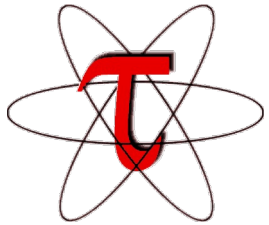
E4S:
A Platform for EDA on Commercial Cloud Platforms

Open Source EDA BoF at DAC 2023
https://open-source-eda-birds-of-a-feather.github.io

7:35 pm – 9:30 pm PDT,
Room 3001, Moscone West, San Francisco, CA



Prof. Sameer Shende
Research Professor and Director,
Performance Research Laboratory, OACISS, University of Oregon
President and Director, ParaTools, Inc.
https://e4s.io/talks/E4S_DAC23.pdf

Challenges

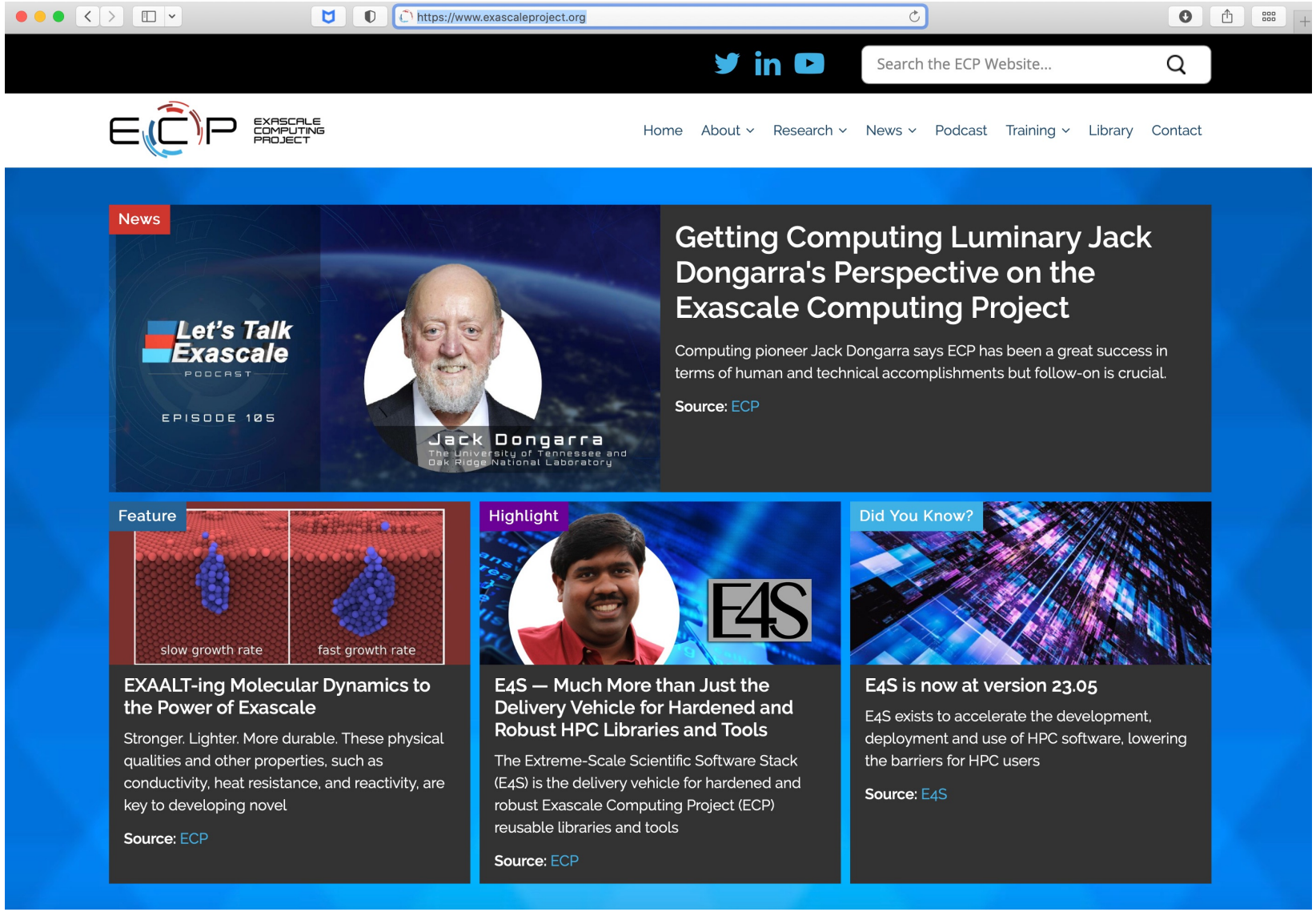
- As our software gets more complex, it is getting harder to install EDA and HPC tools and libraries correctly in an integrated and interoperable software stack to deploy our applications to the cloud platforms!

Key questions

- What EDA tools should we integrate in an open-source software stack targeting commercial cloud platforms?
- Can the Extreme-scale Scientific Software Stack serve as a platform for open-source EDA tool integration?
- How can we build upon what we currently have in E4S?

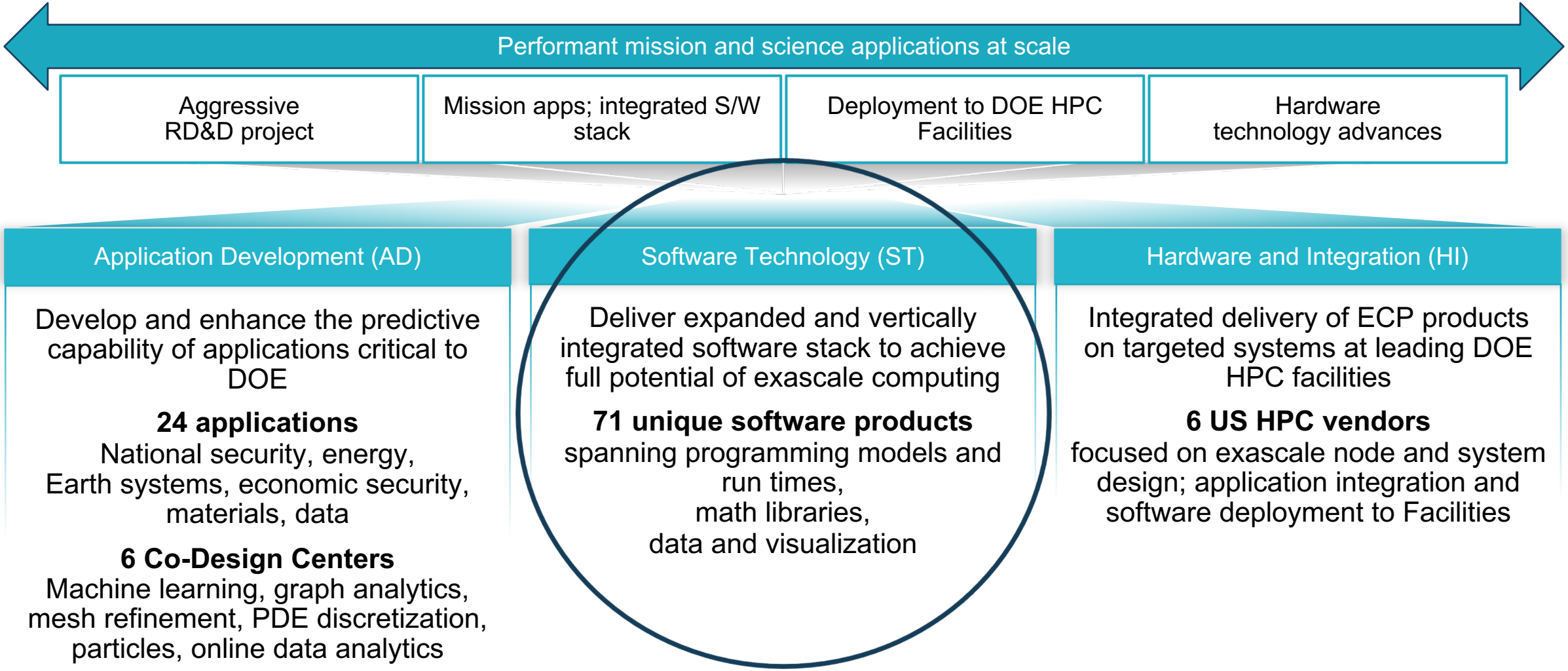
Extreme-scale Scientific Software Stack (E4S)

Exascale Computing Project (ECP)



https://exascaleproject.org

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



US DOE HPC Roadmap to Exascale Systems

2012-2020

2021-2023

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

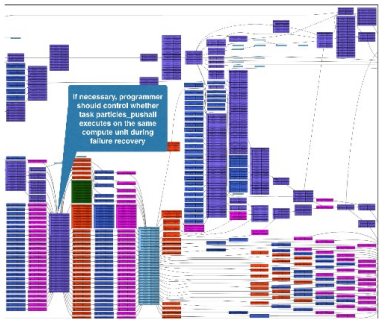
LLNL
HPE/AMD

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



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

https://e4s.io

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

E4S: Extreme-scale Scientific Software Stack

- E4S is a community effort to provide open-source software packages for developing, deploying and running scientific applications on HPC platforms.
- E4S has built a comprehensive, coherent software stack that enables application developers to productively develop highly parallel applications that effectively target diverse exascale architectures.
- E4S provides a curated, Spack based software distribution of 100+ HPC, 50+ EDA (e.g., Xyce), and AI/ML packages (e.g., TensorFlow, PyTorch).
- With E4S Spack binary build caches, E4S supports both bare-metal and containerized deployment for GPU based platforms.
  - X86_64, ppc64le (IBM Power 9), aarch64 (ARM64) with support for GPUs from NVIDIA, AMD, and Intel
  - HPC and AI/ML packages are optimized for GPUs and CPUs.
- Container images on DockerHub and E4S website of pre-built binaries of ECP ST products.
- Base images and full featured containers (with GPU support).
- Commercial support for E4S through ParaTools, Inc. for installation, maintaining an issue tracker, and ECP AD engagement.
  - https://dashboard.e4s.io https://e4s.io/talks/E4S_Support_June23.pdf
- e4s-cl container launch tool allows binary distribution of applications by substituting MPI in the containerized app with the system MPI. e4s-alc is a tool to create custom container images from base images
- Quarterly releases: E4S 23.05 released on May 31, 2023: https://e4s.io/talks/E4S_23.05.pdf
- E4S for commercial cloud platforms: AWS image supports MPI implementations and containers with remote desktop (DCV).
  - Intel MPI, NVHPC, MVAPICH2, MPICH, MPC, OpenMPI

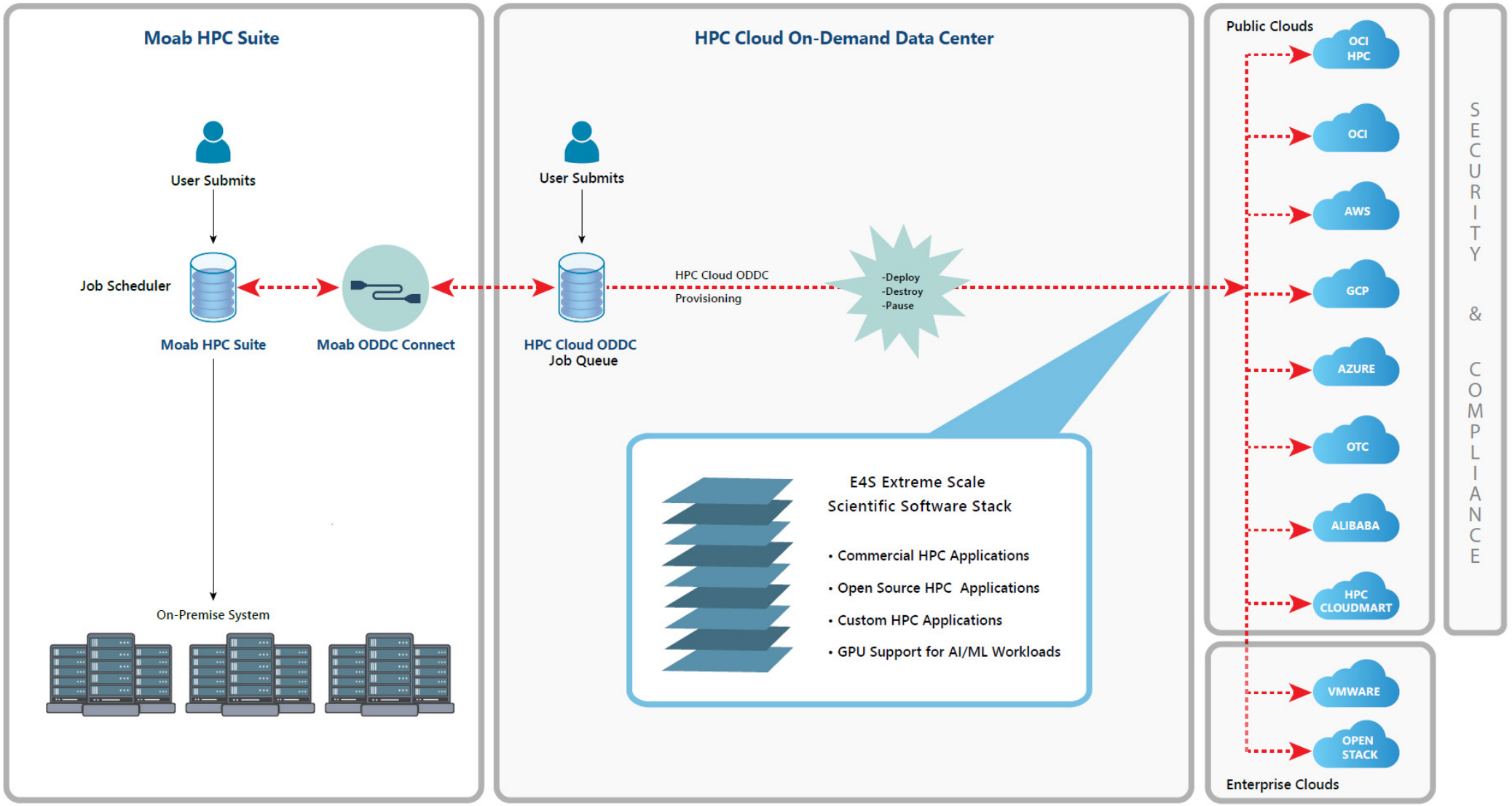
Considerations while deploying HPC/AI workloads to the cloud

- Which cloud provider?
  - AWS, OCI, GCP, Azure, …
  - Why not all?
- HPC and AI/ML workloads need low latency, high bandwidth
  - Which MPI?
- Which image?
  - 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?

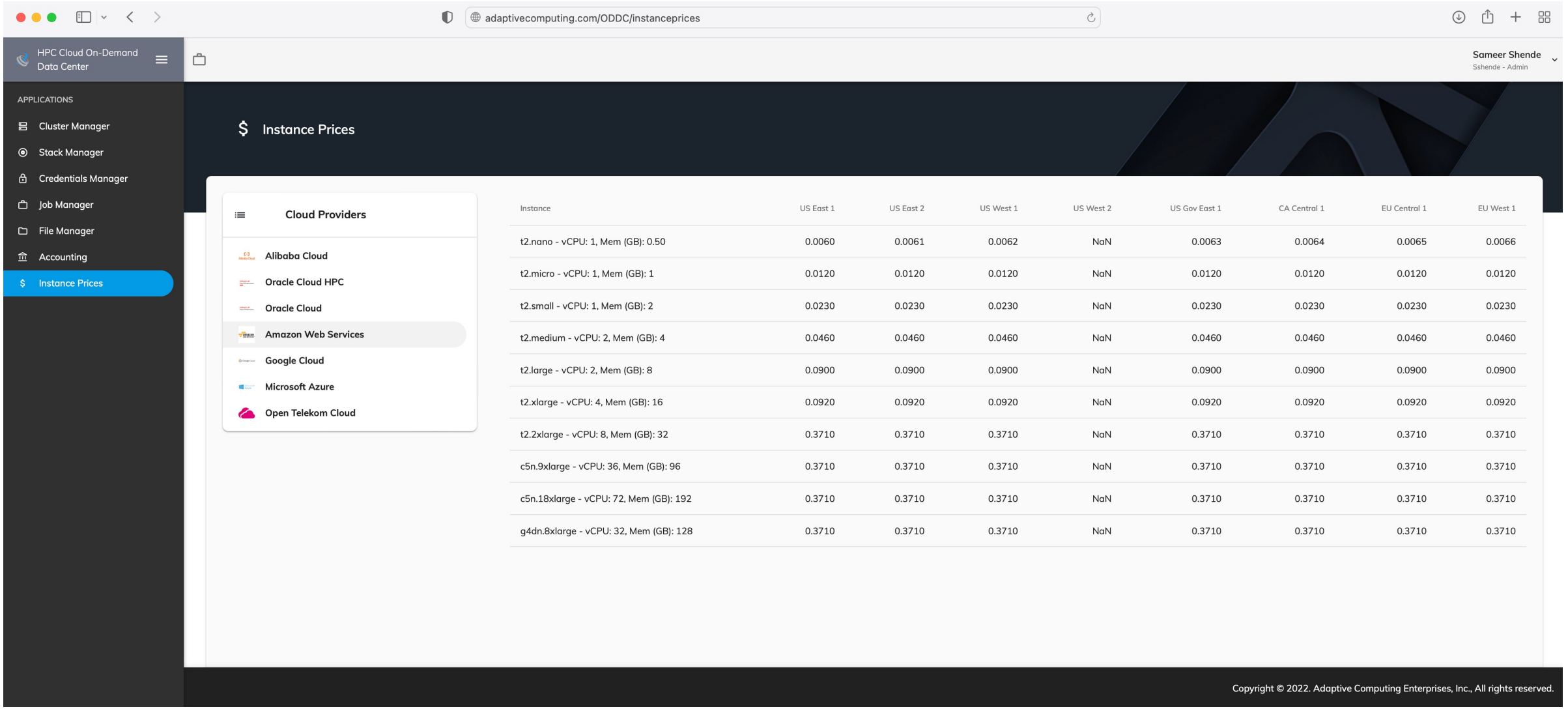
Key considerations for cloud-based deployment for E4S

- 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)
- 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's ODDC interface to launch E4S jobs on multiple cloud providers!

Adaptive Computing's ODDC interface for E4S

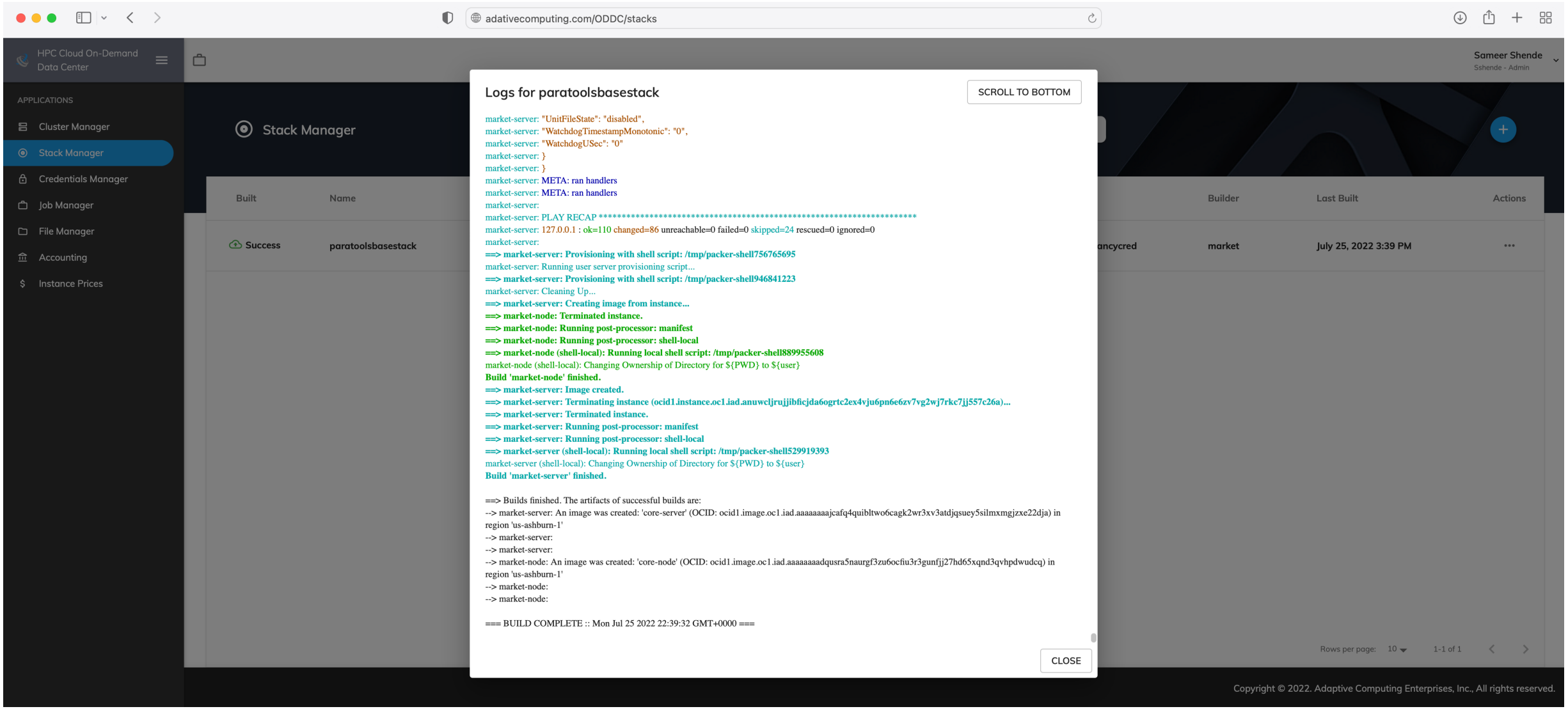


Accessing Multiple Commercial Cloud Providers through ODDC

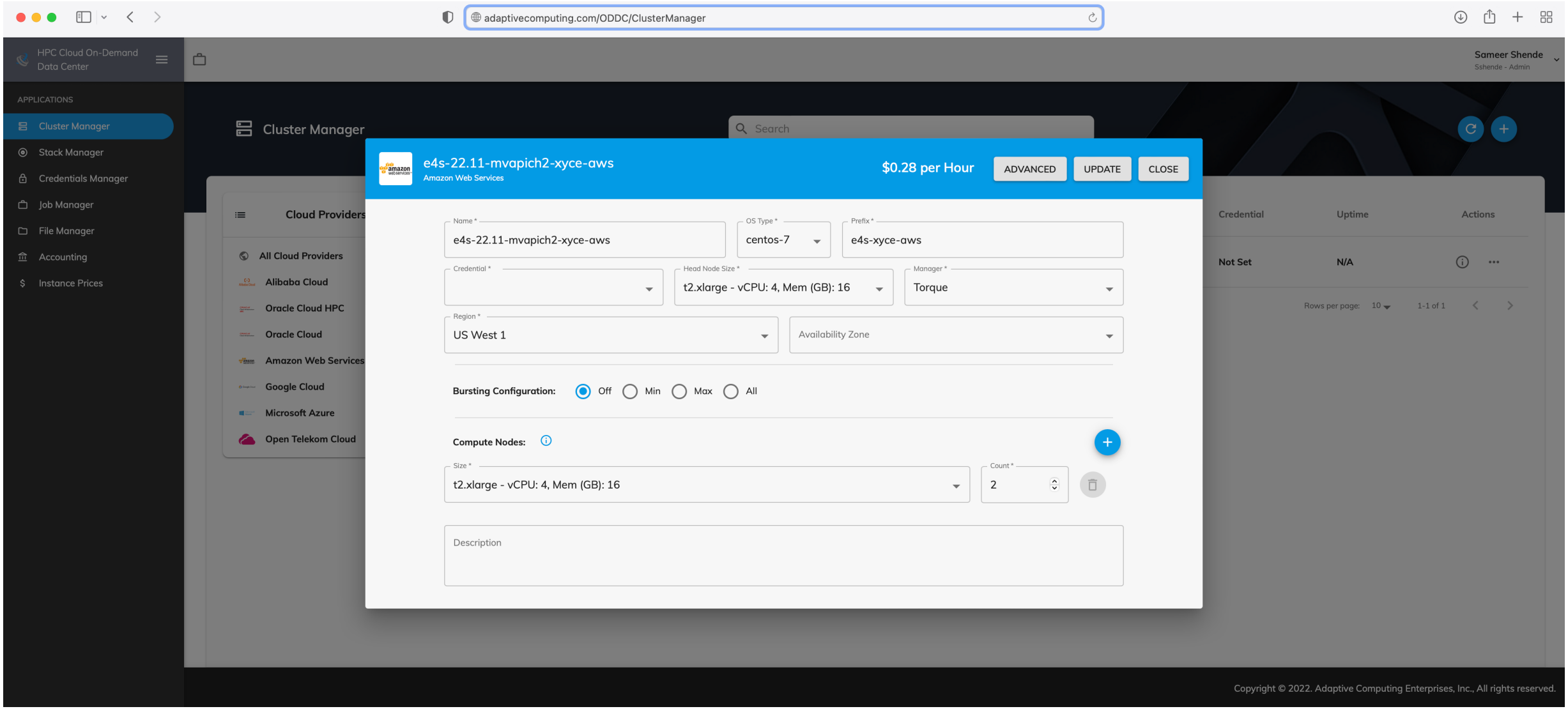


Instance	US East 1	US East 2	US West 1	US West 2	US Gov East 1	CA Central 1	EU Central 1	EU West 1
t2.nano - vCPU: 1, Mem (GB): 0.50	0.0060	0.0061	0.0062	NaN	0.0063	0.0064	0.0065	0.0066
t2.micro - vCPU: 1, Mem (GB): 1	0.0120	0.0120	0.0120	NaN	0.0120	0.0120	0.0120	0.0120
t2.small - vCPU: 1, Mem (GB): 2	0.0230	0.0230	0.0230	NaN	0.0230	0.0230	0.0230	0.0230
t2.medium - vCPU: 2, Mem (GB): 4	0.0460	0.0460	0.0460	NaN	0.0460	0.0460	0.0460	0.0460
t2.large - vCPU: 2, Mem (GB): 8	0.0900	0.0900	0.0900	NaN	0.0900	0.0900	0.0900	0.0900
t2.xlarge - vCPU: 4, Mem (GB): 16	0.0920	0.0920	0.0920	NaN	0.0920	0.0920	0.0920	0.0920
t2.2xlarge - vCPU: 8, Mem (GB): 32	0.3710	0.3710	0.3710	NaN	0.3710	0.3710	0.3710	0.3710
c5n.9xlarge - vCPU: 36, Mem (GB): 96	0.3710	0.3710	0.3710	NaN	0.3710	0.3710	0.3710	0.3710
c5n.18xlarge - vCPU: 72, Mem (GB): 192	0.3710	0.3710	0.3710	NaN	0.3710	0.3710	0.3710	0.3710
g4dn.8xlarge - vCPU: 32, Mem (GB): 128	0.3710	0.3710	0.3710	NaN	0.3710	0.3710	0.3710	0.3710

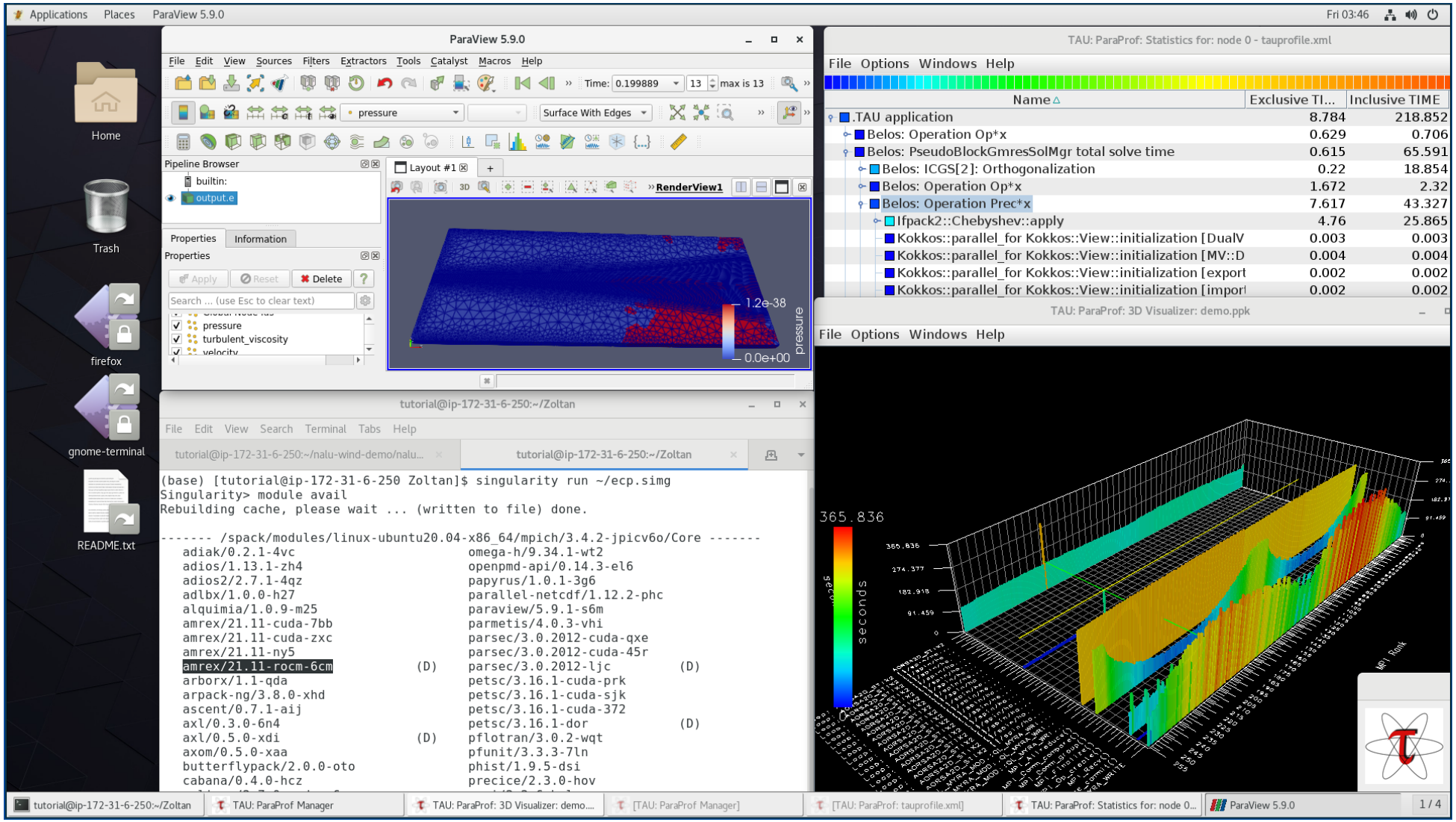
Building an image to deploy on cloud platforms



Choosing an instance on AWS to run the image



E4S 23.05 AWS image: US-West2 (OR)

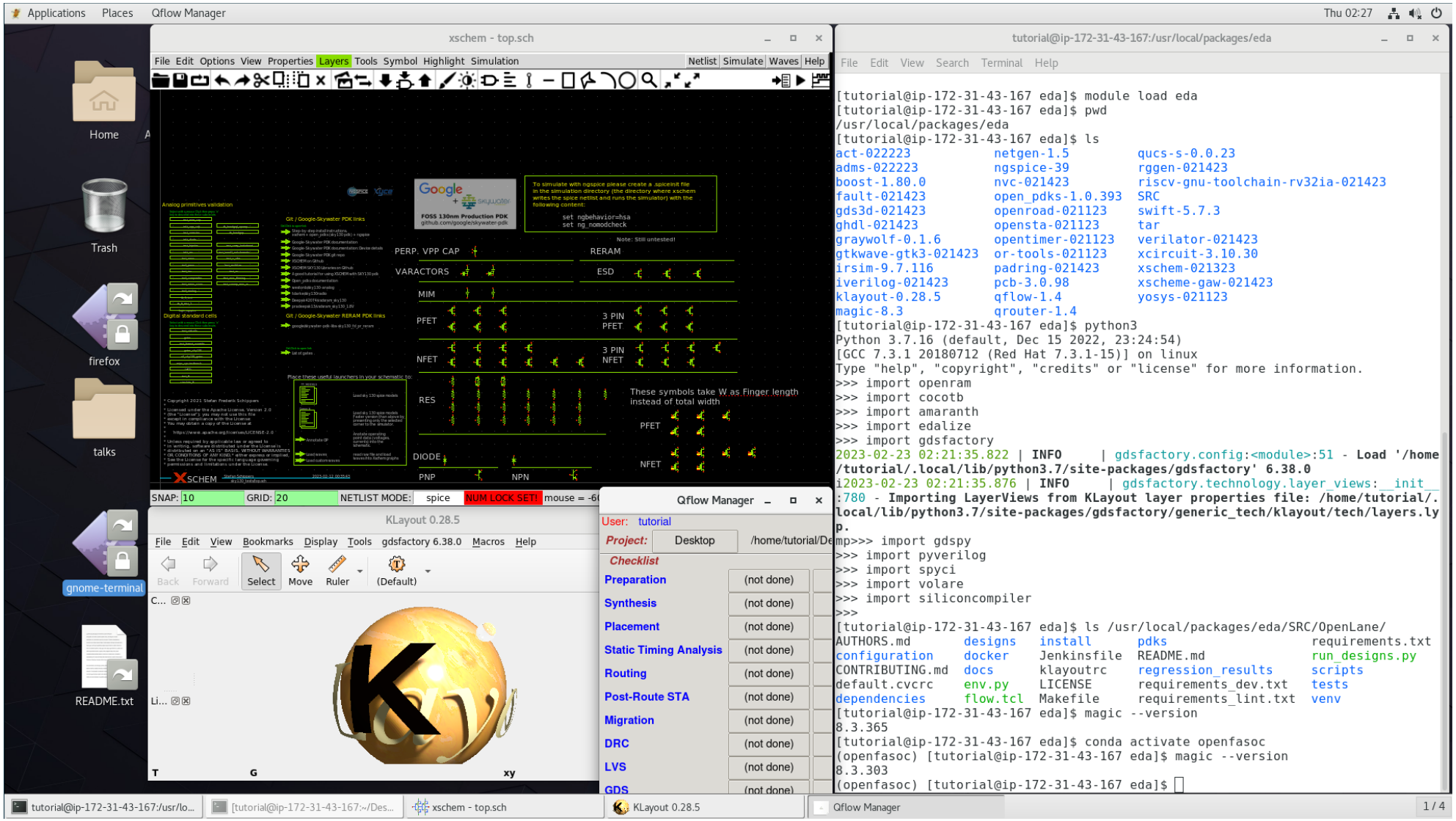


E4S 23.02 AWS

- 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…

E4S for Commercial Cloud Platforms for EDA on AWS

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



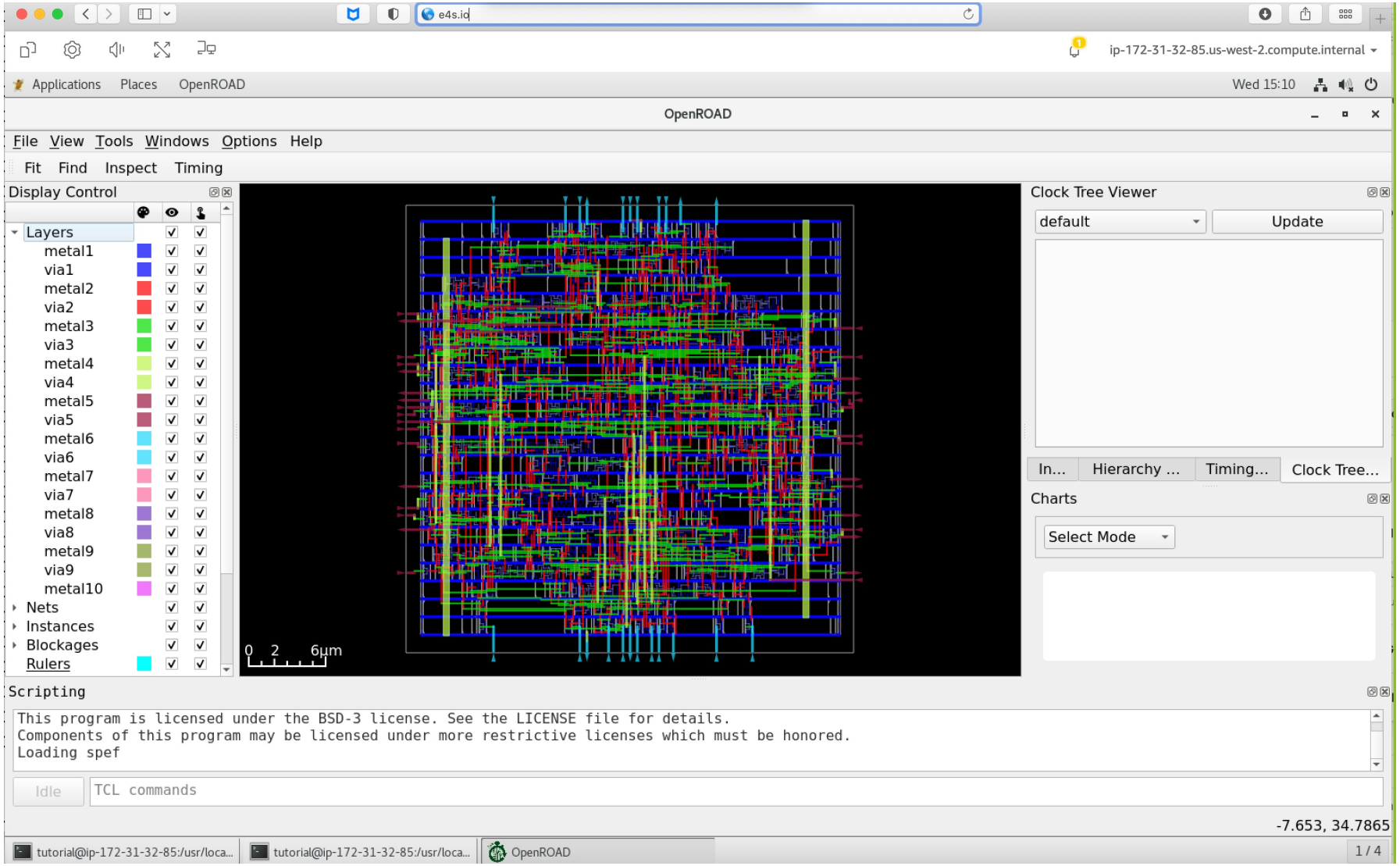
https://e4s.io/eda

E4S EDA on AWS

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

E4S for Commercial Cloud Platforms for EDA on AWS

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



E4S EDA on AWS

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  - Skywater

E4S for Commercial Cloud Platforms for EDA on AWS

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

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

#	Packages currently in E4S	URL
13	Yosys	https://github.com/YosysHQ/yosys
14	Xcircuit	http://opencircuitdesign.com/xcircuit/
15	Graywolf	https://github.com/rubund/graywolf
16	OpenSTA	https://github.com/The-OpenROAD-Project/OpenSTA
17	OpenTimer	https://github.com/OpenTimer/OpenTimer
18	Qrouter	http://opencircuitdesign.com/qrouter/
19	Xscheme	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

https://e4s.io/eda

E4S for Commercial Cloud Platforms for EDA on AWS

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

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

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

https://e4s.io/eda

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

- E4S containers support replacement of MPI libraries using MPICH ABI compatibility layer and Wi4MPI [CEA] for OpenMPI replacement.
- Applications binaries built using E4S can be launched with Singularity using MPI library substitution for efficient inter-node communications.
- e4s-cl is a new tool that simplifies the launch and MPI replacement.
  - e4s-cl init --backend [singularity|shifter|docker] --image <file> --source <startup_cmds.sh>
  - e4s-cl mpirun -np <N> <command>
- Usage:

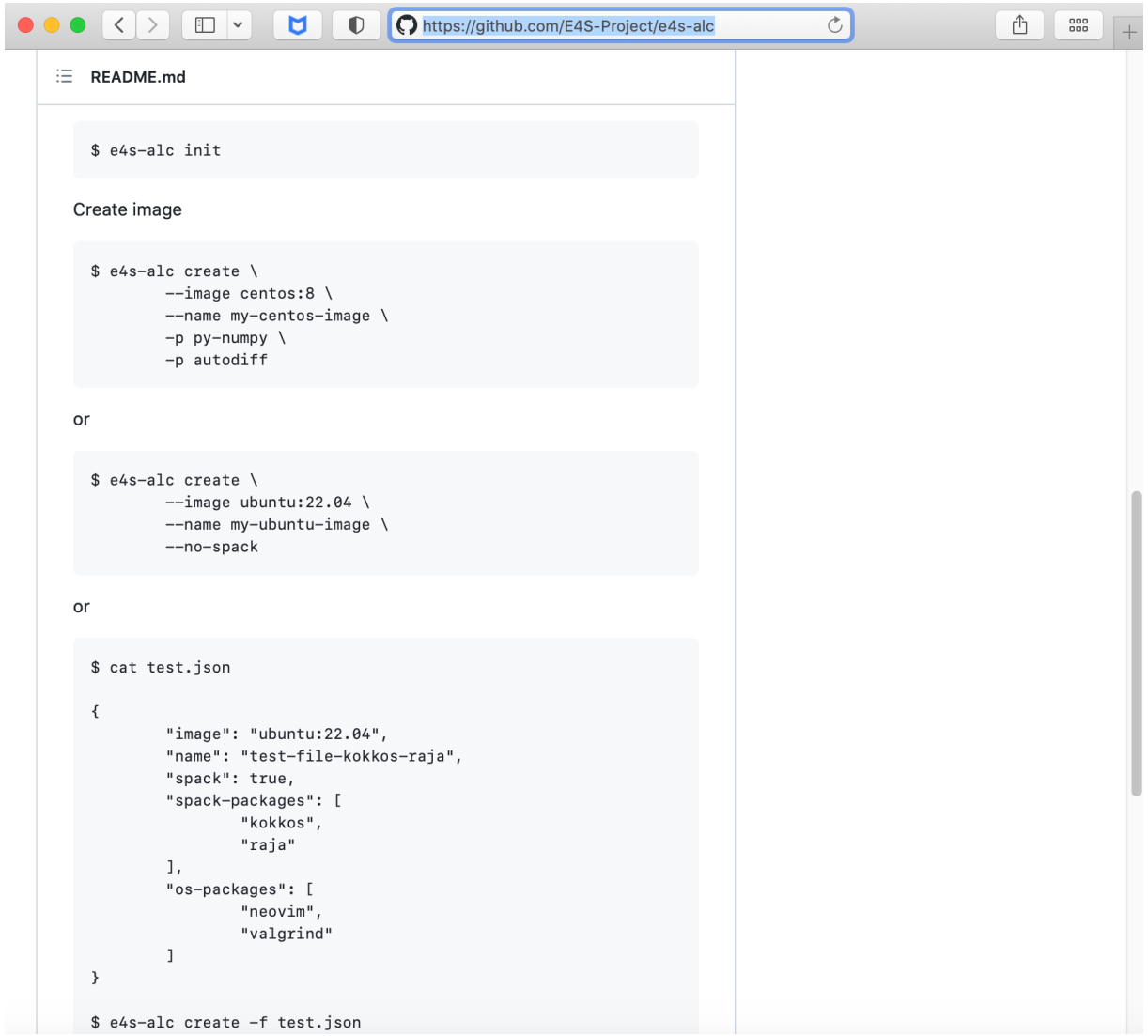
```
e4s-cl init --backend singularity --image ~/images/e4s-gpu-x86.sif --source ~/source.sh

cat ~/source.sh
   . /spack/share/spack/setup-env.sh
   spack load trilinos+cuda cuda_arch=80

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

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

e4s-alc: E4S à la carte – a tool to customize container images



Add packages to a container image:

- Spack packages
- OS packages (yum/apt/zypper)
- Add a tarball to a location
- Create a new container image
- Works with Docker/podman & Singularity/Apptainer!

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

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.
- https://spack.io

Spack is a flexible package manager for HPC

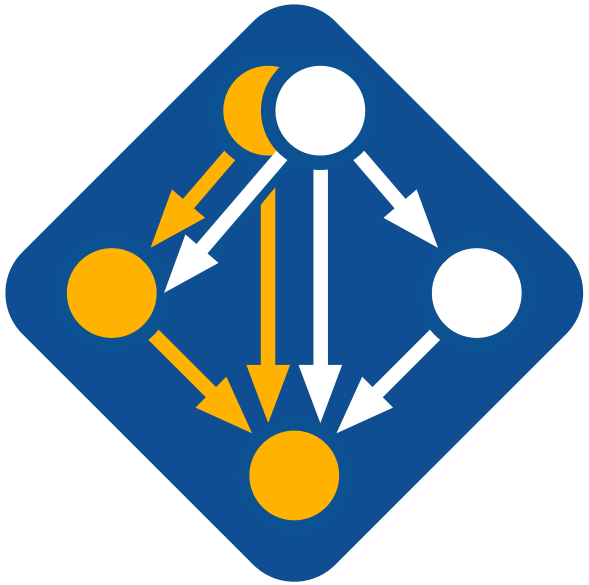
- How to install Spack (works out of the box):

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

- How to install a package:

```
$ spack install tau
```

- TAU and its dependencies are installed within the Spack directory.
- Unlike typical package managers, Spack can also install many variants of the same build.
  - Different compilers
  - Different MPI implementations
  - Different build options



Visit spack.io

github.com/spack/spack

@spackpm

Spack provides the *spec* syntax to describe custom configurations

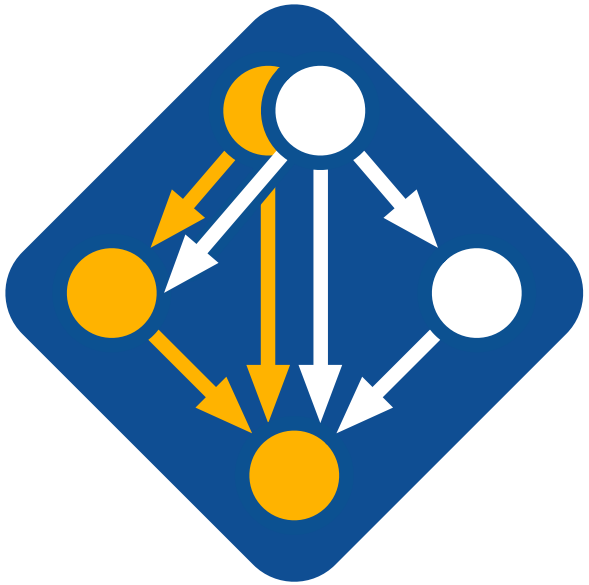
```
$ git clone https://github.com/spack/spack
$ . spack/share/spack/setup-env.sh
$ spack compiler find                                    # set up compilers
$ spack external find                                    # set up external packages
```

```
$ spack install tau                                      unconstrained
$ spack install tau@2.32                                 @ custom version
$ spack install tau@2.32 %gcc@9.3.0                      % custom compiler
$ spack install tau@2.32 %gcc@9.3.0 +rocm                +/- build option
$ spack install tau@2.32 %gcc@9.3.0 +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

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



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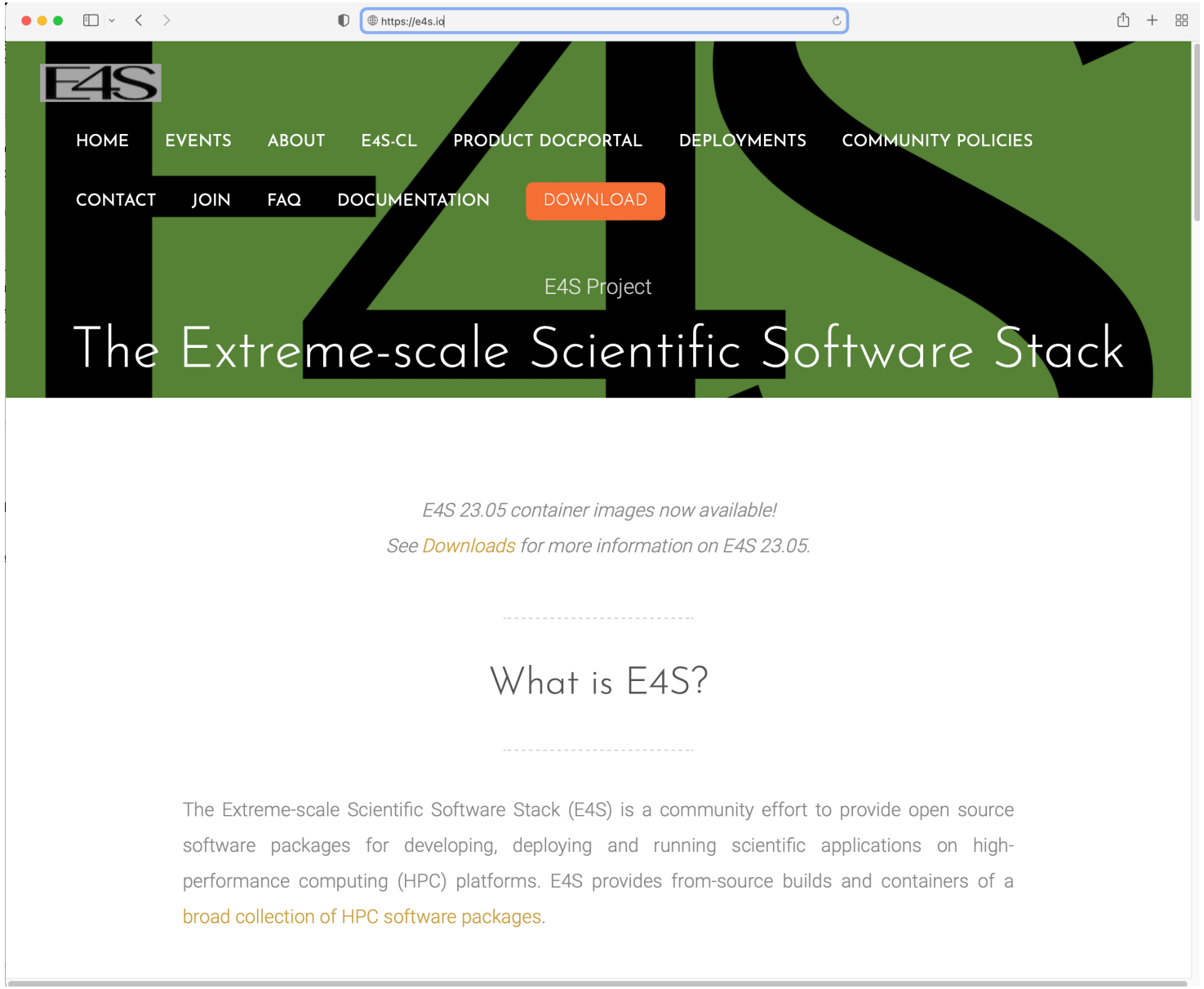
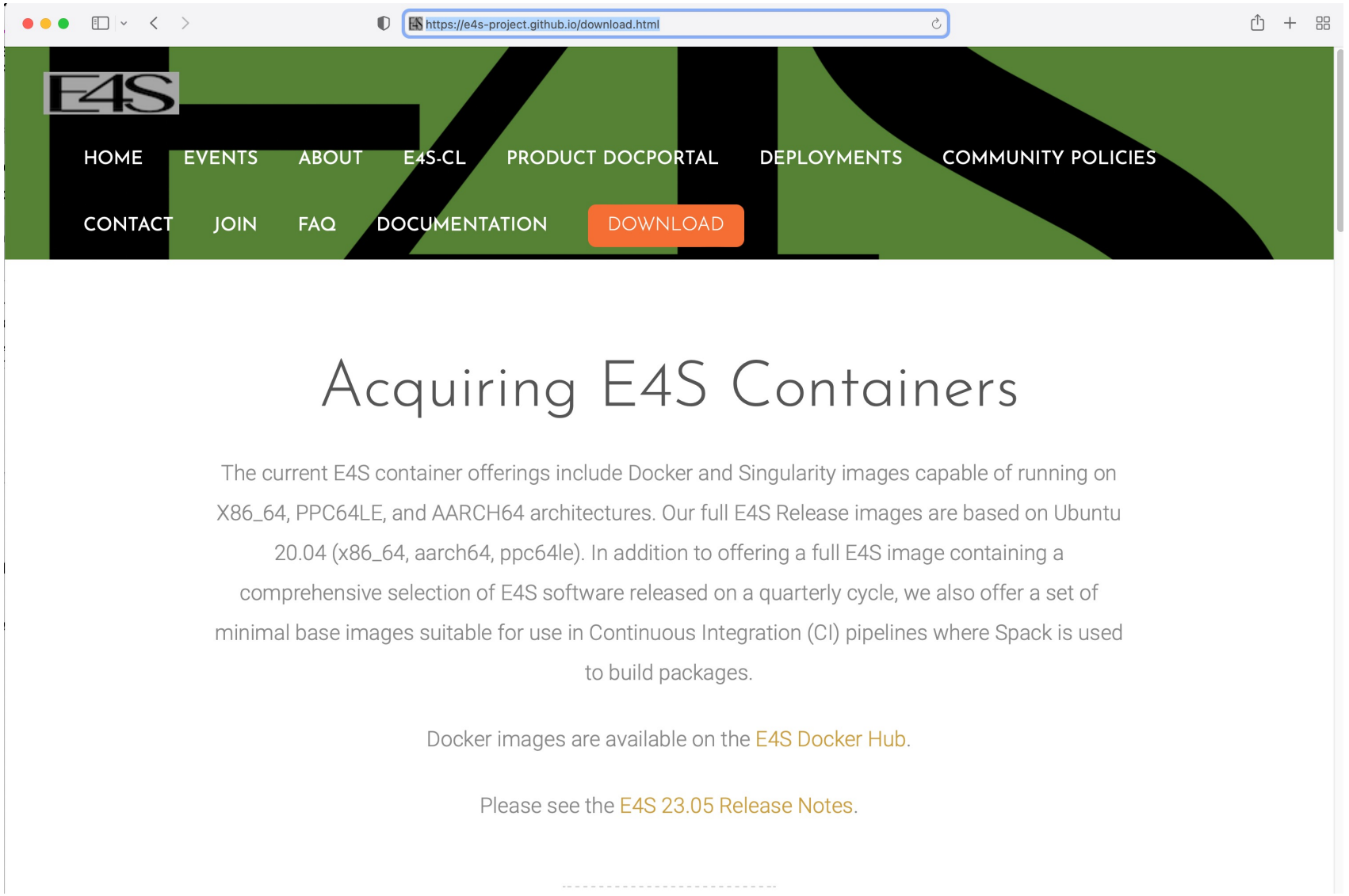
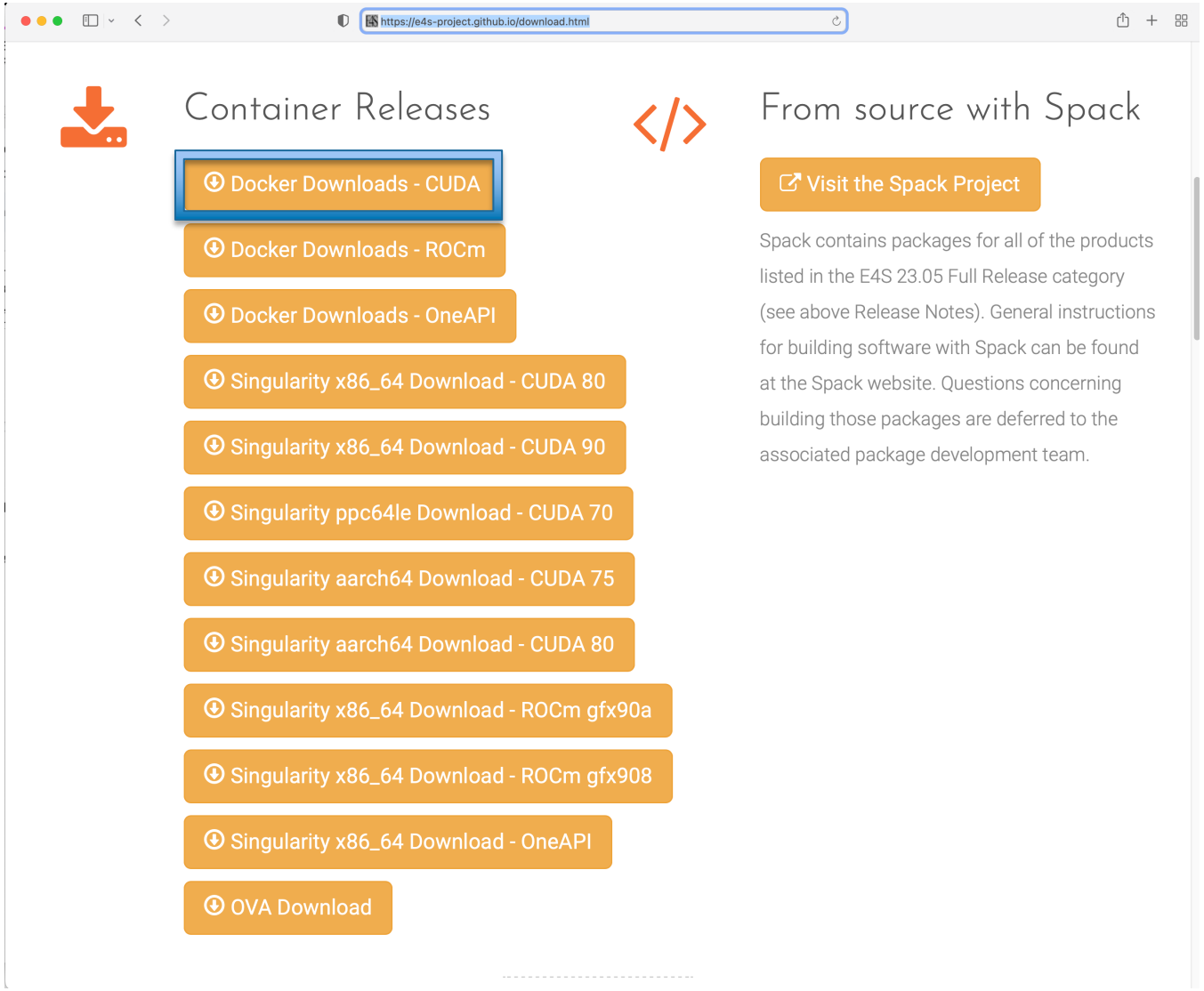
E4S Download from https://e4s.io



E4S Container Download from https://e4s.io



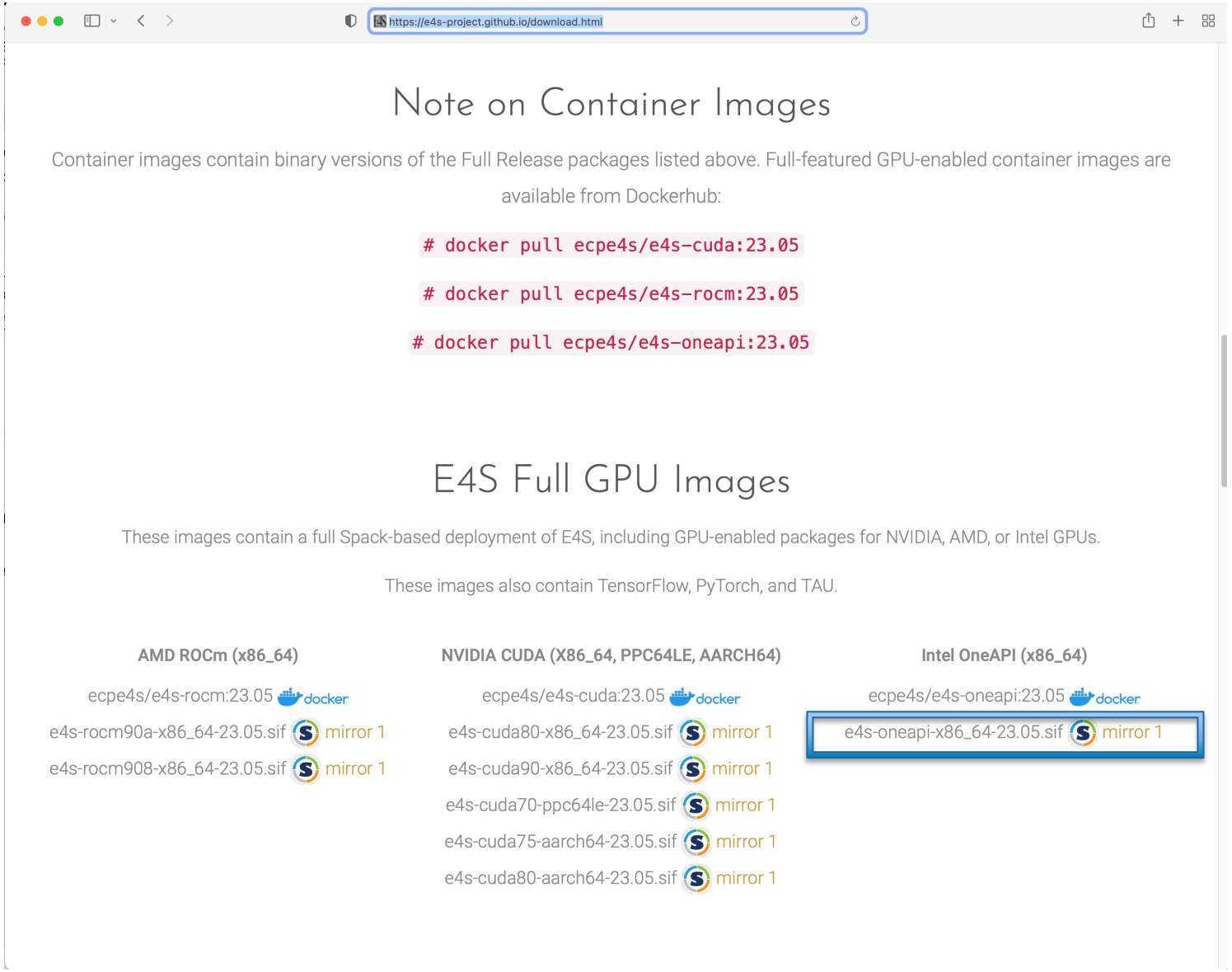
Download E4S 23.05 GPU Container Images: NVIDIA, AMD, Intel



- 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
- 100+ products on 3 architectures

https://e4s.io

Download E4S 23.05 GPU Container Images: AMD, Intel, and NVIDIA

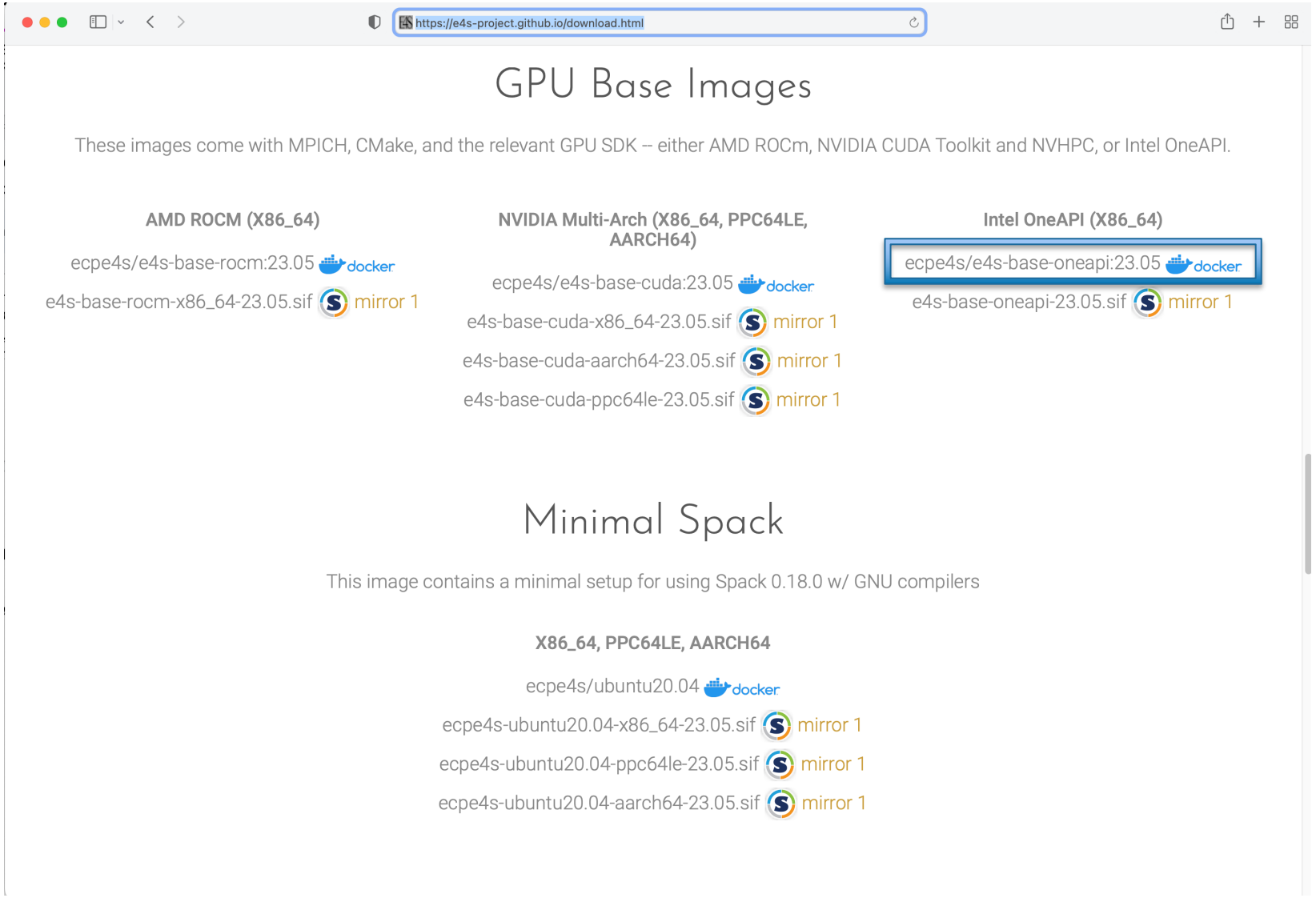


https://e4s.io

Intel Compilers and MPI Libraries Now Accessible in E4S Containers: A Breakthrough Collaboration Driving Productivity and Sustainability

- Background:
  - E4S provides a unified software stack of libraries and tools for portable performance on HPC systems, especially GPU-based systems.
  - E4S promises seamless portability for onsite and cloud-based workflows through its container-based approach.
  - Intel compilers and libraries available in E4S accelerates preparations for Aurora and future Intel-based GPU systems.
  - E4S eliminates the need for separate management of access to Intel compilers and libraries, benefiting users
  - Many important workflows, especially regression testing and turnkey usage for Intel platforms become feasible and easier
- The E4S-Intel agreement makes Intel compilers and MPI libraries available via E4S containers:
  - Enables full testing and execution of HPC libraries and tools on Intel platforms via E4S, including Aurora early access systems
  - Represents a win-win for DOE, Intel, and the broader E4S user community that is developing at other US agencies and industry
- The Intel agreement brings Intel in line with E4S builds that include AMD and NVIDIA tools.
- The E4S-Intel agreement is possible through the partnership of ECP and the E4S commercial provider, ParaTools, Inc.

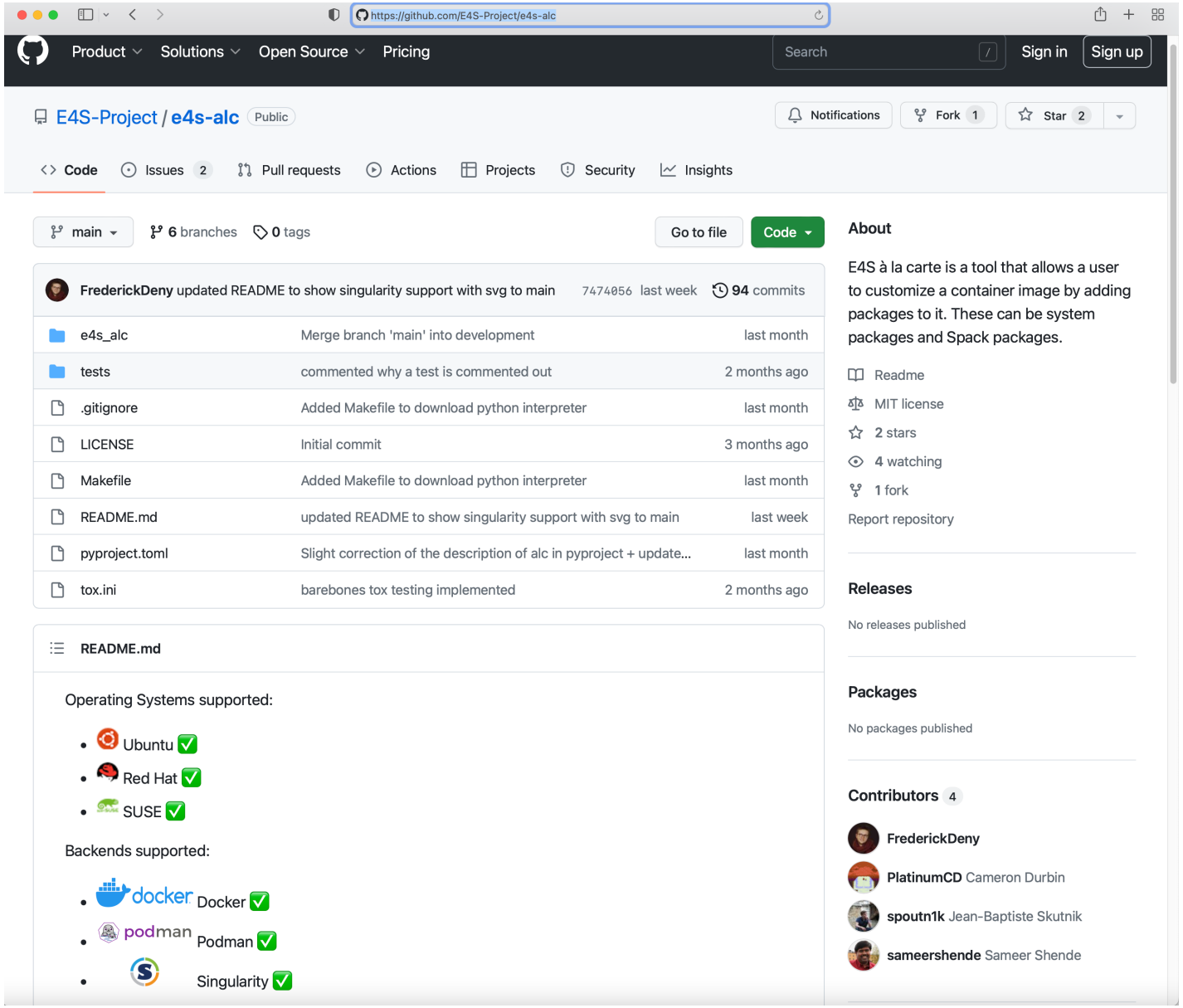
E4S base container images allow users to customize their containers



- Intel oneAPI
- AMD ROCm
- NVIDIA NVHPC and CUDA

https://e4s.io

e4s-alc: a new tool to customize container images

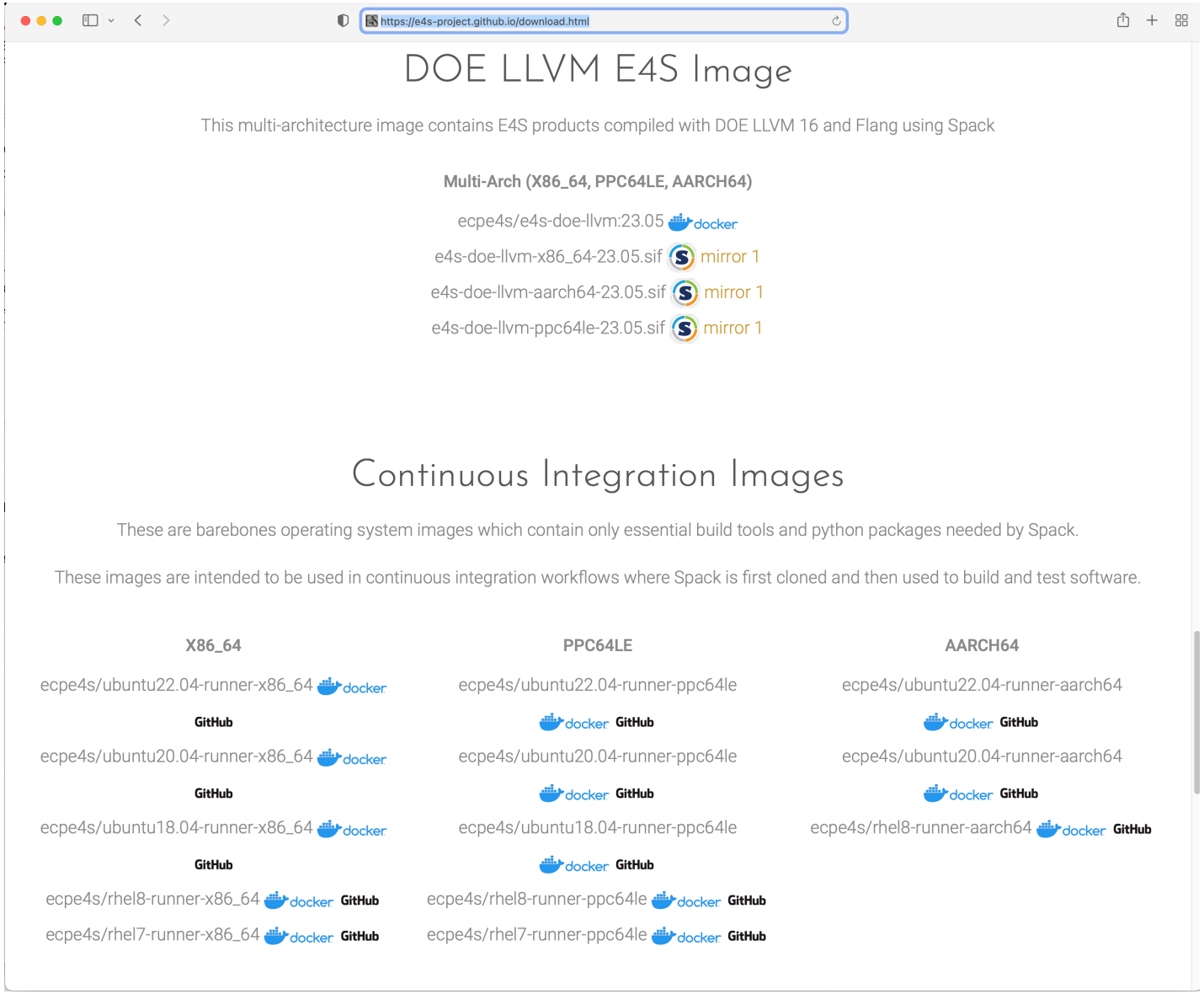


Add to a base image:

- Spack packages
- OS packages
- Tarballs

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

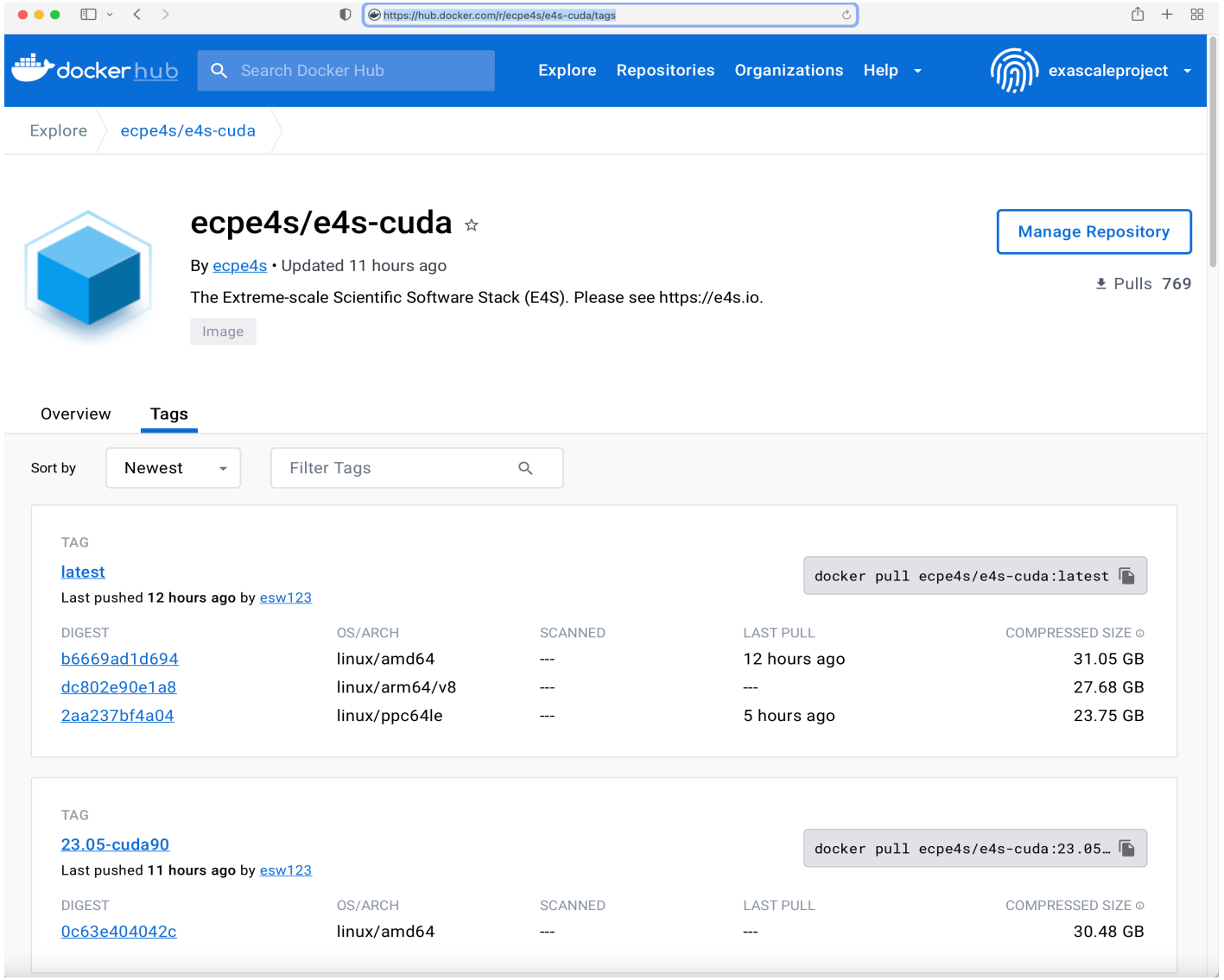
E4S 23.05 DOE LLVM and CI images



https://e4s.io

E4S 23.05 Detailed Documentation for Bare-metal Installation

E4S 23.05 full featured container release on Dockerhub

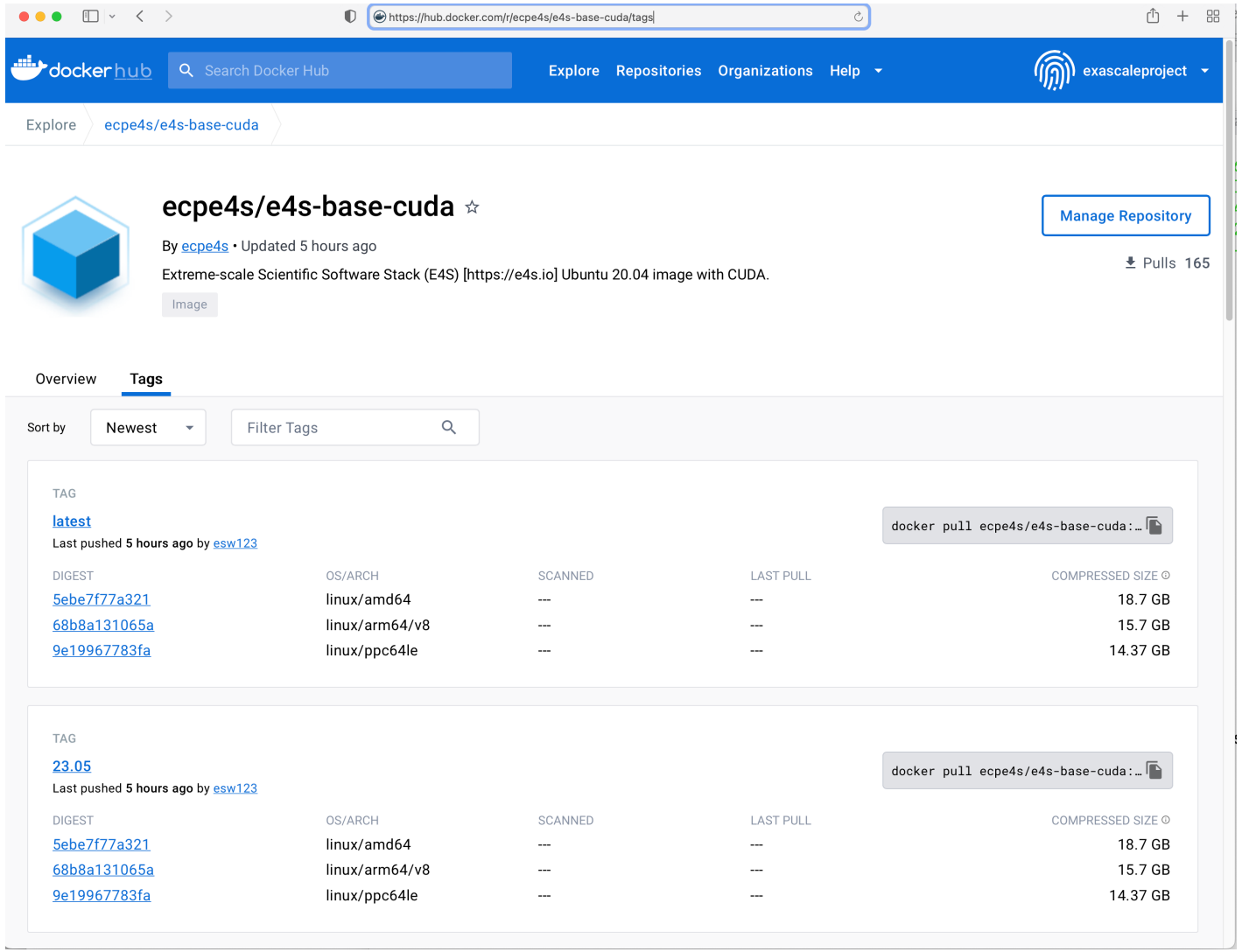


docker pull ecpe4s/e4s-cuda:23.05

Architectures:
- x86_64
- aarch64
- ppc64le

Software:
- CUDA 12.0
- NVHPC 23.3
- oneAPI 2023.1

E4S 23.05 base container release on DockerHub

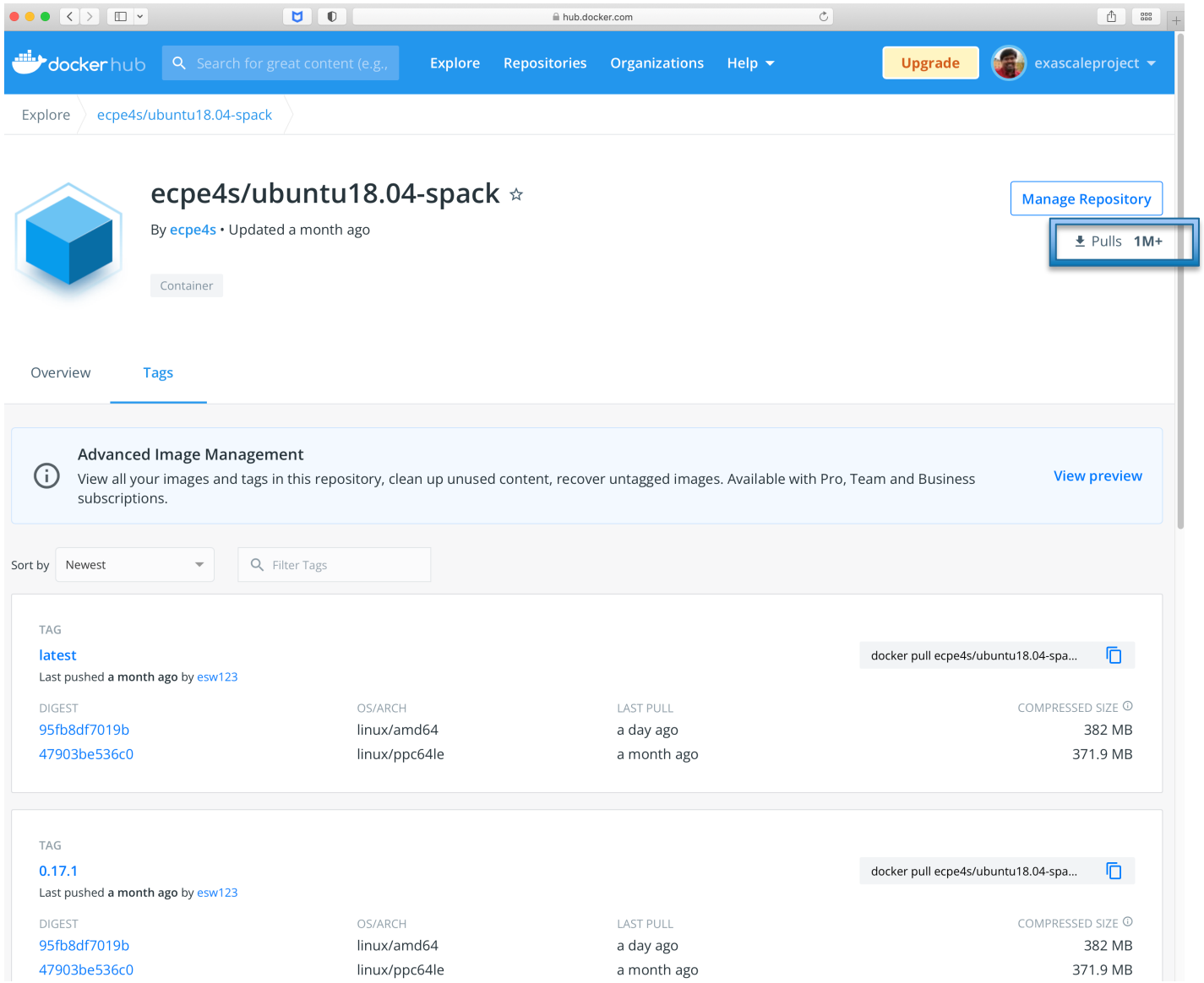


Architectures:
- x86_64
- aarch64
- ppc64le

Software:
- CUDA 12.0
- NVHPC 23.3
- oneAPI 2023.1

docker pull ecpe4s/e4s-base-cuda

Minimal Spack base image on Dockerhub



- Create custom container images
- 1M+ downloads!

23.05 Release: 100+ Official Products + dependencies (gcc, x86_64)

```
 1:  adios2              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/adios2-2.9.0-wr34ihoz2sk6iarctnuyxfhsctxwkvq4
 2:  alquimia            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/alquimia-1.0.10-gba5ayv4ps6ilmh5hc7krkoa4h3ksbvz
 3:  aml                 /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/aml-0.2.0-goqtywxxw2lwciznqkc44paexlucn33v
 4:  amrex               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/amrex-23.05-2syxxbx3xwppc4ut7mbrmlev4ycty4ep
 5:  arborx              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/arborx-1.3-cvlmzk4kzetidsscc4nd4oprdyvcsp3l
 6:  archer              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/archer-2.0.0-vl5rv2ygrh4znug7rdk6jhh6t4nemk5l
 7:  argobots            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/argobots-1.1-f6b6was4pd7d2u2fwvpxdoqffdbate2o
 8:  axom                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/axom-0.7.0-epaxouqc4ul2kppggnhtvnjl6fr3goik
 9:  bolt                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/bolt-2.0-zb4pgmqyozhf3ofvhdo26gpj2hibbc2t
10:  bricks              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/bricks-r0.1-ymuymne4nwfwytzckstwl6macyp6kkk2
11:  butterflypack       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/butterflypack-2.2.2-kzdbd4fzvqfjn575hojafxlen2gzwx2n
12:  cabana              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/cabana-0.5.0-hit7qxj2pwnvgmd5kkaeglbnvqsdgf7n
13:  caliper             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/caliper-2.9.0-cthblsk6ogn43qnufgbxczjvcrawqzab
14:  chai                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/chai-2022.03.0-6gi2vpoxdvy25sat6cdubunutp24i5sk
15:  charliecloud        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/charliecloud-0.32-bmfm6chwp4g6mgnhjgcrh356gusbrzes
16:  conduit             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/conduit-0.8.7-mfdfackt6xuqmyfqdwtiwszivxtrwho2
17:  darshan-runtime     /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/darshan-runtime-3.4.2-nfblomjg6ejmigmmhu3dux6v7iojxnpf
18:  datatransferkit     /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/datatransferkit-3.1-rc3-enk32naiegjk42bex5mvuk3y3mefdef6
19:  dyninst             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/dyninst-12.3.0-k3myl3szf7v3e2jcqoqwwglwyig4444o
20:  ecp-data-vis-sdk    /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/ecp-data-vis-sdk-1.0-s4ya3uqeb2ecyextvb42yprv5zy5l2qk
21:  exaworks            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/exaworks-0.1.0-lxqwv3cswo6pglbycqcacwatuhf6iln2
22:  faodel              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/faodel-1.2108.1-gxc7m6ajdyb2jupcvx5qrvppe4jlcqt6
23:  flecsi              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/flecsi-2.1.0-mfszzzew3vlkejgw43xuakoftuxrqnhm
24:  flit                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/flit-2.1.0-3ptdgvs22o5ng3euhs6eci5nhaq4jctb
25:  flux-sched          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/flux-sched-0.27.0-snqo4rzjtvrmjkdvlkcixuw4vyt4ypie
26:  fortrilinos         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/fortrilinos-2.2.0-dlxz63fh2tljmw2rje5srgfgdbx64adv
27:  gasnet              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/gasnet-2023.3.0-aufps4j5ilwaosagcfyhwe4anrv6uknz
28:  ginkgo              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/ginkgo-1.5.0-4gsh6pioh6qab3d67j7wtfk5qbfz7lnb
29:  globalarrays        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/globalarrays-5.8.2-nzag4ztsjddm67gdurpwtirprgb3rkgz
30:  gotcha              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/gotcha-1.0.4-3rwc6g46qxsit3vswvzi6icv67li57wi
31:  gptune              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/gptune-4.0.0-dyxc7tkwnenjgl2edjqhvyg7eld643xx
32:  h5bench             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/h5bench-1.3-34odudjnlnjbfxl7a44e32gwmuoe6wn6
33:  hdf5                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/hdf5-1.14.1-2-2naucnnhfn57lxmb3dcfls42m4hwdkeg
34:  hdf5-vol-async      /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/hdf5-vol-async-1.5-nwt25ouh2i5vtwvwsaijpnklgowag7ku
35:  heffte              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/heffte-2.3.0-rib3o742d45ng7ukq4qq4vh3lst5dccc
36:  hpctoolkit          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/hpctoolkit-2023.03.01-sbctldelht4ntvzahpd6q5rj23fs25ar
37:  hpx                 /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/hpx-1.9.0-374gqtjzm47p6ea3xsuahpagrq2ogwvy
```

GPU runtimes

- AMD (ROCm)
  - 5.4.3
- NVIDIA (CUDA)
  - 12.0
- NVHPC
  - 23.3
- Intel oneAPI
  - 2023.1

23.05 Release: 100+ Official Products + dependencies (gcc, x86_64)

```
38:  hypre                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/hypre-2.28.0-mozopbseodwvy7r7xklin7jnsuh5s7yi
39:  kokkos               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/kokkos-4.0.01-tgv5irdj4skczex6c2rvfty274vwuyk7
40:  kokkos-kernels       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/kokkos-kernels-3.7.00-2whrnbzjyni42dytgehkubhke2zgaj5u
41:  lammps               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/lammps-20220623.3-cso7xzxuaz5jyld3n6seug2cexxbfnpc
42:  lbann                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/lbann-0.102-hf442maq5bbf5nndr4fqlyhxakdndm23
43:  legion               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/legion-23.03.0-ksb4tvggo6sfcfjiicnszyr5appehqxn
44:  libnrm               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/libnrm-0.1.0-h5ggd2cgai43porp2s2berqrsnki2j6c
45:  libpressio           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/libpressio-0.95.1-h54uerfc7gttwaokywa5cwntylrnklen
46:  libquo               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/libquo-1.3.1-e6ulmqqbtpfcjjypvdqrbpkb4brzkgpf
47:  loki                 /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/loki-0.1.7-a4etdi45t2fbweddhjur5t5p56tiu2ca
48:  magma                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/magma-2.7.1-dapbrjq25hsqg2cztteuusqkismcpnbu
49:  mercury              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/mercury-2.2.0-iap2sil3mo6g6aljjvg34vtnxh2sglof
50:  metall               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/metall-0.25-2xic6pnhpbolhaknalu2qpjnw4bkvemi
51:  mfem                 /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/mfem-4.5.2-2f3kkx62ogbv6bw6sdcybkawubvcyg2n
52:  mgard                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/mgard-2023-03-31-4maqkp6n3e2xshtu2y3tnve5ch7jdb43
53:  mpark-variant        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/mpark-variant-1.4.0-6f25xadnfdzmpweuit4yvpl34katnt4s
54:  mpich                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/mpich-4.1.1-4cbi7qhusseuuh6bcs6lokwgwh6s3itl
55:  mpifileutils         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/mpifileutils-0.11.1-tuy2ycdld67kuv3ppp3diqy4o2bmvhok
56:  nccmp                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/nccmp-1.9.0.1-qmoiwfcpcnknojwspffuvgrw3n3mphzb
57:  nco                  /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/nco-5.1.5-wwe7fm6df3zhc6d6qckvbcyxo5dqawpf
58:  netlib-scalapack     /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/netlib-scalapack-2.2.0-3zhwrxw6f2ohmbnpeec34ksb4h7svs65
59:  nrm                  /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/nrm-0.1.0-47ydygda2r3njdpkxyj4wrfpgfdt2zzl
60:  omega-h              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/omega-h-9.34.13-m2wmv5mmoxpoy622e6tbk7jzey2ufdvi
61:  openfoam             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/openfoam-2206-zftm6f5mhvnhxben2nzeqantgg4lll5d
62:  openmpi              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/openmpi-4.1.5-ed5u3cdcbks6dcve6ftb336v5uhwj4by
63:  openpmd-api          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/openpmd-api-0.15.1-uzamcamznyauzeem57j72gx2ascjpmju
64:  papi                 /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/papi-6.0.0.1-j7dmzprtcei2ifgjykb7rmkbf3gydfk7
65:  papyrus              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/papyrus-1.0.2-kuro7vtc7kh6fot5xmah6awfwgi5chm2
66:  parallel-netcdf      /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/parallel-netcdf-1.12.3-mldyjplnyhw7qiljd327wda7exvpcvtf
67:  paraview             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/paraview-5.11.1-x4aqroj67nfq7gpk7w3pwlxhpfhjyrno
68:  parsec               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/parsec-3.0.2209-wvchc4psqj3uotxff24xyc24xqwprzdg
69:  pdt                  /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/pdt-3.25.1-lx67nrs24pkbnmnj7am3t75swtowtfc5
70:  petsc                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/petsc-3.19.1-bonrfxf3arijwtulzcck4xqyd3ceik63
71:  phist                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/phist-1.11.2-qz36u6cuvuupj3gj5v7hmm4sdbrzdljv
72:  plasma               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/plasma-22.9.29-2qwdll5vjs74mymdiugdhd32iiibm2v3
73:  plumed               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/plumed-2.8.2-oq5243vtzgcl6ex6zookbxqgaeofkzxh
74:  precice              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/precice-2.5.0-b7eniikqkee5veujb5xnuukfnz7wiwm2
75:  pumi                 /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/pumi-2.2.7-57q5bidz4mzlldkfpwaovebwqhvxgps3
76:  py-cinemasci         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-cinemasci-1.3-5tnt5kqnzrin5j5dmse6gdq77mteiiyz
77:  py-jupyterhub        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-jupyterhub-1.4.1-awj3cwfv2d3irsm24dmr37gbhd5xniju
```

23.02 Release: 100 Official Products + dependencies (gcc, x86_64)

78:	py-libensemble	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-libensemble-0.9.3-3d3tb25q2s3pa7uqscw7wlpz5rqmapa5
79:	py-parsl	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-parsl-1.2.0-f7tbq4nmfecdu3nh5fw5zyddwj77zis5
80:	py-radical-saga	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-radical-saga-1.20.0-wffrzdrcdd4cpst42gtqonbjni7m5pqe
81:	qthreads	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/qthreads-1.16-r4ai62sxg3os22n2xfntik7xbcvijgst
82:	quantum-espresso	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/quantum-espresso-7.1-2hw2nzkjwtc4xi3hopd2oesn2ikmcb5e
83:	raja	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/raja-2022.10.4-fffdno3g4c4wm6f2d5rbrehnjgv3ytw4
84:	rempi	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/rempi-1.1.0-bsppojvqc4e4bf7re6u36f75dwo6wnuv
85:	scr	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/scr-3.0.1-4twvdurdxeiv3ipees4y3nk64pmvtrbl
86:	slate	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/slate-2022.07.00-5xkozs6eabgn45t7uttghekbu4lanbwk
87:	slepc	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/slepc-3.19.0-vqy6iy24c5wkpfdsejjgql2bx32vjfbq
88:	stc	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/stc-0.9.0-ocmzafclc6rsl2dop3poqjbnlyyk7vs2
89:	strumpack	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/strumpack-7.1.1-7feghsapq3qe7stmbfodzcytm7tm44lt
90:	sundials	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/sundials-6.5.1-f23kbyw7bsam3cpka2mshks36d236yr3
91:	superlu-dist	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/superlu-dist-8.1.2-ibmrgavx57kcy3fc7wdbcneuhk6axgxv
92:	swig	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/swig-4.1.1-cm45hunq4nk7x4ml756gur5wlakaidha
93:	sz	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/sz-2.1.12.2-bbc3ru73fa67nmr7j4jbv53f6ji5e4xe
94:	tasmanian	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/tasmanian-7.9-4skuz4cxghjjhlhad776xbixk3jvienk
95:	tau	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/tau-2.32-qxwqmtdsjoaxnrjed5mvlolax5ip273z
96:	trilinos	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/trilinos-14.0.0-alm3rf45sel6ahz7ecfs5odq3eziqcah
97:	turbine	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/turbine-1.3.0-sla74mxwn5michnji2aqmrf3gbphfqco
98:	umap	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/umap-2.1.0-de4ftza63dmgjgvv5uhceeunn2dvkqig
99:	umpire	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/umpire-2022.03.1-spprgtmz5vvvsxxhwngyu7dxbghmdpij
100:	unifyfs	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/unifyfs-1.0.1-q4bmwojbzaa2npnbcp2q4flba5u5oshd
101:	upcxx	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/upcxx-2023.3.0-ideeur7hshemz4ahe2col65tiryjfngh
102:	variorum	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/variorum-0.6.0-h3oif6j2nvgq4qzxjx773bjnef5owexx
103:	veloc	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/veloc-1.6-5g5n244a6mo3i3dlcjxxlq7e3l5tv426
104:	visit	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/visit-3.3.3-nt4yv7ecffq2onv5xznqja42uzt6tqlb
105:	vtk-m	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/vtk-m-2.0.0-7rjk76kmxbf4bmyvepvfj5qsclkfz3uw
106:	wannier90	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/wannier90-3.1.0-dbfs2qlo2yvdxjtcb5mn5d2xlnvplnzc
107:	warpx	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/warpx-23.03-f2nbmfppld7xntj2lpwy552upvwj6bq2
108:	xyce	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/xyce-7.6.0-vt3rht5enpklqck7m7d2z7ji64memqwz
109:	zfp	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/zfp-1.0.0-ibmowr23apboprdgjrrp4eyblmibwd2w

Languages:
- Julia with support for MPI, and CUDA
- Python

AI products with GPU support
- Tensorflow
- Pytorch

EDA Tools:
- Xyce

3D Visualization
- Paraview
- VisIt
- TAU's paraprof …

E4S 23.05 adds support for NVIDIA A100 (sm80), V100 (sm70), and H100 (sm90) GPUs

E4S Support for AI/ML frameworks with V100, A100, and H100 GPUs

```
Singularity> python
Python 3.8.10 (default, Nov 14 2022, 12:59:47)
[GCC 9.4.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import numpy
>>> import scipy
>>> import matplotlib
>>> import tensorflow
>>> tensorflow.__version__
'2.12.0'
>>> import torch
>>> torch.__version__
'2.0.0'
>>> torch.cuda.get_device_name(torch.cuda.current_device())
'NVIDIA H100 PCIe'
>>>
```

E4S 23.05 supports NVIDIA H100 GPUs with TensorFlow 2.12.0 and PyTorch 2.0.0

E4S 23.05 container with ROCm: Top level specs

```
Singularity> spack find -x
-- linux-ubuntu20.04-x86_64 / gcc@11.1.0 ------------------------
```

adios@1.13.1	darshan-util@3.4.2	heffte@2.3.0	mpark-variant@1.4.0	py-h5py@3.7.0	sz@2.1.12.2
adios2@2.9.0	datatransferkit@3.1-rc3	heffte@2.3.0	mpich@4.1.1	py-jupyterhub@1.4.1	sz3@3.1.7
alquimia@1.0.10	dyninst@12.3.0	hpctoolkit@2023.03.01	mpifileutils@0.11.1	py-libensemble@0.9.3	tasmanian@7.9
aml@0.2.0	ecp-data-vis-sdk@1.0	hpctoolkit@2023.03.01	nccmp@1.9.0.1	py-petsc4py@3.19.1	tasmanian@7.9
amrex@23.05	ecp-data-vis-sdk@1.0	hpx@1.9.0	nco@5.1.5	py-warpx@23.03	tau@2.32
amrex@23.05	exaworks@0.1.0	hpx@1.9.0	netlib-scalapack@2.2.0	py-warpx@23.03	tau@2.32
arborx@1.3	faodel@1.2108.1	hypre@2.28.0	nrm@0.1.0	py-warpx@23.03	trilinos@13.0.1
arborx@1.3	flecsi@2.1.0	hypre@2.28.0	omega-h@9.34.13	qthreads@1.16	trilinos@14.0.0
archer@2.0.0	flit@2.1.0	kokkos@4.0.01	openfoam@2206	quantum-espresso@7.1	turbine@1.3.0
argobots@1.1	flux-core@0.49.0	kokkos@4.0.01	openmpi@4.1.5	raja@2022.10.4	umap@2.1.0
ascent@0.9.1	fortrilinos@2.2.0	kokkos-kernels@3.7.00	openpmd-api@0.15.1	raja@2022.10.4	umpire@2022.03.1
axom@0.7.0	gasnet@2023.3.0	lammps@20220623.3	papi@6.0.0.1	rempi@1.1.0	umpire@2022.03.1
bolt@2.0	gasnet@2023.3.0	lbann@0.102	papyrus@1.0.2	scr@3.0.1	unifyfs@1.0.1
boost@1.79.0	ginkgo@1.5.0	legion@23.03.0	parallel-netcdf@1.12.3	slate@2022.07.00	upcxx@2023.3.0
bricks@r0.1	ginkgo@1.5.0	libcatalyst@2.0.0-rc3	paraview@5.11.1	slate@2022.07.00	upcxx@2023.3.0
butterflypack@2.2.2	globalarrays@5.8.2	libnrm@0.1.0	paraview@5.11.1	slepc@3.19.0	variorum@0.6.0
cabana@0.5.0	gmp@6.2.1	libpressio@0.95.1	parsec@3.0.2209	slepc@3.19.0	veloc@1.6
cabana@0.5.0	gotcha@1.0.4	libquo@1.3.1	pdt@3.25.1	stc@0.9.0	visit@3.3.3
cabana@0.5.0	gptune@4.0.0	libunwind@1.6.2	petsc@3.19.1	strumpack@7.1.1	vtk-m@1.9.0
caliper@2.9.0	h5bench@1.3	loki@0.1.7	petsc@3.19.1	strumpack@7.1.1	vtk-m@2.0.0
caliper@2.9.0	hdf5@1.12.2	magma@2.7.1	phist@1.11.2	sundials@6.5.1	wannier90@3.1.0
chai@2022.03.0	hdf5@1.14.1-2	mercury@2.2.0	plasma@22.9.29	sundials@6.5.1	xyce@7.6.0
chai@2022.03.0	hdf5-vol-async@1.5	metall@0.25	plumed@2.8.2	superlu@5.3.0	zfp@0.5.5
charliecloud@0.32	hdf5-vol-cache@v1.1	mfem@4.5.2	precice@2.5.0	superlu-dist@8.1.2	
conduit@0.8.7	hdf5-vol-log@1.4.0	mfem@4.5.2	pumi@2.2.7	superlu-dist@8.1.2	
darshan-runtime@3.4.2	hdf5-vol-log@1.4.0	mgard@2023-03-31	py-cinemasci@1.3	swig@4.0.2-fortran	

```
==> 153 installed packages
Singularity>
```

EXASCALE COMPUTING PROJECT

E4S 23.05 : All Spack packages including dependencies!

```
Singularity> spack find
-- linux-ubuntu20.04-x86_64 / gcc@11.1.0 ------------------------
```

adiak@0.2.2
adios@1.13.1
adios2@2.9.0
adios2@2.9.0
adios2@2.9.0
adlbx@1.0.0
alquimia@1.0.10
aluminum@1.3.0
aml@0.2.0
amrex@23.05
amrex@23.05
ant@1.10.13
antlr@2.7.7
arborx@1.3
arborx@1.3
archer@2.0.0
argobots@1.1
arpack-ng@3.9.0
ascent@0.9.1
asio@1.16.1
asio@1.21.0
autoconf@2.69
autoconf-archive@2023.02.20
automake@1.16.5
axl@0.7.1
axl@0.8.0
axom@0.7.0
berkeley-db@18.1.40
binutils@2.40
bison@3.8.2
bitgroomingz@2022-10-14
blaspp@2022.07.00
blaspp@2022.07.00
blt@0.5.2
bolt@2.0
boost@1.79.0
boost@1.79.0
bricks@r0.1
butterflypack@2.2.2
bzip2@1.0.8
c-blosc@1.21.2
ca-certificates-mozilla@2023-01-10
cabana@0.5.0
cabana@0.5.0
cabana@0.5.0
caliper@2.9.0
caliper@2.9.0
camp@2022.10.1
camp@2022.10.1
camp@2022.10.1
cereal@1.3.0
cgal@4.13
chai@2022.03.0
chai@2022.03.0
charliecloud@0.32
clara@1.1.5
cli11@1.9.1
cmake@3.26.3
conduit@0.8.7
conduit@0.8.7
curl@8.0.1
curl@8.0.1
czmq@4.1.1
darshan-runtime@3.4.2
darshan-util@3.4.2
datatransferkit@3.1-rc3
diffutils@3.9
dihydrogen@develop
docbook-xml@4.5
docbook-xsl@1.79.2
double-conversion@3.2.1
dtcmp@1.1.4
dyninst@12.3.0
==> 726 installed packages
Singularity>

ecp-data-vis-sdk@1.0
ecp-data-vis-sdk@1.0
eigen@3.4.0
elfutils@0.189
embree@3.13.1
er@0.2.0
er@0.4.0
exaworks@0.1.0
exmcutils@0.6.0
expat@2.5.0
faodel@1.2108.1
fftw@3.3.10
fftw@3.3.10
fides@1.2.0
findutils@4.9.0
flecsi@2.1.0
flex@2.6.3
flex@2.6.4
flit@2.1.0
flux-core@0.49.0
flux-core@0.49.0
flux-sched@0.27.0
fortrilinos@2.2.0
fpzip@1.3.0
freetype@2.10.2
freetype@2.11.1
gasnet@2023.3.0
gasnet@2023.3.0
gawk@5.2.1
gdbm@1.23
gettext@0.21.1
ginkgo@1.5.0
ginkgo@1.5.0
git@2.40.0
git@2.40.0
gl2ps@1.4.2
glew@2.2.0
glib@2.76.1
globalarrays@5.8.2
glproto@1.4.17
glx@1.4
gmake@4.4.1
gmp@6.2.1
gotcha@1.0.4
gperftools@2.10
gptune@4.0.0
gsl@2.7.1
h5bench@1.3
hdf5@1.8.21
hdf5@1.12.2
hdf5@1.14.1-2
hdf5@1.14.1-2
hdf5-vol-async@1.5
hdf5-vol-cache@v1.1
hdf5-vol-log@1.4.0
hdf5-vol-log@1.4.0
heffte@2.3.0
heffte@2.3.0
help2man@1.49.3
hip@5.4.3
hip@5.4.3
hipblas@5.4.3
hipsolver@5.4.3
hipsparse@5.4.3
hpctoolkit@2023.03.01
hpctoolkit@2023.03.01
hpcviewer@2023.04
hpx@1.9.0
hpx@1.9.0
hsa-rocr-dev@5.4.3
hsa-rocr-dev@5.4.3
hwloc@2.9.1
hydrogen@develop

hypre@2.28.0
hypre@2.28.0
inputproto@2.3.2
intel-tbb@2020.3
intel-tbb@2021.9.0
intel-xed@2022.10.11
ispc@1.19.0
jansson@2.14
jq@1.6
json-c@0.16
jsoncpp@1.9.5
kbproto@1.0.7
kokkos@3.7.00
kokkos@3.7.01
kokkos@4.0.01
kokkos@4.0.01
kokkos@4.0.01
kokkos@4.0.01
kokkos-kernels@3.7.00
krb5@1.20.1
kvtree@1.3.0
kvtree@1.4.0
lammps@20220623.3
lapackpp@2022.07.00
lapackpp@2022.07.00
lbann@0.102
legion@23.03.0
libaec@1.0.6
libarchive@3.6.2
libbsd@0.11.7
libcap@2.68
libcatalyst@2.0.0-rc3
libcircle@0.3.0
libdistributed@0.4.2
libdwarf@20180129
libedit@3.1-20210216
libevent@2.1.12
libfabric@1.18.0
libffi@3.4.4
libfms@0.2.0
libgcrypt@1.10.2
libgit2@1.6.4
libgpg-error@1.47
libiberty@2.40
libice@1.0.9
libiconv@1.17
libidn2@2.3.4
libjpeg-turbo@2.1.5
libmd@1.0.4
libmonitor@2023.03.15
libnrm@0.1.0
libogg@1.3.5
libpciaccess@0.17
libpng@1.6.39
libpressio@0.95.1
libpthread-stubs@0.4
libquo@1.3.1
libsigsegv@2.14
libsm@1.2.3
libsodium@1.0.18
libssh2@1.10.0
libstdcompat@0.0.17
libtheora@1.1.1
libtiff@4.5.0
libtool@2.4.7
libunistring@1.1
libunwind@1.6.2
libx11@1.8.4
libxau@1.0.8
libxcb@1.14
libxcrypt@4.4.33
libxdmcp@1.1.4
libxext@1.3.3

libxml2@2.10.3
libxrandr@1.5.3
libxrender@0.9.10
libxslt@1.1.33
libxt@1.1.5
libyaml@0.2.5
libyogrt@1.33
libzmq@4.3.4
llvm@8.0.0
llvm@15.0.7
llvm-amdgpu@5.4.3
llvm-amdgpu@5.4.3
llvm-openmp-ompt@tr6_forwards
loki@0.1.7
lua@5.3.6
lua@5.3.6
lua@5.4.4
lua-luaposix@36.1
lua-luaposix@36.1
lua-sol2@3.2.3
lwgrp@1.0.5
lz4@1.9.4
lzo@2.10
m4@1.4.19
magma@2.7.1
mbedtls@2.28.2
memkind@1.13.0
mercury@2.1.0
mercury@2.2.0
mesa@22.1.6
mesa-glu@9.0.2
meson@1.1.0
meson@1.1.0
metall@0.25
metis@5.1.0
mfem@4.5.2
mfem@4.5.2
mfem@4.5.2
mgard@2023-03-31
mochi-margo@0.9.6
mpark-variant@1.4.0
mpfr@4.2.0
mpich@4.1.1
mpifileutils@0.11.1
munge@0.5.15
nasm@2.15.05
nccmp@1.9.0.1
nco@5.1.5
ncurses@6.3
netcdf-c@4.9.2
netcdf-c@4.9.2
netcdf-c@4.9.2
netcdf-cxx@4.2
netlib-scalapack@2.2.0
nghttp2@1.52.0
ninja@1.11.1
nlohmann-json@3.11.2
nrm@0.1.0
numactl@2.0.14
omega-h@9.34.13
oniguruma@6.9.8
openblas@0.3.23
openblas@0.3.23
openfoam@2206
openimagedenoise@1.4.3
openjdk@11.0.17_8
openmpi@4.1.5
openpmd-api@0.15.1
openpmd-api@0.15.1
openpmd-api@0.15.1
openssh@9.3p1
openssl@1.1.1t
openturns@1.18

openvkl@1.3.1
ospray@2.10.0
otf2@2.3
pagmo2@2.18.0
papi@6.0.0.1
papyrus@1.0.2
parallel-netcdf@1.12.3
paraview@5.11.1
paraview@5.11.1
parmetis@4.0.3
parsec@3.0.2209
pcre@8.45
pcre2@10.42
pdsh@2.31
pdt@3.25.1
pegtl@3.2.0
perl@5.36.0
perl-data-dumper@2.173
petsc@3.19.1
petsc@3.19.1
pflotran@4.0.1
phist@1.11.2
pigz@2.7
pkgconf@1.9.5
plasma@22.9.29
plumed@2.8.2
pmix@4.2.3
precice@2.5.0
proj@8.1.0
protobuf@3.21.12
pugixml@1.13
pumi@2.2.7
py-alembic@1.5.5
py-anyio@3.6.1
py-apache-libcloud@1.2.1
py-argon2-cffi@21.3.0
py-argon2-cffi@21.3.0
py-argon2-cffi-bindings@21.2.0
py-argon2-cffi-bindings@21.2.0
py-async-generator@1.10
py-attrs@22.2.0
py-attrs@22.2.0
py-autograd@1.3
py-babel@2.10.3
py-backcall@0.2.0
py-bcrypt@3.2.0
py-beautifulsoup4@4.11.1
py-beautifulsoup4@4.11.1
py-bleach@5.0.1
py-bleach@5.0.1
py-bottleneck@1.3.5
py-calver@2022.6.26
py-calver@2022.6.26
py-certifi@2022.12.7
py-certifi@2022.12.7
py-certipy@0.1.3
py-cffi@1.15.1
py-cffi@1.15.1
py-charset-normalizer@2.0.12
py-charset-normalizer@2.0.12
py-cinemasci@1.3
py-cloudpickle@2.2.0
py-colorama@0.4.5
py-configspace@0.4.20
py-cppy@1.1.0
py-cryptography@38.0.1
py-cycler@0.11.0
py-cython@0.29.33
py-cython@0.29.33
py-cython@3.0.0a9
py-debugpy@1.6.6
py-debugpy@1.6.6
py-decorator@5.1.1

py-decorator@5.1.1
py-defusedxml@0.7.1
py-defusedxml@0.7.1
py-deprecation@2.1.0
py-deprecation@2.1.0
py-dill@0.3.6
py-editables@0.3
py-editables@0.3
py-entrypoints@0.4
py-fastjsonschema@2.16.3
py-fastjsonschema@2.16.3
py-filelock@3.5.0
py-filelock@3.5.0
py-flit-core@3.7.1
py-fn-py@0.5.2
py-fonttools@4.37.3
py-future@0.18.2
py-gevent@1.5.0
py-gevent@1.5.0
py-gevent@21.12.0
py-globus-sdk@3.10.1
py-gpy@1.9.9
py-greenlet@1.1.3
py-greenlet@2.0.2
py-greenlet@2.0.2
py-h5py@3.7.0
py-hatch-nodejs-version@0.3.1
py-hatch-nodejs-version@0.3.1
py-hatchling@1.14.0
py-hatchling@1.14.0
py-hpbandster@0.7.4
py-idna@3.4
py-importlib-metadata@6.6.0
py-importlib-metadata@6.6.0
py-importlib-resources@5.12.0
py-importlib-resources@5.12.0
py-ipykernel@6.16.0
py-ipykernel@6.16.0
py-ipyparallel@6.3.0
py-ipython@7.31.1
py-ipython@7.31.1
py-ipython-genutils@0.2.0
py-ipython-genutils@0.2.0
py-ipywidgets@8.0.2
py-jedi@0.18.1
py-jedi@0.18.1
py-jinja2@3.1.2
py-jinja2@3.1.2
py-joblib@1.2.0
py-json5@0.9.10
py-jsonpatch@1.23
py-jsonpointer@1.9
py-jsonschema@2.6.0
py-jsonschema@4.4.0
py-jsonschema@4.4.0
py-jupyter-client@7.3.5
py-jupyter-client@7.3.5
py-jupyter-core@4.11.1
py-jupyter-core@4.11.1
py-jupyter-packaging11@0.11.1
py-jupyter-packaging11@0.12.3
py-jupyter-server@1.13.5
py-jupyter-telemetry@0.1.0
py-jupyterhub@1.4.1
py-jupyterlab@3.2.9
py-jupyterlab-pygments@0.2.2
py-jupyterlab-pygments@0.2.2
py-jupyterlab-server@2.10.3
py-jupyterlab-widgets@3.0.3
py-kiwisolver@1.3.2
py-lhsmdu@1.1
py-libensemble@0.9.3
py-lxml@4.9.1

py-lxml@4.9.1
py-mako@1.2.2
py-mako@1.2.2
py-markupsafe@2.1.1
py-markupsafe@2.1.1
py-matplotlib@3.5.3
py-matplotlib@3.5.3
py-matplotlib-inline@0.1.6
py-matplotlib-inline@0.1.6
py-mistune@2.0.4
py-mistune@2.0.4
py-mpi4py@3.1.4
py-msgpack@1.0.4
py-nbclassic@0.3.5
py-nbclient@0.6.7
py-nbclient@0.6.7
py-nbconvert@7.0.0
py-nbconvert@7.0.0
py-nbformat@5.8.0
py-nbformat@5.8.0
py-nest-asyncio@1.5.6
py-nest-asyncio@1.5.6
py-netifaces@0.10.5
py-netifaces@0.10.5
py-notebook@6.4.12
py-notebook@6.4.12
py-ntplib@0.4.0
py-numcodecs@0.7.3
py-numexpr@2.8.3
py-numpy@1.21.6
py-oauthlib@3.2.1
py-opentuner@0.8.7
py-packaging@23.0
py-pamela@1.0.0
py-pandas@1.3.5
py-pandocfilters@1.5.0
py-pandocfilters@1.5.0
py-paramiko@2.12.0
py-paramz@0.9.5
py-parse@1.18.0
py-parsl@1.2.0
py-parso@0.8.3
py-parso@0.8.3
py-pathspec@0.11.1
py-patsy@0.5.2
py-periodictable@1.5.0
py-petsc4py@3.19.1
py-pexpect@4.8.0
py-pexpect@4.8.0
py-pickleshare@0.7.5
py-pickleshare@0.7.5
py-picmistandard@0.0.22
py-pika@0.13.0
py-pillow@9.5.0
py-pip@23.0
py-pkgconfig@1.5.5
py-pluggy@1.0.0
py-pluggy@1.0.0
py-ply@3.11
py-poetry-core@1.2.0
py-poetry-core@1.2.0
py-prometheus-client@0.14.1
py-prometheus-client@0.14.1
py-prompt-toolkit@3.0.31
py-prompt-toolkit@3.0.31
py-protobuf@4.21.9
py-psij-python@0.1.0.post2
py-psutil@5.9.4
py-psutil@5.9.4
py-ptyprocess@0.7.0
py-py@1.11.0
py-pyaml@21.8.3
py-pybind11@2.10.1

py-pybind11@2.10.1
py-pycparser@2.21
py-pycparser@2.21
py-pyelftools@0.29
py-pygments@2.13.0
py-pygments@2.13.0
py-pyjwt@2.4.0
py-pymongo@3.12.1
py-pymoo@0.5.0
py-pynacl@1.5.0
py-pyopenssl@22.1.0
py-pyparsing@3.0.9
py-pyro4@4.81
py-pyrsistent@0.19.3
py-pyrsistent@0.19.3
py-pystache@0.6.0
py-python-dateutil@2.8.2
py-python-dateutil@2.8.2
py-python-editor@1.0.4
py-python-json-logger@0.1.11
py-pytz@2022.2.1
py-pyyaml@6.0
py-pyyaml@6.0
py-pyzmq@17.1.2
py-pyzmq@25.0.2
py-pyzmq@25.0.2
py-pyzmq@25.0.2
py-radical-entk@1.20.0
py-radical-gtod@1.20.0
py-radical-pilot@1.20.0
py-radical-saga@1.20.0
py-radical-utils@1.20.0
py-regex@2022.8.17
py-requests@2.28.2
py-requests@2.28.2
py-ruamel-yaml@0.17.16
py-ruamel-yaml-clib@0.2.0
py-scikit-learn@1.0.2
py-scikit-optimize@master
py-scipy@1.5.4
py-semantic-version@2.10.0
py-send2trash@1.8.0
py-send2trash@1.8.0
py-serpent@1.40
py-setproctitle@1.1.10
py-setuptools@59.4.0
py-setuptools@67.6.0
py-setuptools-rust@1.5.1
py-setuptools-scm@6.3.2
py-setuptools-scm@6.3.2
py-setuptools-scm-git-archive@1.4
py-six@1.16.0
py-six@1.16.0
py-sniffio@1.3.0
py-soupsieve@2.3.2.post1
py-soupsieve@2.3.2.post1
py-sqlalchemy@1.4.45
py-sqlalchemy@1.4.45
py-statsmodels@0.13.2
py-tblib@1.6.0
py-terminado@0.15.0
py-terminado@0.15.0
py-threadpoolctl@3.1.0
py-tinycss2@1.1.1
py-tinycss2@1.1.1
py-toml@0.10.2
py-tomli@2.0.1
py-tomlkit@0.11.4
py-tomlkit@0.11.4
py-tornado@5.1.1
py-tornado@6.2
py-tornado@6.2
py-traitlets@5.9.0

py-traitlets@5.9.0
py-trove-classifiers@2023.3.9
py-trove-classifiers@2023.3.9
py-typeguard@2.13.3
py-typing-extensions@4.5.0
py-urllib3@1.26.12
py-urllib3@1.26.12
py-vcversioner@2.16.0.0
py-versioneer@0.28
py-warlock@1.3.3
py-warpx@23.03
py-warpx@23.03
py-warpx@23.03
py-wcwidth@0.2.5
py-wcwidth@0.2.5
py-webencodings@0.5.1
py-webencodings@0.5.1
py-websocket-client@1.5.1
py-wheel@0.37.1
py-widgetsnbextension@4.0.3
py-ytopt-autotune@1.1.0
py-zipp@3.8.1
py-zipp@3.8.1
py-zope-event@4.6
py-zope-interface@5.4.0
pygmo@2.18.0
python@3.7.15
qhull@2020.2
qthreads@1.16
quantum-espresso@7.1
raja@2022.10.4
raja@2022.10.4
randrproto@1.5.0
rankstr@0.1.0
rankstr@0.3.0
re2c@2.2
readline@8.2
redset@0.2.0
redset@0.3.0
rempi@1.1.0
renderproto@0.11.1
rkcommon@1.10.0
rocblas@5.4.3
rocfft@5.4.3
rocprim@5.4.3
rocprim@5.4.3
rocprofiler-dev@5.4.3
rocrand@5.4.3
rocrand@5.4.3
rocsolver@5.4.3
rocsparse@5.4.3
rocsparse@5.4.3
rocthrust@5.4.3
rocthrust@5.4.3
roctracer-dev@4.5.3
rust@1.65.0
scotch@7.0.3
scr@3.0.1
sed@4.9
shuffile@0.2.0
shuffile@0.3.0
silo@4.11
slate@2022.07.00
slate@2022.07.00
slepc@3.19.0
slepc@3.19.0
slurm@23-02-1-1
snappy@1.1.10
spath@0.2.0
spath@0.3.0
spdlog@1.11.0
sqlite@3.40.1
stc@0.9.0

strumpack@7.1.1
strumpack@7.1.1
suite-sparse@5.13.0
sundials@6.5.1
sundials@6.5.1
superlu@5.3.0
superlu-dist@7.2.0
superlu-dist@8.1.2
superlu-dist@8.1.2
swig@4.0.2-fortran
swig@4.1.1
sz@1.4.12.3
sz@2.1.12.2
sz@2.1.12.2
sz3@3.1.7
sz3@3.1.7
tar@1.34
tasmanian@7.9
tasmanian@7.9
tau@2.32
tau@2.32
tcl@8.6.12
texinfo@7.0.3
toml11@3.7.1
trilinos@13.0.1
trilinos@13.4.1
trilinos@14.0.0
trilinos@14.0.0
turbine@1.3.0
udunits@2.2.28
umap@2.1.0
umpire@2022.03.1
umpire@2022.03.1
umpire@2022.03.1
umpire@2022.03.1
unifyfs@1.0.1
unzip@6.0
upcxx@2023.3.0
upcxx@2023.3.0
util-linux-uuid@2.38.1
util-macros@1.19.3
variorum@0.6.0
veloc@1.6
visit@3.3.3
vtk@8.1.2
vtk-m@1.9.0
vtk-m@2.0.0
wannier90@3.1.0
warpx@23.03
warpx@23.03
warpx@23.03
xcb-proto@1.15.2
xerces-c@3.2.4
xextproto@7.3.0
xproto@7.0.31
xrandr@1.5.0
xtrans@1.4.0
xyce@7.6.0
xz@5.4.1
yaksa@0.2
yaml-cpp@0.6.3
yaml-cpp@0.7.0
zfp@0.5.5
zfp@1.0.0
zlib@1.2.13
zsh@5.8
zstd@1.5.5
zstd@1.5.5
zstr@1.0.7

726 packages!

E4S 23.05 Intel oneAPI 2023.1: Packages built with Intel compilers

```
Singularity> spack find -x
-- linux-ubuntu20.04-x86_64 / gcc@11.1.0 ------------------------
papi@6.0.0.1

-- linux-ubuntu20.04-x86_64 / oneapi@2023.1.0 -------------------
adios@1.13.1          cabana@0.5.0              gmp@6.2.1              legion@23.03.0       netlib-scalapack@2.2.0  py-libensemble@0.9.3  sz3@3.1.7
aml@0.2.0             cabana@0.5.0              gotcha@1.0.4           libnrm@0.1.0         omega-h@9.34.13         py-petsc4py@3.19.1    tasmanian@7.9
aml@0.2.0             caliper@2.9.0             h5bench@1.3            libquo@1.3.1         openmpi@4.1.5           qthreads@1.16         tau@2.32
amrex@22.12           chai@2022.03.0            hdf5-vol-async@1.5     libunwind@1.6.2      openpmd-api@0.15.1      quantum-espresso@7.1  tau@2.32
amrex@23.05           charliecloud@0.32         hdf5-vol-log@1.4.0     loki@0.1.7           papyrus@1.0.2           raja@2022.10.4        trilinos@13.0.1
arborx@1.3            conduit@0.8.7             heffte@2.3.0           mercury@2.2.0        parsec@3.0.2209         rempi@1.1.0           turbine@1.3.0
arborx@1.3            datatransferkit@3.1-rc3   hpx@1.9.0              metall@0.25          pdt@3.25.1              slate@2022.07.00      umap@2.1.0
archer@2.0.0          exaworks@0.1.0            hypre@2.28.0           mfem@4.5.2           petsc@3.19.1            slepc@3.19.0          umpire@2022.03.1
argobots@1.1          flecsi@2.2.0              kokkos@4.0.01          mgard@2023-03-31     phist@1.11.2            stc@0.9.0             variorum@0.6.0
axom@0.7.0            flit@2.1.0                kokkos@4.0.01          mpark-variant@1.4.0  plasma@22.9.29          strumpack@7.1.1       wannier90@3.1.0
bolt@2.0              flux-core@0.49.0          kokkos-kernels@3.7.00  mpich@4.1.1          plumed@2.8.2            sundials@6.5.1
boost@1.82.0          fortrilinos@2.2.0         kokkos-kernels@3.7.00  mpifileutils@0.11.1  precice@2.5.0           superlu@5.3.0
bricks@r0.1           gasnet@2023.3.0           lammps@20220623.3      nccmp@1.9.0.1        pumi@2.2.7              superlu-dist@8.1.2
butterflypack@2.2.2   globalarrays@5.8.2        lbann@0.102            nco@5.1.5            py-h5py@3.7.0           swig@4.0.2-fortran
```

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

E4S 23.05 Intel oneAPI 2023.1: Packages built with Intel compilers

```
Singularity> module avail

------------------------------------------------------------------ /opt/intel/oneapi/modulefiles -------------------------------------------------------------------
   advisor/latest                compiler32/latest             dnnl-cpu-tbb/latest          inspector/latest                    mpi/latest
   advisor/2023.1.0       (D)    compiler32/2023.1.0    (D)    dnnl-cpu-tbb/2023.1.0 (D)    inspector/2023.1.0           (D)    mpi/2021.9.0     (D)
   ccl/latest                    dal/latest                    dnnl/latest                  intel_ipp_intel64/latest            oclfpga/latest
   ccl/2021.9.0           (D)    dal/2023.1.0           (D)    dnnl/2023.1.0         (D)    intel_ipp_intel64/2021.8.0   (D)    oclfpga/2023.1.0 (D)
   clck/latest                   debugger/latest               dpl/latest                   intel_ippcp_intel64/latest          tbb/latest
   clck/2021.7.3          (D)    debugger/2023.1.0      (D)    dpl/2022.1.0          (D)    intel_ippcp_intel64/2021.7.0 (D)    tbb/2021.9.0     (D)
   compiler-rt/latest            dev-utilities/latest          icc/latest                   itac/latest                         vtune/latest
   compiler-rt/2023.1.0   (D)    dev-utilities/2021.9.0 (D)    icc/2023.1.0          (D)    itac/2021.9.0                (D)    vtune/2023.1.0   (D)
   compiler-rt32/latest          dnnl-cpu-gomp/latest          icc32/latest                 mkl/latest
   compiler-rt32/2023.1.0 (D)    dnnl-cpu-gomp/2023.1.0 (D)    icc32/2023.1.0        (D)    mkl/2023.1.0                 (D)
   compiler/latest               dnnl-cpu-iomp/latest          init_opencl/latest           mkl32/latest
   compiler/2023.1.0      (D)    dnnl-cpu-iomp/2023.1.0 (D)    init_opencl/2023.1.0  (D)    mkl32/2023.1.0               (D)

---------------------------------------------- /spack/share/spack/lmod/linux-ubuntu20.04-x86_64/mpich/4.1.1/Core ----------------------------------------------
   adios/1.13.1                      datatransferkit/3.1-rc3     libnrm/0.1.0              petsc/3.19.1                  strumpack/7.1.1-openmp
   amrex/22.12-sycl                  exaworks/0.1.0              libquo/1.3.1              phist/1.11.2-openmp           sundials/6.5.1
   amrex/23.05               (D)     flecsi/2.2.0                mercury/2.2.0             plumed/2.8.2                  superlu-dist/8.1.2
   arborx/1.3-sycl                   fortrilinos/2.2.0           metall/0.25               precice/2.5.0                 tasmanian/7.9
   arborx/1.3                (D)     globalarrays/5.8.2          mfem/4.5.2                pumi/2.2.7                    tau/2.32-level-zero    (L)
   axom/0.7.0-openmp                 h5bench/1.3                 mpifileutils/0.11.1       py-h5py/3.7.0                 tau/2.32               (D)
   boost/1.82.0                      hdf5-vol-async/1.5          nccmp/1.9.0.1             py-libensemble/0.9.3          trilinos/13.0.1
   bricks/r0.1                       hdf5-vol-log/1.4.0          nco/5.1.5                 py-petsc4py/3.19.1            turbine/1.3.0
   butterflypack/2.2.2-openmp        heffte/2.3.0                netlib-scalapack/2.2.0    quantum-espresso/7.1-openmp   wannier90/3.1.0
   cabana/0.5.0-sycl                 hpx/1.9.0                   omega-h/9.34.13           rempi/1.1.0
   cabana/0.5.0              (D)     hypre/2.28.0                openpmd-api/0.15.1        slate/2022.07.00-openmp
   caliper/2.9.0                     lammps/20220623.3-openmp    papyrus/1.0.2             slepc/3.19.0
   conduit/0.8.7                     lbann/0.102                 parsec/3.0.2209           stc/0.9.0

---------------------------------------------------- /spack/share/spack/lmod/linux-ubuntu20.04-x86_64/Core -----------------------------------------------------
   aml/0.2.0-level-zero       flit/2.1.0                      kokkos/4.0.01-openmp            mpich/4.1.1          (L)    superlu/5.3.0
   aml/0.2.0           (D)    flux-core/0.49.0                kokkos/4.0.01-sycl-openmp (D)   openmpi/4.1.5               swig/4.0.2-fortran
   archer/2.0.0               gasnet/2023.3.0                 legion/23.03.0                  papi/6.0.0.1         (L)    sz3/3.1.7
   argobots/1.1               gmp/6.2.1                       libunwind/1.6.2          (L)    pdt/3.25.1                  umap/2.1.0
   bolt/2.0                   gotcha/1.0.4                    loki/0.1.7                      plasma/22.9.29              umpire/2022.03.1
   chai/2022.03.0             kokkos-kernels/3.7.00-openmp    mgard/2023-03-31-openmp         qthreads/1.16               variorum/0.6.0
   charliecloud/0.32          kokkos-kernels/3.7.00-sycl (D)  mpark-variant/1.4.0             raja/2022.10.4-openmp
```

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

E4S Support for ROCm variants for MI250X (gfx90a) on x86_64

```
Singularity> spack find -x
-- linux-ubuntu20.04-x86_64 / gcc@11.1.0 ------------------------
adios@1.13.1          chai@2022.03.0          gptune@4.0.0          libcatalyst@2.0.0-rc3  openpmd-api@0.15.1     py-warpx@23.03          tasmanian@7.9
adios2@2.9.0          charliecloud@0.32       h5bench@1.3           libnrm@0.1.0           papi@6.0.0.1           qthreads@1.16           tasmanian@7.9
alquimia@1.0.10       conduit@0.8.7           hdf5@1.12.2           libpressio@0.95.1      papyrus@1.0.2          quantum-espresso@7.1    tau@2.32
aml@0.2.0             darshan-runtime@3.4.2   hdf5@1.14.1-2         libquo@1.3.1           parallel-netcdf@1.12.3 raja@2022.10.4          tau@2.32
amrex@23.05           darshan-util@3.4.2      hdf5-vol-async@1.5    libunwind@1.6.2        paraview@5.11.1        raja@2022.10.4          trilinos@13.0.1
amrex@23.05           datatransferkit@3.1-rc3 hdf5-vol-cache@v1.1   loki@0.1.7             paraview@5.11.1        rempi@1.1.0             trilinos@14.0.0
arborx@1.3            dyninst@12.3.0          hdf5-vol-log@1.4.0    magma@2.7.1            parsec@3.0.2209        scr@3.0.1               turbine@1.3.0
arborx@1.3            ecp-data-vis-sdk@1.0    hdf5-vol-log@1.4.0    mercury@2.2.0          pdt@3.25.1             slate@2022.07.00        umap@2.1.0
archer@2.0.0          ecp-data-vis-sdk@1.0    heffte@2.3.0          metall@0.25            petsc@3.19.1           slate@2022.07.00        umpire@2022.03.1
argobots@1.1          exaworks@0.1.0          heffte@2.3.0          mfem@4.5.2             petsc@3.19.1           slepc@3.19.0            umpire@2022.03.1
ascent@0.9.1          faodel@1.2108.1         hpctoolkit@2023.03.01 mfem@4.5.2             phist@1.11.2           slepc@3.19.0            unifyfs@1.0.1
axom@0.7.0            flecsi@2.1.0            hpctoolkit@2023.03.01 mgard@2023-03-31       plasma@22.9.29         stc@0.9.0               upcxx@2023.3.0
bolt@2.0              flit@2.1.0              hpx@1.9.0             mpark-variant@1.4.0    plumed@2.8.2           strumpack@7.1.1         upcxx@2023.3.0
boost@1.79.0          flux-core@0.49.0        hpx@1.9.0             mpich@4.1.1            precice@2.5.0          strumpack@7.1.1         variorum@0.6.0
bricks@r0.1           fortrilinos@2.2.0       hypre@2.28.0          mpifileutils@0.11.1    pumi@2.2.7             sundials@6.5.1          veloc@1.6
butterflypack@2.2.2   gasnet@2023.3.0         hypre@2.28.0          nccmp@1.9.0.1          py-cinemasci@1.3       sundials@6.5.1          visit@3.3.3
cabana@0.5.0          gasnet@2023.3.0         kokkos@4.0.01         nco@5.1.5              py-h5py@3.7.0          superlu@5.3.0           vtk-m@1.9.0
cabana@0.5.0          ginkgo@1.5.0            kokkos@4.0.01         netlib-scalapack@2.2.0 py-jupyterhub@1.4.1    superlu-dist@8.1.2      vtk-m@2.0.0
cabana@0.5.0          ginkgo@1.5.0            kokkos-kernels@3.7.00 nrm@0.1.0              py-libensemble@0.9.3   superlu-dist@8.1.2      wannier90@3.1.0
caliper@2.9.0         globalarrays@5.8.2      lammps@20220623.3     omega-h@9.34.13        py-petsc4py@3.19.1     swig@4.0.2-fortran      xyce@7.6.0
caliper@2.9.0         gmp@6.2.1               lbann@0.102           openfoam@2206          py-warpx@23.03         sz@2.1.12.2             zfp@0.5.5
chai@2022.03.0        gotcha@1.0.4            legion@23.03.0        openmpi@4.1.5          py-warpx@23.03         sz3@3.1.7
==> 153 installed packages
```

E4S 23.05 supports AMD MI100 (gfx908) as well as MI250X (gfx90a) GPUs

E4S Support for ROCm variants for MI250X (gfx90a) on x86_64

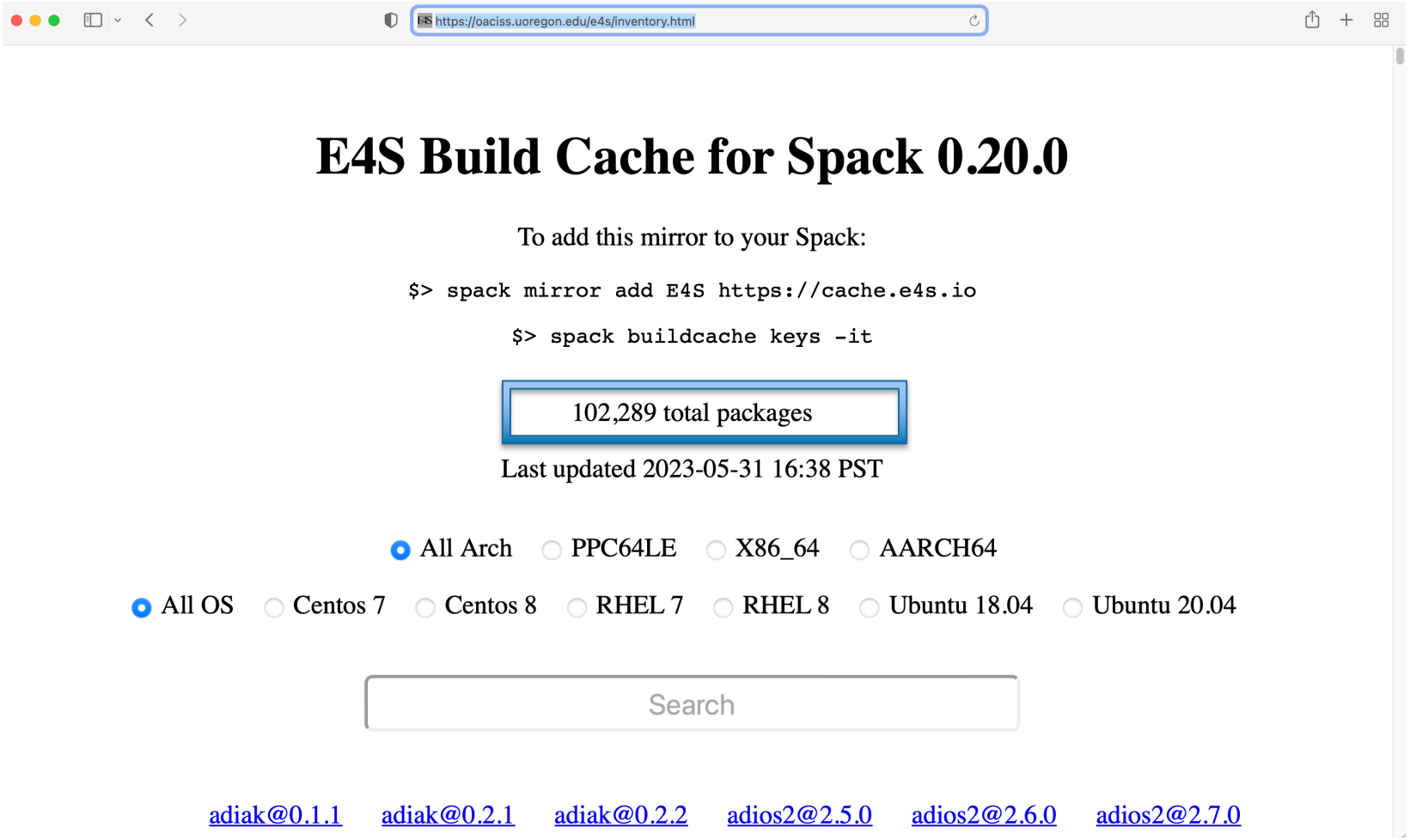
```
Singularity> module avail

------------------------------------------------ /spack/share/spack/lmod/linux-ubuntu20.04-x86_64/mpich/4.1.1/Core ------------------------------------------------
   adios/1.13.1                       ginkgo/1.5.0-openmp        (D)    nccmp/1.9.0.1                          slate/2022.07.00-openmp       (D)
   adios2/2.9.0                       globalarrays/5.8.2                nco/5.1.5                              slepc/3.19.0-gfx908
   alquimia/1.0.10                    gptune/4.0.0                      netlib-scalapack/2.2.0                 slepc/3.19.0                  (D)
   amrex/23.05-gfx908                 h5bench/1.3                       omega-h/9.34.13                        stc/0.9.0
   amrex/23.05                (D)     hdf5-vol-async/1.5                openfoam/2206                          strumpack/7.1.1-gfx908-openmp
   arborx/1.3-gfx908                  hdf5-vol-cache/v1.1               openpmd-api/0.15.1                     strumpack/7.1.1-openmp        (D)
   arborx/1.3                 (D)     hdf5-vol-log/1.4.0                papyrus/1.0.2                          sundials/6.5.1-gfx908
   ascent/0.9.1-openmp                hdf5/1.12.2                       parallel-netcdf/1.12.3                 sundials/6.5.1                (D)
   axom/0.7.0-openmp                  hdf5/1.14.1-2              (D)    paraview/5.11.1-gfx908                 superlu-dist/8.1.2-gfx908
   boost/1.79.0                       heffte/2.3.0-gfx908               paraview/5.11.1                (D)     superlu-dist/8.1.2            (D)
   bricks/r0.1                        heffte/2.3.0               (D)    parsec/3.0.2209                        sz/2.1.12.2
   butterflypack/2.2.2-openmp         hpctoolkit/2023.03.01-rocm        petsc/3.19.1-gfx908                    tasmanian/7.9-gfx908
   cabana/0.5.0-rocm-gfx90a           hpctoolkit/2023.03.01      (D)    petsc/3.19.1                   (D)     tasmanian/7.9                 (D)
   cabana/0.5.0-rocm-gfx908           hpx/1.9.0-gfx908                  phist/1.11.2-openmp                    tau/2.32-rocm                 (L)
   cabana/0.5.0               (D)     hpx/1.9.0                  (D)    plumed/2.8.2                           tau/2.32                      (D)
   caliper/2.9.0-gfx908               hypre/2.28.0-gfx908               precice/2.5.0                          trilinos/13.0.1
   caliper/2.9.0              (D)     hypre/2.28.0               (D)    pumi/2.2.7                             trilinos/14.0.0-gfx908        (D)
   conduit/0.8.7                      lammps/20220623.3-openmp          py-cinemasci/1.3                       turbine/1.3.0
   darshan-runtime/3.4.2              lbann/0.102                       py-h5py/3.7.0                          unifyfs/1.0.1
   datatransferkit/3.1-rc3            libcatalyst/2.0.0-rc3             py-libensemble/0.9.3                   upcxx/2023.3.0-gfx908
   dyninst/12.3.0-openmp              libnrm/0.1.0                      py-petsc4py/3.19.1                     upcxx/2023.3.0                (D)
   ecp-data-vis-sdk/1.0-gfx908        libpressio/0.95.1-openmp          py-warpx/23.03-dims2                   veloc/1.6
   ecp-data-vis-sdk/1.0       (D)     libquo/1.3.1                      py-warpx/23.03-dims3                   visit/3.3.3
   exaworks/0.1.0                     mercury/2.2.0                     py-warpx/23.03-dimsRZ          (D)     vtk-m/1.9.0-openmp
   faodel/1.2108.1                    metall/0.25                       quantum-espresso/7.1-openmp            vtk-m/2.0.0-gfx908            (D)
   flecsi/2.1.0                       mfem/4.5.2-gfx908                 rempi/1.1.0                            wannier90/3.1.0
   fortrilinos/2.2.0                  mfem/4.5.2                 (D)    scr/3.0.1                              xyce/7.6.0
   ginkgo/1.5.0-gfx908-openmp         mpifileutils/0.11.1               slate/2022.07.00-gfx908-openmp

------------------------------------------------------ /spack/share/spack/lmod/linux-ubuntu20.04-x86_64/Core ------------------------------------------------------
   aml/0.2.0                  flux-core/0.49.0                  libunwind/1.6.2         (L)    pdt/3.25.1              (L)    umap/2.1.0
   archer/2.0.0               gasnet/2023.3.0-gfx908            loki/0.1.7                     plasma/22.9.29                 umpire/2022.03.1-gfx908
   argobots/1.1               gasnet/2023.3.0            (D)    magma/2.7.1-gfx908             py-jupyterhub/1.4.1            umpire/2022.03.1       (D)
   bolt/2.0                   gmp/6.2.1                         mgard/2023-03-31-openmp        qthreads/1.16                  variorum/0.6.0
   chai/2022.03.0-gfx908      gotcha/1.0.4                      mpark-variant/1.4.0            raja/2022.10.4-gfx908          zfp/0.5.5
   chai/2022.03.0      (D)    kokkos-kernels/3.7.00-openmp      mpich/4.1.1             (L)    raja/2022.10.4-openmp (D)
   charliecloud/0.32          kokkos/4.0.01-gfx908              nrm/0.1.0                      superlu/5.3.0
   darshan-util/3.4.2         kokkos/4.0.01-openmp       (D)    openmpi/4.1.5                  swig/4.0.2-fortran
   flit/2.1.0                 legion/23.03.0                    papi/6.0.0.1            (L)    sz3/3.1.7
```

E4S 23.05 supports AMD MI100 (gfx908) as well as MI250X (gfx90a) GPUs

E4S 23.05 DOE LLVM Release: x86_64, ppc64le, and aarch64

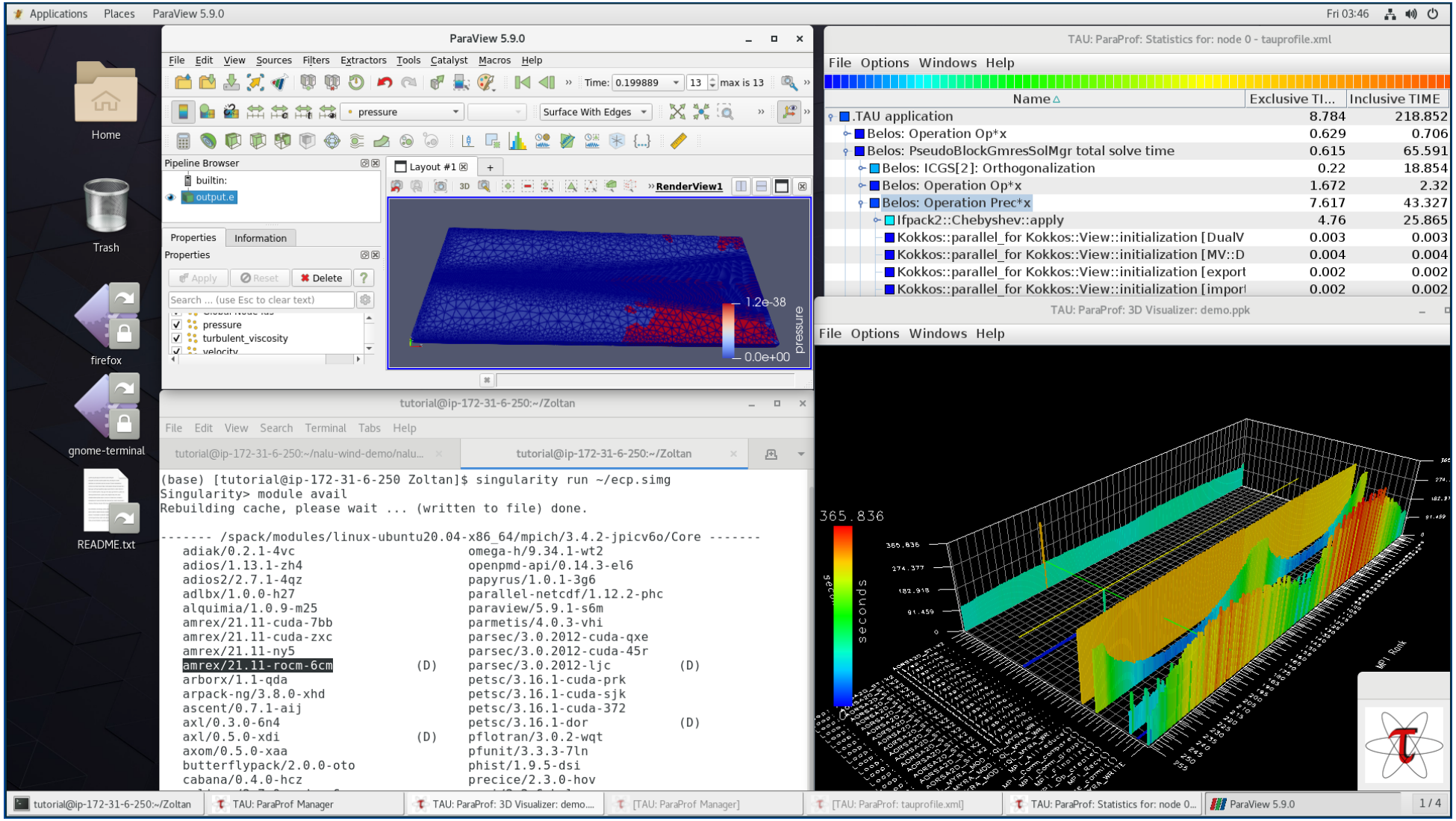
```
Singularity> spack find -x
-- linux-ubuntu20.04-x86_64 / clang@16.0.2 ----------------------
adios@1.13.1  cabana@0.5.0       globalarrays@5.8.2  heffte@2.3.0     mfem@4.5.2           parsec@3.0.2209  sundials@6.5.1      umpire@2022.03.1
aml@0.2.0     chai@2022.03.0     gmp@6.2.1           hypre@2.28.0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

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

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

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

Singularity> spack find -x
-- linux-ubuntu20.04-aarch64 / clang@16.0.2 ---------------------
adios@1.13.1  cabana@0.5.0       globalarrays@5.8.2  heffte@2.3.0     mfem@4.5.2           parsec@3.0.2209  sundials@6.5.1      umpire@2022.03.1
aml@0.2.0     chai@2022.03.0     gmp@6.2.1           hypre@2.28.0     mpark-variant@1.4.0  pdt@3.25.1       superlu@5.3.0       upcxx@2023.3.0
amrex@23.05   charliecloud@0.32  gotcha@1.0.4        legion@23.03.0   mpich@4.1.1          plumed@2.8.2     swig@4.0.2-fortran
arborx@1.3    flit@2.1.0         h5bench@1.3         libnrm@0.1.0     nccmp@1.9.0.1        pumi@2.2.7       tasmanian@7.9
argobots@1.1  flux-core@0.49.0   hdf5-vol-async@1.5  libquo@1.3.1     nco@5.1.5            qthreads@1.16    turbine@1.3.0
bolt@2.0      gasnet@2023.3.0    hdf5-vol-log@1.4.0  libunwind@1.6.2  papyrus@1.0.2        stc@0.9.0        umap@2.1.0

-- linux-ubuntu20.04-aarch64 / gcc@11.1.0 -----------------------
cmake@3.26.3  llvm-doe@16.0.2
```

E4S Build Cache for Spack 0.19.1 hosted at U. Oregon



- Over 100K binaries!
- No need to recompile from source code.

E4S 23.02 AWS image: US-West2 (OR)

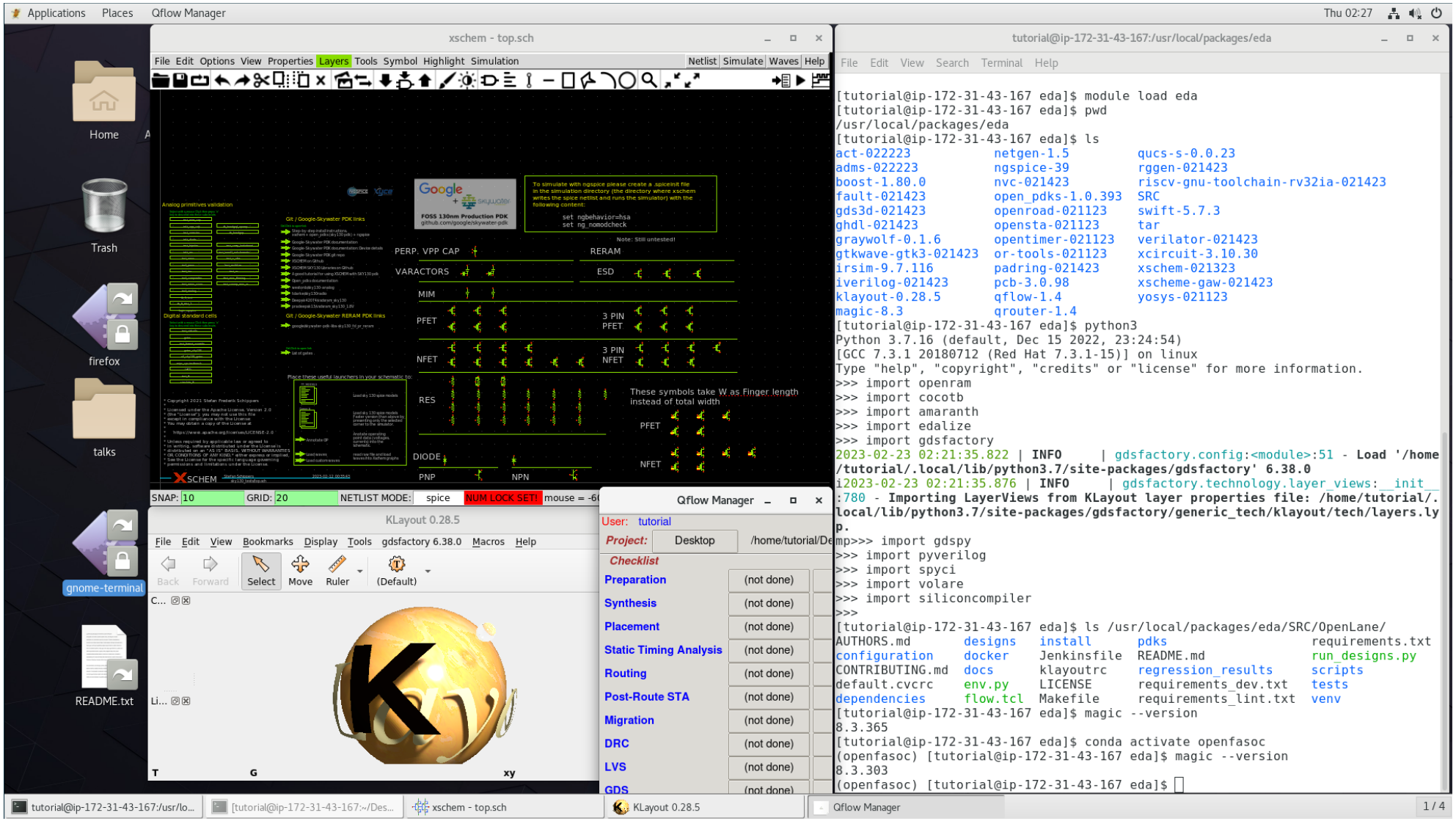


E4S 23.02 AWS

- 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…

E4S for Commercial Cloud Platforms for EDA on AWS

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



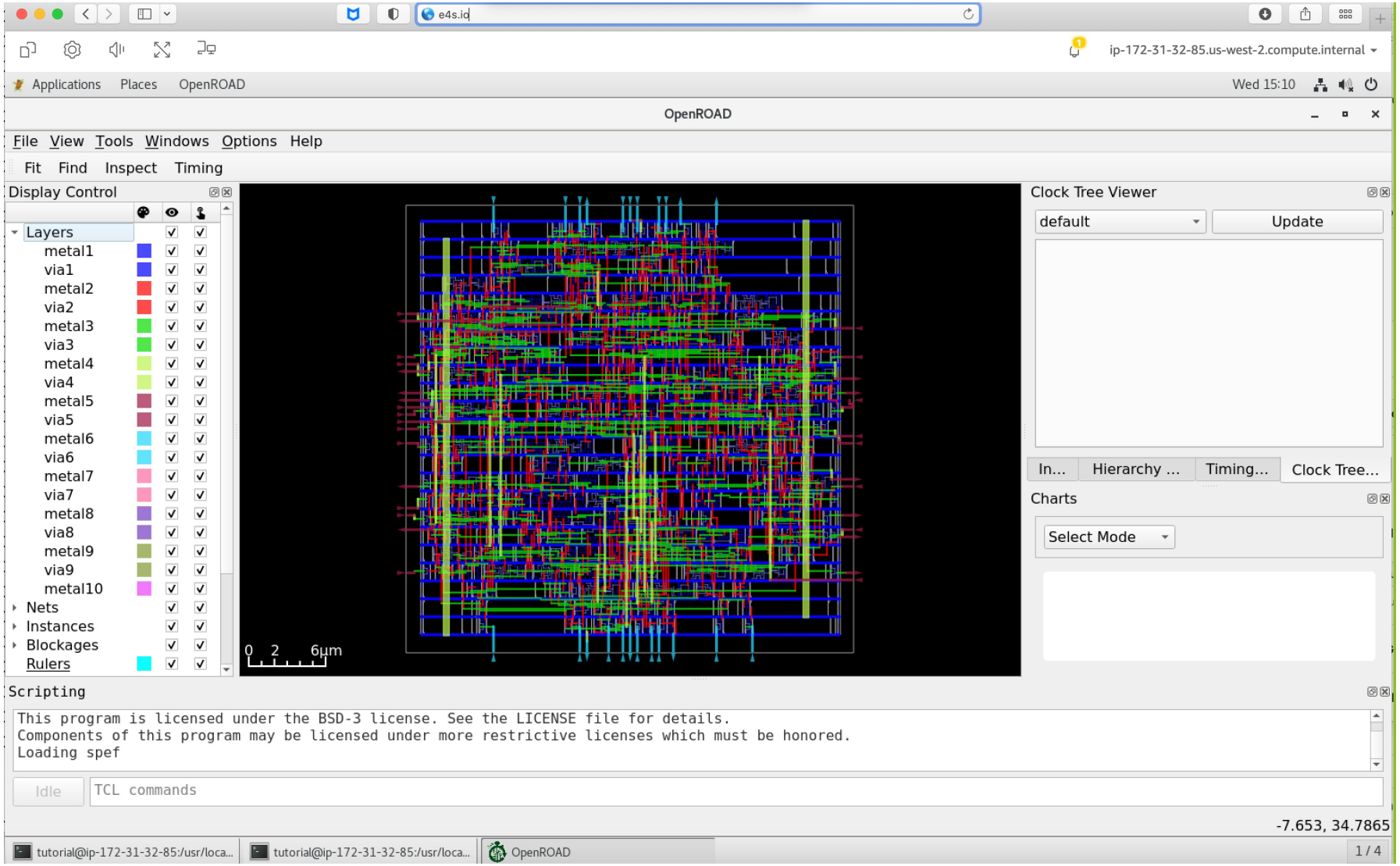
https://e4s.io/eda

E4S EDA on AWS

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

E4S for Commercial Cloud Platforms for EDA on AWS

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



E4S EDA on AWS

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  - Gdstk
  - Silicon compiler
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- PDKs
  - GF
  - Skywater

E4S for Commercial Cloud Platforms for EDA on AWS

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

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

#	Packages currently in E4S	URL
13	Yosys	https://github.com/YosysHQ/yosys
14	Xcircuit	http://opencircuitdesign.com/xcircuit/
15	Graywolf	https://github.com/rubund/graywolf
16	OpenSTA	https://github.com/The-OpenROAD-Project/OpenSTA
17	OpenTimer	https://github.com/OpenTimer/OpenTimer
18	Qrouter	http://opencircuitdesign.com/qrouter/
19	Xscheme	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

https://e4s.io/eda

E4S for Commercial Cloud Platforms for EDA on AWS

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

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

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

https://e4s.io/eda

Can E4S help provide a stable platform for EDA on Cloud?

- 50+ open source EDA packages available on AWS
- Using DCV for a remote desktop in E4S is efficient
- Scalable, multi-node capability using commercial cloud platform specific network adapters (e.g., EFA on AWS)
- Platform for workforce development, training workshops
- What are we missing?

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.