Performance Evaluation of GPU-accelerated HPC and AI applications using HPCToolkit, TAU, and ParaTools Pro for E4S™

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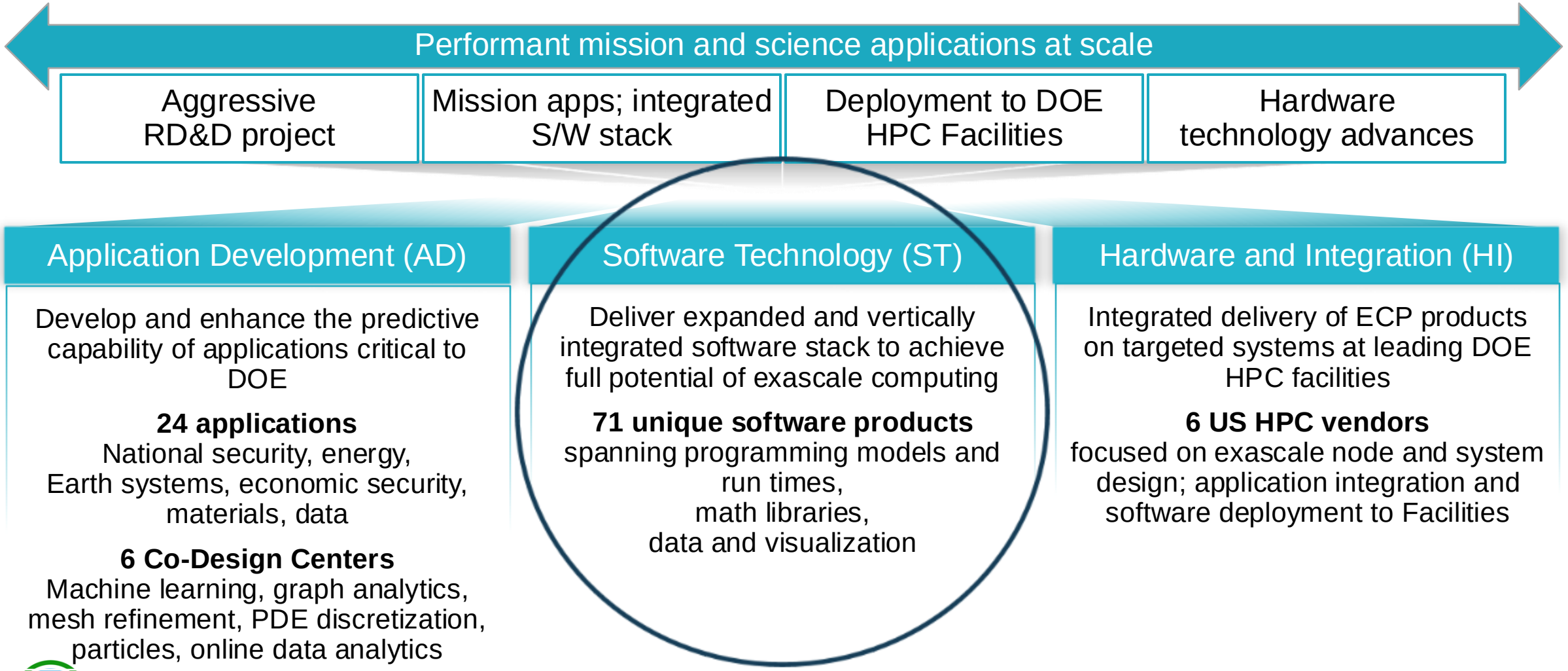
Presentation at EnergyHPC conference, Rice U., Houston

February 27, 2025

https://tinyurl.com/e4stut

U.S. DEPARTMENT OF ENERGY | Office of Science

ECP's holistic approach uses co-design and integration to achieve exascale computing



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US DOE HPC Roadmap to Exascale Systems

2012-2020 | **2021-2025**

decommissioned

ORNL
Cray/AMD/NVIDIA

ANL
IBM BG/Q

ANL
Cray/Intel KNL

LBNL
Cray/Intel Xeon/KNL

ORNL
IBM/NVIDIA

ORNL
HPE/AMD

Exascale Systems

ANL
Intel/HPE

LBNL
HPE/AMD/NVIDIA

LLNL
IBM BG/Q

LANL/SNL
Cray/Intel Xeon/KNL

LLNL
IBM/NVIDIA

LANL/SNL
HPE/Intel

LLNL
HPE/AMD

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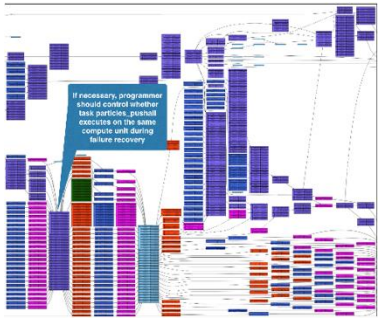
ECP **Software Technology (ST)**

Goal

Build a comprehensive, coherent software stack that enables application developers to productively develop highly parallel applications that effectively target diverse exascale architectures

- Prepare SW stack for scalability with massive on-node parallelism
- Extend existing capabilities when possible, develop new when not
- Guide, and complement, and integrate with vendor efforts
- Develop and deliver high-quality and robust software products



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E4S: Extreme-scale Scientific Software Stack

https://e4s.io

About E4S

- 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 120+ HPC (OpenFOAM, Gromacs, Nek5000, LAMMPS), EDA (e.g., Xyce), and AI/ML packages (e.g., NVIDIA NeMo™, HuggingFace Hub, TensorFlow, PyTorch, TorchBraid, Scikit-Learn, Pandas, JAX, Horovod, LBANN with support for GPUs).
- Base images and full featured containers (with GPU support) and DOE LLVM containers.
- Commercial support for E4S through ParaTools, Inc. for installation, maintaining an issue tracker, and ECP AD engagement.
- E4S for commercial cloud platforms: Adaptive Computing's ODDC with ParaTools Pro for E4S™ image for AWS, GCP, Azure.
- 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.
- e4s-chain-spack.sh to chain two Spack instances allows us to install new packages in home directory and use other tools.
- e4s-cl container launch tool allows binary distribution of applications by swapping MPI in the containerized app w/ system MPI.
- e4s-alc is an à la carte tool to customize container images by adding system and Spack packages to an existing image.

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Argonne NATIONAL LABORATORY · BERKELEY LAB · Brookhaven National Laboratory · kitware · Lawrence Livermore National Laboratory · Los Alamos NATIONAL LABORATORY · OAK RIDGE National Laboratory · Pacific Northwest · ParaTools · Sandia National Laboratories · SUSTAINABLE HORIZONS INSTITUTE

Reproducibility of scientific results using E4S containers

- E4S has built and distributed 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-alc is an à-la-carte tool to customize container images by adding system and Spack packages to an existing image.
- e4s-chain-spack.sh to chain two Spack instances allows us to install new packages in home directory and use other tools.
- e4s-cl container launch tool allows binary distribution of applications by swapping MPI in the containerized app with system MPI.
- Using containers to take a snapshot of a working scientific model for reproducibility.
- Hands-on exercises on building a working container with MPI and using it on an HPC system.

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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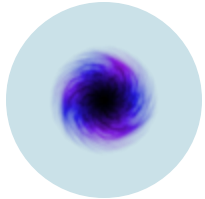
E4S: Better quality, documentation, testing, integration, delivery, building & use

Delivering HPC software to facilities, vendors, agencies, industry, international partners in a brand-new way

Quality Commitment
Community policies, improvement



DocPortal
Single portal to all E4S product info

Portfolio testing
Especially leadership platforms

Curated collection
The end of dependency hell

Quarterly releases
Release 24.11 – November

Build caches
10X build time improvement

Turnkey stack
A new user experience

https://e4s.io

E4S Strategy Group
US agencies, industry, international

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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)

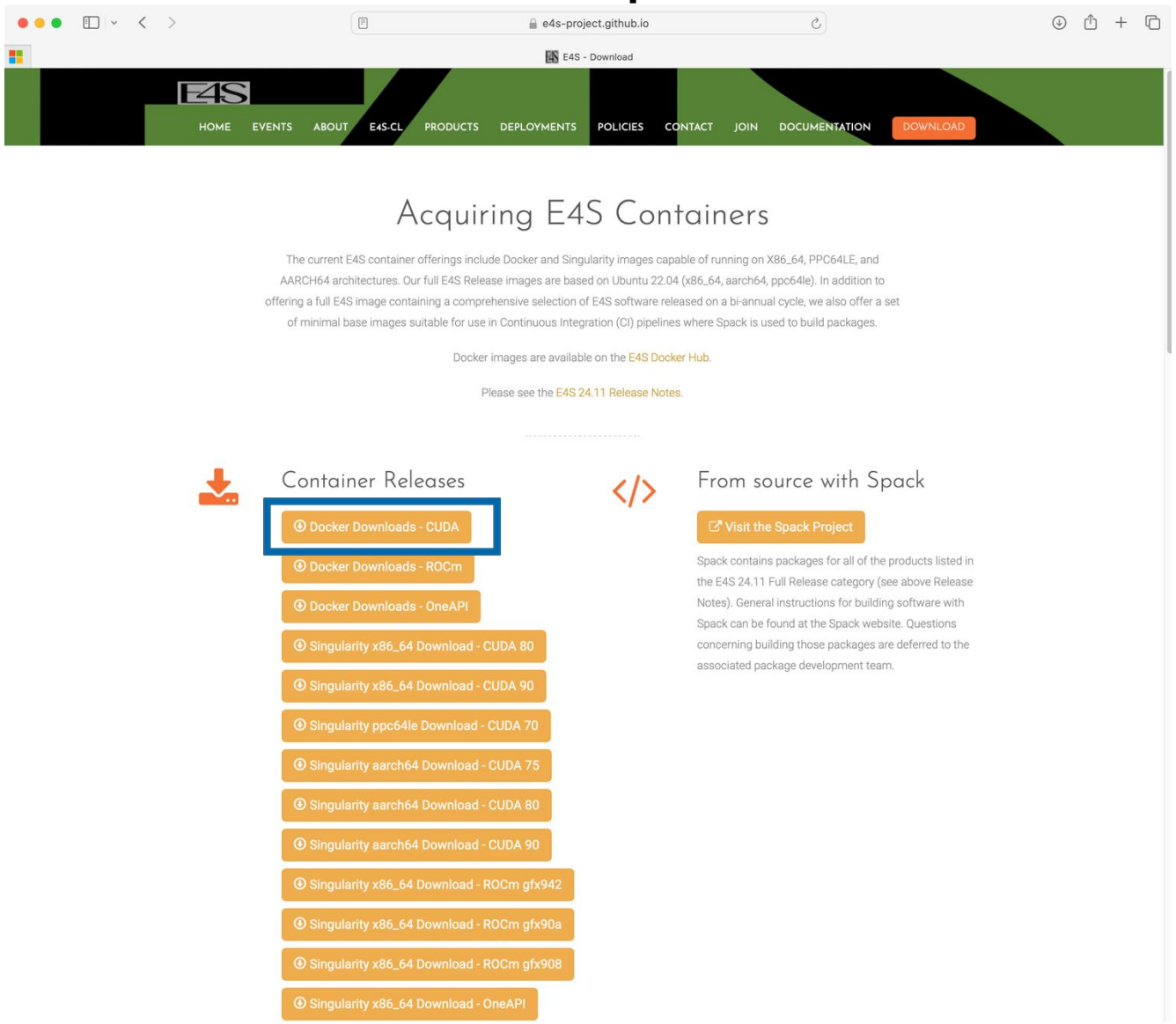
Also include other products .e.g.,
AI: NVIDIA NeMo™, DeepHyper, TorchBraid, Scikit-Learn, JAX, PyTorch, TensorFlow, Horovod, LBANN
Co-Design: AMReX, Cabana, MFEM
EDA: Xyce

PESO

E4S Download from https://e4s.io

PESO

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

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

```
 1: adios2           /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/adios2-2.10.1-rp2yih6nctfwonm7nv3rgefjxqydda4j
 2: alquimia         /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/alquimia-1.1.0-ko37njvqldmohhnihg5rnuk2qllfftgd
 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
 8: axom             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/axom-0.9.0-ksr6mvkn256ummrzmstshusediyx4fst
 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
17: chapel           /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/chapel-2.2.0-4r2cezcrg7nxwssp2muw4p7cp2zr4mxx
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
29: exago            /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/exago-1.6.0-ed4r6b3rpuff3mjy7m55linfijb6zgzt
30: exaworks         /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/exaworks-0.1.0-7ifhre632qydkhipyqm6pd5unwn4ch4u
31: faodel           /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/faodel-1.2108.1-m323gnsgvffuabsvefkrp264phzypy4z
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33: flecsi           /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/flecsi-2.3.0-p5wlwxz3fw7yalfbitqeze7gjtx4bmbn
34: flit             /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/flit-2.1.0-t4bb2k5wzypjwfna252tjik344ag6sme
35: flux-core        /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/flux-core-0.66.0-a73mo2pilzum6lzzkugp7hfmy5nn5ex4
36: flux-sched       /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/flux-sched-0.36.1-qbewzrfine24nrjuv7xh34b4jucutcry
37: fortrilinos      /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/fortrilinos-2.3.0-qudhrrp3agu3f2jym4ziey37asswolmq
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

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
50:  hpctoolkit          /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/hpctoolkit-2024.01.1-frwgnvqbcru6w3wqra5cp7amshjd6fey
51:  hpx                 /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/hpx-1.10.0-pam2qt2ggxdjku2nrjd2eskliefwoe3j
52:  hypre               /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/hypre-2.32.0-zkijq2mug7eqjcxbpk7fuuwq44xsol7i
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63:  libquo              /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/libquo-1.4-b23b2c2gxo2k6gbd3b3sbqlhjwfapxef
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71:  mpich               /usr/local/mpich/install/mpich
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73:  nccmp               /spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/nccmp-1.9.1.0-wxmr6dvro3sa4w63ssc6emnaqyucz3af
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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
```

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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 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
- PyTorch: 2.3.0
- NVIDIA NeMo™: 2.0.0rc1
- NVHPC 24.9
- CUDA 12.2.2
- CuDNN 8.9.7.29, 9.5.0
- NCCL 2.20.3
- TensorRT 8.6.1.6

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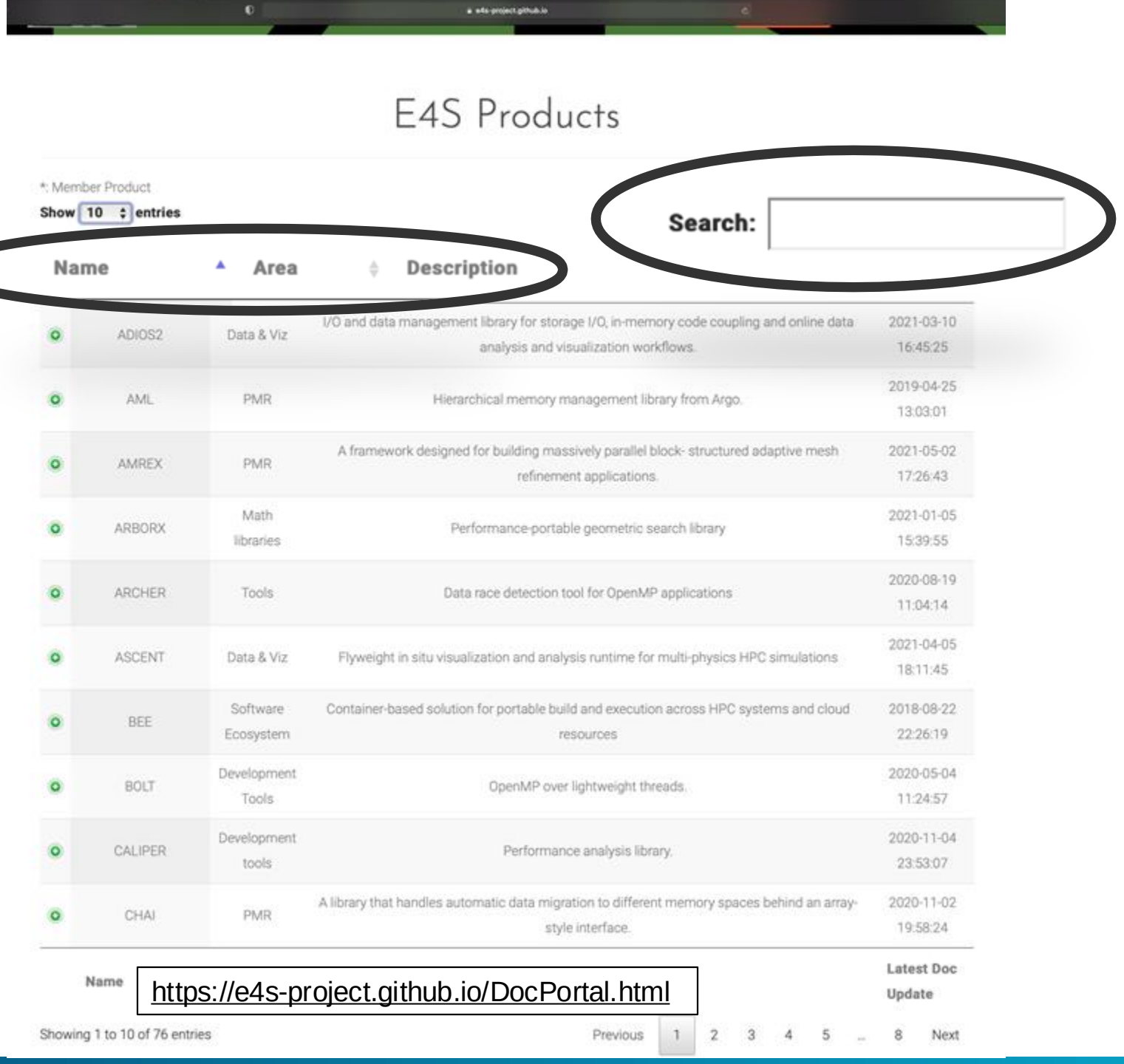
E4S 24.11 Support for GPUs: NVIDIA

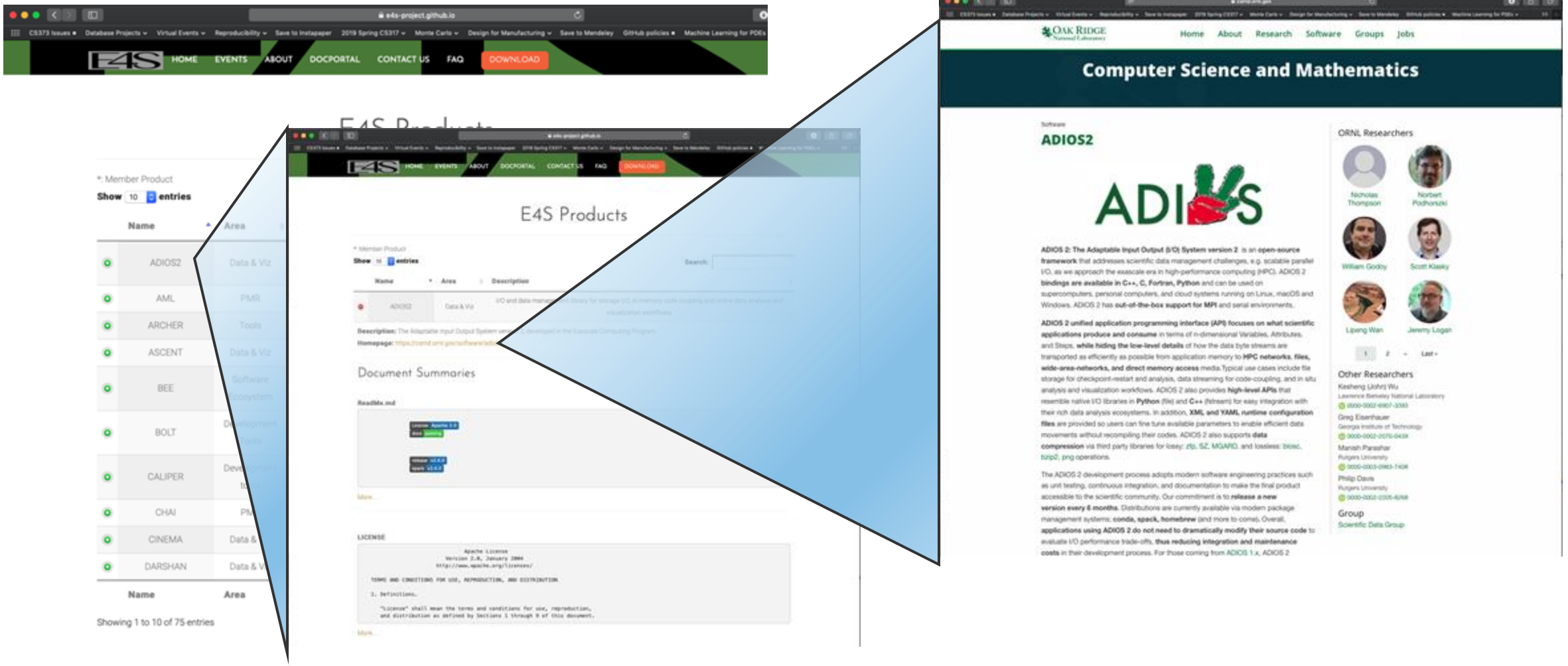
```
$ singularity run --nv e4s-24.11-cuda90-arm64.sif
Singularity> spack find -x +cuda
-- linux-ubuntu24.04-aarch64 / gcc@13.2.0 ------------------------
adios2@2.10.1  caliper@2.11.0       flecsi@2.3.0      hpctoolkit@2024.01.1  legion@24.09.0     petsc@3.22.0      sundials@7.1.1      umpire@2024.07.0
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 DocPortal

- Single point of access
- All E4S products
- Summary Info
  - Name
  - Functional Area
  - Description
  - License
- Searchable
- Sortable
- Rendered daily from repos

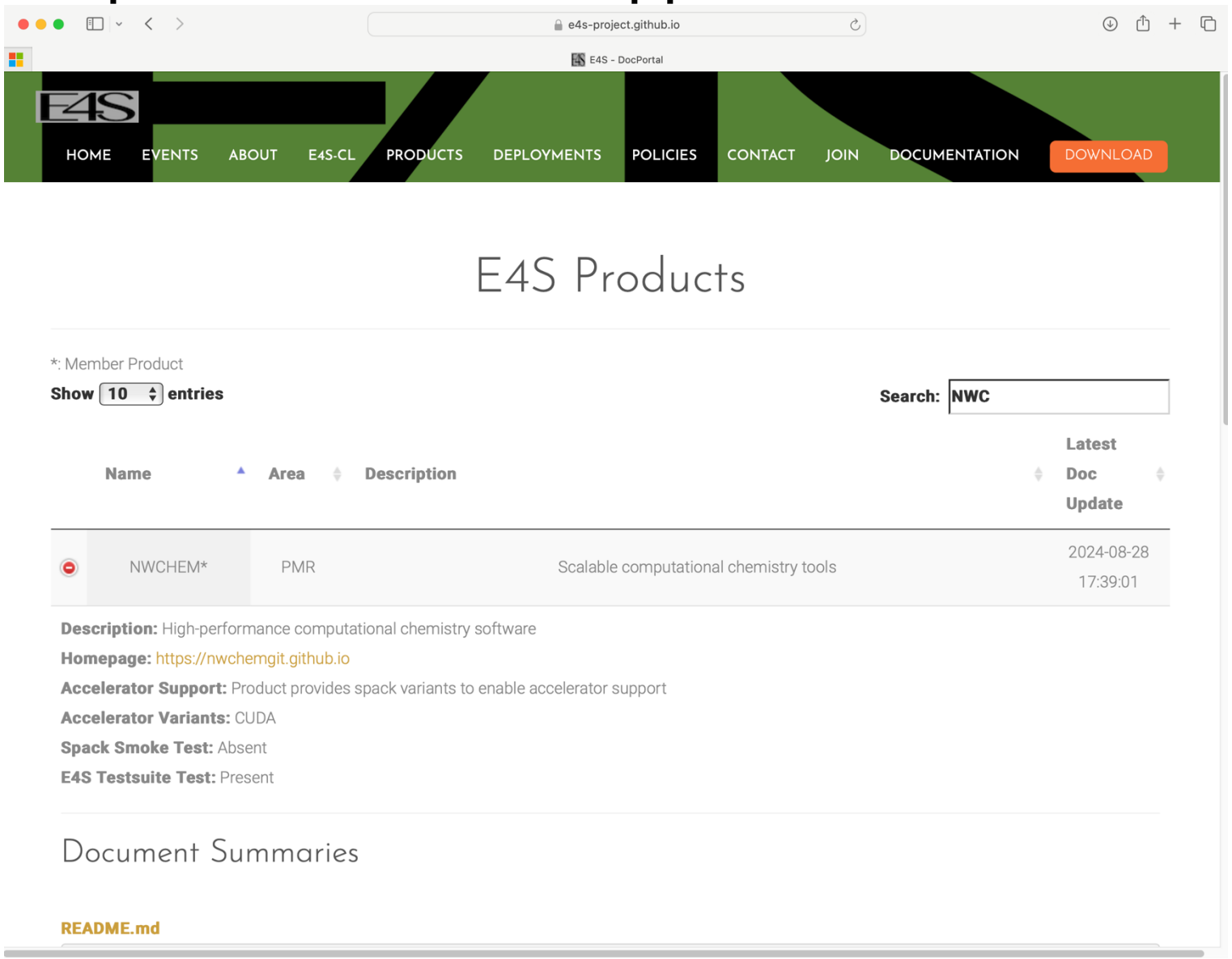


Goal: All E4S product documentation accessible from single portal on E4S.io (working mock webpage below)



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

E4S DocPortal updated with new applications and AI/ML tools



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@13.0.1

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

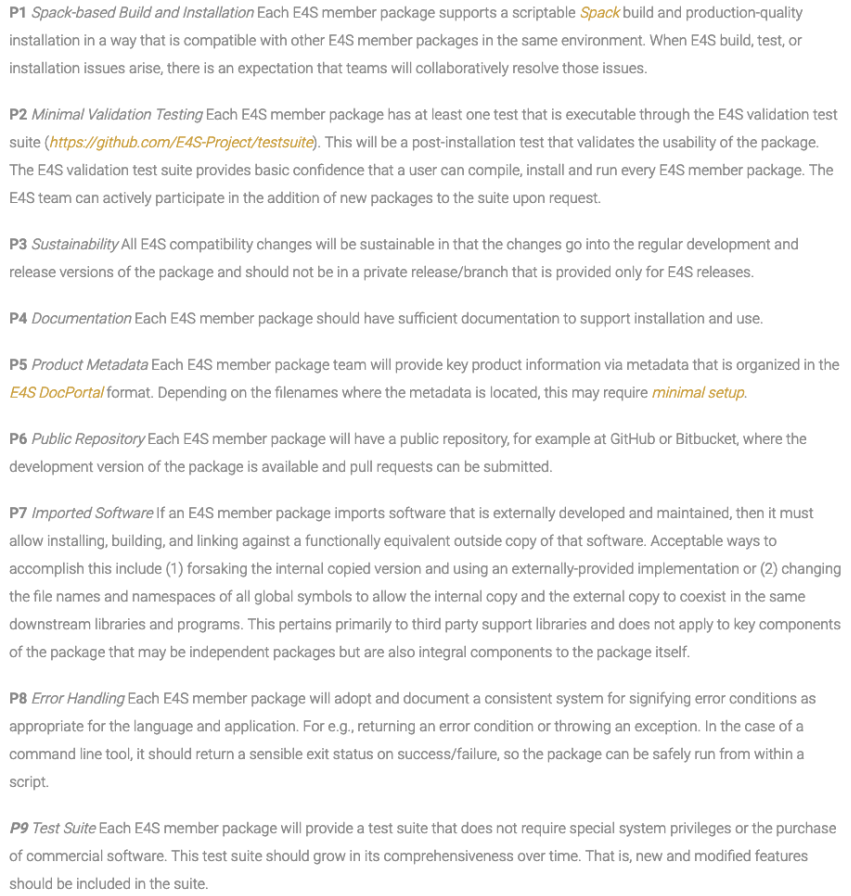
https://github.com/E4S-Project/e4s-cl

PESO

E4S Community Policies Version 1

A Commitment to Quality Improvement

- Will serve as membership criteria for E4S
  - Membership is not required for *inclusion* in E4S
  - Also includes forward-looking draft policies
- Purpose: enhance sustainability and interoperability
- Topics cover building, testing, documentation, accessibility, error handling and more
- Multi-year effort led by SDK team
  - Included representation from across ST
  - Multiple rounds of feedback incorporated from ST leadership and membership
- Modeled after xSDK Community Policies
- https://e4s-project.github.io/policies.html



P1 *Spack-based Build and Installation* Each E4S member package supports a scriptable *Spack* build and production-quality installation in a way that is compatible with other E4S member packages in the same environment. When E4S build, test, or installation issues arise, there is an expectation that teams will collaboratively resolve those issues.

P2 *Minimal Validation Testing* Each E4S member package has at least one test that is executable through the E4S validation test suite (*https://github.com/E4S-Project/testsuite*). This will be a post-installation test that validates the usability of the package. The E4S validation test suite provides basic confidence that a user can compile, install and run every E4S member package. The E4S team can actively participate in the addition of new packages to the suite upon request.

P3 *Sustainability* All E4S compatibility changes will be sustainable in that the changes go into the regular development and release versions of the package and should not be in a private release/branch that is provided only for E4S releases.

P4 *Documentation* Each E4S member package should have sufficient documentation to support installation and use.

P5 *Product Metadata* Each E4S member package team will provide key product information via metadata that is organized in the *E4S DocPortal* format. Depending on the filenames where the metadata is located, this may require *minimal setup*.

P6 *Public Repository* Each E4S member package will have a public repository, for example at GitHub or Bitbucket, where the development version of the package is available and pull requests can be submitted.

P7 *Imported Software* If an E4S member package imports software that is externally developed and maintained, then it must allow installing, building, and linking against a functionally equivalent outside copy of that software. Acceptable ways to accomplish this include (1) forsaking the internal copied version and using an externally-provided implementation or (2) changing the file names and namespaces of all global symbols to allow the internal copy and the external copy to coexist in the same downstream libraries and programs. This pertains primarily to third party support libraries and does not apply to key components of the package that may be independent packages but are also integral components to the package itself.

P8 *Error Handling* Each E4S member package will adopt and document a consistent system for signifying error conditions as appropriate for the language and application. For e.g., returning an error condition or throwing an exception. In the case of a command line tool, it should return a sensible exit status on success/failure, so the package can be safely run from within a script.

P9 *Test Suite* Each E4S member package will provide a test suite that does not require special system privileges or the purchase of commercial software. This test suite should grow in its comprehensiveness over time. That is, new and modified features should be included in the suite.

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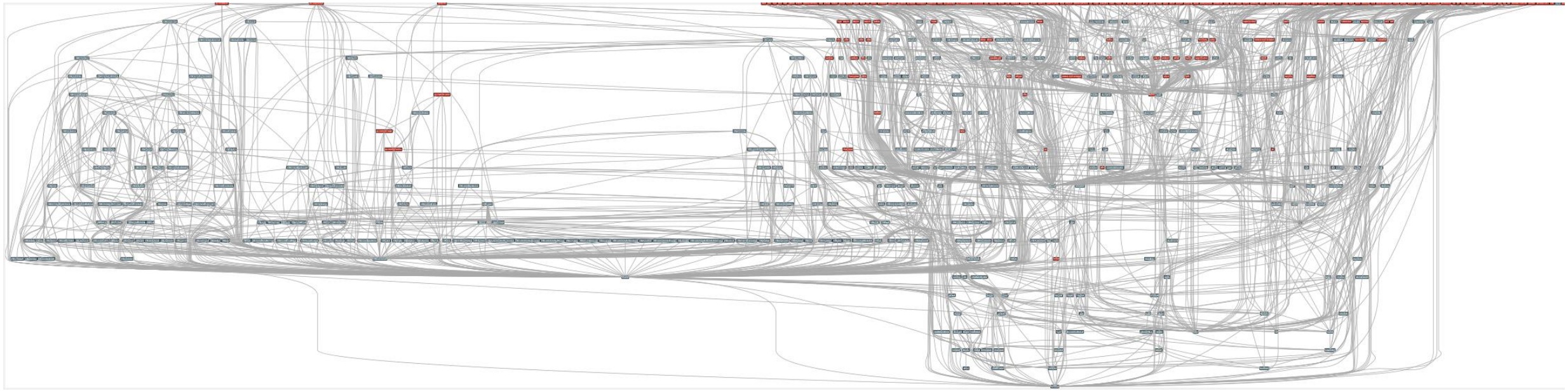
Spack

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

Managing large software installations: E4S



- Red boxes are the packages in it (about 100)
- Blue boxes are what *else* you need to build it (about 600)
- It’s infeasible to build and integrate all of this manually

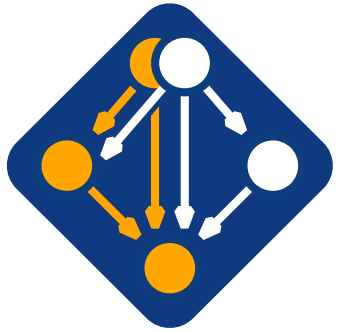
Spack enables software distribution for HPC

No installation required: clone and go

```
$ git clone https://github.com/spack/spack
$ source spack/share/spack/setup-env.sh
$ spack compiler find
$ spack external find
```

```
$ spack install tau                                                    unconstrained
$ spack install tau@2.34                                               @ custom version
$ spack install tau@2.34 %gcc@11.2.0                                   % custom compiler
$ spack install tau@2.34 %gcc@11.2.0 +mpi+python+pthreads              +/- build option
$ spack install tau@2.34 %gcc@11.2.0 +mpi ^mvapich2@2.3~wrapperrpath ^ dependency information
```

- Each expression is a ***spec*** for a particular configuration
  - Each clause adds a constraint to the spec
  - Constraints are optional – specify only what you need.
  - Customize install on the command line!
- Spec syntax is recursive
  - Full control over the combinatorial build space



github.com/spack/spack

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The Spack community is growing rapidly

- **Spack simplifies HPC software for:**
  - Users
  - Developers
  - Cluster installations
  - The largest HPC facilities
- **Spack is central to ECP's software strategy**
  - Enable software reuse for developers and users
  - Allow the facilities to consume the entire ECP stack
- **The roadmap is packed with new features:**
  - Building the ECP software distribution
  - Better workflows for building containers
  - Stacks for facilities
  - Chains for rapid dev workflow
  - Optimized binaries
  - Better dependency resolution

Visit spack.io

github.com/spack/spack

@spackpm

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ParaTools Pro for E4S™: Using E4S on Cloud Platforms

Considerations while deploying HPC/AI workloads to the cloud

- Which cloud provider?
  - AWS, OCI, GCP, Azure, …
  - Why not all?
- HPC and AI/ML workloads need low latency, high bandwidth
  - Which MPI?
- Which image?
  - Remote desktop accelerated by GPU, integration with batch schedulers (SLURM, Torque)
  - Base Ubuntu without HPC tools or libraries? Too steep a learning curve
- Provisioning and building the image on different cloud providers
  - Command line interfaces can be cumbersome to use
- Bursting to the cloud from on-prem clusters using batch submission scripts?

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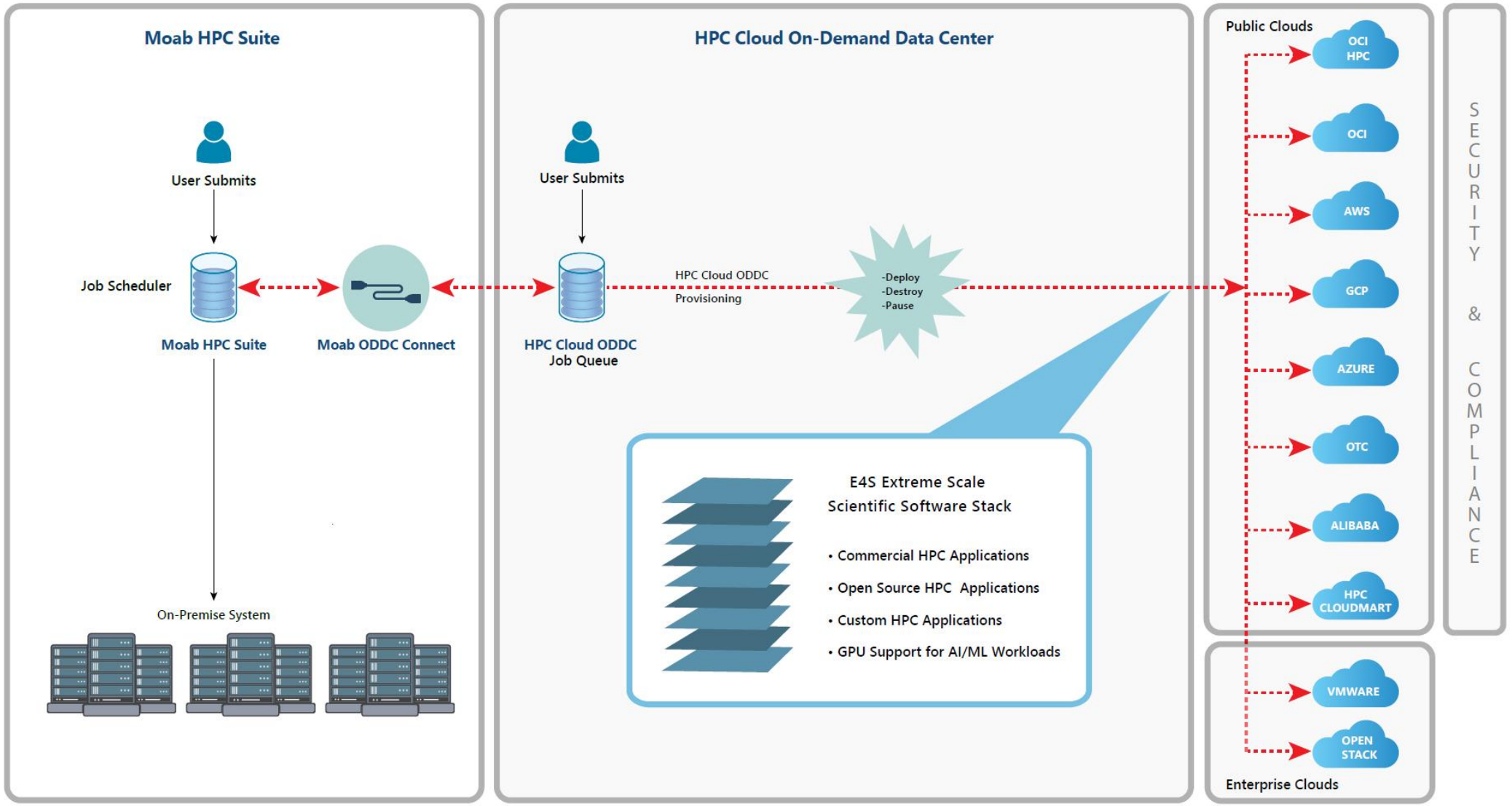
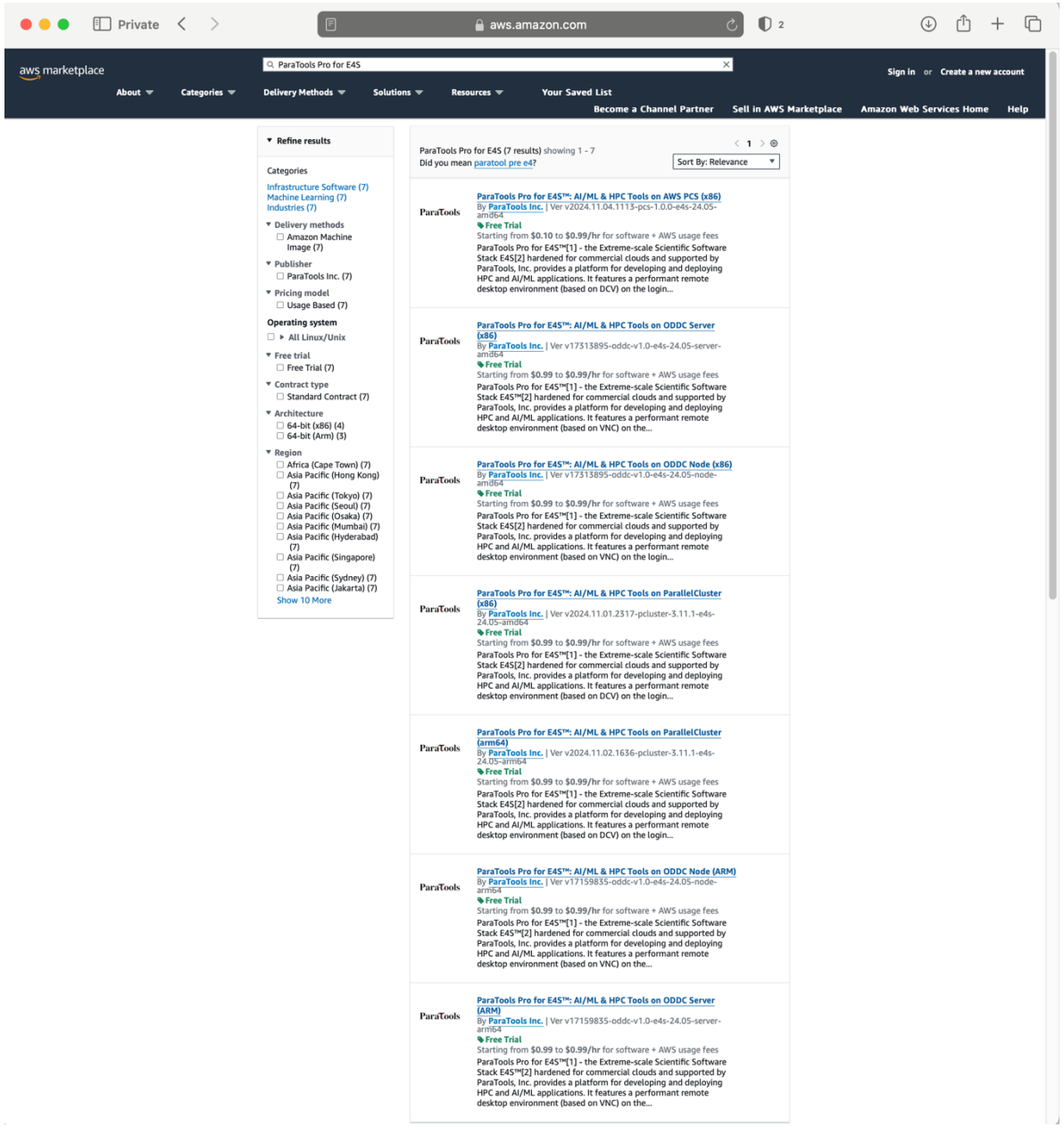
Key considerations for cloud-based deployment for E4S

- MPI - the core inter-node communication library has several implementations
  - Intel MPI, MVAPICH2-X, OpenMPI
  - Interfacing MPI with the job scheduling package (MOAB, Torque, SLURM)
- Cloud providers have different inter-node network adapters:
  - Elastic Fabric Adapter (EFA) on AWS
  - Infiniband on Azure
  - Mellanox Connect-X 5 Ethernet (ROCE) on Oracle Cloud Infrastructure (OCI)
  - IPU on Google Cloud (GCP)
- Intra-node communication with XPMEM (driver and kernel module support is critical)
- GPU Direct Async (GDR) support for communication between GPUs in MVPICH-Plus release
- ParaTools, Inc. building E4S optimized with MVAPICH-Plus for AWS, OCI, GCP, and Azure
- Using Adaptive Computing, Inc.’s ODDC interface to launch E4S jobs on multiple cloud providers!

Adaptive Computing's ODDC with ParaTools Pro for E4S™



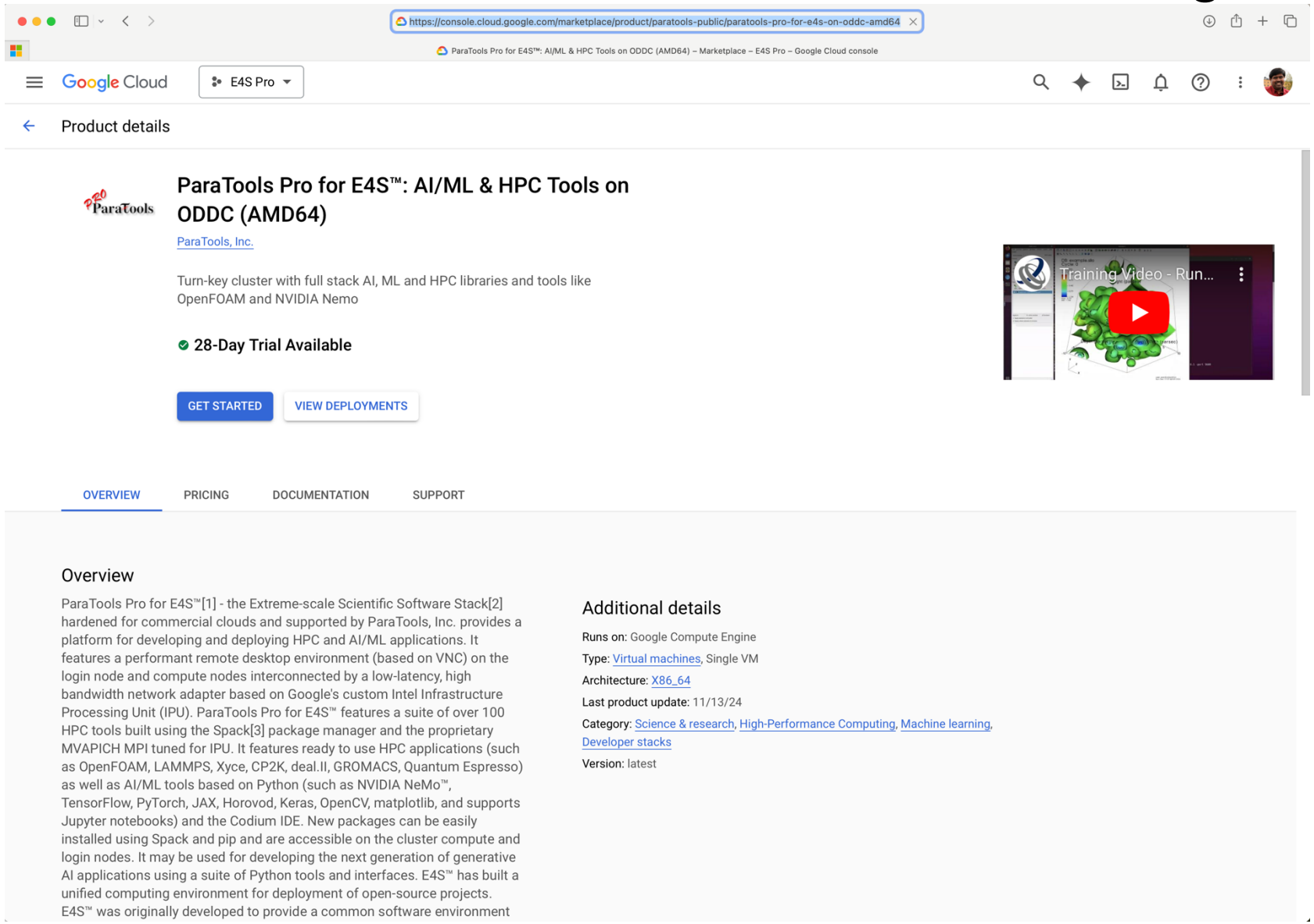
ParaTools Pro for E4S™*: Available in AWS, Google Cloud, Azure



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

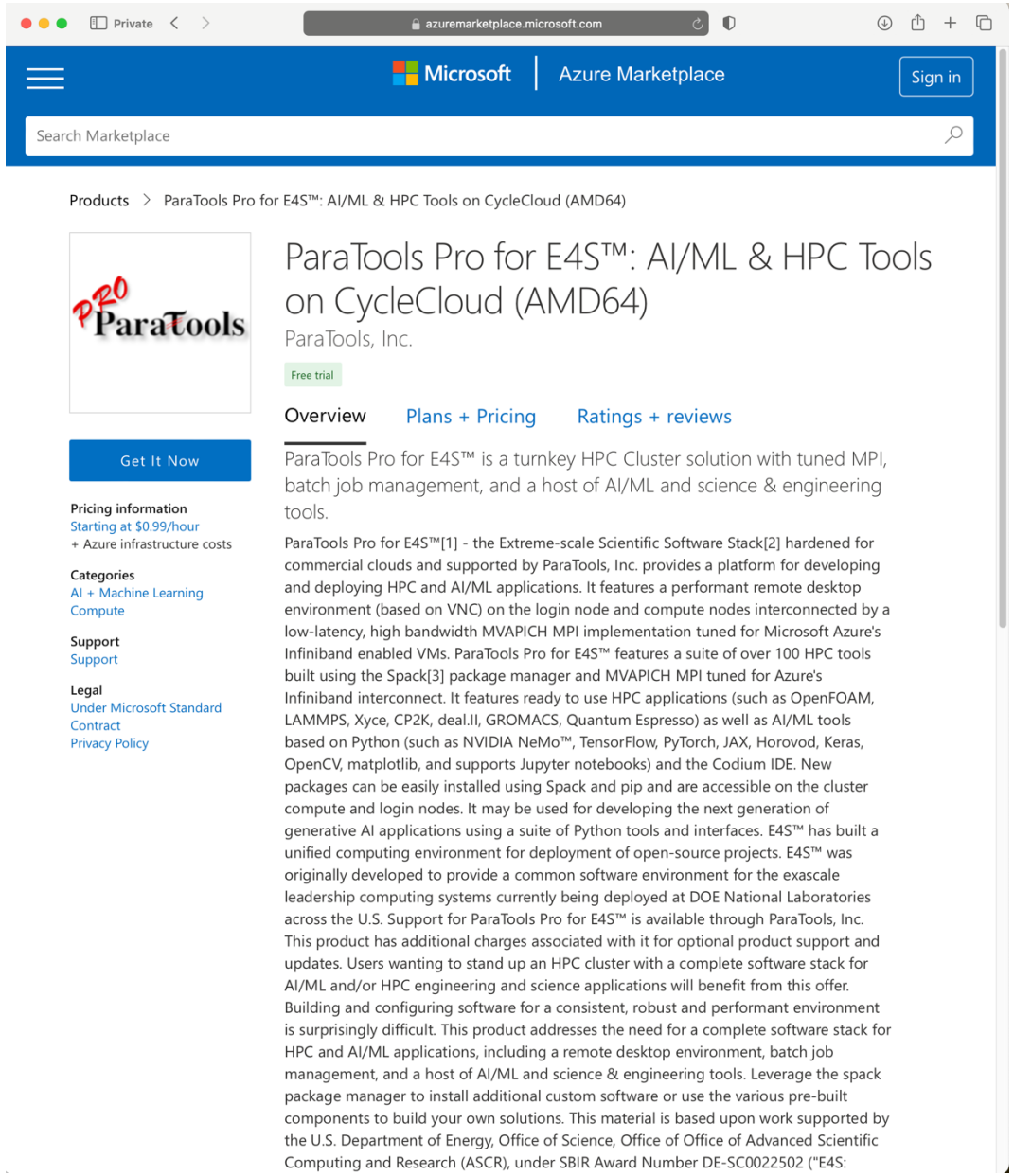
* Supported by DOE SBIR Phase I and II DE-SC0022502

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



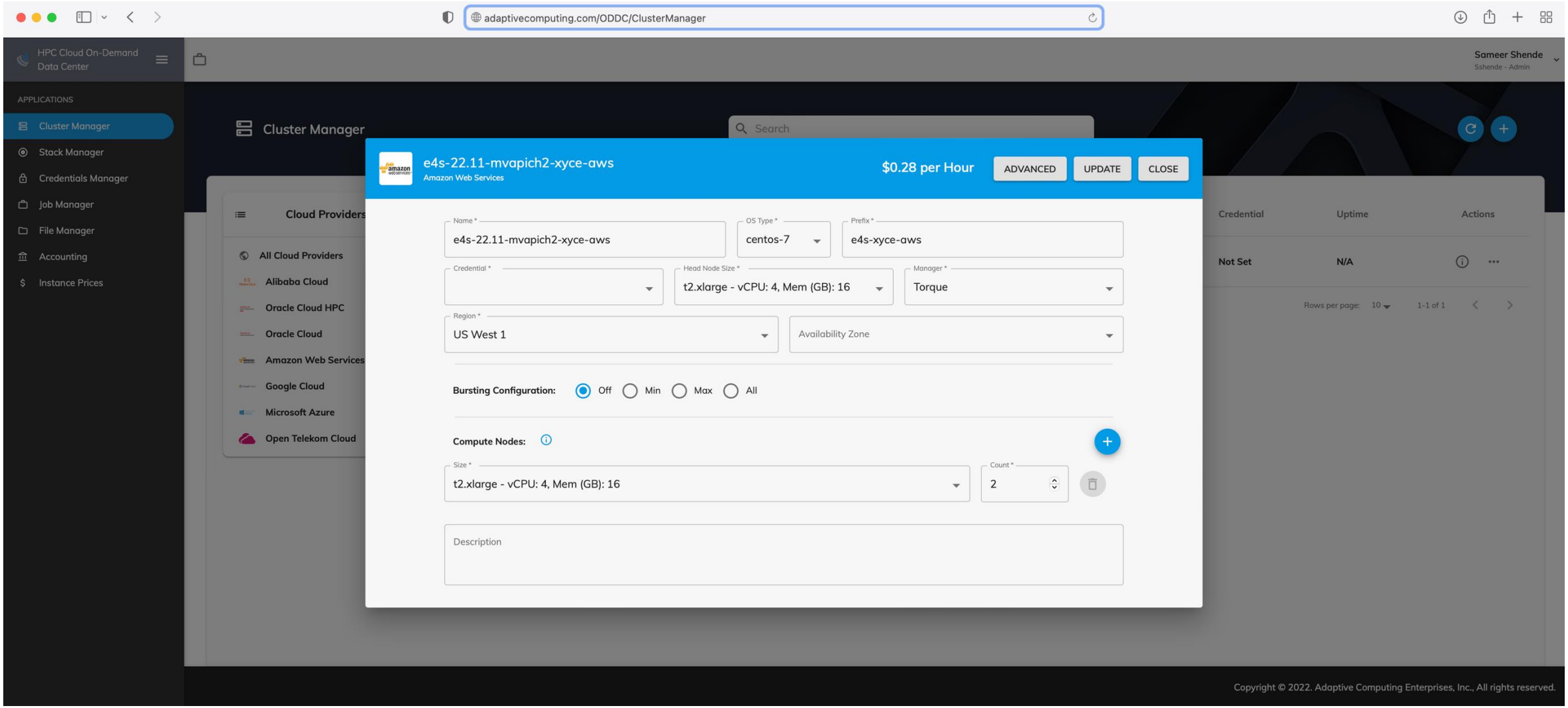
Google Cloud Marketplace

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



Azure Marketplace listing

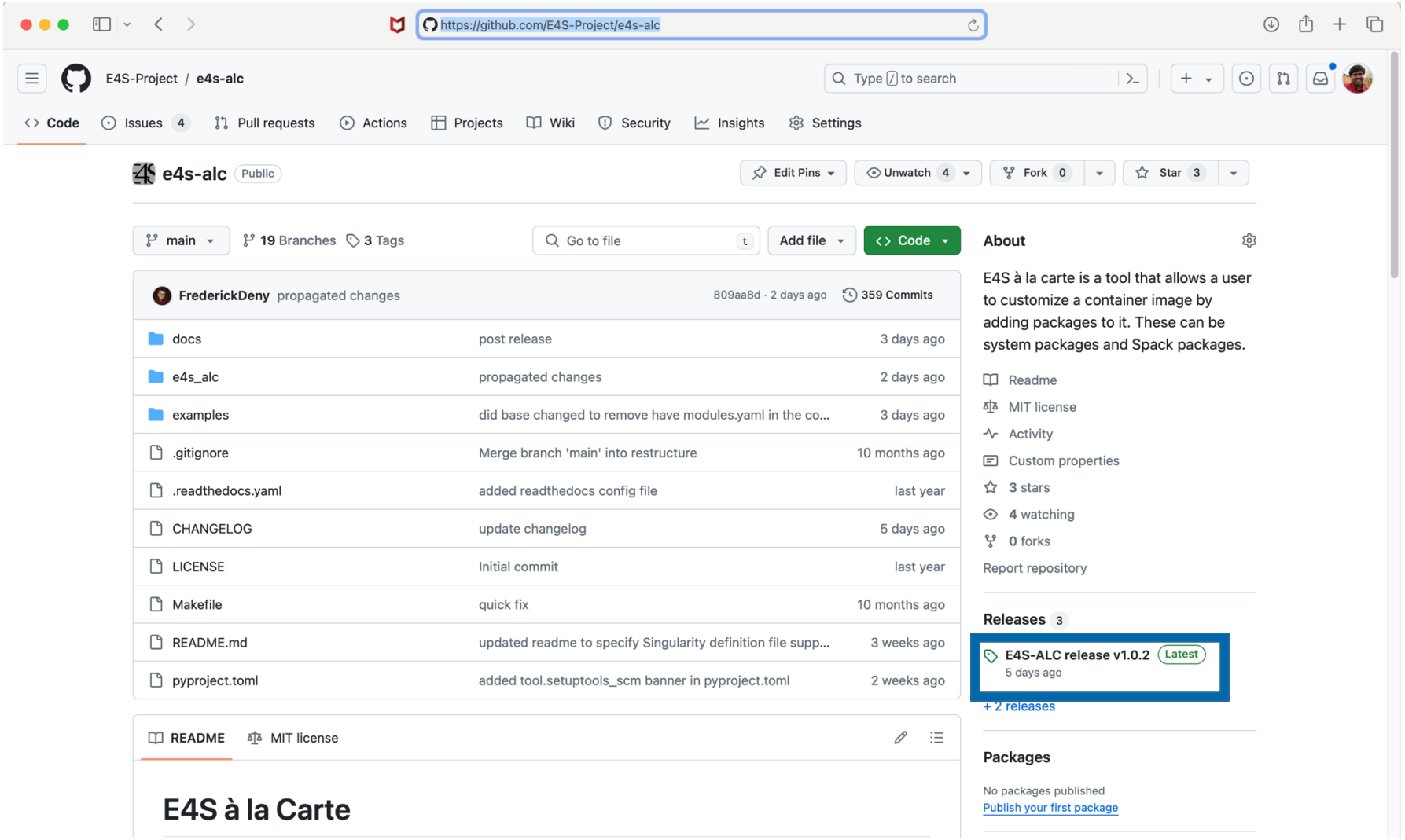
Choosing an instance on AWS to run the image using Heidi



Using ParaTools Pro for E4S image on AWS with Adaptive Computing's Heidi Workshops (ODDC)

STEP 1: Click on Student tab at:
https://paratools.adaptivecomputing.com
Firefox recommended.

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

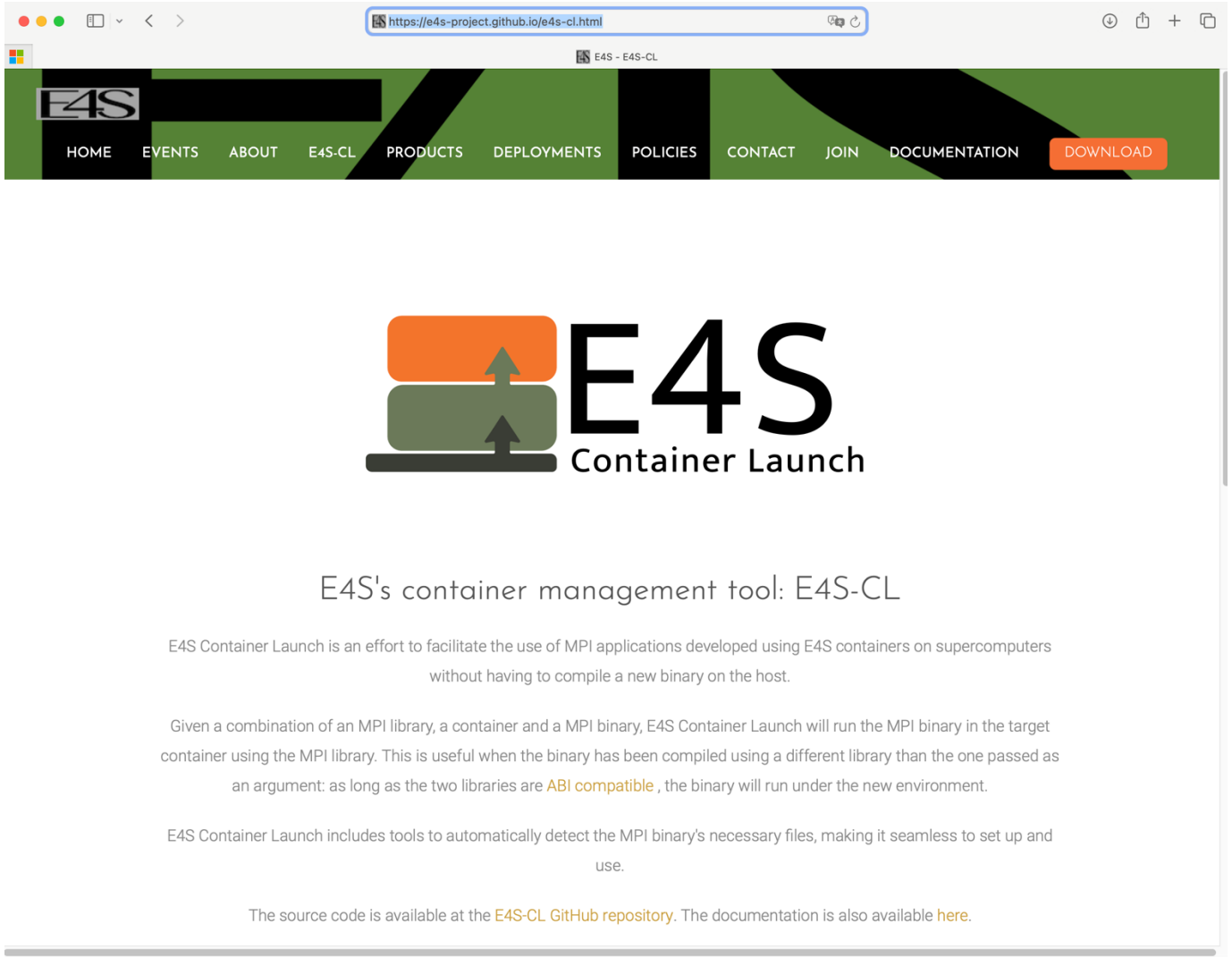


Add to a base image:

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

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

E4S Container Launch tool: e4s-cl



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e4s-cl: A tool to simplify the launch of MPI jobs in E4S containers

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  - 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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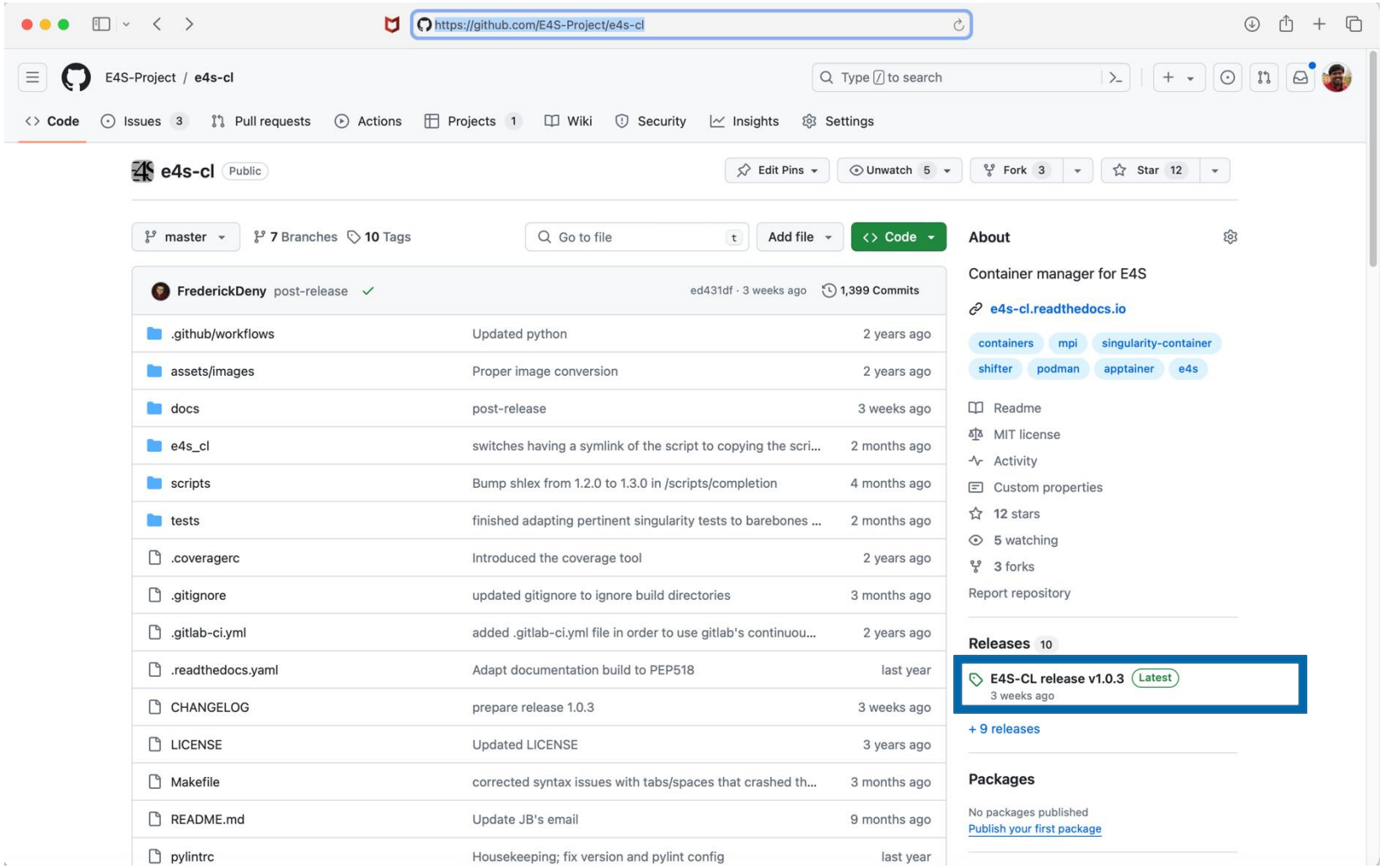
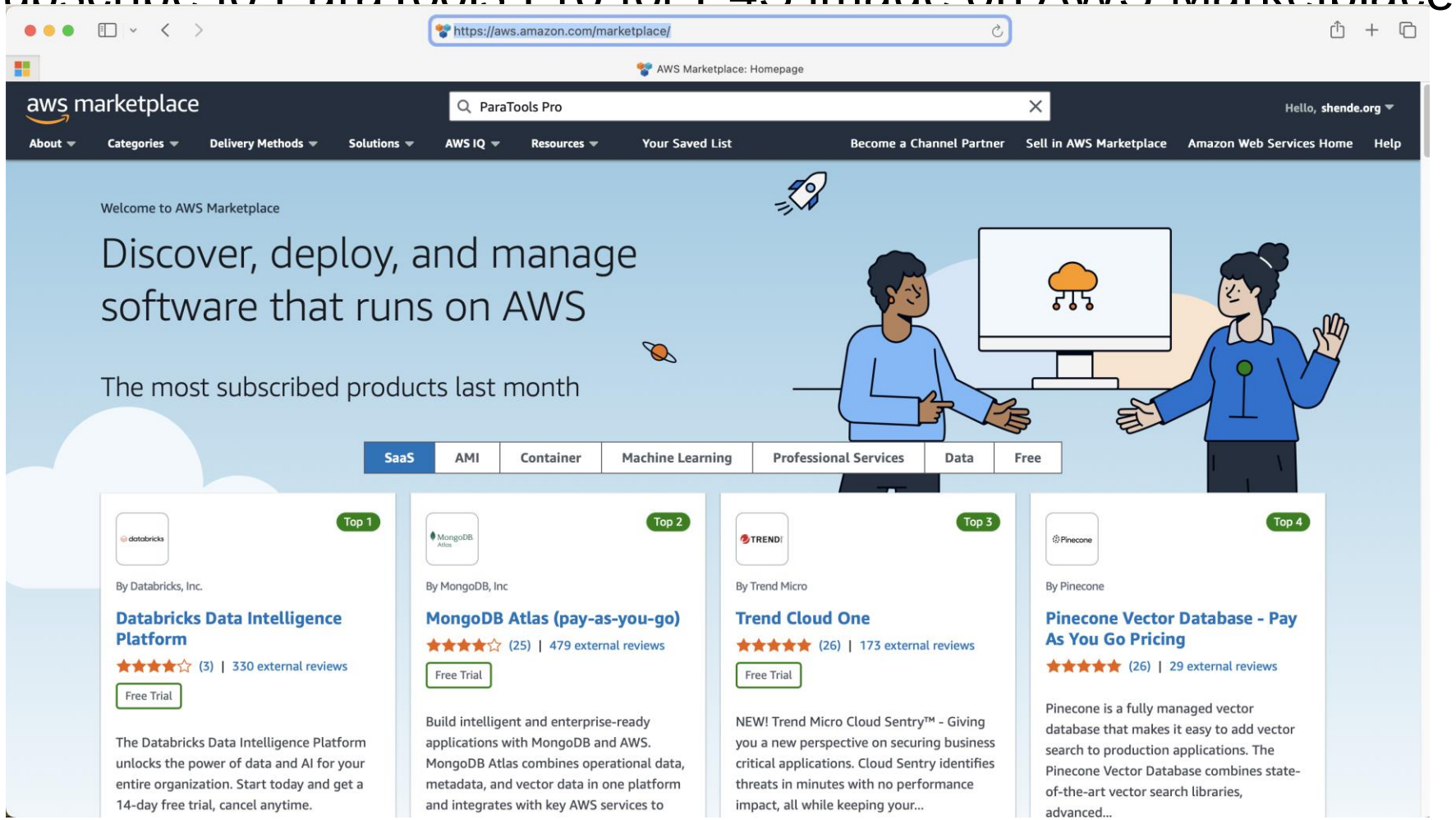
Release of e4s-cl on GitHub



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

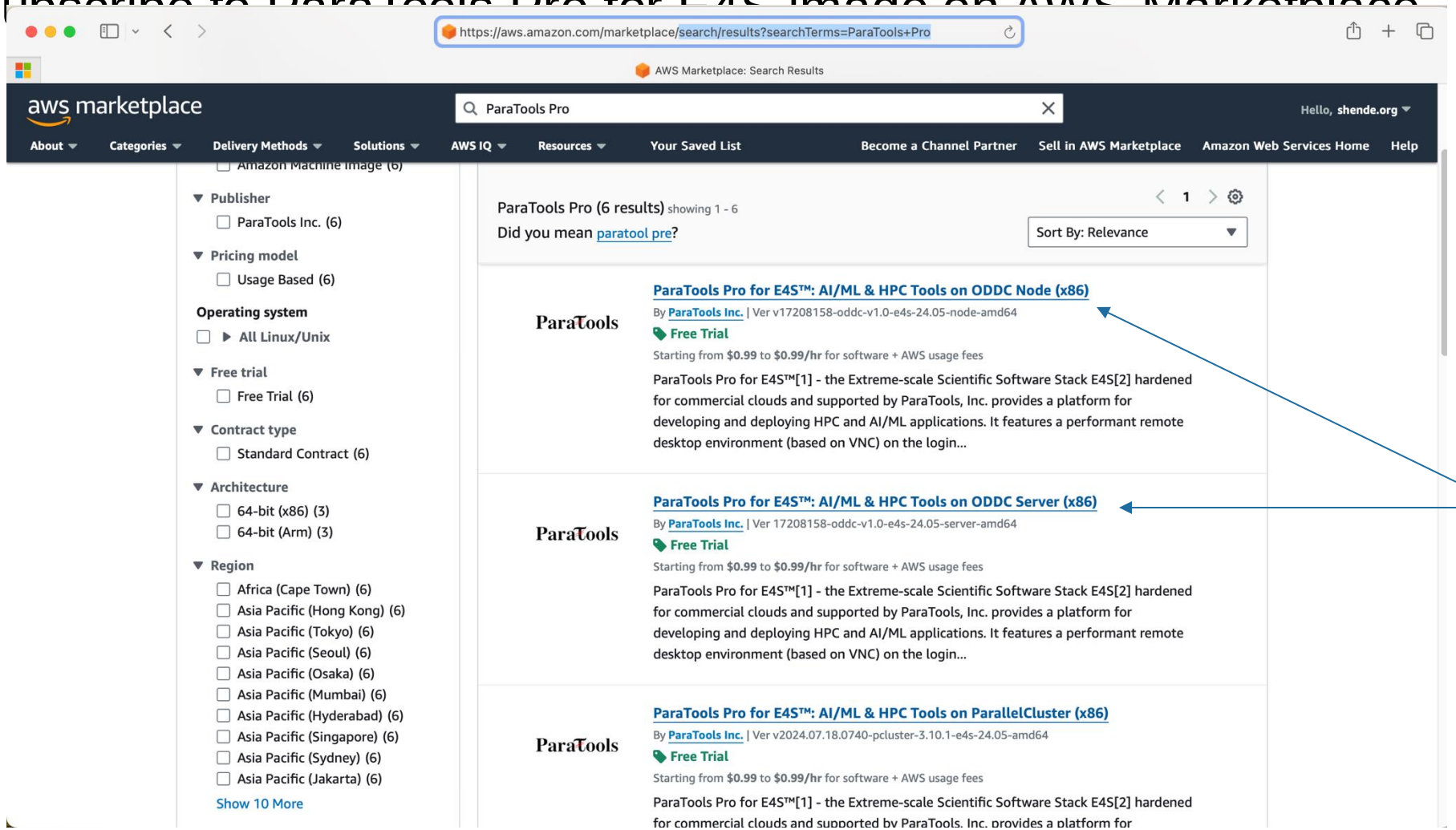
Using your own AWS credentials with ODDC

STEP 1: Subscribe to ParaTools Pro for E4S image on AWS Marketplace



Go to https://aws.amazon.com/marketplace
Login, then search for ParaTools Pro

STEP 1: Subscribe to ParaTools Pro for E4S image on AWS Marketplace

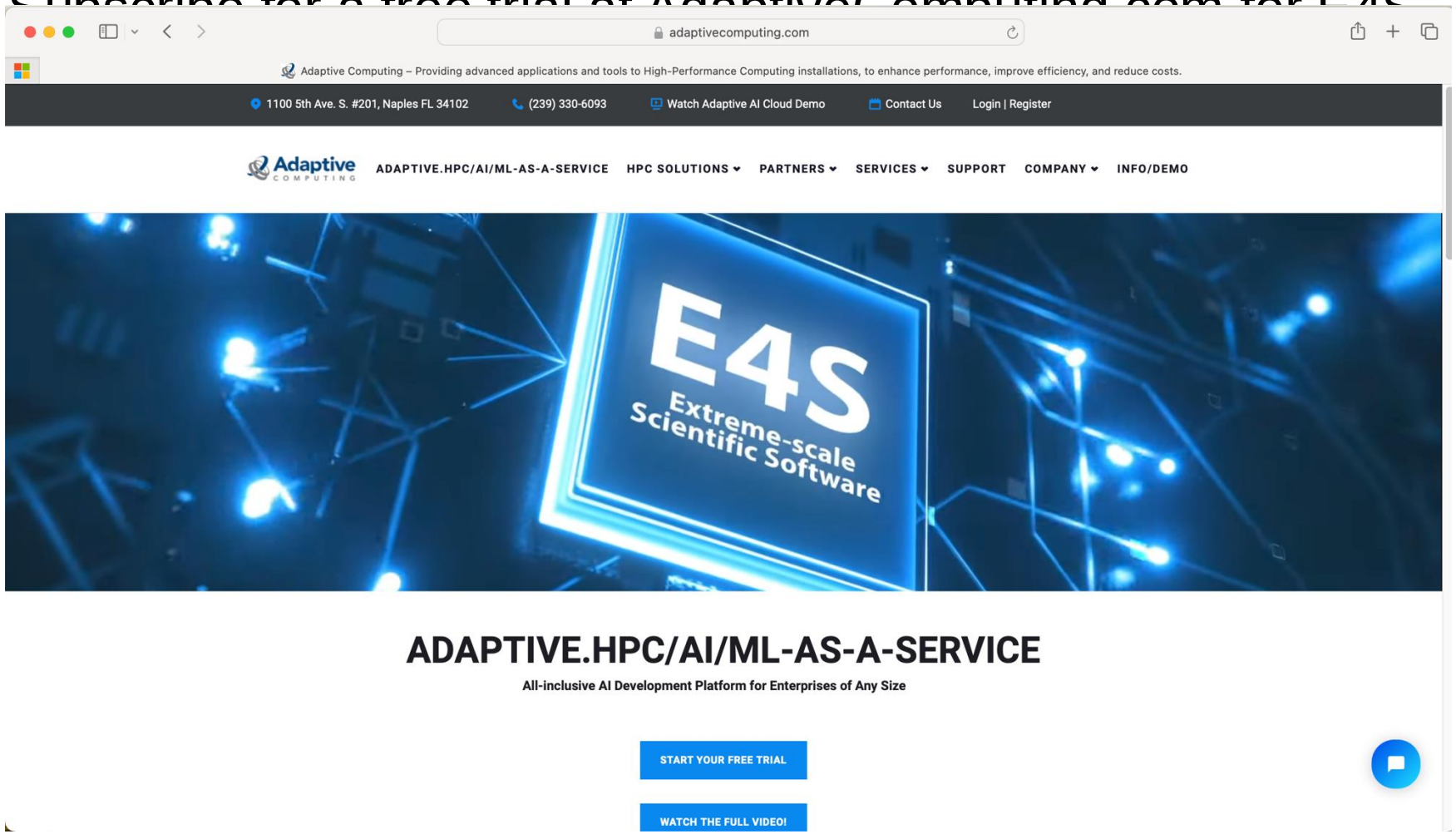


Free trial for 31 days!

Click on ODDC Server (x86) click subscribe

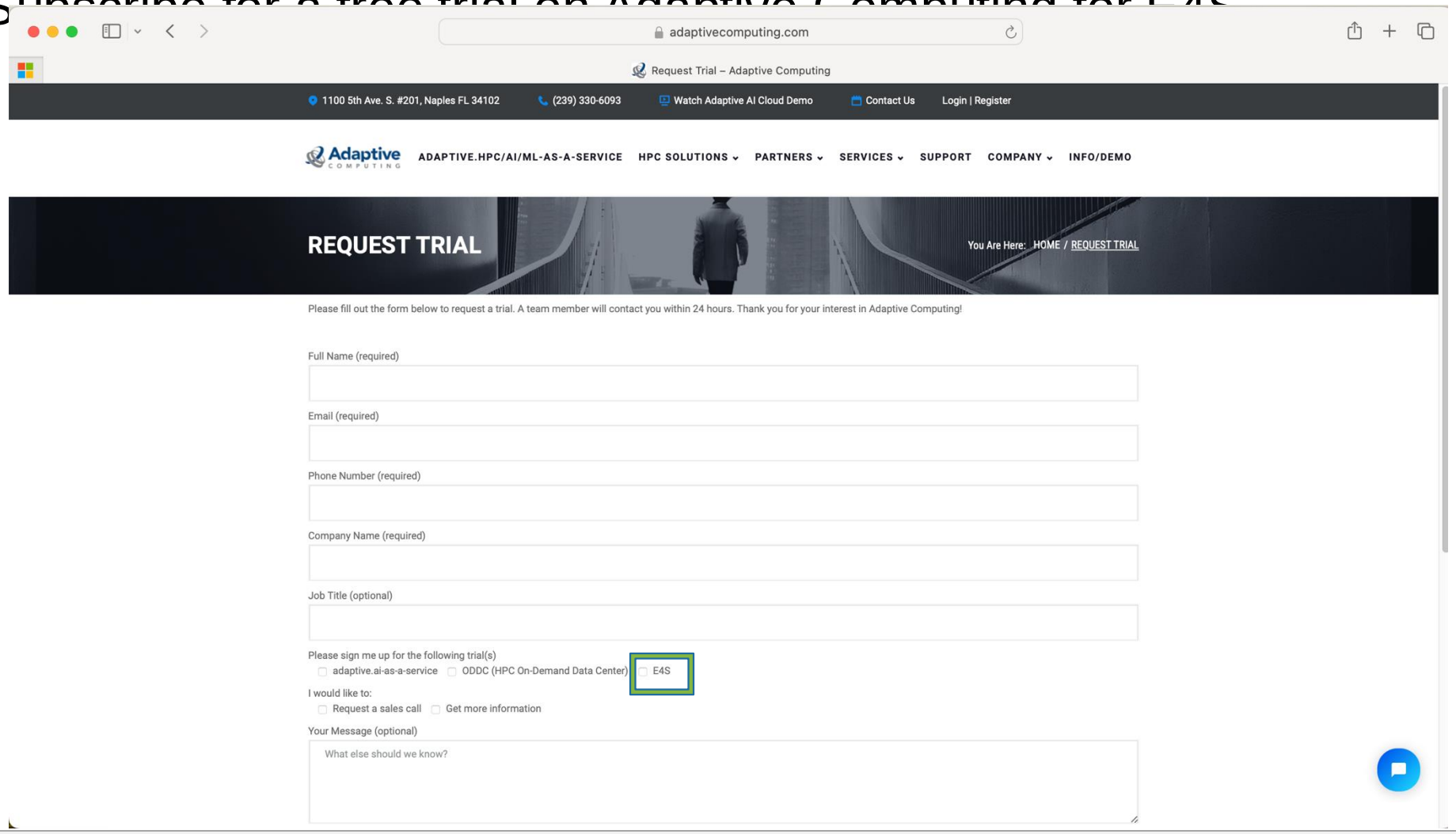
Click on ODDC Node (x86) click subscribe

STEP 2: Subscribe for a free trial at AdaptiveComputing.com for E4S



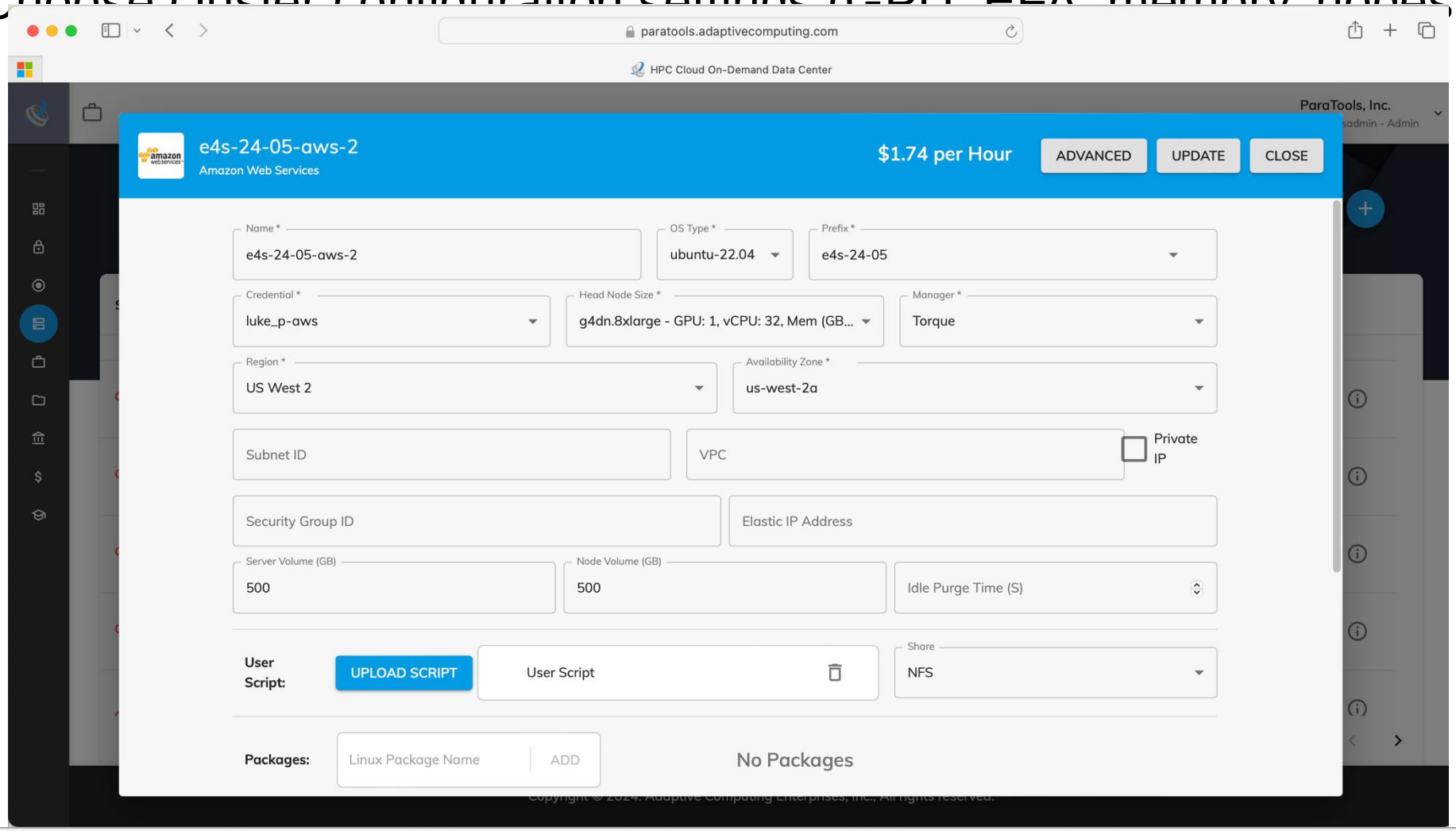
Go to https://adaptivecomputing.com
Click on "Start your free trial"

STEP 2: Subscribe for a free trial on Adaptive Computing for E4S



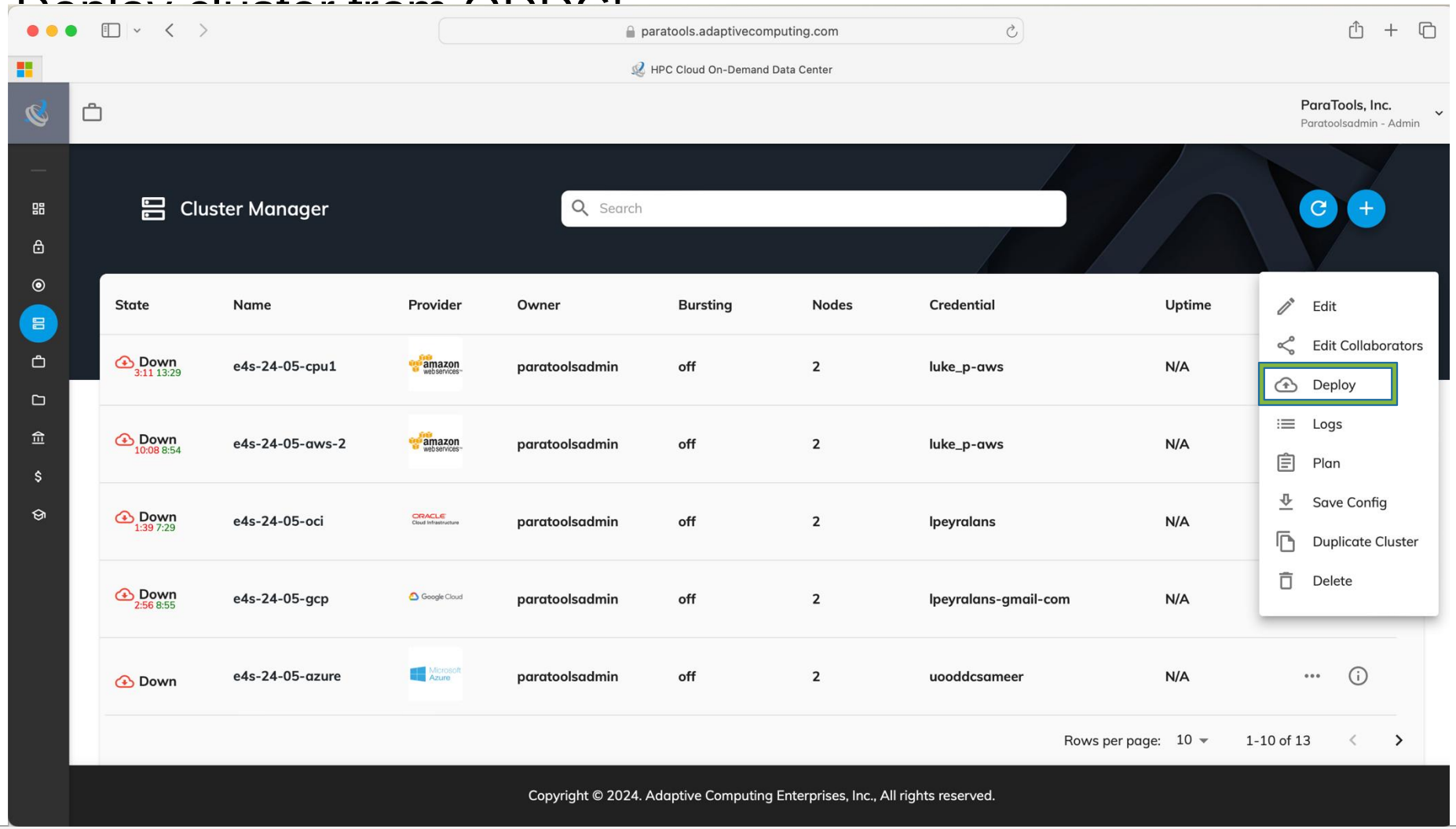
Fill out the form and check the E4S box

STEP 3: Choose cluster configuration settings (GPU, EFA, memory, nodes, shape)



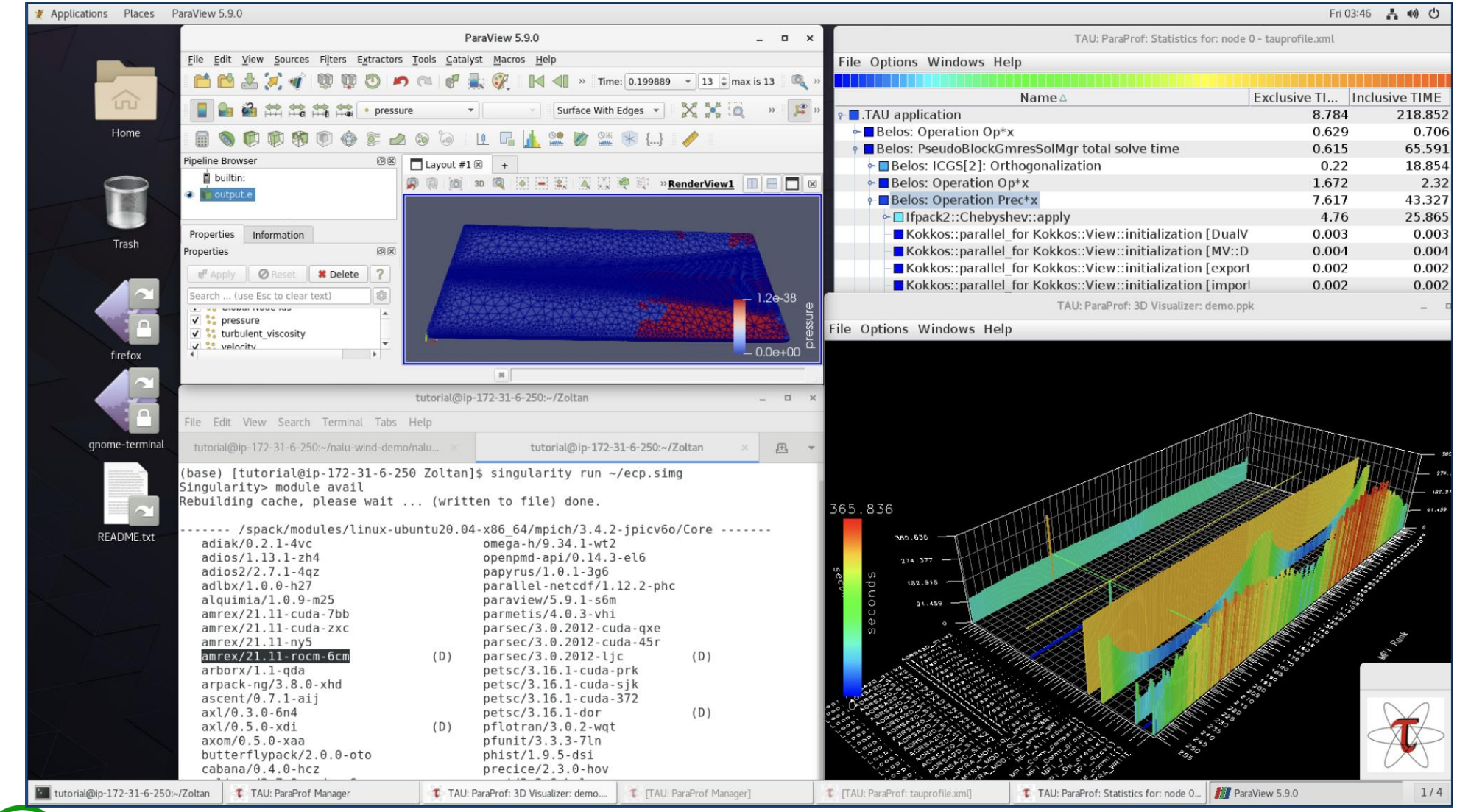
Once login is setup with their help, go to cluster configuration and edit cluster

STEP 4: Deploy cluster from ODDC!



Right click on the cluster, edit collaborators and then click Deploy, click on deployed cluster

E4S 24.11 AWS image: US-West2 (OR)

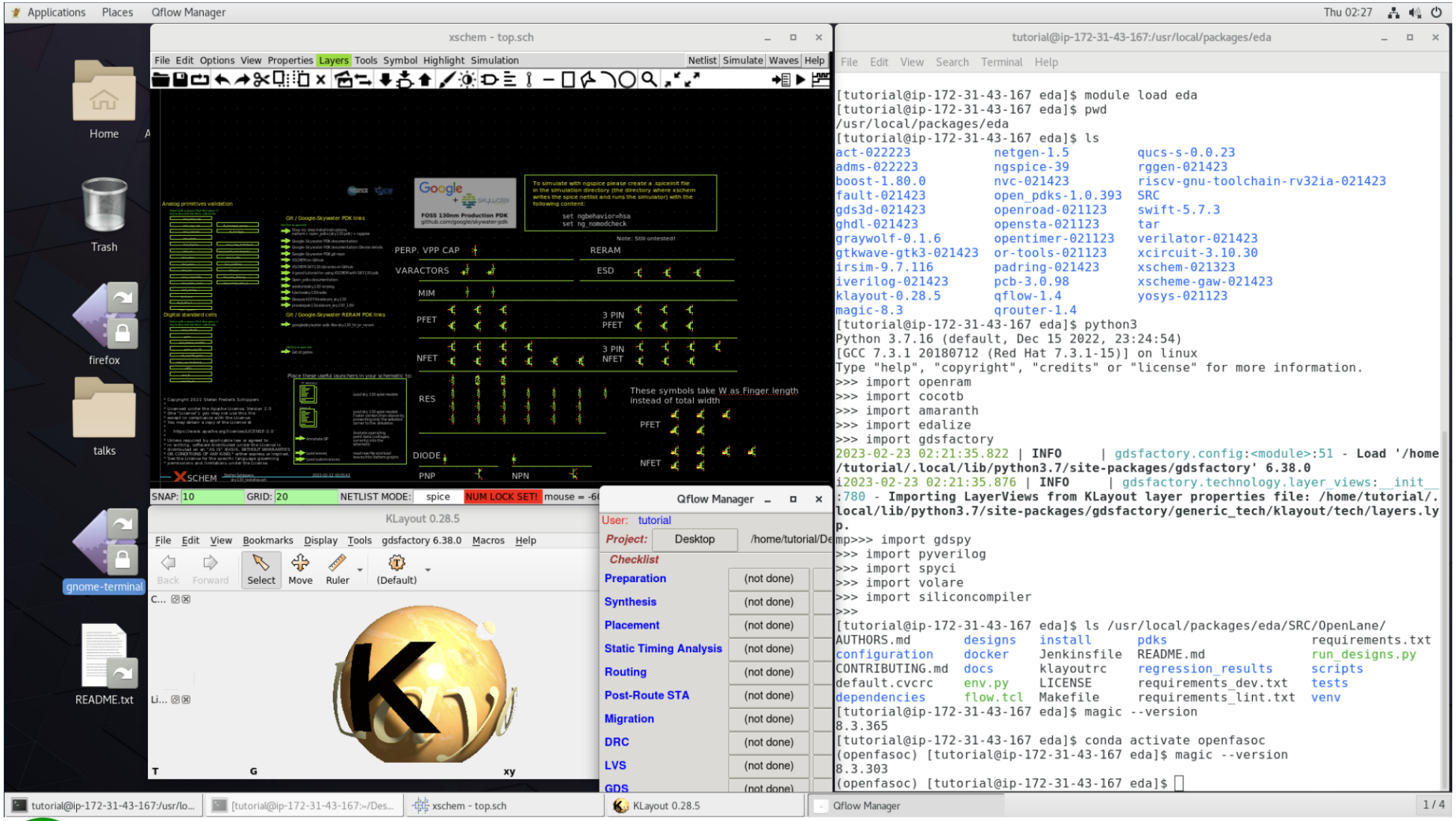


E4S 24.11 AWS

- Intel oneAPI
- CUDA
- NVHPC
- ROCm
- AWS DCV
- Spack Build Cache
- ECP: Nalu-Wind
- Trilinos 13.4.0
- OpenFOAM
- ParaView
- TAU
- Docker
- Shifter
- Charliecloud
- E4S Singularity
- EDA tools…

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
- OpenFASOC
- iVerilog
- Gtkwave
- Irsim
- Qrouter
- Fault
- GDS3D
- Rggen
- Python tools
  - Cocotb
  - Amaranth
  - Edalize
  - Gdsfactory
  - Gdspy
  - OpenRAM
  - Gdstk
  - Silicon compiler
  - Volare …
- PDKs
  - GF
  - Skywater

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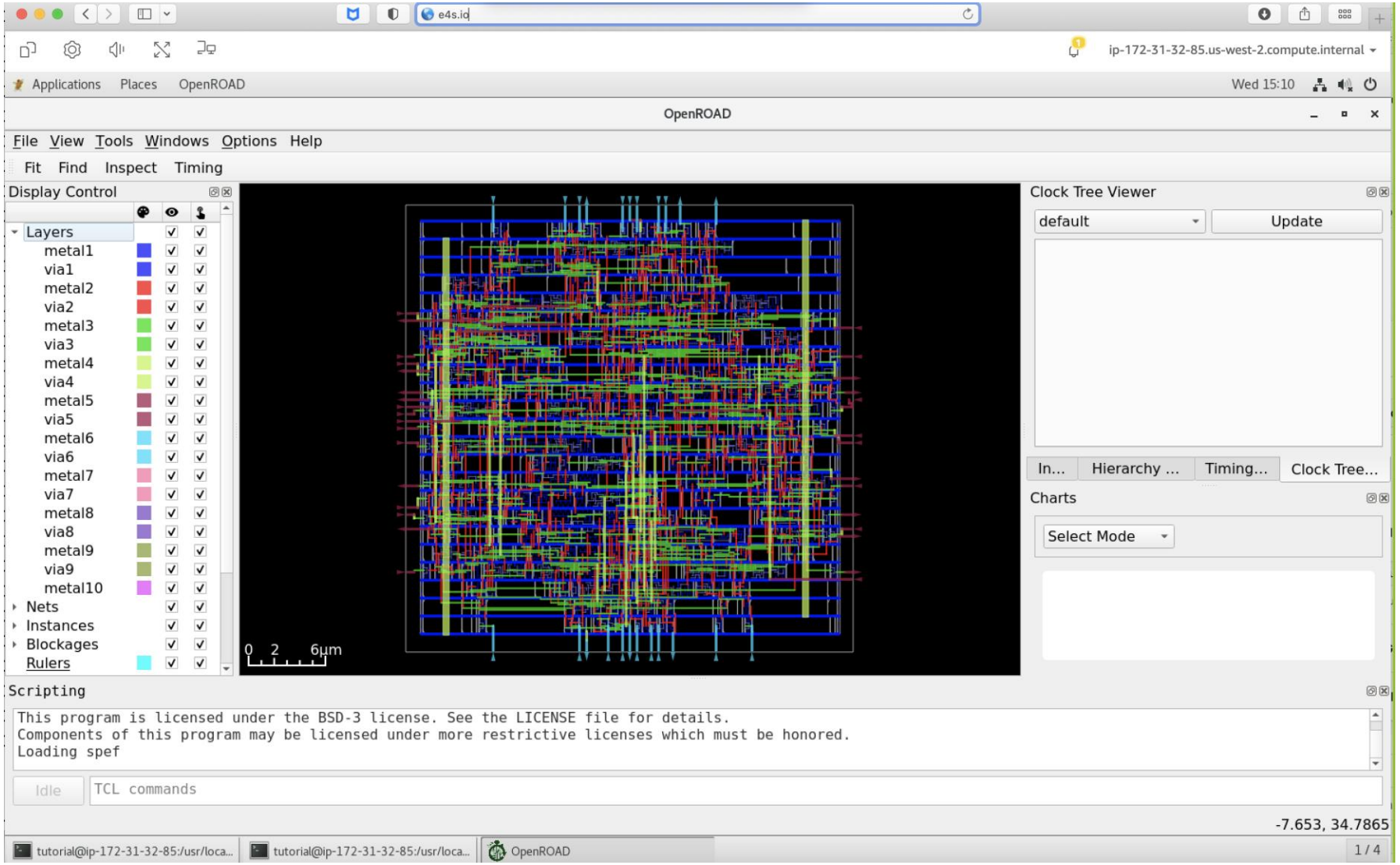
Free to use public AMI on AWS: ami-0e752117cfa13cb9b in the US-West-2 (Oregon) region

E4S for Commercial Cloud Platforms for EDA on AWS

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



E4S EDA on AWS

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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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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

Support Acknowledgements

- US Department of Energy (DOE)
  - ANL
  - Office of Science contracts, ECP
  - SciDAC, LBL contracts
  - LLNL-LANL-SNL ASC/NNSA contract
  - Battelle, PNNL and ORNL contract
- NASA SBIR
- Department of Defense (DoD)
  - PETTT, HPCMP
- National Science Foundation (NSF)
  - SI2-SSI, Glassbox
- CEA, France
- Industry: AWS, AMD, IBM, ARM, Intel, NVIDIA
- Partners:
  - University of Oregon
  - The Ohio State University
  - ParaTools, Inc.
  - University of Tennessee, Knoxville
  - T.U. Dresden, GWT
  - Jülich Supercomputing Center

Acknowledgment

- *This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research, Next-Generation Scientific Software Technologies program, under contract number DE-AC02-06CH11357. DOE SBIR DE-SC0022502.*

- https://science.osti.gov/ascr
- https://pesoproject.org
- https://ascr-step.org
- https://hpsf.io
- https://www.energy.gov/technologytransitions/sbirsttr

PESO

Thank you

https://www.exascaleproject.org

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

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

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