

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



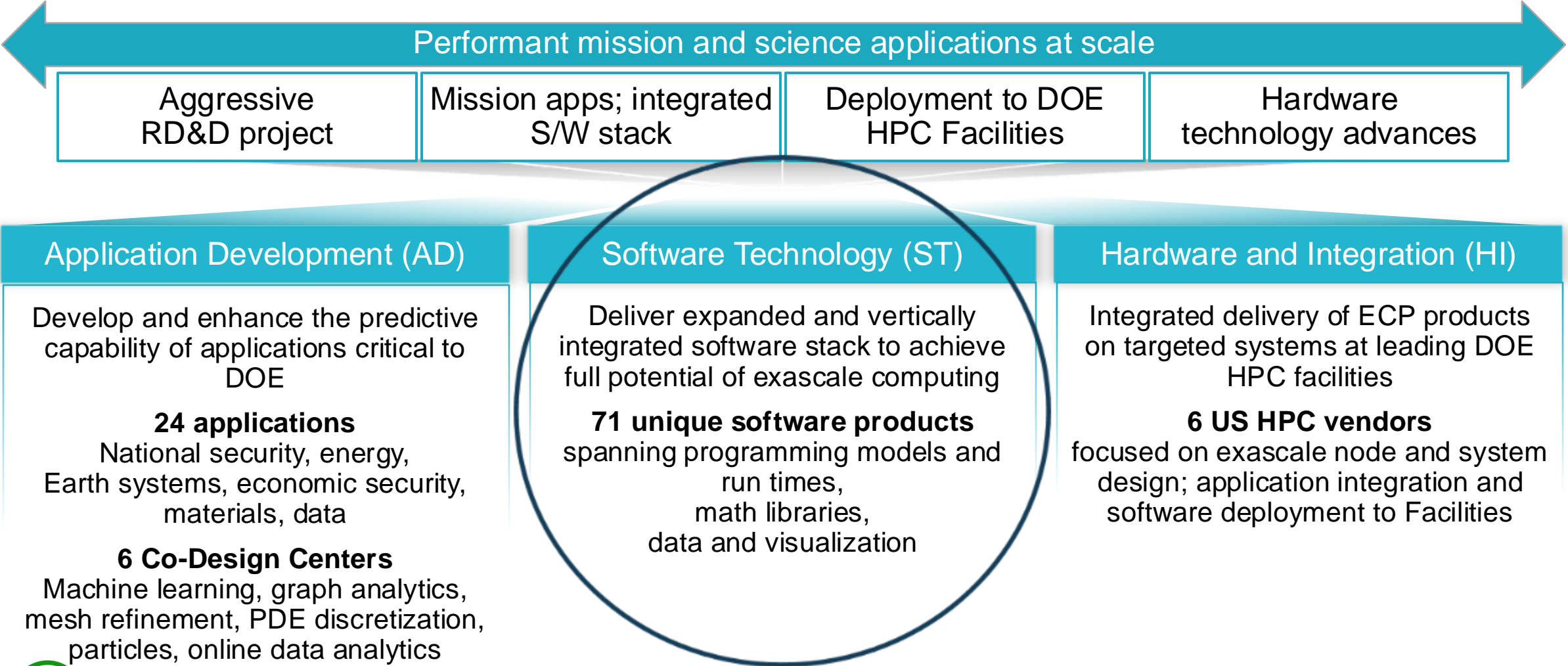
<https://tinyurl.com/e4stut>



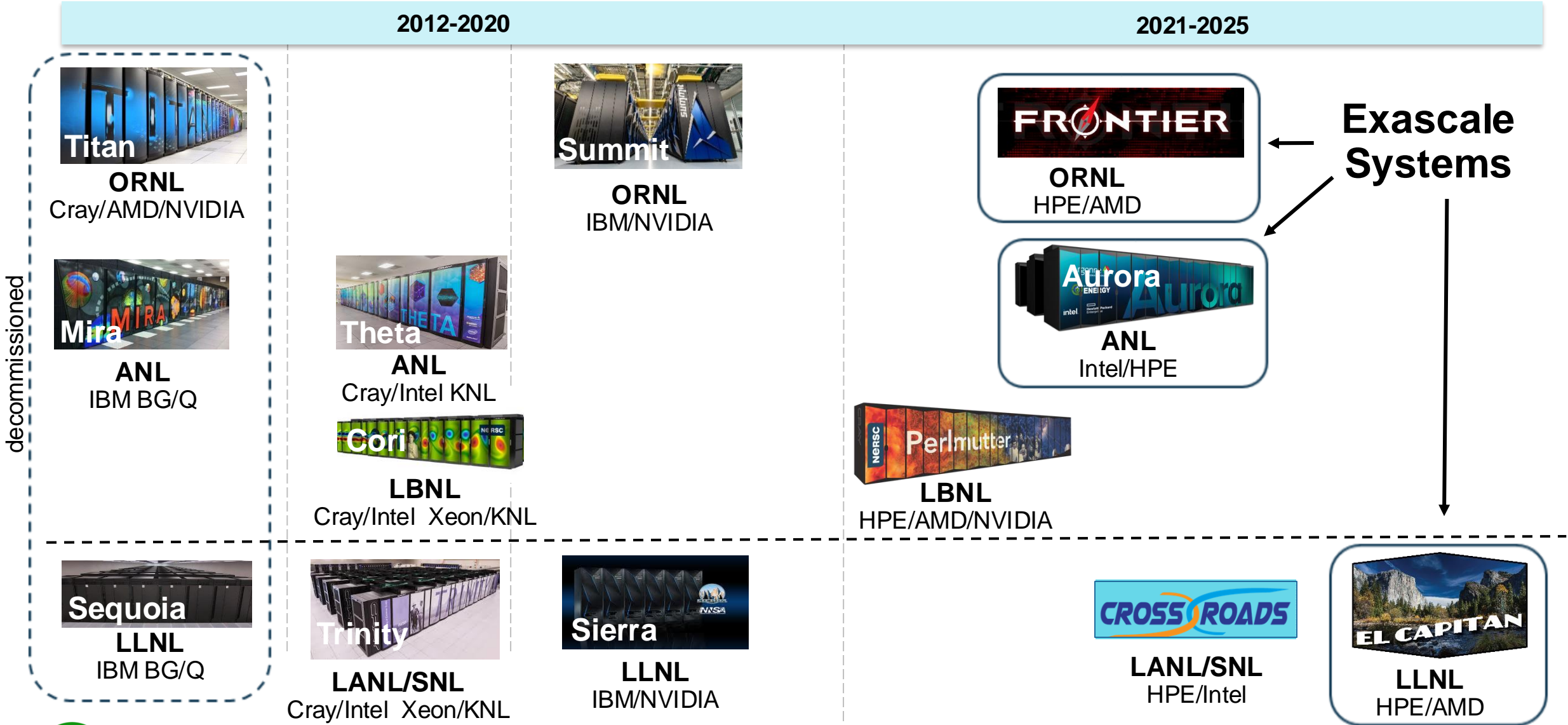
U.S. DEPARTMENT OF
ENERGY

Office of
Science

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



US DOE HPC Roadmap to Exascale Systems



ECP Software Technology (ST)

Goal

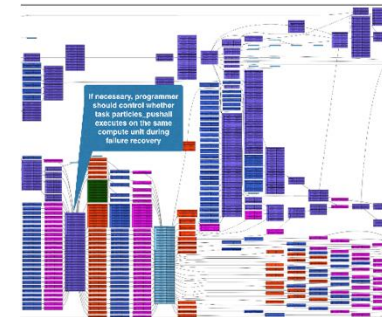
Build a comprehensive, coherent software stack that enables application developers to productively develop highly parallel applications that effectively target diverse exascale architectures

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



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.



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?

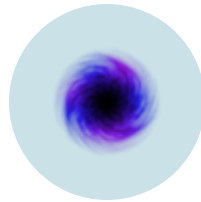
- E4S includes 132+ HPC packages on ARM, x86_64, and ppc64le platforms, 132K+ binaries in E4S build Cache.
- E4S improves support for a cross-platform AI/ML software stack including packages like NVIDIA NeMo™, Huggingface_hub, DeepHyper, Google.generativeai (Gemini API), OpenAI (API), TorchBraid, Pandas, 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>

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

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>

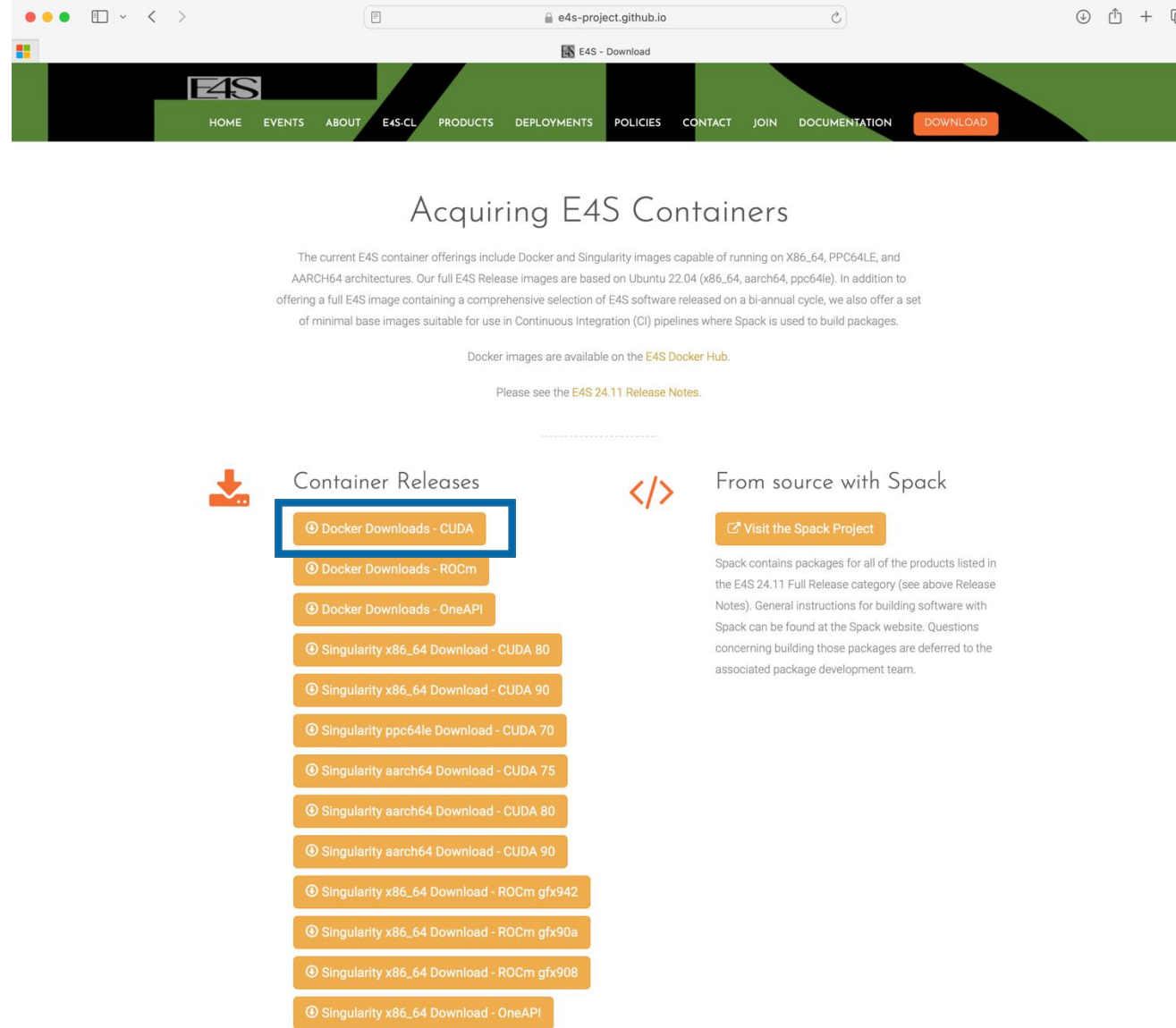
Lead: Sameer Shende
(U Oregon)

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

E4S 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

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-ko37njvqlmohhnhg5rnuk2qllfftg
3: aml	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/aml-0.2.1-um7i2rjzcwvuuvdcv2b65glxxtigwgp
4: amrex	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/amrex-24.10-qj6rcrnpr25y2cgjwdoj2epxqjz15aue
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-xaeozuhghlsrop5dvvdv4kg7xsjazwiyt
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-0.7.0-3tmy6mngjng347yg6nobbcajq4ypiz6aw
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-igtbsjmxf75vksiskskv3cxlois5d4
16: chai	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/chai-2024.07.0-7i44tof2afbfy7hgbqqw16chvge3n2oj
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-rpajcg3ekrpzceaqqddluoaf56rjjf63
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-h23rriorxiw6hh5w6b6b2ctad46vbbsn
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-9.5.1-7goorigib4zmobwddrrrtzvbvs3quggi
25: dyninst	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/dyninst-13.0.0-dhrv3i7ne73qxs4zncdbiwu67sojttha
26: e4s-alc	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/e4s-alc-1.0.2-7nffclxyawkf3rihrvnyjj3n7blf6vpv
27: e4s-cl	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/e4s-cl-1.0.4-kqi6ddd5n5l3qaamfubqdcz7zbjss
28: ecp-data-vis-sdk	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/ecp-data-vis-sdk-1.0-kv6y4i5hwnnu46xond4axik4acyu2rzz
29: exago	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/exago-1.6.0-ed4r6b3rpuff3mjy7m55linfijb6zgt
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-m323gnsqvffuabsvefkrp264phzypy4z
32: fftx	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/fftx-1.2.0-dav33uy6zv3slf7j4sdwn6ok2w5cpgyk
33: flecsi	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/flecsi-2.3.0-p5wlwxz3fw7yalfbtqeze7gjt4bmbn
34: flit	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/flit-2.1.0-t4bb2k5wzypjwfn252tjik344ag6sme
35: flux-core	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/flux-core-0.66.0-a73mo2pilzum6lzzkugp7hfm5nn5ex4
36: flux-sched	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/flux-sched-0.36.1-qbewzrfine24nrjuv7xh34b4jucutcry
37: fortilinos	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/fortilinos-2.3.0-qudhrp3agu3f2jym4ziey37asswolmq
38: gasnet	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/gasnet-2024.5.0-a6mbvkjs4m7fdxcqv5o423sktdgtmmb
39: ginkgo	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/ginkgo-1.8.0-qpn6kl7mlbesvmkzct46raa7hmdhd6y
40: globalarrays	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/globalarrays-5.8.2-5byrunc5uqpdvstblfkuo62v7liiiktm
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-yzr7cb2u343pzmf4sallvbtbn34pqxys
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-pvq4cwhbezgrp4kt4jt4zwnbdbupfrr

- 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/hdf5-1.14.5-6gftpz5y6pewmq4htrv4pvysux2ucb5m
46: hdf5-vol-cache	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/hdf5-vol-cache-v1.1-mdjhbzwgeuu4oae15776dg2rdnstztow
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-n4cczmu374zwbgtq6ivj7tftgkbes7w
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
53: kokkos	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/kokkos-4.4.01-c3n77su7hdchooilrbpnu4ynfu6fh5mp
54: kokkos-kernels	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/kokkos-kernels-4.4.01-4poyng2zk3rimtzae46flfss5wgttdv6
55: laghos	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/laghos-3.1-n6qjtg7vafR56z65cxdhxcpkqoyjts5
56: lammps	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/lammps-20240829-ls3cye1fkyknefcvzx2jzs4drqj7pgc6
57: lapackpp	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/lapackpp-2024.05.31-3xzdtn7bw75ak7yk3bwuk4yih4nr5qk
58: lbann	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/lbann-0.104-iyv6v42avt74jghrn7ol4z6y2zjdsposy
59: legion	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/legion-24.09.0-t6bxt7a27psf3gm2butya4uzf6q7hg2e
60: libcatalyst	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/libcatalyst-2.0.0-wmryn2xoazqxcliwr5zsuptya6t7c3r7
61: libnrm	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/libnrm-0.1.0-cn5g3aojvk3h43voedsaaktgwuetzgte
62: libpressio	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/libpressio-0.99.4-hnscophslfa7qcelldjh5otilcnkomth3
63: libquo	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/libquo-1.4-b23b2c2gx02k6gbd3b3sbqlhjwfpaxef
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-nsase6ghkwatq2qps2hin7x2mqcgwvi
68: mfem	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/mfem-4.7.0-eajr2n3ulhejyvxvfbocapubz3qmf6ee
69: mgard	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/mgard-2023-12-09-fxzwqezvoxiasigz4acdvr3ytquxbx
70: mpark-variant	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/mpark-variant-1.4.0-sfrlscq4242fhkn7utnp545jh432opx6
71: mpich	/usr/local/mpich/install/mpich
72: mpiutils	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/mpiutils-0.11.1-nwd2qjjxnm4cbnwkhuitzjvks5kunt7q
73: nccmp	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/nccmp-1.9.1.0-wxmr6dvro3sa4w63ssc6emnaqyuc3af
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-dnczmmqys75oxvb67g2cdyeyo5shkhdg
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-4.6.1-46yy72aftgzzgn6il4t175lsfhvrx7wt
78: netlib-scalapack	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/netlib-scalapack-2.2.0-zdskhgrbnit2p66ocwvorx3yny64am
79: nrm	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/nrm-0.1.0-22bucvue7af0qppfei7mjbntniztokob2
80: nwchem	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/nwchem-7.2.3-bhf6p5dpfhceizb455b7yzecehchyw6
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: openpmc-api	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/openpmc-api-0.16.0-3wdhvkspqg3zyruqr6yxo2ymfcojpbz1
85: papi	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/papi-7.1.0-y2r2j4wpyzx16bswtoujx5vlkmvzsui4
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-5.13.1-57dbd2bnczh6boehiho55cyjzeceb2zv

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-hkyu7eadk3ompvl26qbs43ig7ubbr5
90:	pdt	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/pdt-3.25.2-njatamqvcoenbaqcfykut236pgpzm5
91:	petsc	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/petsc-3.22.0-xqaokru57p65fnujzhe46oibuz2cj6iyy
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-o7prc6wqlx46tvwb27ewr7ggxkteti
96:	pruners-ninja	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/pruners-ninja-1.0.1-bxhxm47tfeam32hcgqtubqosia3arjw
97:	pumi	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/pumi-2.2.8-obeabm7tgu154yydoefxvl4bk3p6wo6p
98:	py-cinemas	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/py-cinemas-1.3-juxfpomndnt7nxagyqoikzwmi2lqhdz
99:	py-deepphyper	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/py-deepphyper-0.6.0-l7wuzhvl3rbdao7aqxggckfpfcmle5f
100:	py-jupyterhub	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/py-jupyterhub-1.4.1-q6v3kng5b2uv7my6b2jwo1bx5hjqaaju
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-2023.08.21-6qv2sz36iww2iaqbizmgbvvrq4wctyf
103:	py-radical-saga	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/py-radical-saga-1.47.0-h6ilsdskhrcswaubyhq1gmvuakz2rmx
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-gxjb4l6ebquee4cd3s6wtbl5ay5hkrek
106:	raja	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/raja-2024.07.0-x5umeqy7y6dkbg24gvynfynuhthbrstgk
107:	rempi	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/rempi-1.1.0-wc7zoqyhjpwooti6w3tfhakfvzfjn6j7
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-2024.05.31-2ecdrykid477yd3n2bp2m2mp2jxeapla
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-ybrlxcfyjztiof2umiea6bpw4ashzjcr
112:	strumpack	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/strumpack-7.2.0-fsg63gootalx7gyjjwzlvfvrorygb
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-jccuenwobtjuovmu4fry2trf6zdpwue
115:	swig	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/swig-4.1.1-gnw7j6q5wdctjirbqwc62rtrjfigfn
116:	sz3	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/sz3-3.2.0-jkh6xikf24u7twxqormgcrv2ephey3j
117:	tasmanian	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/tasmanian-8.0-g7c3luju2qnluvul5vgxjrhczaqlqsymg
118:	tau	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/tau-2.34-77jqzvfzwxge47jxgh3dctiikh4ihhni
119:	trilinos	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/trilinos-16.0.0-pi4g4hlvnmkxehtczq5irbhp2towxfs
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-s5vkv5g44qmltngwpo7rr3pgiy55ed4d
122:	umpire	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/umpire-2024.07.0-76aq7phrhfeh5t3rk6q3pzyfmtcpn
123:	unifyfs	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/unifyfs-2.0-0a6yjlvt2nkfti5mf6dvi5etbh45fwv4
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-ryt7oqpkh2yhnznoc33esdcxnnztcoap
126:	veloc	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/veloc-1.7-6yqgctazcu3tazt6iir62bj3rtyen
127:	visit	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/visit-3.3.3-xeoojeuxgi3o4dl5iyxudwv6bbvkavagv
128:	vtk-m	/spack/opt/spack/linux-ubuntu22.04-x86_64/gcc-11.4.0/vtk-m-2.2.0-z4p7ayhzobpfaqkooxptmmhx7wlh7yl
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-jw3bykeqmnqxsjfhc4vb3pmijqcofrt
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-2021.11.0-2qi2xp2qs4kxwddgnibhixhgjmwnvngvo)
[+] /spack/opt/spack/linux-ubuntu22.04-x86_64/oneapi-2024.0.2/gmake-4.4.1-zpg4uz3bbxf4ljfzxm5uhhepceiwdwd
[+] /spack/opt/spack/linux-ubuntu22.04-x86_64/oneapi-2024.0.2/boost-1.84.0-zualrbbig6f5cvkjif227s3mebjfnov
==> Installing valgrind-3.20.0-7t4aj3mw3fokiyun6ofcjpgxaj6teseas [4/4]
==> No binary for valgrind-3.20.0-7t4aj3mw3fokiyun6ofcjpgxaj6teseas 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-3.20.0-7t4aj3mw3fokiyun6ofcjpgxaj6teseas
    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-3.20.0-7t4aj3mw3fokiyun6ofcjpgxaj6teseas
Singularity> spack load valgrind
Singularity> which valgrind
/home/users/sameer/tmp/spack/opt/spack/linux-ubuntu22.04-x86_64/oneapi-2024.0.2/valgrind-3.20.0-7t4aj3mw3fokiyun6ofcjpgxaj6teseas/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

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 openfoam@2312 qthreads@1.18 trilinos@16.0.0
aml@0.2.1 dealii@9.5.1 gromacs@2024.3 libnrm@0.1.0 openmpi@5.0.5 quantum-espresso@7.3.1 trilinos@16.0.0
amrex@24.10 dyninst@13.0.0 h5bench@1.4 libpressio@0.99.4 openpmd-api@0.16.0 raja@2024.07.0 turbine@1.3.0
amrex@24.10 e4s-alc@1.0.2 hdf5@1.12.3 libpressio@0.99.4 papirus@1.0.2 raja@2024.07.0 umap@2.1.1
arborx@1.7 e4s-cl@1.0.4 hdf5@1.14.5 libquo@1.4 parallel-netcdf@1.12.3 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 papi@7.1.0 umpire@2024.07.0
argobots@1.2 exago@1.6.0 hdf5-vol-cache@v1.1 loki@0.1.7 papyrus@1.0.2 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 vtk-m@2.2.0
axom@0.9.0 faodel@1.2108.1 heffte@2.4.0 metall@0.28 parsec@3.0.2209 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 wannier90@3.1.0
boost@1.79.0 fftx@1.2.0 hpctoolkit@2024.01.1 mfem@4.7.0 pdt@3.25.2 warpx@24.10
butterflypack@2.4.0 flecsi@2.3.0 hpctoolkit@2024.01.1 mgard@2023-12-09 petsc@3.22.0 wps@4.5
cabana@0.7.0 flecsi@2.3.0 hpx@1.10.0 mgard@2023-12-09 petsc@3.22.0 wrf@4.5.2
cabana@0.7.0 flit@2.1.0 hpx@1.10.0 mpark-variant@1.4.0 phist@1.12.1 plasma@24.8.7 xyce@7.8.0
caliper@2.11.0 flux-core@0.66.0 hypre@2.32.0 mpich@4.2.3 plumed@2.9.2 superlu@5.3.0 zfp@0.5.5
caliper@2.11.0 flux-core@0.66.0 hypre@2.32.0 mpiutils@0.11.1 precice@3.1.2 superlu-dist@8.2.1 zfp@1.0.0
chai@2024.07.0 fpm@0.10.0 kokkos@4.4.01 nco@5.2.4 pruners-ninja@1.0.1 superlu-dist@8.2.1
chai@2024.07.0 gasnet@2024.5.0 kokkos-kernels@4.4.01 nek5000@19.0 pumi@2.2.8 swig@4.0.2-fortran
chapel@2.2.0 ginkgo@1.8.0 kokkos-kernels@4.4.01 nekbone@17.0 py-cinemasci@1.7.0 sz@2.1.12.5
charliecloud@0.38 ginkgo@1.8.0 kokkos-kernels@4.4.01 netcdf-fortran@4.6.1 py-deeppy@0.6.0 sz3@3.2.0
conduit@0.9.2 globalarrays@5.8.2 laghos@3.1 netlib-scalapack@2.2.0 py-h5py@3.11.0 tasmanian@8.0
cuda@12.6.2 glvis@4.2 lammps@20240829
==> 170 installed packages
```

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○	AML	PMR	Hierarchical memory management library from Argo.	2019-04-25 13:03:01
○	AMREX	PMR	A framework designed for building massively parallel block-structured adaptive mesh refinement applications.	2021-05-02 17:26:43
○	ARBORX	Math libraries	Performance-portable geometric search library	2021-01-05 15:39:55
○	ARCHER	Tools	Data race detection tool for OpenMP applications	2020-08-19 11:04:14
○	ASCENT	Data & Viz	Flyweight in situ visualization and analysis runtime for multi-physics HPC simulations	2021-04-05 18:11:45
○	BEE	Software Ecosystem	Container-based solution for portable build and execution across HPC systems and cloud resources	2018-08-22 22:26:19
○	BOLT	Development Tools	OpenMP over lightweight threads.	2020-05-04 11:24:57
○	CALIPER	Development tools	Performance analysis library.	2020-11-04 23:53:07
○	CHAI	PMR	A library that handles automatic data migration to different memory spaces behind an array-style interface.	2020-11-02 19:58:24

Name <https://e4s-project.github.io/DocPortal.html> Latest Doc Update

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AML	PMR
ARCHER	Tools
ASCENT	Data & Viz
BEE	Software ecosystem
BOLT	Development tools
CALIPER	Development tools
CHAI	PMR
CINEMA	Data & Viz
DARSHAN	Data & Viz

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HOME

EVENTS

ABOUT

DOCPORTAL

CONTACT US

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Search:

Name	Area	Description
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Description: The Adaptable Input Output System (ADIOS) is developed in the Exascale Computing Program.

Homepage: <https://portal.oakridge.gov/docportal/>

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ADIOS2

ADIOS2

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About

Research

Software


Groups

Jobs

Computer Science and Mathematics

Software

ADIOS2



ADIOS 2: The Adaptable Input Output (I/O) System version 2 is an open-source framework that addresses scientific data management challenges, e.g. scalable parallel I/O, as we approach the exascale era in high-performance computing (HPC). ADIOS 2 bindings are available in C++, C, Fortran, Python and can be used on supercomputers, personal computers, and cloud systems running on Linux, macOS and Windows. ADIOS 2 has out-of-the-box support for MPI and serial environments.

ADIOS 2 unified application programming interface (API) focuses on what scientific applications produce and consume in terms of n-dimensional Variables, Attributes, and Steps, while hiding the low-level details of how the data byte streams are transported as efficiently as possible from application memory to HPC networks, files, wide-area networks, and direct memory access media. Typical use cases include file storage for checkpoint-restart and analysis, data streaming for code-coupling, and in situ analysis and visualization workflows. ADIOS 2 also provides high-level APIs that resemble native I/O libraries in Python (file) and C++ (stream) for easy integration with their rich data analysis ecosystems. In addition, XML and YAML runtime configuration files are provided so users can fine tune available parameters to enable efficient data movements without recompiling their codes. ADIOS 2 also supports data compression via third party libraries for lossy: zfp, SZ, MQAPIO, and lossless: brotli, lz4, png operations.

The ADIOS 2 development process adopts modern software engineering practices such as unit testing, continuous integration, and documentation to make the final product accessible to the scientific community. Our commitment is to release a new version every 6 months. Distributions are currently available via modern package management systems: conda, spack, homebrew (and more to come). Overall, applications using ADIOS 2 do not need to dramatically modify their source code to evaluate I/O performance trade-offs, thus reducing integration and maintenance costs in their development process. For those coming from ADIOS 1.x, ADIOS 2

OAK Ridge

Researchers

Nicholas Thompson

Norbert Podhorszki

William Goddy

Scott Klasky

Liping Wan

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9092-0902-0070-4968

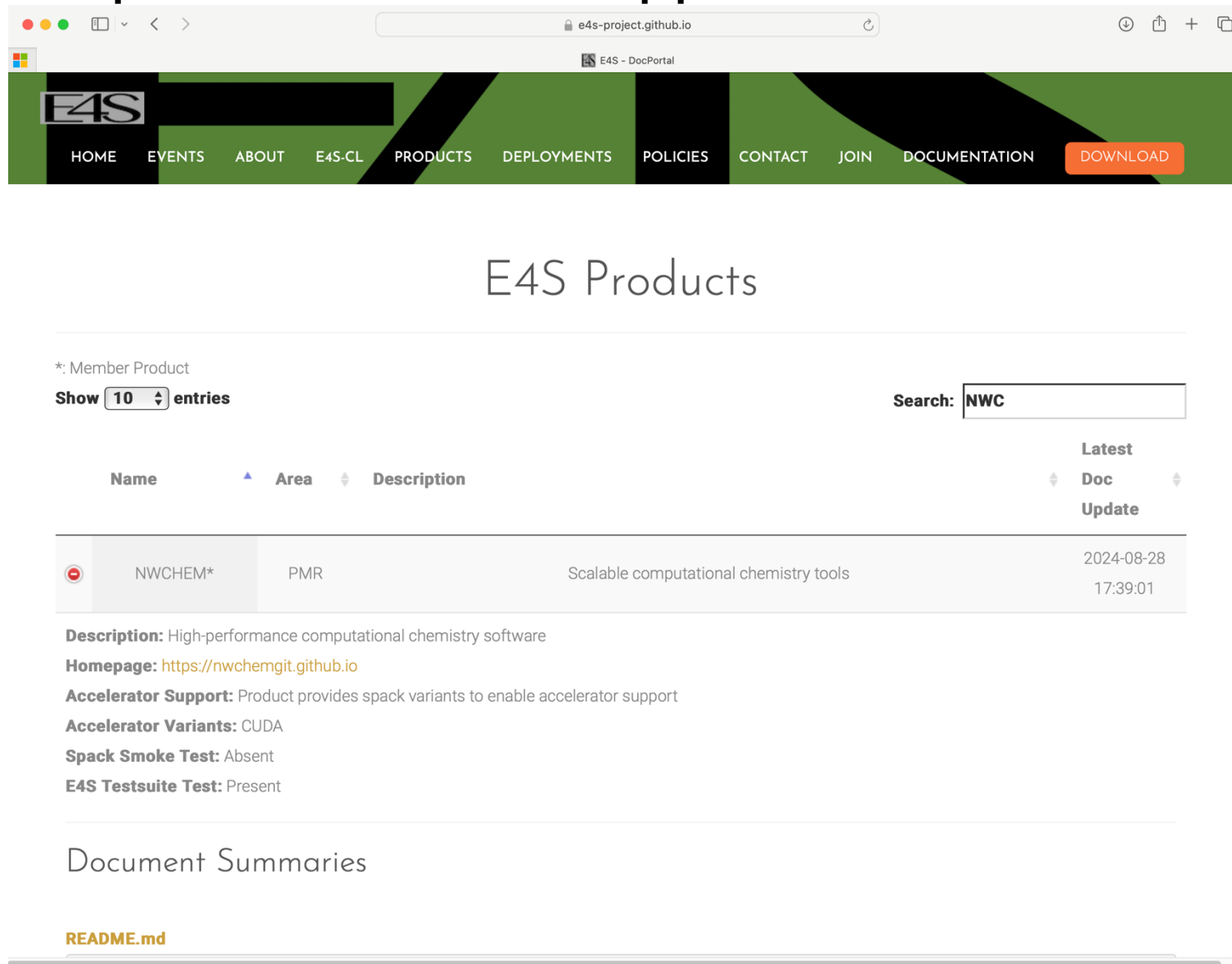
Group

Scientific Data Group



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

E4S DocPortal updated with new applications and AI/ML tools



The screenshot shows the E4S DocPortal website. The browser address bar displays 'e4s-project.github.io'. The website has a green and black header with the E4S logo and a navigation menu: HOME, EVENTS, ABOUT, E4S-CL, PRODUCTS, DEPLOYMENTS, POLICIES, CONTACT, JOIN, DOCUMENTATION, and a DOWNLOAD button. The main content area is titled 'E4S Products'. Below the title, there is a search bar with 'NWC' entered. A table lists products, with 'NWCHEM*' highlighted. The table columns are Name, Area, Description, and Latest Doc Update. Below the table, there is a section for 'Document Summaries' with a link to 'README.md'.

*: Member Product

Show 10 entries

Search: NWC

Name	Area	Description	Latest Doc Update
NWCHEM*	PMR	Scalable computational chemistry tools	2024-08-28 17:39:01

Description: High-performance computational chemistry software
Homepage: <https://nwchemgit.github.io>
Accelerator Support: Product provides spack variants to enable accelerator support
Accelerator Variants: CUDA
Spack Smoke Test: Absent
E4S Testsuite Test: Present

Document Summaries

[README.md](#)

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>

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.

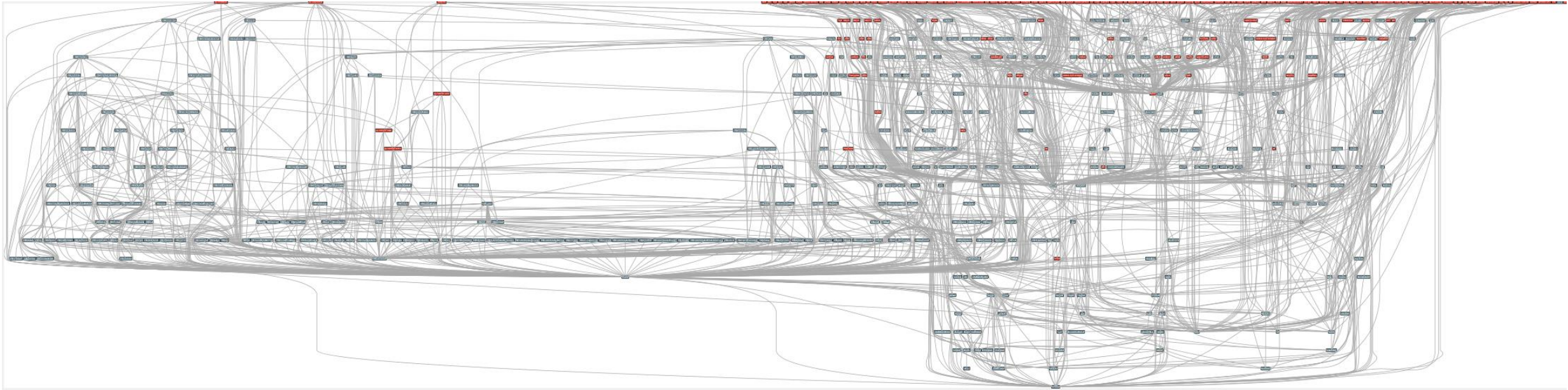
P8 Error Handling Each E4S member package will adopt and document a consistent system for signifying error conditions as appropriate for the language and application. For e.g., returning an error condition or throwing an exception. In the case of a command line tool, it should return a sensible exit 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.

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 *e/se* 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
$ spack install tau@2.34
$ spack install tau@2.34 %gcc@11.2.0
$ spack install tau@2.34 %gcc@11.2.0 +mpi+python+pthread
$ spack install tau@2.34 %gcc@11.2.0 +mpi ^mvapich2@2.3~wrapperrpath ^ dependency information
```

unconstrained
@ custom version
% custom compiler
+/- build option

- 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

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](https://twitter.com/spackpm)

ParaTools Pro for E4S™: Using E4S on Cloud Platforms



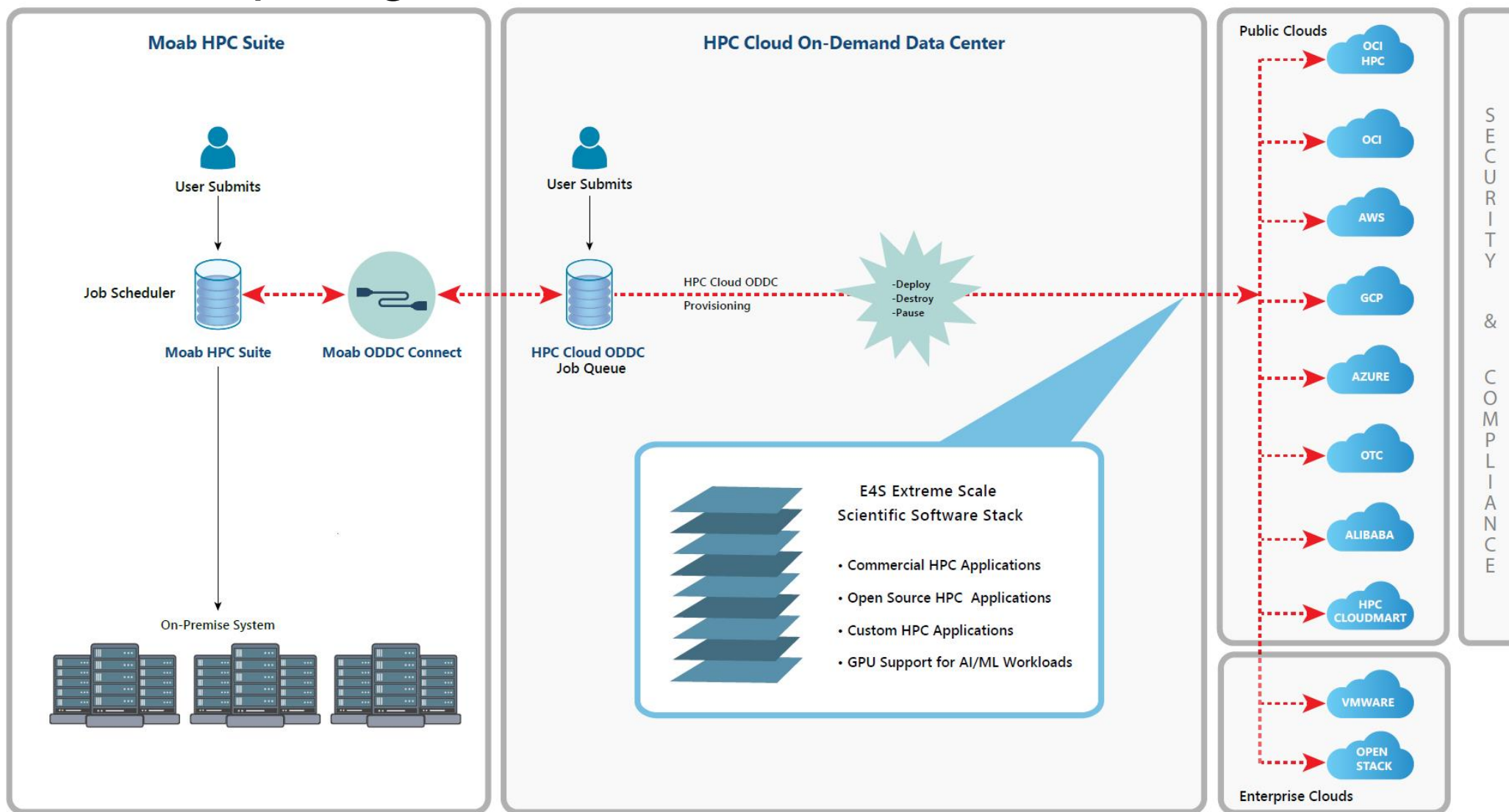
Considerations while deploying HPC/AI workloads to the cloud

- 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?

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

The screenshot shows the AWS Marketplace interface. The search bar at the top contains 'ParaTools Pro for E4S'. The left sidebar has filters for Categories (Infrastructure Software, Machine Learning, Industries), Delivery methods (Amazon Machine Image), Publisher (ParaTools Inc.), Pricing model (Usage Based), Operating system (All Linux/Unix), Free trial (Free Trial), Contract type (Standard Contract), Architecture (64-bit x86, 64-bit Arm), and Region (Africa, Asia Pacific, Europe, North America, South America). The main content area displays a list of ParaTools Pro for E4S products. Each product listing includes the product name, version, and a 'Free Trial' button. The products listed are:

- ParaTools Pro for E4S™: AI/ML & HPC Tools on AWS PCS (x86)
- ParaTools Pro for E4S™: AI/ML & HPC Tools on ODDC Server (x86)
- ParaTools Pro for E4S™: AI/ML & HPC Tools on ODDC Node (x86)
- ParaTools Pro for E4S™: AI/ML & HPC Tools on ParallelCluster (x86)
- ParaTools Pro for E4S™: AI/ML & HPC Tools on ParallelCluster (ARM)
- ParaTools Pro for E4S™: AI/ML & HPC Tools on ODDC Node (ARM)
- ParaTools Pro for E4S™: AI/ML & HPC Tools on ODDC Server (ARM)

- 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

E4S Pro

Product details

ParaTools Pro

ParaTools, Inc.

Turn-key cluster with full stack AI, ML and HPC libraries and tools like OpenFOAM and NVIDIA Nemo

28-Day Trial Available

GET STARTED

VIEW DEPLOYMENTS

Training Video - Run...

OVERVIEW

PRICING

DOCUMENTATION

SUPPORT

Overview

ParaTools Pro for E4S™[1] - the Extreme-scale Scientific Software Stack[2] hardened for commercial clouds and supported by ParaTools, Inc. provides a platform for developing and deploying HPC and AI/ML applications. It features a performant remote desktop environment (based on VNC) on the login node and compute nodes interconnected by a low-latency, high bandwidth network adapter based on Google's custom Intel Infrastructure Processing Unit (IPU). ParaTools Pro for E4S™ features a suite of over 100 HPC tools built using the Spack[3] package manager and the proprietary MVAPICH MPI tuned for IPU. It features ready to use HPC applications (such as OpenFOAM, LAMMPS, Xyce, CP2K, deal.II, GROMACS, Quantum Espresso) as well as AI/ML tools based on Python (such as NVIDIA NeMo™, TensorFlow, PyTorch, JAX, Horovod, Keras, OpenCV, matplotlib, and supports Jupyter notebooks) and the Codium IDE. New packages can be easily installed using Spack and pip and are accessible on the cluster compute and login nodes. It may be used for developing the next generation of generative AI applications using a suite of Python tools and interfaces. E4S™ has built a unified computing environment for deployment of open-source projects. E4S™ was originally developed to provide a common software environment

Additional details

Runs on: Google Compute Engine

Type: [Virtual machines](#), Single VM

Architecture: [X86_64](#)

Last product update: 11/13/24

Category: [Science & research](#), [High-Performance Computing](#), [Machine learning](#), [Developer stacks](#)

Version: latest

Google Cloud Marketplace

The logo for PESO, featuring the letters 'PESO' in a bold, sans-serif font. To the right of the text is a circular emblem composed of three concentric arcs in green, blue, and orange, suggesting a globe or a stylized 'P'.

32

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

Private

azuremarketplace.microsoft.com


Microsoft

Azure Marketplace

Sign in

Search Marketplace

Products > ParaTools Pro for E4S™: AI/ML & HPC Tools on CycleCloud (AMD64)



Get It Now

Pricing information

Starting at \$0.99/hour

+ Azure infrastructure costs

Categories

AI + Machine Learning

Compute

Support

Support

Legal

Under Microsoft Standard Contract

Privacy Policy

ParaTools Pro for E4S™: AI/ML & HPC Tools on CycleCloud (AMD64)

ParaTools, Inc.

Free trial

Overview

Plans + Pricing

Ratings + reviews

ParaTools Pro for E4S™ is a turnkey HPC Cluster solution with tuned MPI, batch job management, and a host of AI/ML and science & engineering tools.

ParaTools Pro for E4S™[1] - the Extreme-scale Scientific Software Stack[2] hardened for commercial clouds and supported by ParaTools, Inc. provides a platform for developing and deploying HPC and AI/ML applications. It features a performant remote desktop environment (based on VNC) on the login node and compute nodes interconnected by a low-latency, high bandwidth MVAPICH MPI implementation tuned for Microsoft Azure's Infiniband enabled VMs. ParaTools Pro for E4S™ features a suite of over 100 HPC tools built using the Spack[3] package manager and MVAPICH MPI tuned for Azure's Infiniband interconnect. It features ready to use HPC applications (such as OpenFOAM, LAMMPS, Xyce, CP2K, deal.II, GROMACS, Quantum Espresso) as well as AI/ML tools based on Python (such as NVIDIA NeMo™, TensorFlow, PyTorch, JAX, Horovod, Keras, OpenCV, matplotlib, and supports Jupyter notebooks) and the Codium IDE. New packages can be easily installed using Spack and pip and are accessible on the cluster compute and login nodes. It may be used for developing the next generation of generative AI applications using a suite of Python tools and interfaces. E4S™ has built a unified computing environment for deployment of open-source projects. E4S™ was originally developed to provide a common software environment for the exascale leadership computing systems currently being deployed at DOE National Laboratories across the U.S. Support for ParaTools Pro for E4S™ is available through ParaTools, Inc. This product has additional charges associated with it for optional product support and updates. Users wanting to stand up an HPC cluster with a complete software stack for AI/ML and/or HPC engineering and science applications will benefit from this offer. Building and configuring software for a consistent, robust and performant environment is surprisingly difficult. This product addresses the need for a complete software stack for HPC and AI/ML applications, including a remote desktop environment, batch job management, and a host of AI/ML and science & engineering tools. Leverage the spack package manager to install additional custom software or use the various pre-built components to build your own solutions. This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Office of Advanced Scientific Computing and Research (ASCR), under SBIR Award Number DE-SC0022502 ("E4S:

Azure Marketplace listing

The logo for PESO (PetaScale Extreme Scale Operations) features the word "PESO" in a bold, sans-serif font. To the right of the text is a circular graphic composed of three concentric arcs in blue, green, and orange, suggesting a globe or a network.

33

Choosing an instance on AWS to run the image using Heidi

adaptivecomputing.com/ODDC/ClusterManager

Sameer Shende
Sshende - Admin

Cluster Manager

Stack Manager
Credentials Manager
Job Manager
File Manager
Accounting
Instance Prices

Cluster Manager

Cloud Providers

All Cloud Providers

Alibaba Cloud

Oracle Cloud HPC

Oracle Cloud

Amazon Web Services

Google Cloud

Microsoft Azure

Open Telekom Cloud

Search

e4s-22.11-mvapich2-xyce-aws

Amazon Web Services

\$0.28 per Hour

ADVANCED

UPDATE

CLOSE

Name *

e4s-22.11-mvapich2-xyce-aws

OS Type *

centos-7

Prefix *

e4s-xyce-aws

Credential *

Head Node Size *

t2.xlarge - vCPU: 4, Mem (GB): 16

Manager *

Torque

Region *

US West 1

Availability Zone

Bursting Configuration:

☒ Off ☐ Min ☐ Max ☐ All

Compute Nodes:

Size *

t2.xlarge - vCPU: 4, Mem (GB): 16

Count *

2

Description

Credential

Uptime

Actions

Not Set

N/A

Rows per page: 10

1-1 of 1

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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

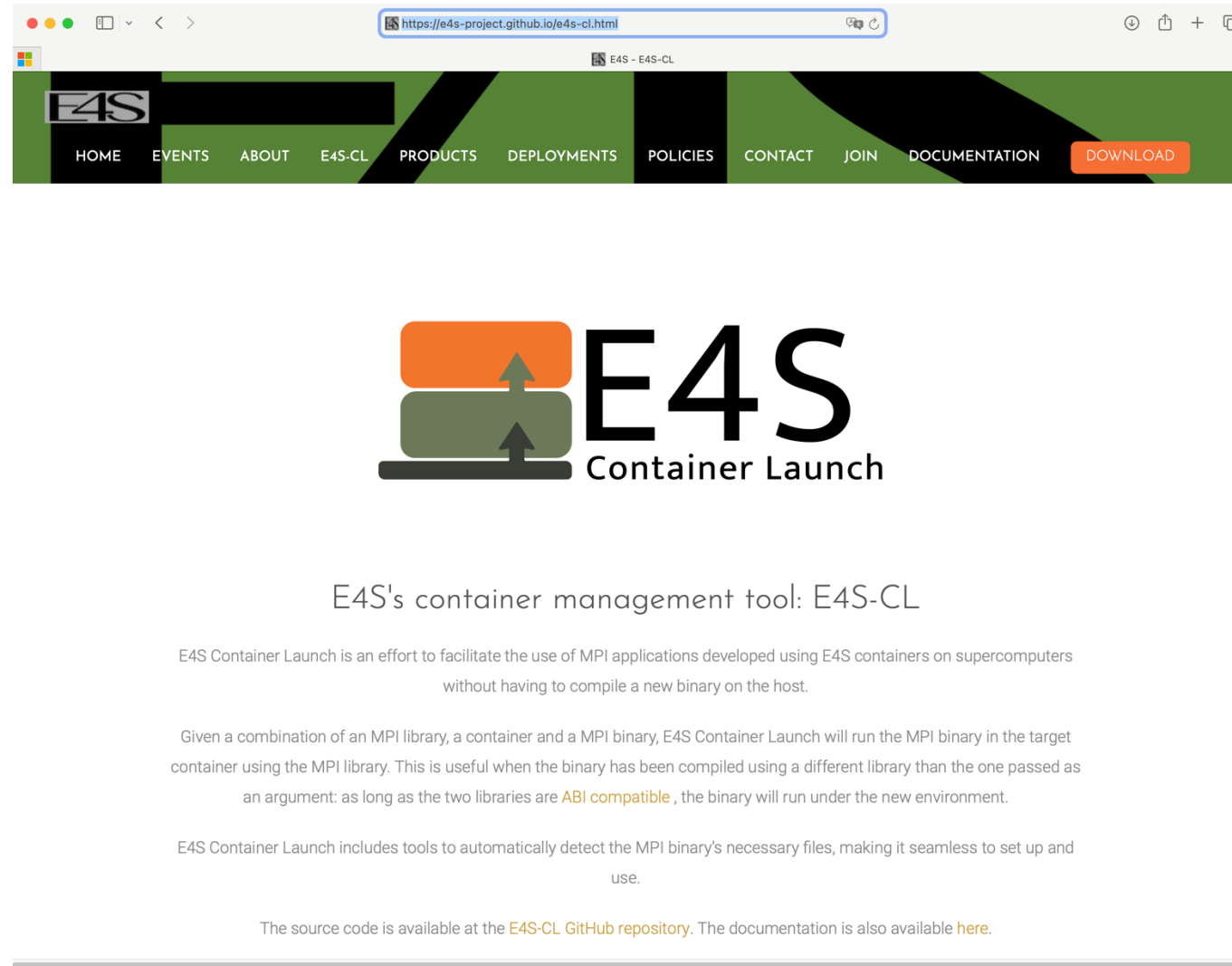
The screenshot displays the GitHub repository for E4S-Project/e4s-alc. The repository is public and has 3 stars and 4 watchers. The latest release is E4S-ALC release v1.0.2, which is highlighted with a blue box and labeled 'Latest'. The repository structure includes a README, a MIT license, and various files and folders. The README section is titled 'E4S à la Carte'.

File/Folder	Commit Message	Time Ago
docs	post release	3 days ago
e4s_alc	propagated changes	2 days ago
examples	did base changed to remove have modules.yaml in the co...	3 days ago
.gitignore	Merge branch 'main' into restructure	10 months ago
.readthedocs.yaml	added readthedocs config file	last year
CHANGELOG	update changelog	5 days ago
LICENSE	Initial commit	last year
Makefile	quick fix	10 months ago
README.md	updated readme to specify Singularity definition file supp...	3 weeks ago
pyproject.toml	added tool.setuptools_scm banner in pyproject.toml	2 weeks ago

Add to a base image:

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

E4S Container Launch tool: 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
```



Release of e4s-cl on GitHub

The screenshot displays the GitHub repository page for `E4S-Project/e4s-cl`. The repository is public and has 12 stars, 3 forks, and 5 unwatchers. The commit history shows a recent commit by `FrederickDeny` titled "post-release" with 1,399 commits. The repository structure includes folders like `.github/workflows`, `assets/images`, `docs`, `e4s_cl`, `scripts`, and `tests`, as well as files like `.coveragerc`, `.gitignore`, `.gitlab-ci.yml`, `.readthedocs.yaml`, `CHANGELOG`, `LICENSE`, `Makefile`, `README.md`, and `pylintrc`.

The right sidebar shows the repository's "About" section, including the description "Container manager for E4S", the website `e4s-cl.readthedocs.io`, and various tags like `containers`, `mpi`, `singularity-container`, `shifter`, `podman`, `apptainer`, and `e4s`. It also lists 12 stars, 5 watchers, and 3 forks.

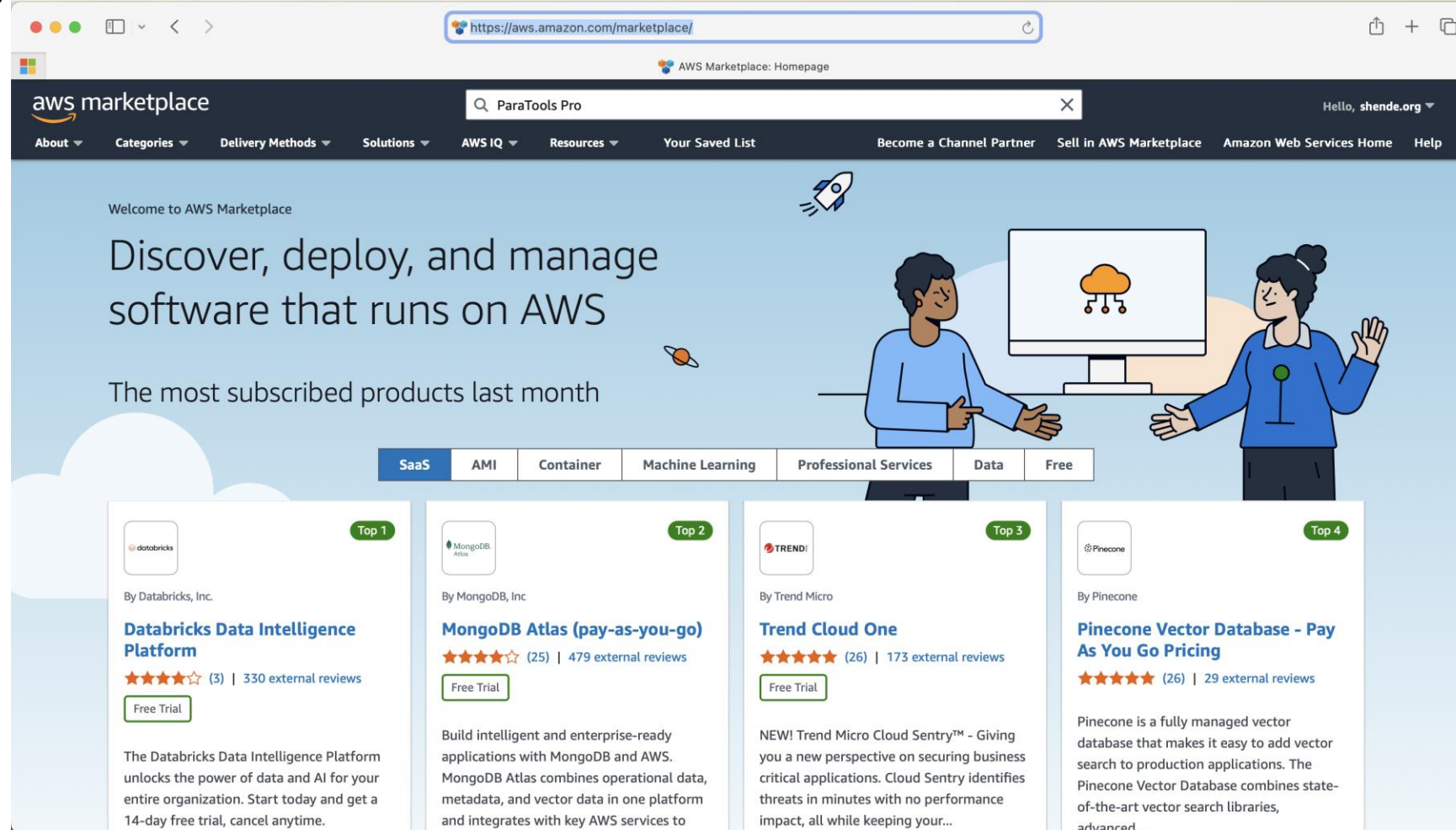
The "Releases" section shows 10 releases, with the latest release, `E4S-CL release v1.0.3`, highlighted by a blue box. This release was published 3 weeks ago and is marked as the "Latest" version. There are 9 other releases available.

The "Packages" section indicates that no packages have been published yet, with a link to "Publish your first package".

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

Using your own AWS credentials with ODDC

STEP 1: Subscribe to ParaTools Pro for F4S 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

aws marketplace

ParaTools Pro

Hello, shende.org

About Categories Delivery Methods Solutions AWS IQ Resources Your Saved List Become a Channel Partner Sell in AWS Marketplace Amazon Web Services Home Help

Amazon Machine Image (6)

Publisher

- ☐ ParaTools Inc. (6)

Pricing model

- ☐ Usage Based (6)

Operating system

- ☐ All Linux/Unix

Free trial

- ☐ Free Trial (6)

Contract type

- ☐ Standard Contract (6)

Architecture

- ☐ 64-bit (x86) (3)
- ☐ 64-bit (Arm) (3)

Region

- ☐ Africa (Cape Town) (6)
- ☐ Asia Pacific (Hong Kong) (6)
- ☐ Asia Pacific (Tokyo) (6)
- ☐ Asia Pacific (Seoul) (6)
- ☐ Asia Pacific (Osaka) (6)
- ☐ Asia Pacific (Mumbai) (6)
- ☐ Asia Pacific (Hyderabad) (6)
- ☐ Asia Pacific (Singapore) (6)
- ☐ Asia Pacific (Sydney) (6)
- ☐ Asia Pacific (Jakarta) (6)

Show 10 More

ParaTools Pro (6 results) showing 1 - 6

Did you mean [paratool pre?](#)

Sort By: Relevance

ParaTools

[ParaTools Pro for E4S™: AI/ML & HPC Tools on ODDC Node \(x86\)](#)

By [ParaTools Inc.](#) | Ver v17208158-oddc-v1.0-e4s-24.05-node-amd64

Free Trial

Starting from \$0.99 to \$0.99/hr for software + AWS usage fees

ParaTools Pro for E4S™[1] - the Extreme-scale Scientific Software Stack E4S[2] hardened for commercial clouds and supported by ParaTools, Inc. provides a platform for developing and deploying HPC and AI/ML applications. It features a performant remote desktop environment (based on VNC) on the login...

ParaTools

[ParaTools Pro for E4S™: AI/ML & HPC Tools on ODDC Server \(x86\)](#)

By [ParaTools Inc.](#) | Ver 17208158-oddc-v1.0-e4s-24.05-server-amd64

Free Trial

Starting from \$0.99 to \$0.99/hr for software + AWS usage fees

ParaTools Pro for E4S™[1] - the Extreme-scale Scientific Software Stack E4S[2] hardened for commercial clouds and supported by ParaTools, Inc. provides a platform for developing and deploying HPC and AI/ML applications. It features a performant remote desktop environment (based on VNC) on the login...

ParaTools

[ParaTools Pro for E4S™: AI/ML & HPC Tools on ParallelCluster \(x86\)](#)

By [ParaTools Inc.](#) | Ver v2024.07.18.0740-pcluster-3.10.1-e4s-24.05-amd64

Free Trial

Starting from \$0.99 to \$0.99/hr for software + AWS usage fees

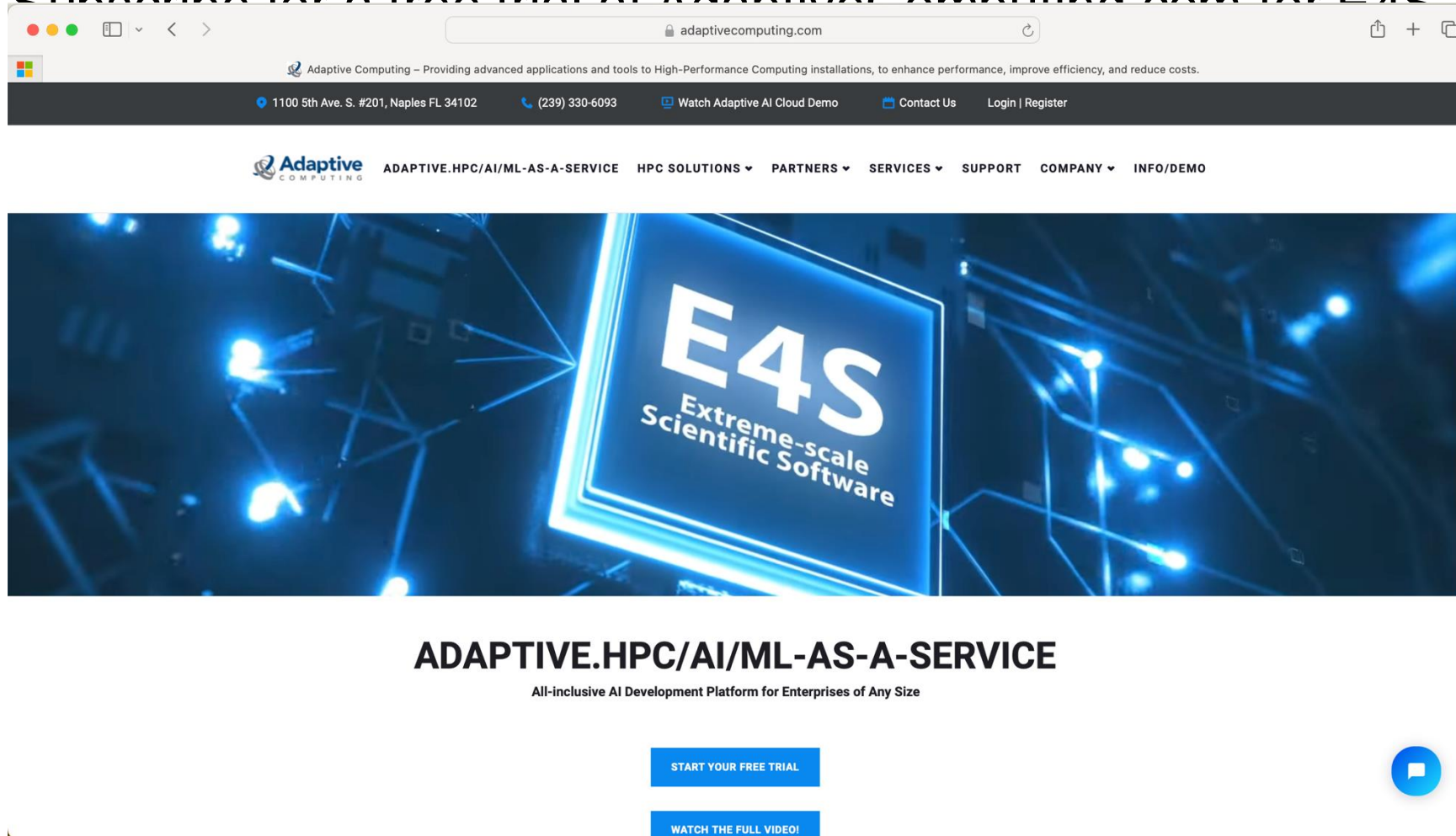
ParaTools Pro for E4S™[1] - the Extreme-scale Scientific Software Stack E4S[2] hardened for commercial clouds and supported by ParaTools, Inc. provides a platform for

Free trial for 31 days!

Click on ODDC Server (x86) click subscribe

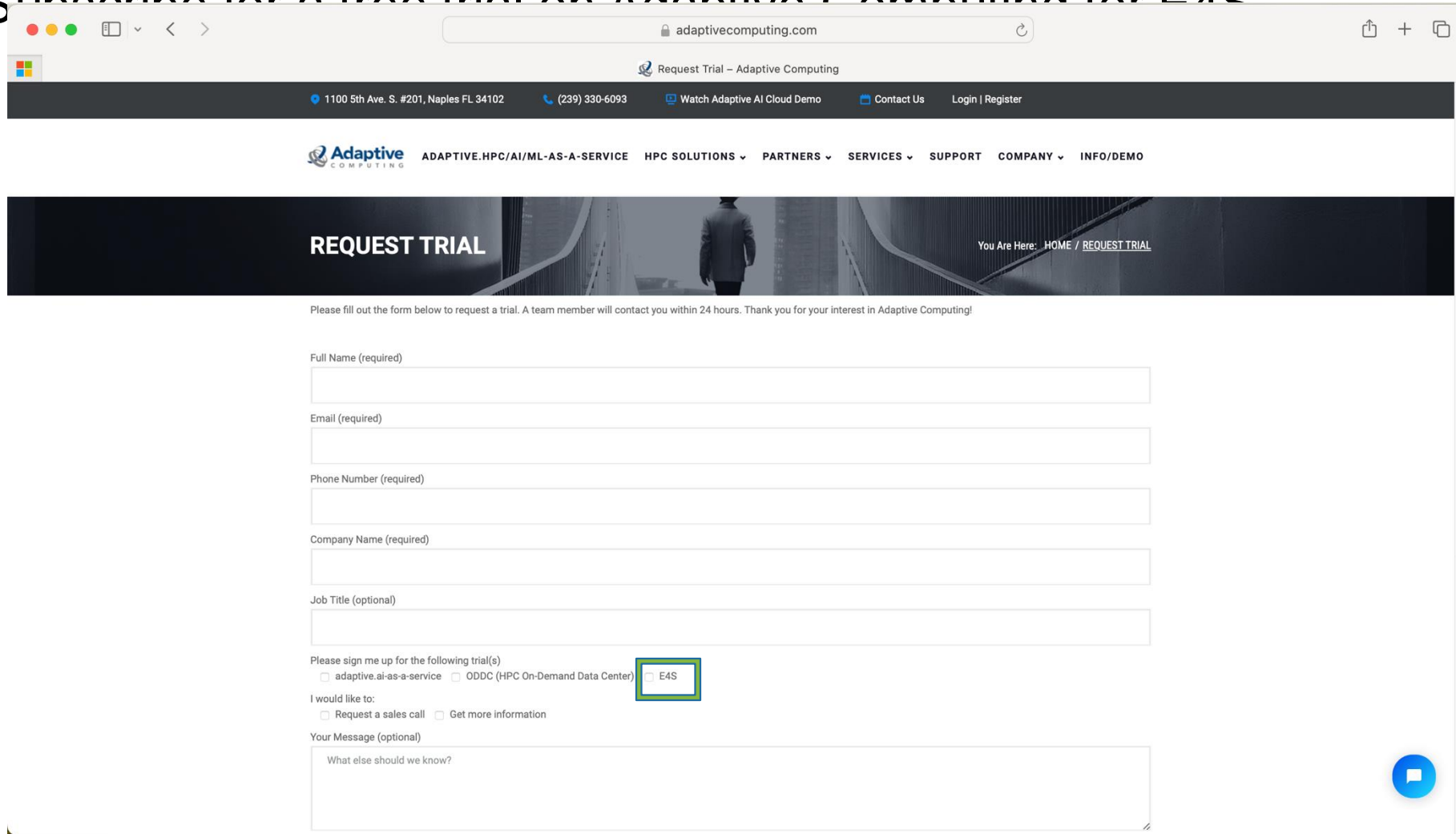
Click on ODDC Node (x86) click subscribe

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



adaptivecomputing.com

Request Trial – Adaptive Computing

1100 5th Ave. S. #201, Naples FL 34102 (239) 330-6093 Watch Adaptive AI Cloud Demo Contact Us Login | Register

Adaptive COMPUTING ADAPTIVE.HPC/AI/ML-AS-A-SERVICE HPC SOLUTIONS PARTNERS SERVICES SUPPORT COMPANY INFO/DEMO

REQUEST TRIAL

You Are Here: [HOME](#) / [REQUEST TRIAL](#)

Please fill out the form below to request a trial. A team member will contact you within 24 hours. Thank you for your interest in Adaptive Computing!

Full Name (required)

Email (required)

Phone Number (required)

Company Name (required)

Job Title (optional)

Please sign me up for the following trial(s)

☐ adaptive.ai-as-a-service ☐ ODDC (HPC On-Demand Data Center) ☒ E4S

I would like to:

☐ Request a sales call ☐ Get more information

Your Message (optional)

What else should we know?

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

The screenshot shows the ParaTools AWS cluster configuration interface. The browser address bar displays `paratools.adaptivecomputing.com`. The page title is "HPC Cloud On-Demand Data Center". The main header bar is blue and contains the Amazon logo, the cluster name "e4s-24-05-aws-2", the price "\$1.74 per Hour", and buttons for "ADVANCED", "UPDATE", and "CLOSE".

The configuration form includes the following fields:

- Name ***: e4s-24-05-aws-2
- OS Type ***: ubuntu-22.04
- Prefix ***: e4s-24-05
- Credential ***: luke_p-aws
- Head Node Size ***: g4dn.8xlarge - GPU: 1, vCPU: 32, Mem (GB...
- Manager ***: Torque
- Region ***: US West 2
- Availability Zone ***: us-west-2a
- Subnet ID**: (empty)
- VPC**: (empty)
- Private IP**: ☐
- Security Group ID**: (empty)
- Elastic IP Address**: (empty)
- Server Volume (GB)**: 500
- Node Volume (GB)**: 500
- Idle Purge Time (S)**: (empty)
- User Script**: (empty) with an "UPLOAD SCRIPT" button
- Share**: NFS
- Packages**: A table with columns "Linux Package Name" and "ADD". The table is currently empty, with the text "No Packages" displayed below it.

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

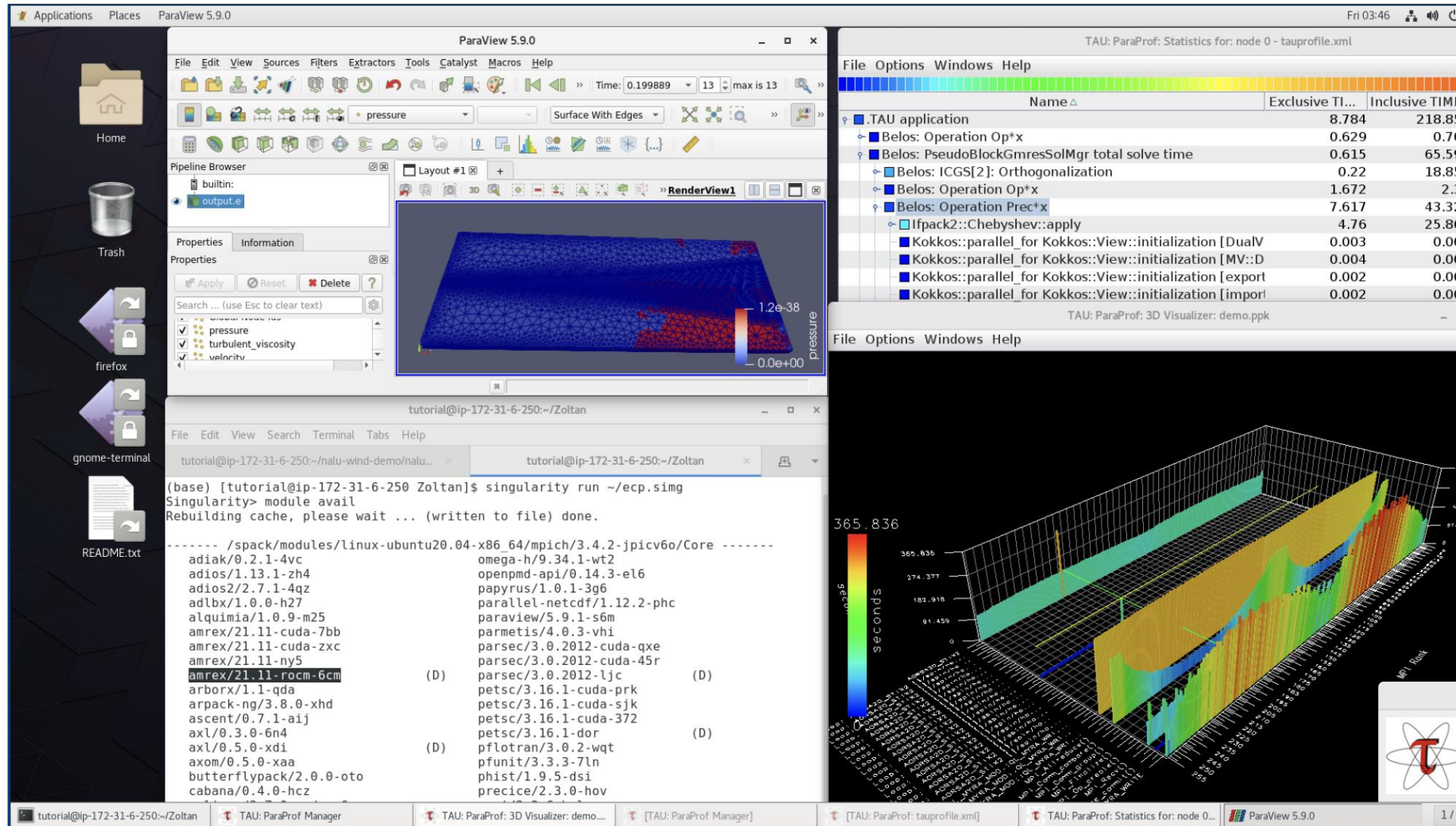
STEP 4: Deploy cluster from ODDCI

The screenshot shows the ParaTools Cluster Manager interface. At the top, the browser address bar displays 'paratools.adaptivecomputing.com'. The page header includes 'HPC Cloud On-Demand Data Center' and 'ParaTools, Inc. Paratoolsadmin - Admin'. The main section is titled 'Cluster Manager' and features a search bar. Below this is a table of clusters with the following columns: State, Name, Provider, Owner, Bursting, Nodes, Credential, and Uptime. The table lists five clusters, all with a 'Down' status. A context menu is open over the first cluster, showing options: Edit, Edit Collaborators, Deploy (highlighted with a green box), Logs, Plan, Save Config, Duplicate Cluster, and Delete. The footer of the interface shows 'Copyright © 2024. Adaptive Computing Enterprises, Inc., All rights reserved.'

State	Name	Provider	Owner	Bursting	Nodes	Credential	Uptime
Down 3:11 13:29	e4s-24-05-cpu1	amazon web services	paratoolsadmin	off	2	luke_p-aws	N/A
Down 10:08 8:54	e4s-24-05-aws-2	amazon web services	paratoolsadmin	off	2	luke_p-aws	N/A
Down 1:39 7:29	e4s-24-05-oci	ORACLE Cloud Infrastructure	paratoolsadmin	off	2	lpeyrans	N/A
Down 2:56 8:55	e4s-24-05-gcp	Google Cloud	paratoolsadmin	off	2	lpeyrans-gmail-com	N/A
Down	e4s-24-05-azure	Microsoft Azure	paratoolsadmin	off	2	uooddcsameer	N/A

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

The screenshot displays the E4S HPC Software Ecosystem interface on AWS. The main window shows a terminal with a list of installed packages, including act, adms, boost, fault, gds3d, ghdl, graywolf, gtkwave, irsim, iverilog, klayout, magic, netgen, ngspice, nvc, open_pdks, openroad, opensta, opentimer, or-tools, padring, pcb, qflow, qrouter, qucs-s, rggen, riscv-gnu-toolchain, swift, tar, verilator, xcircuit, xschem, xscheme-gaw, and yosys. The Qflow Manager window shows a project status table with columns for Project, Checklist, Preparation, Synthesis, Placement, Static Timing Analysis, Routing, Post-Route STA, Migration, DRC, LVS, and GDS, all marked as '(not done)'. The background shows a desktop environment with a file manager, a terminal, and a Qflow Manager window.

E4S EDA on AWS

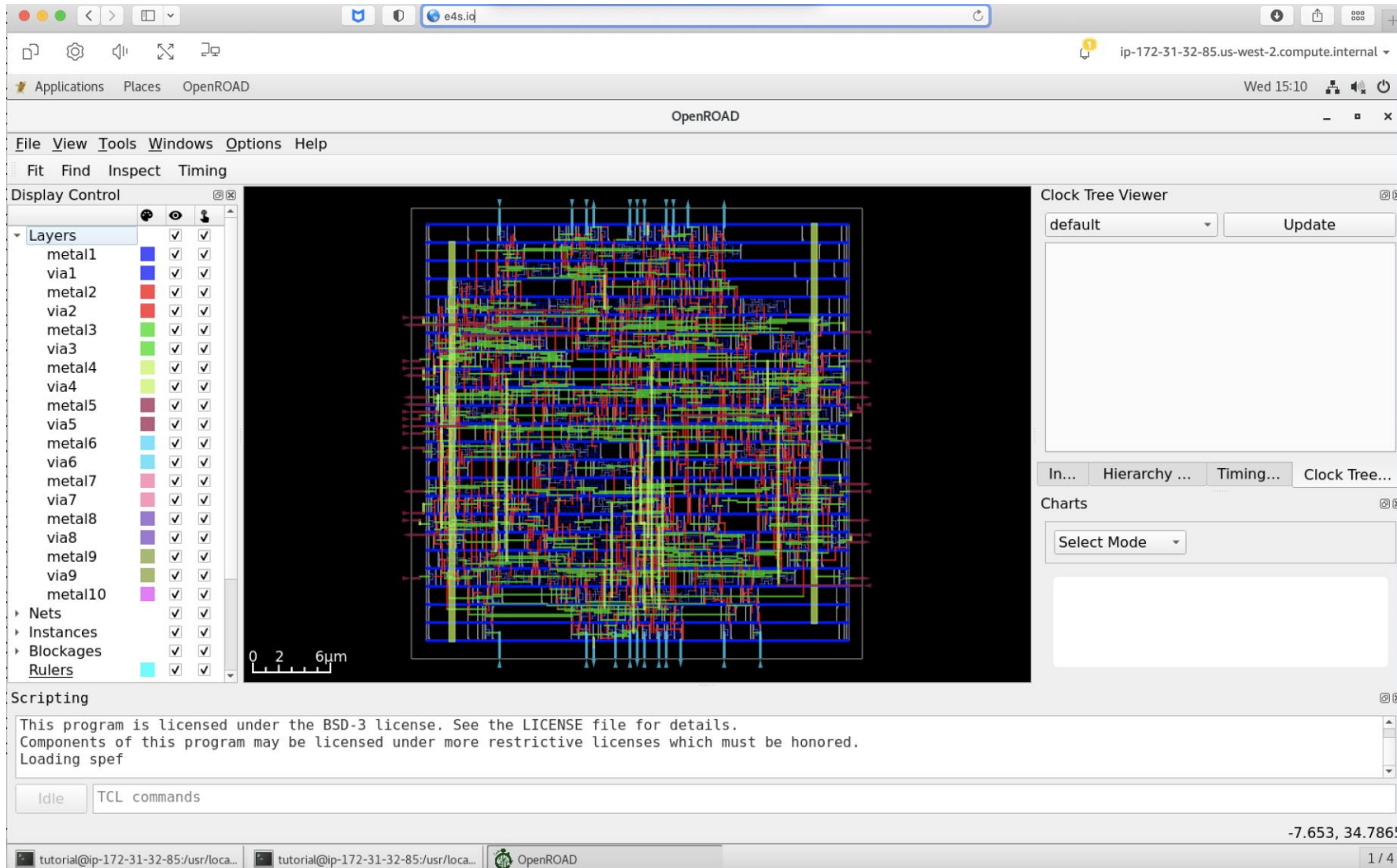
- Magic
- ACT
- Klayout
- Qflow
- Xschem
- Xcircuit
- Yosys
- Volator
- OpenROAD
- OpenLane
- OpenFASOC
- iVerilog
- Gtkwave
- Irsim
- Qrouter
- Fault
- GDS3D
- Rggen
- Python tools
 - Cocotb
 - Amaranth
 - Edalize
 - Gdsfactory
 - Gdspys
 - OpenRAM
 - Gdstk
 - Silicon compiler
 - Volare ...
- PDKs
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



Free to use public AML 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

- Magic
- ACT
- Klayout
- Qflow
- Xschem
- Xcircuit
- Yosys
- Volator
- OpenROAD
- OpenLane
- OpenFASOC
- iVerilog
- Gtkwave
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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

#	Packages currently in E4S	URL	#	Packages currently in E4S	URL
1	Magic	http://opencircuitdesign.com/magic/	13	Yosys	https://github.com/YosysHQ/yosys
2	Xyce	https://xyce.sandia.gov	14	Xcircuit	http://opencircuitdesign.com/xcircuit/
3	NGSPICE	https://ngspice.sourceforge.io	15	Graywolf	https://github.com/rubund/graywolf
4	KLayout	https://www.klayout.de	16	OpenSTA	https://github.com/The-OpenROAD-Project/OpenSTA
5	Qflow	http://opencircuitdesign.com/qflow	17	OpenTimer	https://github.com/OpenTimer/OpenTimer
6	OR-Tools	https://developers.google.com/optimization	18	Qrouter	http://opencircuitdesign.com/qrouter/
7	IRSIM	http://opencircuitdesign.com/irsim/	19	Xschem	https://github.com/silicon-vlsi-org/eda-xschem
8	OpenROAD	https://github.com/The-OpenROAD-Project/OpenROAD	20	RISC-V GNU Toolchain	https://github.com/riscv-collab/riscv-gnu-toolchain
9	OpenLane	https://openlane.readthedocs.io/	21	Fault: Design for Test	https://github.com/AUCOHL/Fault
10	OpenFASOC	https://openfasoc.readthedocs.io/	22	NVC	https://github.com/nickg/nvc
11	Open_PDKs	http://opencircuitdesign.com/open_pdk/	23	Amaranth	https://github.com/amaranth-lang/amaranth
12	Netgen	http://opencircuitdesign.com/netgen/	24	Cocotb	https://github.com/cocotb/cocotb

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

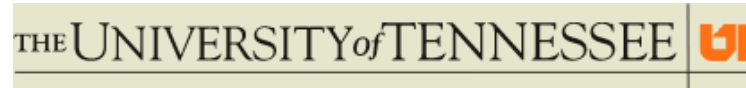
#	Packages currently in E4S	URL
37	Padring	https://github.com/donn/padring
38	Pyverilog	https://github.com/PyHDI/Pyverilog
39	OpenRAM	https://github.com/VLSIDA/OpenRAM
40	Rggen	https://github.com/rggen/rggen
41	Spysi	https://github.com/gmagno/spysi
42	Volare	https://github.com/efabless/volare
43	Siliconcompiler	https://github.com/siliconcompiler/siliconcompiler
44	Verilator	https://github.com/verilator/verilator
45	Sky130	SkyWater Technologies 130nm CMOS PDK
46	Actflow	https://github.com/asynclsi/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/asynclsi/xcell.git



<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.*



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- <https://pesoproject.org>
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- <https://hpsf.io>
- <https://www.energy.gov/technologytransitions/sbirsttr>



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.

