrc
51:	kokkos	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/kokkos-4.4.01-bhwpf6axl36kgnn5awwwecztjk7w2psm
52:	kokkos-kernels	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/kokkos-kernels-4.4.01-kgcy62uqqlmfmbpe5gplrtdmjmrql6xg
53:	laghos	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/laghos-3.1-quke7bb7qqcr44imwnirjorwm3a7mr2b
54:	lammps	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/lammps-20240829-rg43zylkewq6tu7xf6uskeqm6y2ijygj
55:	lapackpp	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/lapackpp-2024.05.31-2g5xojbw5k2t232zxubh5cuqlzi7mtjf
56:	lbann	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/lbann-0.104-m7mmym73du63eavguchvgqoswcojub5u
57:	legion	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/legion-24.09.0-mu5frjd6vjhfulej2shjn2ybcawpfuvc
58:	libcatalyst	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/libcatalyst-2.0.0-rxcc2qzjp6xbpj3udunalvwbmswuxvpl
59:	libnrm	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/libnrm-0.1.0-jountnamzsk4tm7kww2rudq5qxyertnk
60:	libpressio	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/libpressio-0.99.4-m6o5fuqd4khcvhz2pksmbdhz7uos3dk7
61:	libquo	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/libquo-1.4-pxxknwgw3f3m5zvjj6jm5yvbtrm26ytr
62:	loki	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/loki-0.1.7-yquemaz4btjwl5fbdmggiwltnqih6fls
63:	mercury	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/mercury-2.3.1-rotzw4h5niopjw7plwdfiz63l6tazq6a
64:	metall	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/metall-0.28-7ncszghxamojlf6eeduac7koobv3ode2
65:	mfem	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/mfem-4.7.0-wppazl6kfl3fvo2uda2rlgwi3hrgzckq
66:	mgard	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/mgard-2023-12-09-fwvokiwsctfdxib7cnthqomhcwgvnknw
67:	mpark-variant	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/mpark-variant-1.4.0-q7rhw4nvhnvww7ky6d6tq2vxl6etprvn
68:	mpich	/usr/local/mpich/install/mpich
69:	mpifileutils	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/mpifileutils-0.11.1-ac3hvo6gz2wy7aqn3lc5vcqmnq5c7e6x
70:	nccmp	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/nccmp-1.9.1.0-fout3hezgnisgw2foiq7yrntzqujnzyx
71:	nco	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/nco-5.2.4-aqdnxhbp64fbhgo5gooz3snh5vohgudq
72:	netcdf-c	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/netcdf-c-4.9.2-jr2qau2hfqdisjuiqca7thsgfn3i33ad
73:	nek5000	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/nek5000-19.0-fe6yqolwjim7rh3pdirpldlmg5dk4pol
74:	nekbone	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/nekbone-17.0-bvukc2hvrxyqa32rcbwpqnyw4xo5lz3d
75:	netcdf-fortran	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/netcdf-fortran-4.6.1-kpxrpdoccbkiiuyptfiwpvtyjndryzln
76:	netlib-scalapack	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/netlib-scalapack-2.2.0-nw7hho6apabwylokozqxl2ypizs6at34
77:	nrm	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/nrm-0.1.0-unxk5bcajj4n4uvl4vge72dhw24hm6th
78:	nwchem	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/nwchem-7.2.3-fyv5qeyvrdqktsneni3vuzdqyxlaoe3v
79:	omega-h	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/omega-h-9.34.13-6cbbyl4xc2dmoygzscjq4sfmxetwudp4
80:	openfoam	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/openfoam-2312-ye34vs2opwhhoykiet2szwjkp32afoja
81:	openmpi	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/openmpi-5.0.5-cvmwqdo34wt5bsu2ig6kld4jpczte7mu
82:	openpmd-api	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/openpmd-api-0.16.0-zlvbqqor55y7uvkt2jay2gjy5owfzf7a
83:	papi	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/papi-7.1.0-nsre64j5tfawwfpui5na47siszwmi3xz
84:	papyrus	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/papyrus-1.0.2-xy6ft4q3g4mj772vnq2qogt34pncmqnm
85:	parallel-netcdf	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/parallel-netcdf-1.12.3-5cib6tbitk6okqjixdggqm2um3k3bsdm
86:	parmetis	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/parmetis-4.0.3-znjebgbvf4bffgxb6ttzetfkyrcvhgh3
87:	paraview	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/paraview-5.13.1-lgcutv5loxs65jw5oegerq3dhzmrdhpt
88:	parsec	/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/parsec-3.0.2209-uoy6oihnwnbcbf7ovhygyjxs4vmdsghy

PESO

24.11 Release: 132+ Official Products + dependencies (gcc, aarch64)

```
  89:  pdt              /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/pdt-3.25.2-koinyddzls6ty4krh64nweaj2kttihej
  90:  petsc            /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/petsc-3.22.0-ubjxafwef4cdcwgdyk2rkk74bg2rjm75
  91:  phist            /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/phist-1.12.1-46h26zpw5tcn23k7xeu46gvy5vijilcr
  92:  plasma           /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/plasma-24.8.7-wevzkzqzksjxeo7hyvtxigk4j5kuu6ri
  93:  plumed           /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/plumed-2.9.2-yl4tngo3c5gmanxafk3wqcylxftfil3o
  94:  precice          /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/precice-3.1.2-olxj43a2u5lojqraeyprhbvfn5l2ohnf
  95:  pruners-ninja    /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/pruners-ninja-1.0.1-odhusldwcr2u34gc2d3lwlrxvp46gemv
  96:  pumi             /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/pumi-2.2.8-klt7xv6pzq7p7g3bvmgtw4dix2f6nay4
  97:  py-cinemasci     /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/py-cinemasci-1.7.0-rz3ntnojrhlncfwa2gwy2x42vmgmn6co
  98:  py-deephyper     /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/py-deephyper-0.6.0-rccdemevdjyphrj36zmt6wd5t4k6cwqw
  99:  py-h5py          /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/py-h5py-3.11.0-etwmwyfdoyutfshgiazad2h7koby727k
 100:  py-jupyterhub    /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/py-jupyterhub-1.4.1-znymkdteo6gqtfiigx4dhmgq32buhfla
 101:  py-libensemble   /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/py-libensemble-1.4.2-aitbbqjrvmjv4wtjraqbp7bmiuy6yzrm
 102:  py-parsl         /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/py-parsl-2023.08.21-nn2pqnur2x3nfsilhha76uhitpkfzid4
 103:  py-petsc4py      /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/py-petsc4py-3.22.0-ynphsjixnnrn6vm2olcei22vfccfahis
 104:  py-radical-saga  /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/py-radical-saga-1.47.0-rpycb2zc2jxosmvsuqesrxbtzkegqjsa
 105:  qthreads         /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/qthreads-1.18-s7yetoaobxtpsbdsf4qqndgw2gnjsz7l
 106:  quantum-espresso /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/quantum-espresso-7.3.1-ld4zep63stbrw3sf4lt4kbgqcpgl62n4
 107:  raja             /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/raja-2024.07.0-gbnncy7uclzab7ad6tcbz4qqo5ly6xlh
 108:  rempi            /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/rempi-1.1.0-f7fkildds2ol5arx5uoonxm3rthg4joh
 109:  scr              /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/scr-3.0.1-wvzhobqnjrk3n5cx5jxw27vx2hwvrq7g
 110:  slate            /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/slate-2024.05.31-ckbjbsn3gjbftheg5pqejsik4yt6qaoz
 111:  slepc            /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/slepc-3.22.0-rt3advwqk7ybsom7zprn7jsx4ynfyndy
 112:  stc              /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/stc-0.9.0-llrbtru73muy4f2fmbnvge7u35bkdzw6
 113:  strumpack        /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/strumpack-7.2.0-tacqhg4t5vsbpt3j6hjg33mkqeomestg
 114:  sundials         /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/sundials-7.1.1-nh56tksv3yxbewftjhg4kqcafnwza6kv
 115:  superlu-dist     /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/superlu-dist-8.2.1-7xtjpavrbp7e5zyhzue2f5ztbzvf7bfn
 116:  swig             /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/swig-4.1.1-fryz5s46ebpbwapeoi7inyoduy26mtq3
 117:  sz3              /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/sz3-3.2.0-gw5kyymrsbwvhtv4or2z7tjuveh33m6g
 118:  tasmanian        /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/tasmanian-8.0-w6qz23ifechplcknnpias6uwohkfirlp
 119:  tau              /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/tau-2.34-e3mwx4cpoycczxkoxgwdg7jivqqfni6z
 120:  trilinos         /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/trilinos-16.0.0-mac54ev43aobbtelp2vhqgghaqpa2odg
 121:  turbine          /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/turbine-1.3.0-zy2cdktwfxrej6u6oyavhnpxezzjixn5
 122:  umap             /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/umap-2.1.1-fm6vlkx2qrz7xv3jcc4zqtv5753tgjmk
 123:  umpire           /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/umpire-2024.07.0-gibrrcd7yow6xhrkp5yktugzceqtf4oe
 124:  upcxx            /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/upcxx-2023.9.0-bfq7tbzayvgmfnj34tygn4a57p42mtgg
 125:  veloc            /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/veloc-1.7-3ze3quase6hfq53a2qdlodahaqftrqtv
 126:  vtk-m            /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/vtk-m-2.2.0-po5nhcf5braqwuekongz6i6vnepztl4b
 127:  wannier90        /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/wannier90-3.1.0-sji77j4rusktqaqzcb4vffxruao5sifn
 128:  warpx            /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/warpx-24.10-pmo4aofkxr4vtzvd6ofpwt457t6jns7a
 129:  wps              /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/wps-4.5-4tb2cpnvua7elbnseyt2n3xp3as4j2dp
 130:  wrf              /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/wrf-4.5.2-piy4bzwuni7vegxdwdvlsmu7g474as34
 131:  xyce             /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/xyce-7.8.0-u4e4fksa52hwpqdstoufkgdrvzeibngl
 132:  zfp              /spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/zfp-1.0.0-elvm6ohuxazehbgnpewklitgi4cnmwp3
```

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E4S Support for GPUs: CUDA on aarch64

```
$ singularity run --nv e4s-24.11-cuda90-arm64.sif
Singularity> nvidia-smi
Fri Nov 15 20:18:04 2024
+-----------------------------------------------------------------------------------------+
| NVIDIA-SMI 550.54.15              Driver Version: 550.54.15      CUDA Version: 12.4     |
|-----------------------------------------+------------------------+----------------------+
| 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   24C    P0             84W /  700W |     139MiB /  97871MiB |      0%      Default |
|                                         |                        |             Disabled |
+-----------------------------------------+------------------------+----------------------+

+-----------------------------------------------------------------------------------------+
| Processes:                                                                              |
|  GPU   GI   CI        PID   Type   Process name                              GPU Memory |
|        ID   ID                                                               Usage      |
|=========================================================================================|
|    0   N/A  N/A      3666      G   /usr/libexec/Xorg                              4MiB |
+-----------------------------------------------------------------------------------------+
Singularity> python
Python 3.10.15 (main, Sep  7 2024, 18:35:38) [GCC 13.2.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import torch
>>> torch.__version__
'2.5.0'
>>> torch.cuda.get_arch_list()
['sm_75', 'sm_80', 'sm_90']
>>> torch.cuda.get_device_name(0)
'NVIDIA GH200 480GB'
>>>
Singularity> grep _NAME /etc/os-release
PRETTY_NAME="Ubuntu 24.04.1 LTS"
```

- GCC 13.2.0
- CUDA compilers 12.6
- NVHPC 24.9

```
$  singularity run --nv e4s-24.11-cuda90-arm64.sif
Singularity> gcc --version | grep gcc
gcc (Ubuntu 13.2.0-23ubuntu4) 13.2.0
Singularity> nvcc --version | grep release
Cuda compilation tools, release 12.6, V12.6.77
Singularity> nvidia-smi | grep CUDA
| NVIDIA-SMI 550.54.15              Driver Version: 550.54.15      CUDA Version: 12.4     |
Singularity> spack location -i nvhpc
/spack/opt/spack/linux-ubuntu24.04-aarch64/gcc-13.2.0/nvhpc-24.9-exv2h4m5h5onejh6zf33uqsyhog2lenz
Singularity>
```

E4S 24.11 supports CUDA architectures 75 (T4), 80 (A100), as well as 90 (H100/GH200)

E4S Support for GPUs: CUDA on aarch64 (modules)

```
$ singularity run --nv e4s-24.11-cuda90-arm64.sif
Singularity> spack find -x +cuda
-- linux-ubuntu24.04-aarch64 / gcc@13.2.0 ------------------------
adios2@2.10.1  caliper@2.11.0       flecsi@2.3.0      hpctoolkit@2024.01.1  legion@24.09.0     petsc@3.22.0      sundials@7.1.1      umpire@2024.07.0
amrex@24.10    chai@2024.07.0       flux-core@0.66.0  hpx@1.10.0            libpressio@0.99.4  raja@2024.07.0    superlu-dist@8.2.1  vtk-m@2.2.0
arborx@1.7     cusz@0.6.0           ginkgo@1.8.0      hypre@2.32.0          mfem@4.7.0         slate@2024.05.31  tasmanian@8.0       zfp@0.5.5
axom@0.9.0     ecp-data-vis-sdk@1.0 gromacs@2024.3    kokkos@4.4.01         mgard@2023-12-09   slepc@3.22.0      tau@2.34
cabana@0.7.0   fftx@1.2.0           heffte@2.4.0      kokkos-kernels@4.4.01 parsec@3.0.2209    strumpack@7.2.0   trilinos@16.0.0
==> 38 installed packages
Singularity> spack find -x
-- linux-ubuntu24.04-aarch64 / gcc@13.2.0 ------------------------
adios@1.13.1          cusz@0.6.0             gmp@6.3.0              lbann@0.104           nrm@0.1.0             py-jupyterhub@1.4.1     tasmanian@8.0
adios2@2.10.1         darshan-runtime@3.4.5  gotcha@1.0.7           legion@24.09.0        nvhpc@24.9            py-libensemble@1.4.2    tau@2.34
adios2@2.10.1         darshan-util@3.4.5     gptune@4.0.0           legion@24.09.0        nwchem@7.2.3          py-petsc4py@3.22.0      tau@2.34
alquimia@1.1.0        datatransferkit@3.1.1  gromacs@2024.3         libcatalyst@2.0.0     omega-h@9.34.13       qthreads@1.18           trilinos@16.0.0
aml@0.2.1             dealii@9.5.1           gromacs@2024.3         libnrm@0.1.0          openfoam@2312         quantum-espresso@7.3.1  trilinos@16.0.0
amrex@24.10           dyninst@13.0.0         h5bench@1.4            libpressio@0.99.4     openmpi@5.0.5         raja@2024.07.0          turbine@1.3.0
amrex@24.10           e4s-alc@1.0.2          hdf5@1.12.3            libpressio@0.99.4     openpmd-api@0.16.0    raja@2024.07.0          umap@2.1.1
arborx@1.7            e4s-cl@1.0.4           hdf5@1.14.5            libquo@1.4            papi@7.1.0            rempi@1.1.0             umpire@2024.07.0
arborx@1.7            ecp-data-vis-sdk@1.0   hdf5-vol-async@1.7     libunwind@1.6.2       papyrus@1.0.2         scr@3.0.1               umpire@2024.07.0
argobots@1.2          exago@1.6.0            hdf5-vol-cache@v1.1    loki@0.1.7            parallel-netcdf@1.12.3 slate@2024.05.31       upcxx@2023.9.0
ascent@0.9.3          exaworks@0.1.0         hdf5-vol-log@1.4.0     mercury@2.3.1         paraview@5.13.1       slate@2024.05.31        veloc@1.7
axom@0.9.0            faodel@1.2108.1        heffte@2.4.0           metall@0.28           parsec@3.0.2209       slepc@3.22.0            vtk-m@2.2.0
axom@0.9.0            fftx@1.2.0             heffte@2.4.0           mfem@4.7.0            parsec@3.0.2209       slepc@3.22.0            vtk-m@2.2.0
boost@1.79.0          fftx@1.2.0             hpctoolkit@2024.01.1   mfem@4.7.0            pdt@3.25.2            stc@0.9.0               wannier90@3.1.0
butterflypack@2.4.0   flecsi@2.3.0           hpctoolkit@2024.01.1   mgard@2023-12-09      petsc@3.22.0          strumpack@7.2.0         warpx@24.10
cabana@0.7.0          flecsi@2.3.0           hpx@1.10.0             mgard@2023-12-09      petsc@3.22.0          strumpack@7.2.0         wps@4.5
cabana@0.7.0          flit@2.1.0             hpx@1.10.0             mpark-variant@1.4.0   phist@1.12.1          sundials@7.1.1          wrf@4.5.2
caliper@2.11.0        flux-core@0.66.0       hypre@2.32.0           mpich@4.2.3           plasma@24.8.7         sundials@7.1.1          xyce@7.8.0
caliper@2.11.0        flux-core@0.66.0       hypre@2.32.0           mpifileutils@0.11.1   plumed@2.9.2          superlu@5.3.0           zfp@0.5.5
chai@2024.07.0        fpm@0.10.0             kokkos@4.4.01          nccmp@1.9.1.0         precice@3.1.2         superlu-dist@8.2.1      zfp@1.0.0
chai@2024.07.0        gasnet@2024.5.0        kokkos@4.4.01          nco@5.2.4             pruners-ninja@1.0.1   superlu-dist@8.2.1
chapel@2.2.0          ginkgo@1.8.0           kokkos-kernels@4.4.01  nek5000@19.0          pumi@2.2.8            swig@4.0.2-fortran
charliecloud@0.38     ginkgo@1.8.0           kokkos-kernels@4.4.01  nekbone@17.0          py-cinemasci@1.7.0    sz@2.1.12.5
conduit@0.9.2         globalarrays@5.8.2     laghos@3.1             netcdf-fortran@4.6.1  py-deephyper@0.6.0    sz3@3.2.0
cuda@12.6.2           glvis@4.2              lammps@20240829        netlib-scalapack@2.2.0 py-h5py@3.11.0       tasmanian@8.0
==> 170 installed packages
```

E4S 24.11 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
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-aarch64 / gcc@11.1.0 -----------------------
cmake@3.26.3  llvm-doe@16.0.2
```

24.11 Release: 132+ Official Products + dependencies (gcc, ppc64le)

```
 1:  adios2              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/adios2-2.10.1-hsu62svr6m4sbgva4kdmrx3xf344l4kt
 2:  alquimia            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/alquimia-1.1.0-h6lpvoigip4khrisjg4wr4bkjcfwxmcw
 3:  aml                 /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/aml-0.2.1-lmufmaijeqzxkmul6jns5jqiy4s2dnlp
 4:  amrex               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/amrex-24.10-ytwvv6lp7qseuoumpoj4ohef3efspuoq
 5:  arborx              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/arborx-1.7-habrdgteu5vnqyqoklfpqwmhuyuoa7ij
 6:  argobots            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/argobots-1.2-vm5qzmmgdojsplhtqxc37fazqwqynptl
 7:  ascent              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/ascent-0.9.3-nglsxm6mjpwdzbrlie4c2lufgnlst2py
 8:  axom                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/axom-0.9.0-bkptof7nzosyunpukgtbyz5wl5wvkbrp
 9:  bolt                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/bolt-2.0-75ezw3co7nb2qknkmfwtmnw2fynrb2gv
10:  blaspp              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/blaspp-2024.05.31-r2hufnnz7bkcbhfrtddj4vgjilhg4l74
11:  bricks              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/bricks-2023.08.25-ztlcihsngb6izuwuwcqgjphipwh5uyt4
12:  butterflypack       /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/butterflypack-2.4.0-roeftx745y6nzp5yceaakfqejo3kpevi
13:  cabana              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/cabana-0.7.0-63fwupauhlcvssd7gaifidvjptkzrgnr
14:  caliper             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/caliper-2.11.0-urvwlpxty65vhcqvoohievkb3fbrhcpg
15:  camp                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/camp-2024.07.0-dkgh2anxyob4uqm4eefttkfvq6touyzk
16:  chai                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/chai-2024.07.0-e35trzi7nuctyedfbqkjwcu3betklvn2
17:  chapel              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/chapel-2.2.0-rszkvlvqh7n6kxtf55c7kuja35pnc73r
18:  charliecloud        /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/charliecloud-0.38-sdcp53qyyyr6booxtarcjnjb5ynmutim
19:  conduit             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/conduit-0.9.2-4vpkogqzxlbqojmuyhyzj46izsskbes7
20:  cp2k                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/cp2k-2024.3-fwzyk5bfbcltehi53x3teiejho2fejle
21:  cusz                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/cusz-0.6.0-dmd3rbjguowt6xlaywdj35hckfjga7ls
22:  darshan-runtime     /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/darshan-runtime-3.4.5-bspq5kogwoww53igm6gqujdwgcfaw3vy
23:  datatransferkit     /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/datatransferkit-3.1.1-qatcto4lbfi7oqjmzaqqfpendrohtvop
24:  dyninst             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/dyninst-13.0.0-qn7uyivhvep5xxfjzkyyvz4pbjncgrom
25:  e4s-alc             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/e4s-alc-1.0.2-4dbjrt6vm4artaszzwu3ibbqpyoo2izj
26:  e4s-cl              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/e4s-cl-1.0.4-norzqqymywbmwgol6mqlghf4267zjouh
27:  ecp-data-vis-sdk    /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/ecp-data-vis-sdk-1.0-h5r3wyvquuvkvhzv7badbjxz6og6in5w
28:  exago               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/exago-1.6.0-zownbeujxnmkn3x7yafctlcn3wwn7lr2
29:  exaworks            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/exaworks-0.1.0-n4etyjnygvxv4t7oa732sxpwe5rsxsp3
30:  faodel              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/faodel-1.2108.1-ihszcnxtfb4kb4m7oxml6u2siqv2koez
31:  flecsi              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/flecsi-2.3.0-4apfchqnzd4yzq6gdakh7zd35vwajldw
32:  flit                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/flit-2.1.0-vcqrupxseyq4agygpaod7wq7xr6bp3l2
33:  flux-core           /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/flux-core-0.66.0-d7efjojvu6yi7irrx3jwruqxh223tpac
34:  flux-sched          /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/flux-sched-0.36.1-uymkbcjwzmlmtlqgcoxgucpzsnqwhp5q
35:  fortrilinos         /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/fortrilinos-2.3.0-6mzfaadlkgsdwifdn2srw7zbs2xkqoot
36:  gasnet              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/gasnet-2024.5.0-26lx6lgeibqmsmad3577yvqzad36akig
37:  ginkgo              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/ginkgo-1.8.0-nlwuccnbbzjwce3tmunbyetkpkh5wdmj
38:  globalarrays        /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/globalarrays-5.8.2-pue6ng6vpdlhcyx3cfkznydbzl7itjnm
39:  gotcha              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/gotcha-1.0.7-enee4hf3ebt6wvo6mtzjql35a7unc24t
40:  gptune              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/gptune-4.0.0-t2iqmp3iv6k2ykqn6yc4bucs57kzqug7
41:  gromacs             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/gromacs-2024.3-hluif34mtghx4d52taeoekoqxyzwj7db
42:  h5bench             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/h5bench-1.4-6zfclcxjkl24jdkldq2iwolcnrt2rr22
43:  hdf5                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hdf5-1.14.5-xmj5lgxx3pstds5oisxgbdixvhy77ddd
44:  hdf5-vol-cache      /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hdf5-vol-cache-v1.1-5xnckg3p777cwbe5ovyt7atb4oaocfjz
```

GPU runtimes for IBM Power
- CUDA 12.4

Languages
- Chapel
- Julia with MPI and CUDA
- Python
- Rust

EDA Tools
- Xyce

CFD Tools
- OpenFOAM
- Nek5000

AI packages for NVIDIA GPU
- TensorFlow
- PyTorch
- LBANN

24.11 Release: 132+ Official Products + dependencies (gcc, ppc64le)

45:	hdf5-vol-async	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hdf5-vol-async-1.7-xhq5xjc7cizn7oktqvlwfgzol26oey7d
46:	hdf5-vol-log	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hdf5-vol-log-1.4.0-bx4fhebxxiayulsb6o46oxkyk5n2p5u3
47:	heffte	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/heffte-2.4.0-3mmkre7rnm7ben26z7h7yand45cbzvfv
48:	hiop	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hiop-1.0.0-vyvovtludzpjrffb3rxyb7ocuxm65lgk
49:	hpctoolkit	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hpctoolkit-2024.01.1-35ovi25hy6vnjjqfj4qb2im5bo7ccagk
50:	hpx	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hpx-1.10.0-cruy66mk42kdabso4kd6zm7pade3quc6
51:	hypre	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hypre-2.32.0-fcevpjf3vvjxnirffso6qdxzftywww2k
52:	kokkos	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/kokkos-4.4.01-yqexqrle6bsbolkfs62mmdeuer4bnfu3
53:	kokkos-kernels	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/kokkos-kernels-4.4.01-2iwxtadwavfytldono5fzquj2ncn67xz
54:	laghos	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/laghos-3.1-p7m57gqb74l4yenpwkclwouvop5uz2jr
55:	lammps	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/lammps-20240829-tdh7ddtcsrzyhfp5jaexamn3cdxumpor
56:	lapackpp	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/lapackpp-2024.05.31-lbmowmqsuq6kpskncdomqf5oum4mkn57
57:	lbann	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/lbann-0.104-s2xx6esrl5hnbebtjmoczkapqjachznz
58:	legion	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/legion-24.09.0-t66k5wfiufu77rb2fjs5v43mc4gea2tw
59:	libcatalyst	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/libcatalyst-2.0.0-jgjfpseqaidgo5axtigeiggzmm6clhsg
60:	libnrm	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/libnrm-0.1.0-k547zygow45ieyusmwat4f4yfw4nobkw
61:	libpressio	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/libpressio-0.99.4-6xe6yg4or2ikvdxucy4g4bvkhfqb4ykp
62:	libquo	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/libquo-1.4-sny422tzxqwvs3rpsizgnbzyr3pesiyt
63:	loki	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/loki-0.1.7-4nvbe3d5hpffc5x4plyo3cjxr5hsjnlq
64:	magma	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/magma-2.8.0-bdr4axcl6ewdxc3qcwsqubpu5jiyhj3r
65:	mercury	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mercury-2.3.1-473dp4kdnvuwrea57s2za6ivxhpu4phu
66:	metall	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/metall-0.28-qjentgvnfh4v5poqvnip4lex7vzaozbm
67:	mfem	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mfem-4.7.0-hbduv3ppp6ruymtp4c5waaw5x4rwqbau
68:	mgard	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mgard-2023-12-09-vimux6h77ahy4iszzdgms3wylrrqzjsb
69:	mpark-variant	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mpark-variant-1.4.0-liafspyuxgqv7x6ts4tlmgingvacme44
70:	mpich	/usr/local/mpich/install/mpich
71:	mpifileutils	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mpifileutils-0.11.1-w7p4scf6eapb4mhi52yimrskeq6yhfwd
72:	nccmp	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/nccmp-1.9.1.0-2lstifrfv27ymol5fzaq7qnfdy2eza2r
73:	nco	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/nco-5.2.4-74rdwu2hpjrrihxhcepwhbtsyji6xsns
74:	netcdf-c	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/netcdf-c-4.9.2-chd7f2phnus2554vdkyc6dvbf7lkhg3q
75:	nek5000	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/nek5000-19.0-bcfj5i37ra5judy76gvuf5wsbwytdscv
76:	nekbone	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/nekbone-17.0-n2bdc7ft6slb4xl6q26gjrljroqs2qh3
77:	netcdf-fortran	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/netcdf-fortran-4.6.1-giso75hz2byzfj64zzyypxjlg3sfr2m2
78:	netlib-scalapack	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/netlib-scalapack-2.2.0-kp3unzrs2dokm4bgvqynislpii5tufb7
79:	nrm	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/nrm-0.1.0-cw7q2pna52lltmrx7how5ldxyf4zlglu
80:	nwchem	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/nwchem-7.2.3-y75j6dwulnvyxbj4w6bxz2kw4ieuopxy
81:	omega-h	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/omega-h-9.34.13-3bktjjtyjufm6iqit6itoyp4wjdjrkcw
82:	openfoam	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/openfoam-2312-d7mmkv45mxq52r7bayftocm2nc7z5z37
83:	openmpi	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/openmpi-5.0.5-ew4sj3574aezp662x34bpnjc6ongoplh
84:	openpmd-api	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/openpmd-api-0.16.0-hi2p6aq3kcepirljhgn6sk2lhbrys2fk
85:	papi	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/papi-7.1.0-ffcmjx72xb7eewjeydueo4vpim2lg222
86:	papyrus	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/papyrus-1.0.2-nptlau3dhy3bd4zap4hf45ojfurxchnq
87:	parallel-netcdf	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/parallel-netcdf-1.12.3-7ickoaqrfnwhz2j4glmxc4ifsgdcy6n2
88:	paraview	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/paraview-5.13.1-y7d4uqqbkjoqteesrgb2yr73laehqlpg

PESO

24.11 Release: 132+ Official Products + dependencies (gcc, ppc64le)

```
 89:  parsec              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/parsec-3.0.2209-nyvdrkzibfimnj7skiw5gp7qeamqwer3
 90:  pdt                 /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/pdt-3.25.2-ausduslzarfnpwbgboctyalzpjh64kro
 91:  petsc               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/petsc-3.22.0-qxcq5joourav6uvrwpl7ccmgzk5kttpj
 92:  plasma              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/plasma-24.8.7-inugxhvtidbbw7y5puevrduecmw3uevh
 93:  plumed              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/plumed-2.9.2-6gviybo7dsqzhfouxsejhwdhx5ph3wjg
 94:  precice             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/precice-3.1.2-gknuctavf2ipqwipcwu3fmztsavllbor
 95:  pruners-ninja       /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/pruners-ninja-1.0.1-ooc2eaick55jddykuhabrffnvqioyaib
 96:  pumi                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/pumi-2.2.8-cxmxkzklocgdjz43gjuafjiii5khgoam
 97:  py-cinemasci        /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-cinemasci-1.3-moyypjcitdedmbo2uskqam5eoj62ohdc
 98:  py-deephyper        /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-deephyper-0.6.0-scsiogzqieoylyeelfz4fbxfakj4zx6c
 99:  py-jupyterhub       /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-jupyterhub-1.4.1-rydtejgkdlckgicryt6jve4wensndbk7
100:  py-libensemble      /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-libensemble-1.4.2-lmnravrku4hyhyphtxwo2amd5obue3he
101:  py-parsl            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-parsl-2023.08.21-zvrne2uzxclcf4wm5phq4eyjpoi4gk4y
102:  py-radical-saga     /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-radical-saga-1.47.0-27md5k33liojnjjt3yfzqavhzwagvnf2
103:  qthreads            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/qthreads-1.18-4ayiuz3br7b5itshqhlfc6v2eeikyfsg
104:  quantum-espresso    /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/quantum-espresso-7.3.1-eqxhtjsvd3ou7qx65xd4jmmn45cj6t4k
105:  raja                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/raja-2024.07.0-d5gw6nvfnofhix452lxovxbrcwa42ob3
106:  rempi               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/rempi-1.1.0-wrou73egedgmo5rmm6d7pojiv5qqsqhc
107:  scr                 /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/scr-3.0.1-5rug3f3abb3v6brs7niqr3tzamt6cqlf
108:  slate               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/slate-2024.05.31-bgorjkljdea2yuksrzh5mk5vuj3wrjkc
109:  slepc               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/slepc-3.22.0-pgmndfpoybhbvai4crq5tvn2d2n45xcg
110:  stc                 /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/stc-0.9.0-ys6m24eg7coafr4nbhlk3pdvdqc7azfa
111:  strumpack           /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/strumpack-7.2.0-im4og4xi6yjc62q2fgou6t4jbsvtdref
112:  sundials            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/sundials-7.1.1-to4njfsisowjeqgnmiqb36sj55k64kdu
113:  superlu-dist        /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/superlu-dist-8.2.1-x6apzll6wntegcqo2h7wmfv6o5yva7on
114:  swig                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/swig-4.1.1-7hqq6zog5kqkgxjkjm4ed4rs6uvvazuy
115:  sz                  /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/sz-2.1.12.5-vhumozmdw3vrmiiqwbz3njmisxv7537g
116:  sz3                 /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/sz3-3.2.0-4wcu3ghqf4htq2izroru4jolrdcvj65m
117:  tasmanian           /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/tasmanian-8.0-imtc6tlsjfctwl4xvk6b5t4dgvzbmfgv
118:  tau                 /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/tau-2.34-2kini77w2qsvyuj4m76qmmjz5bvjl7pq
119:  trilinos            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/trilinos-16.0.0-fvwodnaj2px7lgb6ylt2ksnhq2k7bsbu
120:  turbine             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/turbine-1.3.0-btrukr622ux24w7l7a52itiecgaz4moq
121:  umap                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/umap-2.1.1-x7lqkworhk67yy4scqr4cdrt6j2dmutk
122:  umpire              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/umpire-2024.07.0-oqkdktfgu6vlrklzkhivqhh3oxr3lpdt
123:  unifyfs             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/unifyfs-2.0-gg6hfukpulmxzcdwtugajbv6owt2hzv6
124:  upcxx               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/upcxx-2023.9.0-glgrp5yfjbxbefxsf6tvnitha2emulio
125:  veloc               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/veloc-1.7-vwz64aohu2cmu5iagmu7jqpd6jxwrcfy
126:  visit               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/visit-3.3.3-gcpciu747gjyyowma6gadzvfv7ggi4xm
127:  vtk-m               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/vtk-m-2.2.0-vjzc2lu5nmkvz3jhee24mrivklxjyjb6
128:  wannier90           /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/wannier90-3.1.0-arp23qjl2743logudeosmd2czbl3x566
129:  warpx               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/warpx-24.10-swedvbr4a7qzlufvreoppdcczevgukr4
130:  wrf                 /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/wrf-4.5.2-qt7ieck35roet6oykuh3d7j4aitsehht
131:  xyce                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/xyce-7.8.0-5wevw7vyew35a73a4rkmupbvsjuq7xf5
132:  zfp                 /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/zfp-1.0.0-xperbvmaqboxfxpdvapwmsrxd3mgq5k2
```

Supports
IBM Power10 and
Power 9 processors

E4S 24.11 Support for GPUs: NVIDIA CUDA on IBM ppc64le

```
Singularity> spack find +cuda
-- linux-ubuntu20.04-ppc64le / gcc@9.4.0 ------------------------
adios2@2.10.1      camp@0.2.3           flecsi@2.3.0         hwloc@2.11.1          legion@24.09.0    parsec@3.0.2209   strumpack@7.2.0     umpire@2024.07.0
amrex@24.10        camp@2024.07.0       flux-core@0.66.0     hypre@2.32.0          magma@2.8.0       petsc@3.22.0      sundials@7.1.1      upcxx@2023.9.0
arborx@1.7         camp@2024.07.0       ginkgo@1.8.0         kokkos@4.4.01         mfem@4.7.0        petsc@3.22.0      superlu-dist@8.2.1  vtk-m@2.2.0
axom@0.9.0         chai@2024.07.0       gromacs@2024.3       kokkos@4.4.01         mgard@2023-12-09  raja@0.14.0       tasmanian@8.0       zfp@0.5.5
blaspp@2024.05.31  cusz@0.6.0           heffte@2.4.0         kokkos@4.4.01         nvcomp@2.2.0      raja@2024.07.0    tau@2.34
bricks@2023.08.25  ecp-data-vis-sdk@1.0 hiop@1.0.0           kokkos-kernels@4.4.01 omega-h@9.34.13   raja@2024.07.0    umpire@6.0.0
cabana@0.7.0       exago@1.6.0          hpctoolkit@2024.01.1 lammps@20240829       papi@7.1.0        slate@2024.05.31  umpire@2024.07.0
caliper@2.11.0     fftx@1.2.0           hpx@1.10.0           lapackpp@2024.05.31   paraview@5.13.1   slepc@3.22.0      umpire@2024.07.0
==> 60 installed packages
Singularity> spack find -x
-- linux-ubuntu20.04-ppc64le / gcc@9.4.0 ------------------------
adios@1.13.1         cp2k@2024.3            globalarrays@5.8.2     lammps@20240829       netlib-scalapack@2.2.0  py-jupyterhub@1.4.1     tau@2.34
adios2@2.7.1         cusz@0.6.0             glvis@4.2              lammps@20240829       nrm@0.1.0               py-libensemble@1.4.2    trilinos@13.0.1
adios2@2.10.1        darshan-runtime@3.4.5  gmp@6.3.0              lbann@0.104           nwchem@7.2.3            py-petsc4py@3.22.0      trilinos@16.0.0
alquimia@1.1.0       darshan-util@3.4.5     gotcha@1.0.7           legion@24.09.0        omega-h@9.34.13         qthreads@1.18           turbine@1.3.0
aml@0.2.1            datatransferkit@3.1.1  gptune@4.0.0           legion@24.09.0        omega-h@9.34.13         quantum-espresso@7.3.1  umap@2.1.1
amrex@24.10          dyninst@13.0.0         gromacs@2024.3         libcatalyst@2.0.0     openfoam@2312           raja@2024.07.0          umpire@2024.07.0
amrex@24.10          e4s-alc@1.0.2          gromacs@2024.3         libcatalyst@2.0.0     openmpi@5.0.5           raja@2024.07.0          umpire@2024.07.0
arborx@1.7           e4s-cl@1.0.4           h5bench@1.4            libnrm@0.1.0          openpmd-api@0.16.0      rempi@1.1.0             unifyfs@2.0
arborx@1.7           ecp-data-vis-sdk@1.0   hdf5@1.12.3            libpressio@0.99.4     papi@7.1.0              scr@3.0.1               upcxx@2023.9.0
argobots@1.2         ecp-data-vis-sdk@1.0   hdf5@1.14.5            libquo@1.4            papi@7.1.0              slate@2024.05.31        upcxx@2023.9.0
ascent@0.9.3         exago@1.6.0            hdf5-vol-async@1.7     libunwind@1.6.2       papyrus@1.0.2           slate@2024.05.31        veloc@1.7
axom@0.9.0           exago@1.6.0            hdf5-vol-cache@v1.1    loki@0.1.7            parallel-netcdf@1.12.3  slepc@3.22.0            visit@3.3.3
axom@0.9.0           exaworks@0.1.0         hdf5-vol-log@1.4.0     magma@2.8.0           paraview@5.13.1         slepc@3.22.0            vtk-m@2.2.0
bolt@2.0             faodel@1.2108.1        hdf5-vol-log@1.4.0     mercury@2.3.1         paraview@5.13.1         stc@0.9.0               vtk-m@2.2.0
boost@1.86.0         fftx@1.2.0             heffte@2.4.0           metall@0.28           parsec@3.0.2209         strumpack@7.2.0         wannier90@3.1.0
bricks@2023.08.25    fftx@1.2.0             heffte@2.4.0           mfem@4.7.0            parsec@3.0.2209         strumpack@7.2.0         warpx@24.10
bricks@2023.08.25    flecsi@2.3.0           hpctoolkit@2024.01.1   mfem@4.7.0            pdt@3.25.2              sundials@7.1.1          wps@4.5
butterflypack@2.4.0  flecsi@2.3.0           hpctoolkit@2024.01.1   mgard@2023-12-09      petsc@3.22.0            sundials@7.1.1          wrf@4.5.2
cabana@0.7.0         flit@2.1.0             hpx@1.10.0             mgard@2023-12-09      petsc@3.22.0            superlu@5.3.0           xyce@7.8.0
cabana@0.7.0         flux-core@0.66.0       hpx@1.10.0             mpark-variant@1.4.0   plasma@24.8.7           superlu-dist@8.2.1      zfp@0.5.5
caliper@2.11.0       flux-core@0.66.0       hypre@2.32.0           mpich@4.2.3           plumed@2.9.2            superlu-dist@8.2.1      zfp@0.5.5
caliper@2.11.0       fortrilinos@2.3.0      hypre@2.32.0           mpifileutils@0.11.1   precice@3.1.2           swig@4.0.2-fortran
chai@2024.07.0       fpm@0.10.0             kokkos@4.4.01          nccmp@1.9.1.0         pruners-ninja@1.0.1     sz@2.1.12.5
chai@2024.07.0       gasnet@2024.5.0        kokkos@4.4.01          nco@5.2.4             pumi@2.2.8              sz3@3.2.0
chapel@2.2.0         geopm-runtime@3.1.0    kokkos-kernels@4.4.01  nek5000@19.0          py-cinemasci@1.3        tasmanian@8.0
charliecloud@0.38    ginkgo@1.8.0           kokkos-kernels@4.4.01  nekbone@17.0          py-deephyper@0.6.0      tasmanian@8.0
conduit@0.9.2        ginkgo@1.8.0           laghos@3.1             netcdf-fortran@4.6.1  py-h5py@3.11.0          tau@2.34
==> 183 installed packages
Singularity>
```

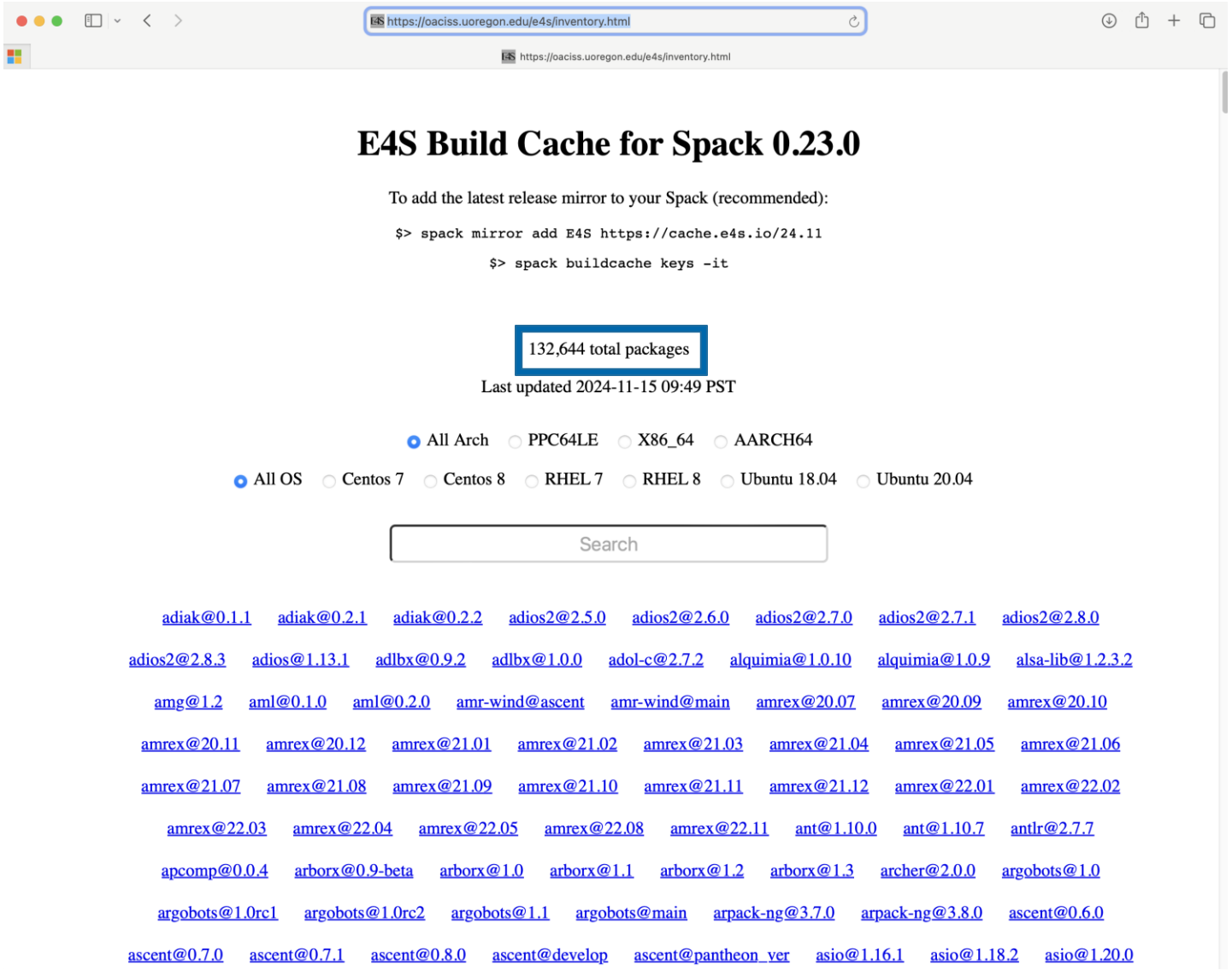
E4S 24.11 Support for GPUs: NVIDIA CUDA on ppc64le (modules)

```
$ singularity run --nv e4s-24.11-cuda70-ppc64.sif
Singularity> module avail

---------------------------------------------------------- /spack/share/spack/lmod/linux-ubuntu20.04-ppc64le/mpich/4.2.3-mhjxbgs/Core ----------------------------------------
   adios/1.13.1                      ecp-data-vis-sdk/1.0          (D)    hpx/1.10.0-cuda70                 openfoam/2312                     strumpack/7.2.0-openmp    (D)
   adios2/2.7.1                      exago/1.6.0-cuda70                   hpx/1.10.0                 (D)    openpmd-api/0.16.0                sundials/7.1.1-cuda70
   adios2/2.10.1-cuda70       (D)    exago/1.6.0                   (D)    hypre/2.32.0-cuda70               papyrus/1.0.2                     sundials/7.1.1            (D)
   alquimia/1.1.0                    exaworks/0.1.0                       hypre/2.32.0               (D)    parallel-netcdf/1.12.3            superlu-dist/8.2.1-cuda70
   amrex/24.10-cuda70                faodel/1.2108.1                      laghos/3.1                        paraview/5.13.1-cuda70            superlu-dist/8.2.1        (D)
   amrex/24.10                (D)    flecsi/2.3.0-cuda70                  lammps/20240829-cuda70-openmp     paraview/5.13.1            (D)    sz/2.1.12.5
   arborx/1.7-cuda70                 flecsi/2.3.0                  (D)    lammps/20240829-openmp     (D)    parsec/3.0.2209-cuda70            tasmanian/8.0-cuda70
   arborx/1.7                 (D)    fortrilinos/2.3.0                    lbann/0.104                       parsec/3.0.2209            (D)    tasmanian/8.0             (D)
   ascent/0.9.3-openmp               geopm-runtime/3.1.0-openmp           libcatalyst/2.0.0                 petsc/3.22.0-cuda70               tau/2.34-cuda
   axom/0.9.0-cuda70-openmp          ginkgo/1.8.0-cuda70-openmp           libcatalyst/2.0.0-zlib-new (D)    petsc/3.22.0               (D)    tau/2.34                  (D)
   axom/0.9.0-openmp          (D)    ginkgo/1.8.0-openmp           (D)    libnrm/0.1.0                      plumed/2.9.2                      trilinos/13.0.1
   boost/1.86.0                      globalarrays/5.8.2                   libpressio/0.99.4-openmp          precice/3.1.2                     trilinos/16.0.0           (D)
   bricks/2023.08.25-cuda            glvis/4.2                            libquo/1.4                        pruners-ninja/1.0.1               turbine/1.3.0
   bricks/2023.08.25          (D)    gptune/4.0.0                         mercury/2.3.1                     pumi/2.2.8                        umpire/2024.07.0-cuda70
   butterflypack/2.4.0-openmp        gromacs/2024.3-cuda70-openmp         metall/0.28                       py-cinemasci/1.3                  umpire/2024.07.0          (D)
   cabana/0.7.0-cuda70               gromacs/2024.3-openmp         (D)    mfem/4.7.0-cuda70                 py-h5py/3.11.0                    unifyfs/2.0
   cabana/0.7.0               (D)    h5bench/1.4                          mfem/4.7.0                 (D)    py-libensemble/1.4.2              upcxx/2023.9.0-cuda70
   caliper/2.11.0-cuda70             hdf5-vol-async/1.7                   mpifileutils/0.11.1               py-petsc4py/3.22.0                upcxx/2023.9.0            (D)
   caliper/2.11.0             (D)    hdf5-vol-cache/v1.1                  nccmp/1.9.1.0                     quantum-espresso/7.3.1-openmp     veloc/1.7
   chai/2024.07.0-cuda70             hdf5-vol-log/1.4.0-threadsafe        nco/5.2.4                         rempi/1.1.0                       visit/3.3.3
   chai/2024.07.0             (D)    hdf5-vol-log/1.4.0            (D)    nek5000/19.0                      scr/3.0.1                         vtk-m/2.2.0-cuda70-openmp
   conduit/0.9.2                     hdf5/1.12.3                          nekbone/17.0                      slate/2024.05.31-cuda70-openmp    vtk-m/2.2.0-openmp        (D)
   cp2k/2024.3-openmp                hdf5/1.14.5                   (D)    netcdf-fortran/4.6.1              slate/2024.05.31-openmp    (D)    wannier90/3.1.0
   darshan-runtime/3.4.5             heffte/2.4.0-cuda70                  netlib-scalapack/2.2.0            slepc/3.22.0-cuda70               warpx/24.10
   datatransferkit/3.1.1             heffte/2.4.0                  (D)    nwchem/7.2.3                      slepc/3.22.0               (D)    wps/4.5
   dyninst/13.0.0-openmp             hpctoolkit/2024.01.1-cuda            omega-h/9.34.13-cuda70            stc/0.9.0                         wrf/4.5.2
   ecp-data-vis-sdk/1.0-cuda70       hpctoolkit/2024.01.1          (D)    omega-h/9.34.13            (D)    strumpack/7.2.0-cuda70-openmp     xyce/7.8.0

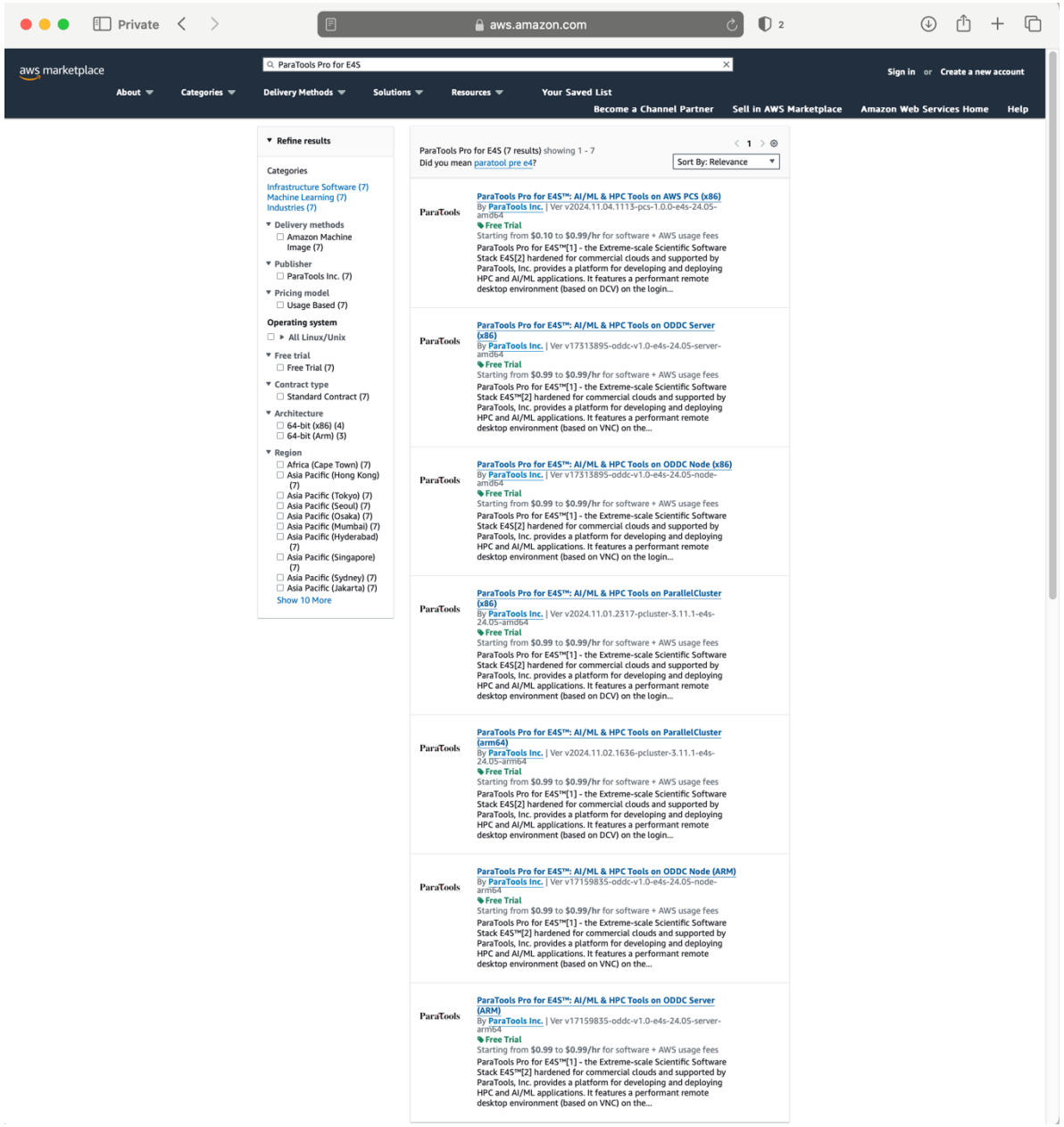
---------------------------------------------------------------------- /spack/share/spack/lmod/linux-ubuntu20.04-ppc64le/Core ----------------------------------------------------
   aml/0.2.1             e4s-cl/1.0.4                gmp/6.3.0                          libunwind/1.6.2                    openmpi/5.0.5             raja/2024.07.0-cuda70
   argobots/1.2          fftx/1.2.0-cuda70           gotcha/1.0.7                       loki/0.1.7                         papi/7.1.0-cuda           raja/2024.07.0        (D)
   bolt/2.0              fftx/1.2.0           (D)    kokkos-kernels/4.4.01-cuda70       magma/2.8.0-cuda70                 papi/7.1.0          (D)   superlu/5.3.0
   chapel/2.2.0          flit/2.1.0                  kokkos-kernels/4.4.01-openmp (D)   mgard/2023-12-09-cuda70-openmp     pdt/3.25.2                swig/4.0.2-fortran
   charliecloud/0.38     flux-core/0.66.0-cuda       kokkos/4.4.01-cuda70               mgard/2023-12-09-openmp       (D)  plasma/24.8.7             sz3/3.2.0
   cusz/0.6.0-cuda70     flux-core/0.66.0     (D)    kokkos/4.4.01-openmp         (D)   mpark-variant/1.4.0                py-deephyper/0.6.0        umap/2.1.1
   darshan-util/3.4.5    fpm/0.10.0-openmp           legion/24.09.0-cuda70              mpich/4.2.3                   (L)  py-jupyterhub/1.4.1       zfp/0.5.5-cuda70
   e4s-alc/1.0.2         gasnet/2024.5.0             legion/24.09.0               (D)   nrm/0.1.0                          qthreads/1.18             zfp/0.5.5             (D)
```

E4S Build Cache for Spack 0.23.0 hosted at U. Oregon



- Over 132K binaries!
- No need to recompile from source code

ParaTools Pro for E4S™*: Available in AWS, Google Cloud, Azure



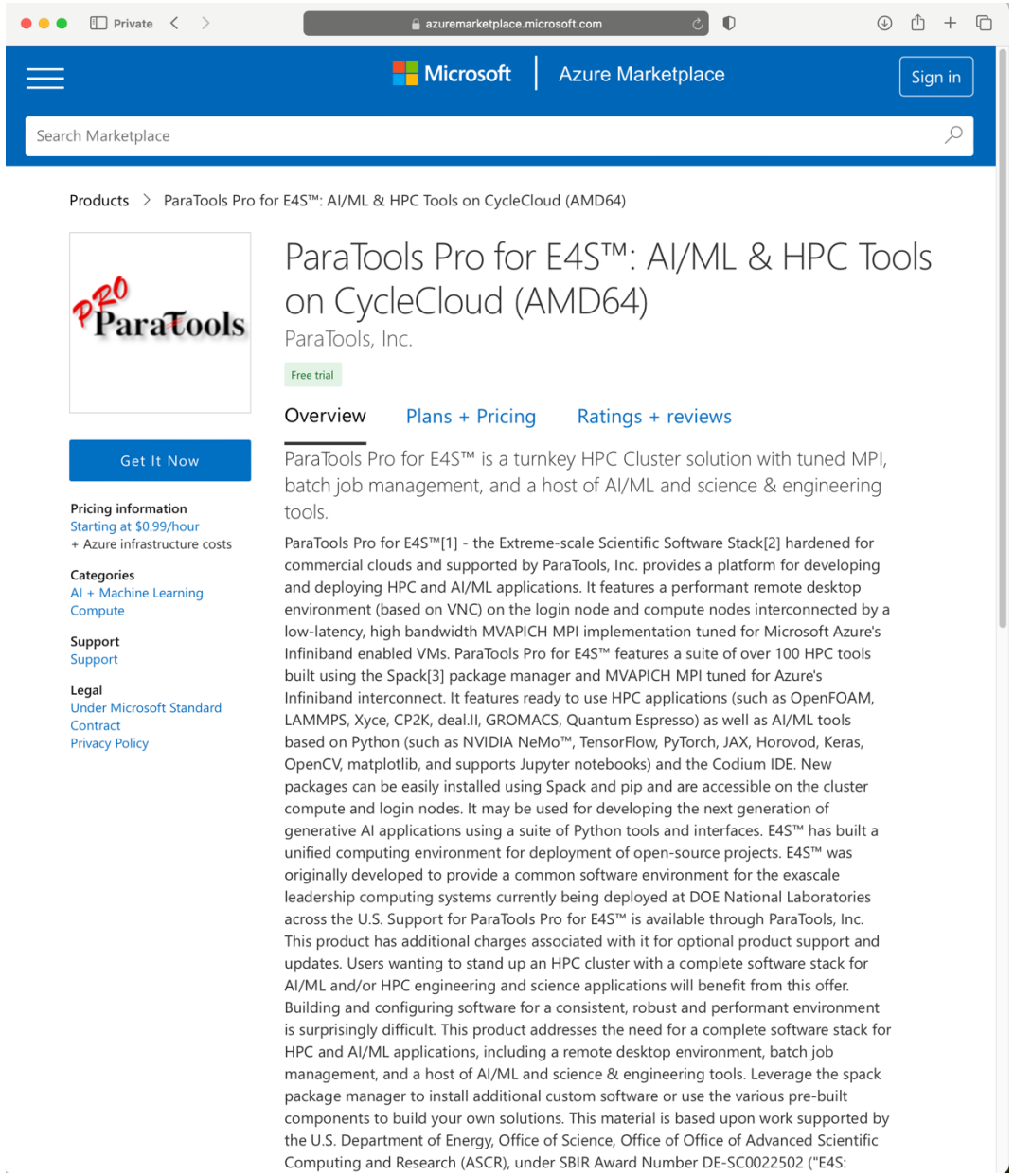
- AWS Marketplace listing
- Support for SLURM and Torque
- GPU accelerated remote desktop
- Compute nodes with GPUs
- Commercial image with support

* Supported by DOE SBIR Phase I and II DE-SC0022502

ParaTools Pro for E4S™: Available in AWS, Google Cloud, Azure

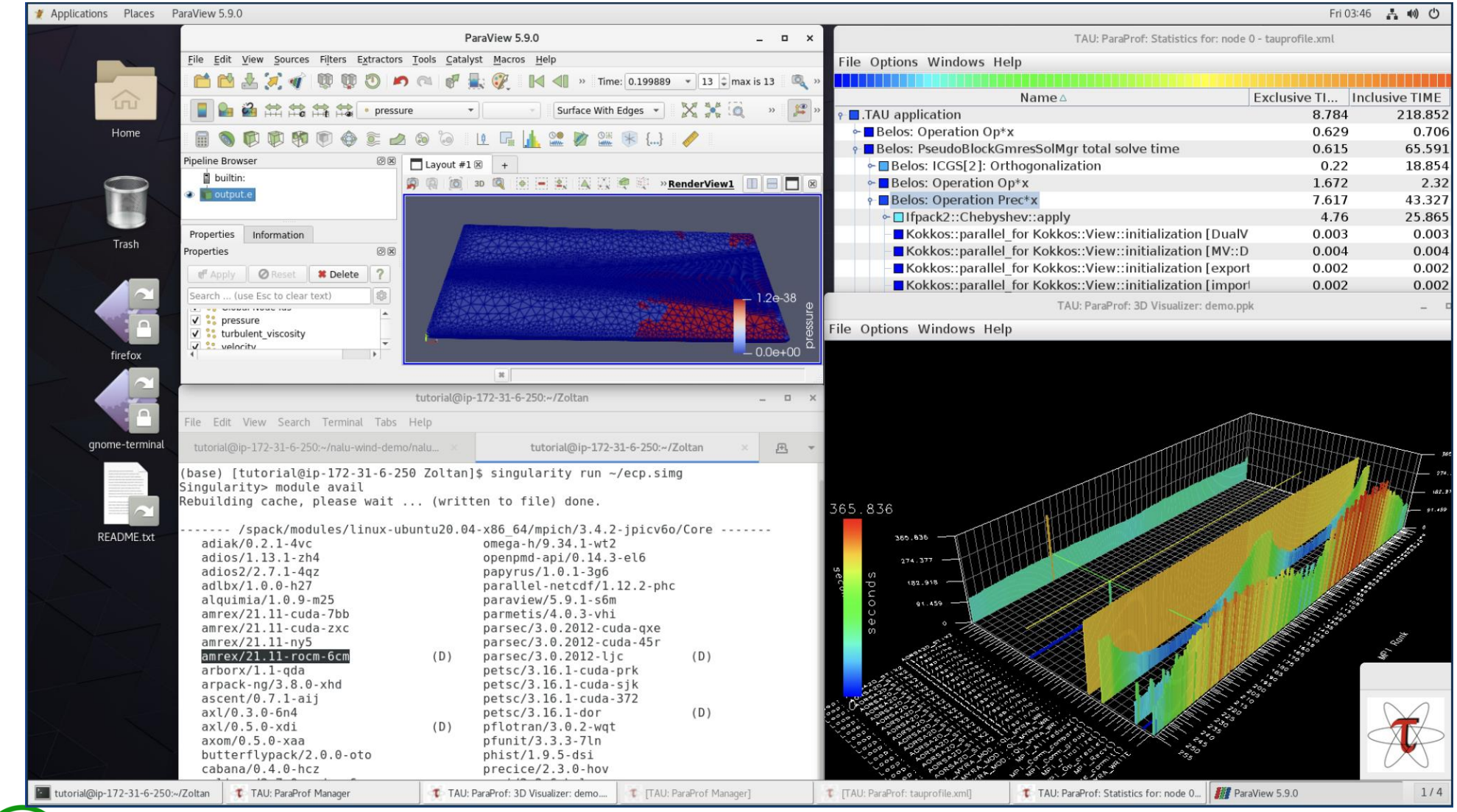
Google Cloud Marketplace

ParaTools Pro for E4S™: Available in AWS, Google Cloud, Azure



Azure Marketplace listing

E4S 24.11 AWS image: ami-0e752117cfa13cb9b in US-West-2 (OR)

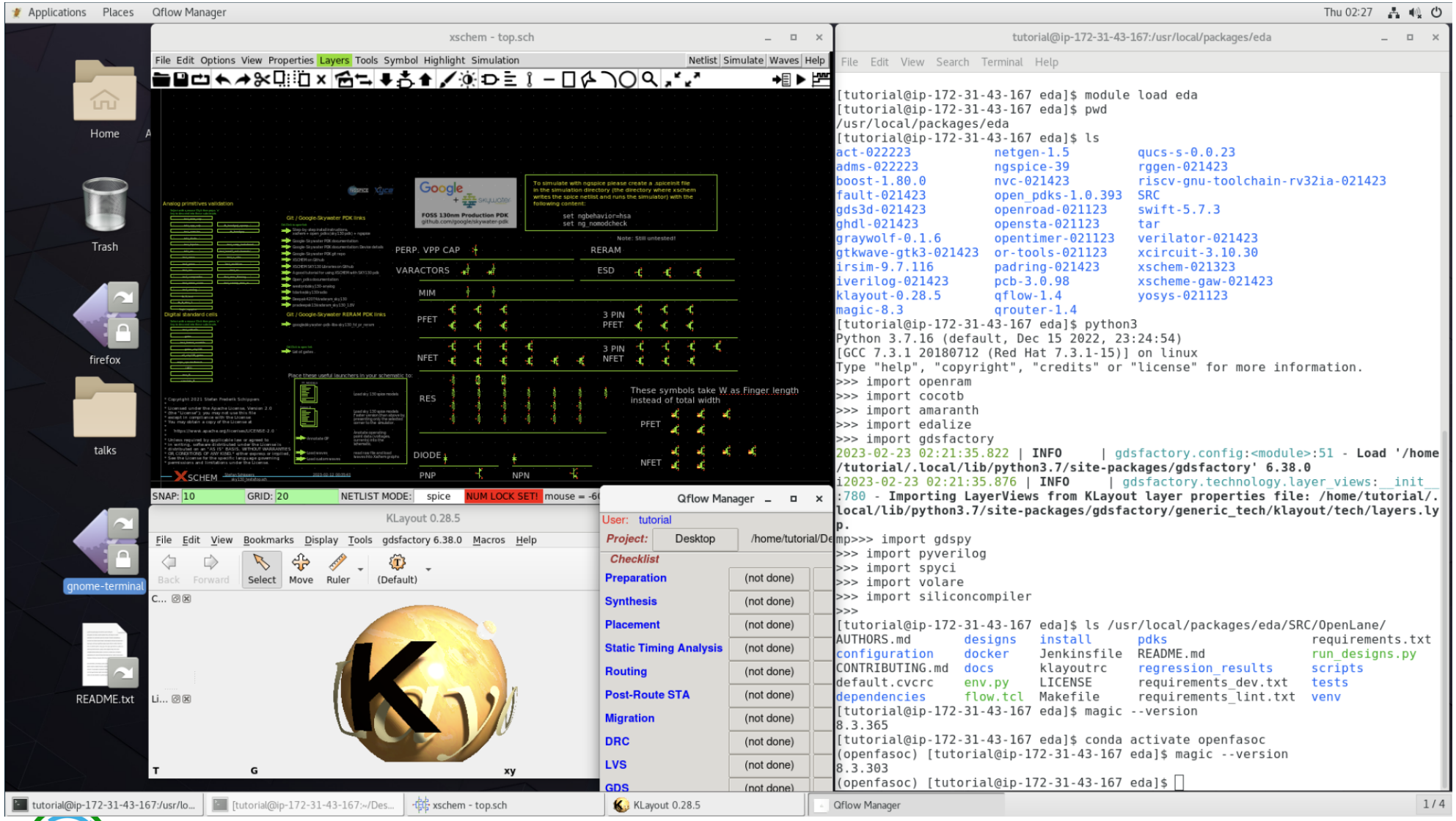


E4S AWS

- 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



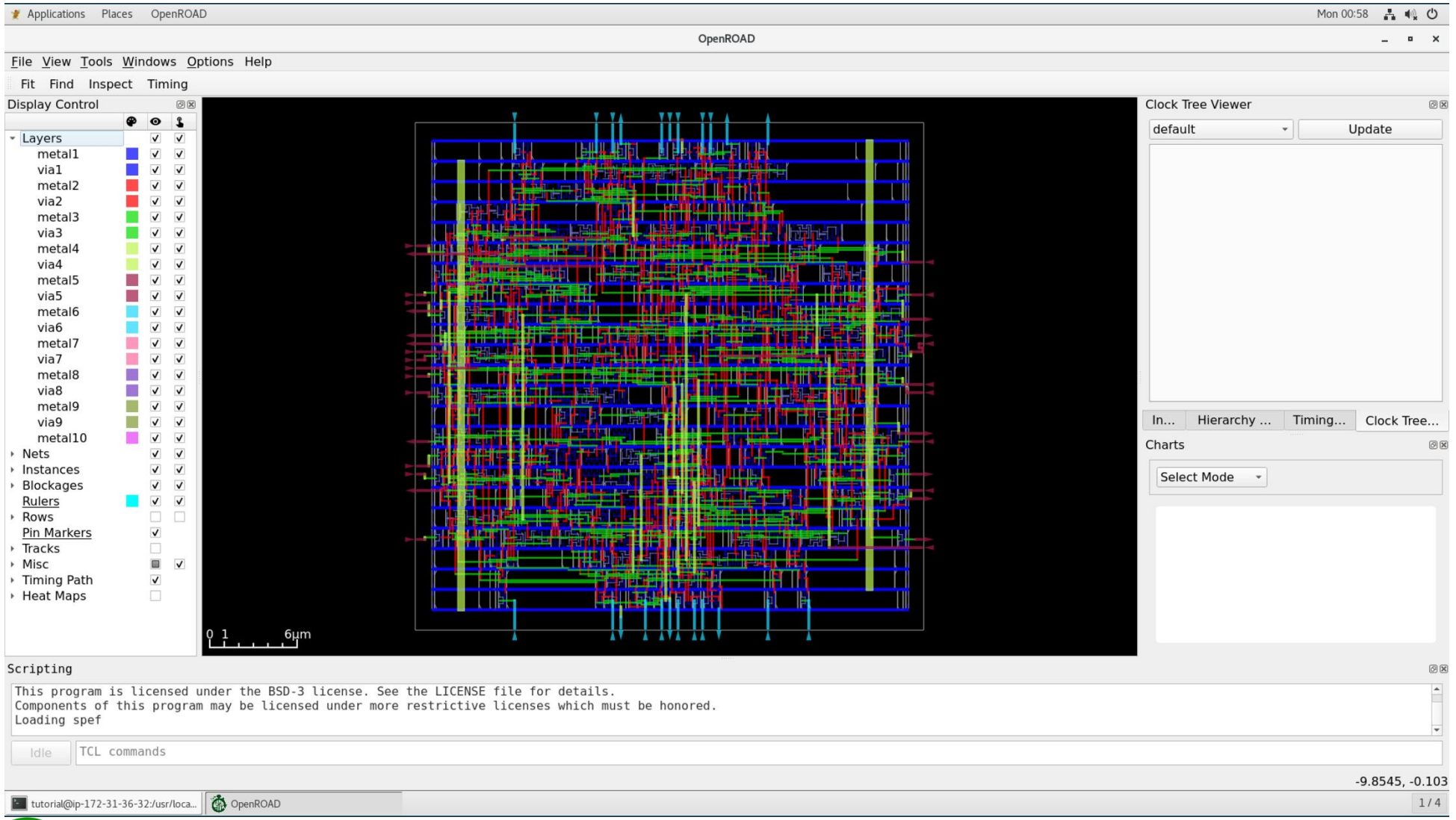
E4S EDA on AWS

- 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

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. Microwatt CPU (IBM) in OpenROAD.



OpenROAD GUI

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

#	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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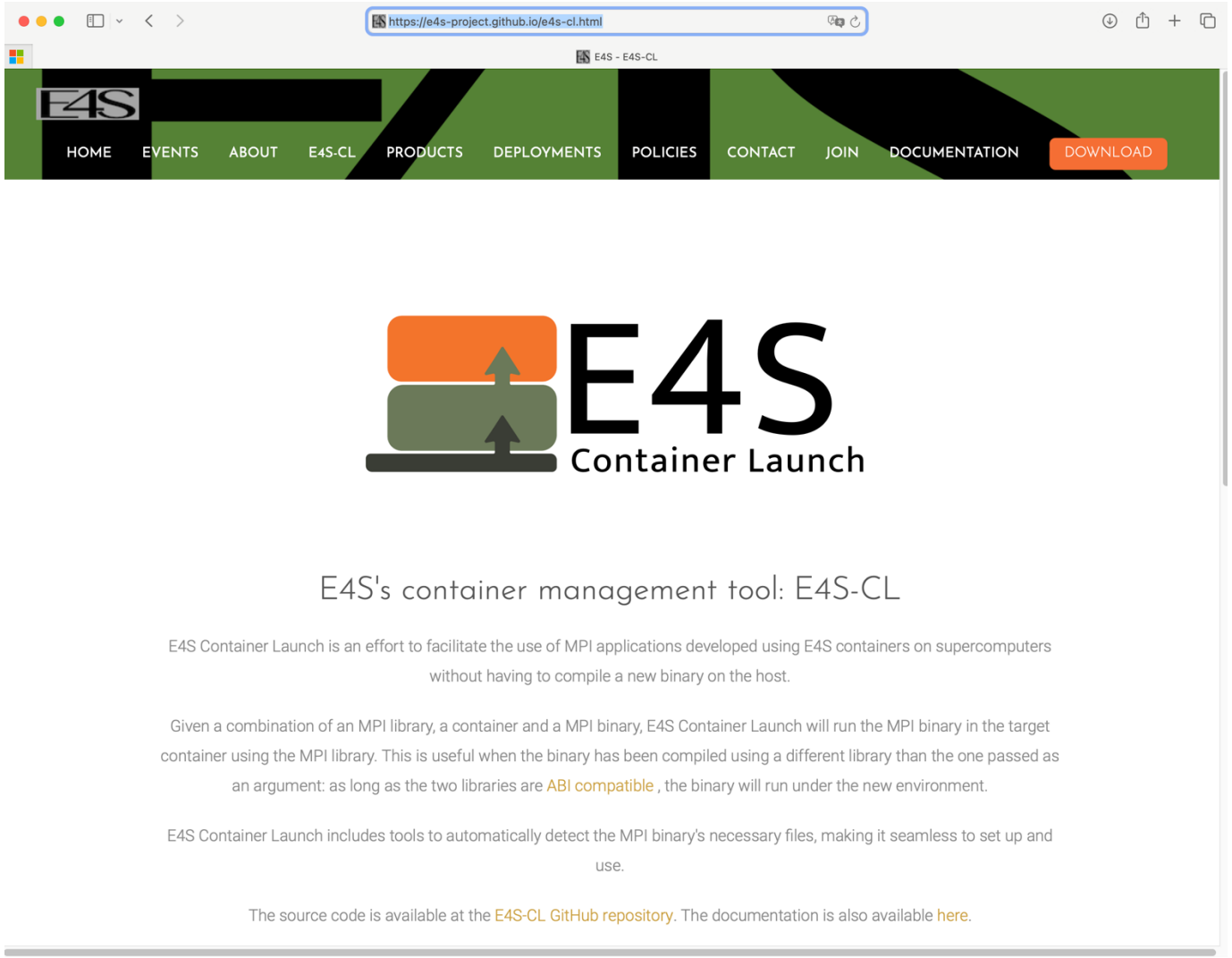
https://e4s.io/eda

E4S Container Launch tool: e4s-cl



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

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
```

E4S Container Launch

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

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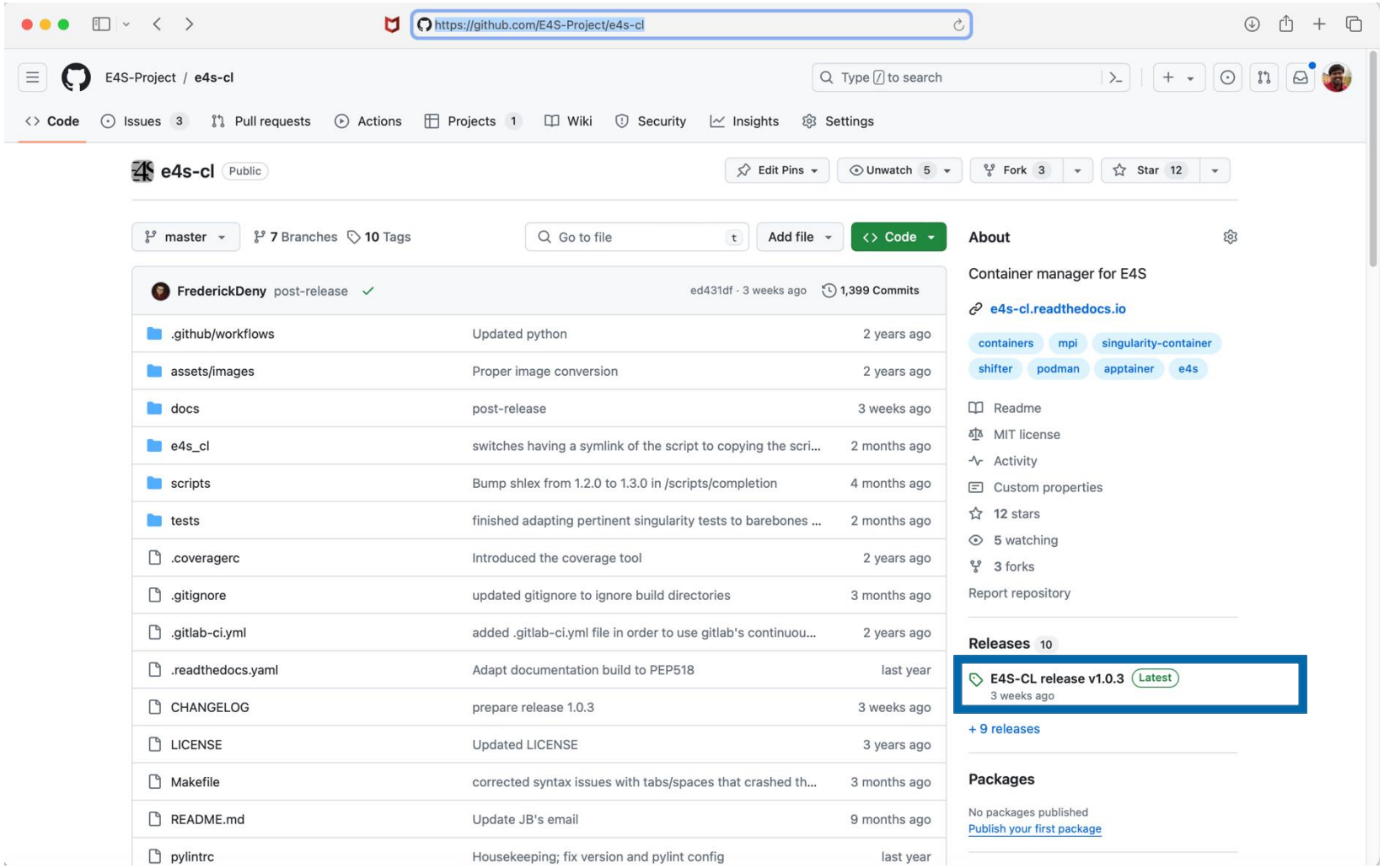
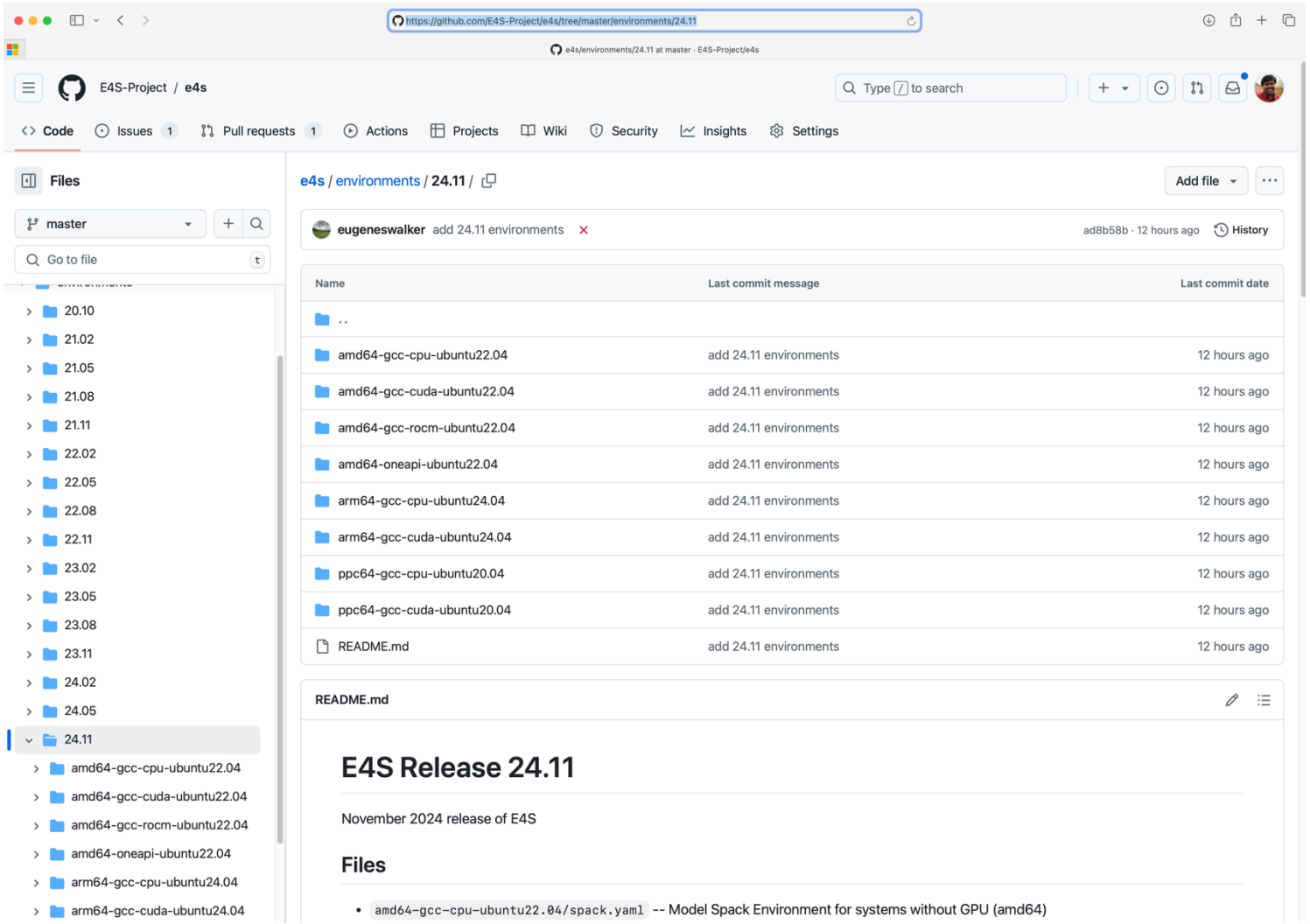
Release of e4s-cl on GitHub



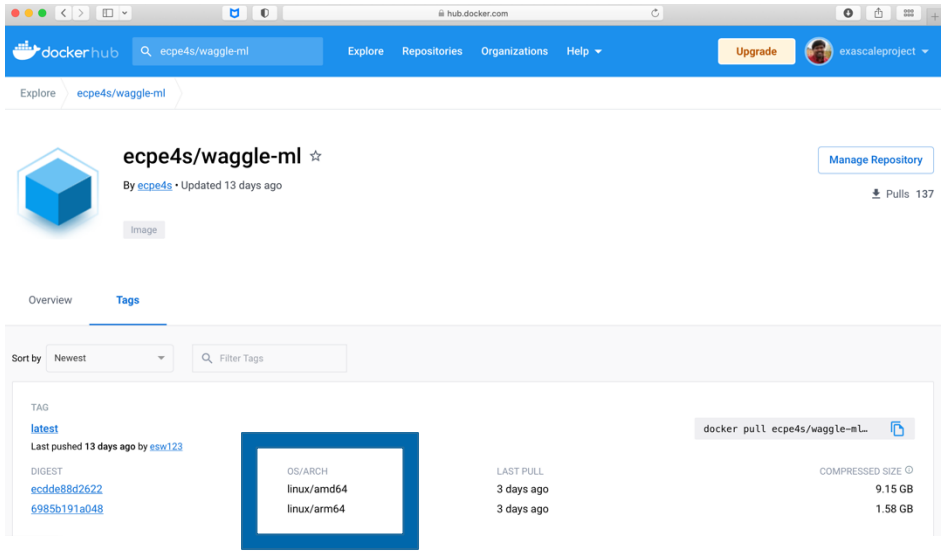
https://github.com/E4S-Project/e4s-cl

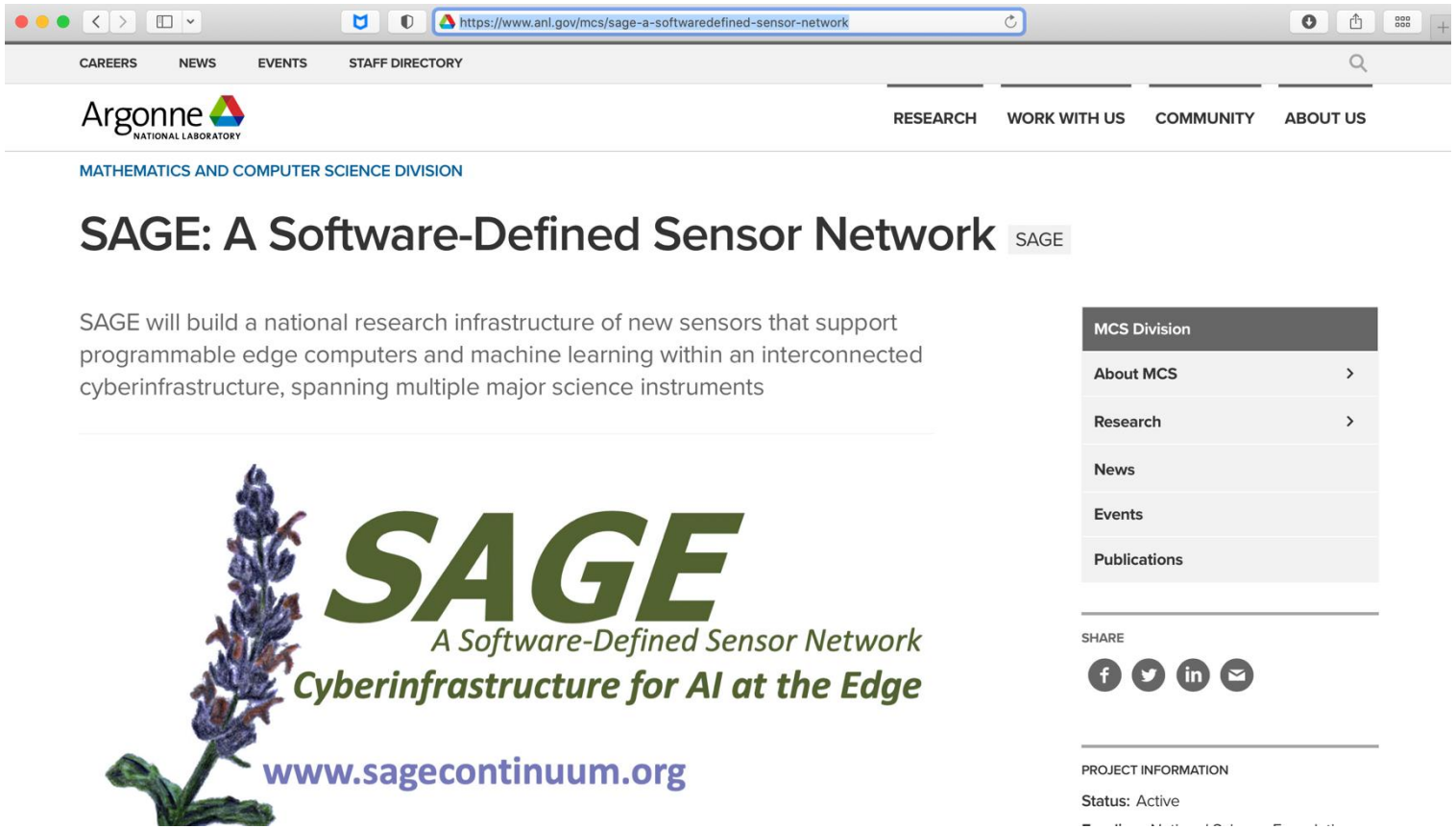
E4S: Open Source Development on GitHub



https://github.com/E4S-Project

Release of custom E4S images: Waggle and SAGE projects





% docker pull ecpe4s/waggle-ml

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- https://science.osti.gov/ascr
- https://pesoproject.org
- https://hpsf.io

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Thank you

https://www.exascaleproject.org

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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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