E4S: The Extreme-scale Scientific Software Stack Release 25.11

Release 25.11 notes

November 14, 2025

High Performance Software Foundation

E4S Team

https://e4s.io

E4S 25.11: What's New?

https://e4s.io

- E4S includes 125+ HPC-AI packages on aarch64, x86_64, and ppc64le platforms.
- All new website [https://e4s.io] with an OpenAI based chatbot to simplify access to E4S documentation.
- Support for NVIDIA Blackwell on x86_64 and aarch64 (Grace-Blackwell) architectures.
- Support for Rocky Linux 9.6 with Hopper and Blackwell (x86_64 and aarch64), Ubuntu 24.04 LTS.
- Spack 1.0.2 [https://spack.io] integration.
- All new E4S Spack build cache [https://cache.e4s.io/25.11] with over 7500 optimized binaries.
- AI software stack with Python 3.12.11 including packages like NVIDIA BioNeMo™, NVIDIA NeMo™, Google Agent Development Kit (adk), Vllm, HuggingFace CLI, TensorFlow, PyTorch, Google.genai (Gemini API), OpenAI (API), TorchBraid, Pandas, Scikit-Learn, JAX, OpenCV, LBANN and Codium, Jupyter, and Marimo notebooks.
- HPC Applications include: CP2K, DealII, FFTX, GROMACS, LAMMPS, Nek500, Nekbone, NWChem, OpenFOAM, WarpX, WRF, Quantum Espresso, and Xyce with GPU support where available.
- CUDA upgraded to 12.9 (aarch64, x86_64), ROCm upgraded to 6.4.3, oneAPI upgraded to 2025.2.
- Adaptive Computing's Heidi web-based platform for multi-user, multi-node, ParaTools Pro for E4S™ cloud images on AWS, Microsoft Azure, Google Cloud, IBM Cloud, and OCI with NVIDIA GPUs with SLURM or Torque.
  - https://adaptivecomputing.com/ and https://paratoolspro.com

E4S Spack Integration

- E4S is a curated, Spack based distribution of HPC-AI software.
- Major Changes in Spack 1.0.2
  - Compilers as First-Class Dependencies: Compilers are now treated as proper dependencies in the concretization process, leading to clearer and more reproducible environments.
  - Stable Package API: Spack 1.0 introduces a stable API for package development, improving long-term maintainability and easing contributions.
  - Concurrent Builds: Builds can now run concurrently, leveraging parallel jobs and increasing throughput on multi-core machines.
  - Updated Install Tree Layout: The default install tree format is revamped for better organization and reproducibility.
  - Content-Addressed Build Caches: Binary caches now use content-based addressing, improving the reliability and provenance of shared binaries.
  - Improved Git Provenance: Enhanced mirroring and fetching mechanisms for package sources and dependencies.

Visit spack.io

github.com/spack/spack

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E4S: Extreme-scale Scientific Software Stack

https://e4s.io

About E4S

- E4S is an **ecosystem for science** and a community effort to provide open-source software packages for developing, deploying and running scientific applications on HPC platforms.
- E4S has built a comprehensive, coherent software stack that enables application developers to productively develop highly parallel applications that effectively target diverse exascale architectures.
- E4S provides a curated, Spack based software distribution of 125+ HPC (TAU, Trilinos, PETSc,OpenFOAM, Gromacs, Nek5000, LAMMPS), EDA (e.g., Xyce), and AI/ML packages (e.g., Google ADK, NVIDIA NeMo™, NVIDIA BioNeMo™, Vllm, HuggingFace CLI, TensorFlow, PyTorch, OpenCV, TorchBraid, Scikit-Learn, Pandas, JAX, LBANN optimized for GPUs where available).
- 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 clouds: Adaptive Computing's Heidi with ParaTools Pro for E4S™ image for **AWS, GCP, IBM Cloud, Azure, OCI.**
- 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 CPUs and GPUs from NVIDIA, AMD, and Intel
  - 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.
- E4S 25.11 released on November 14, 2025: https://e4s.io/talks/E4S_25.11.pdf

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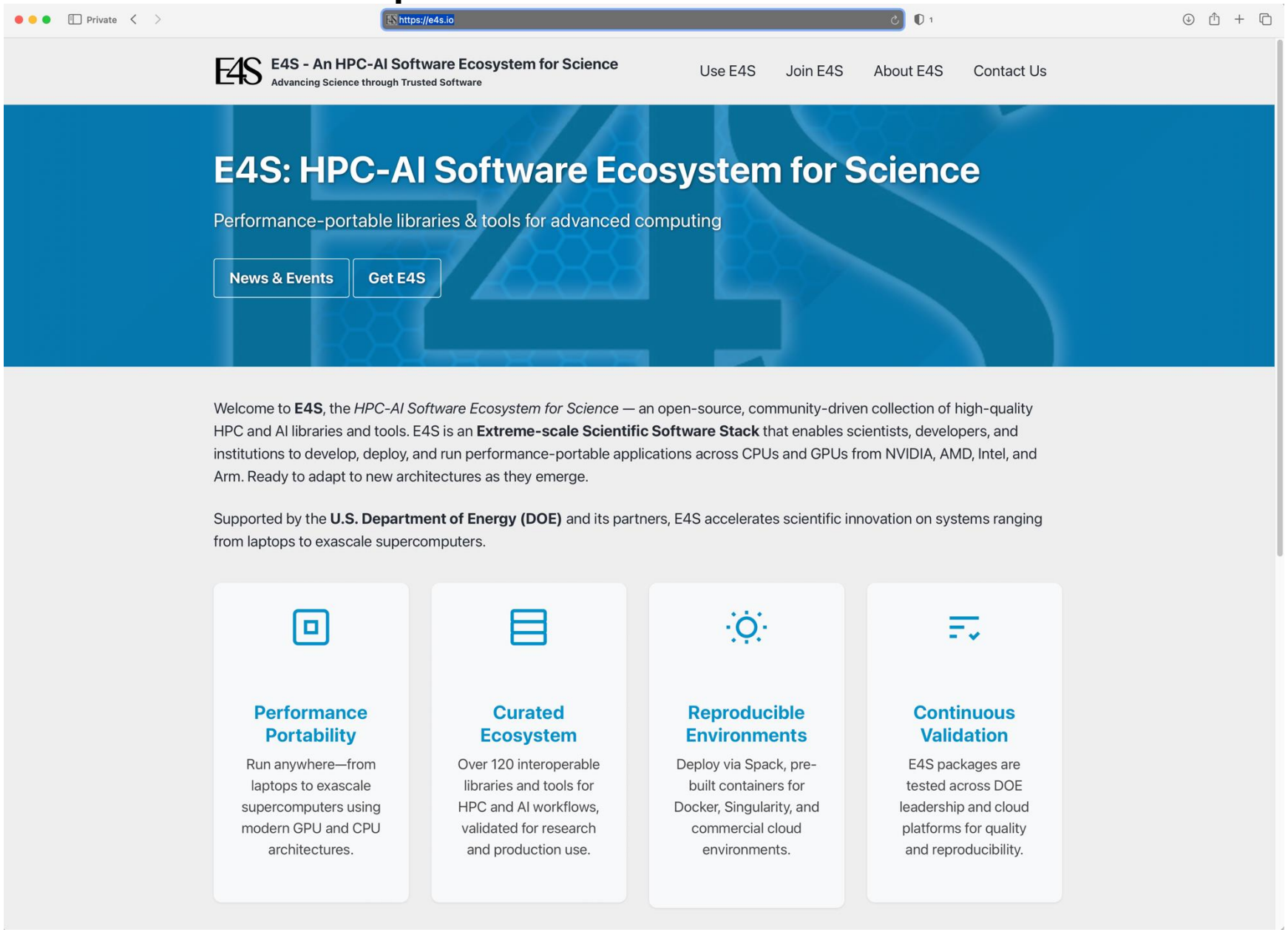
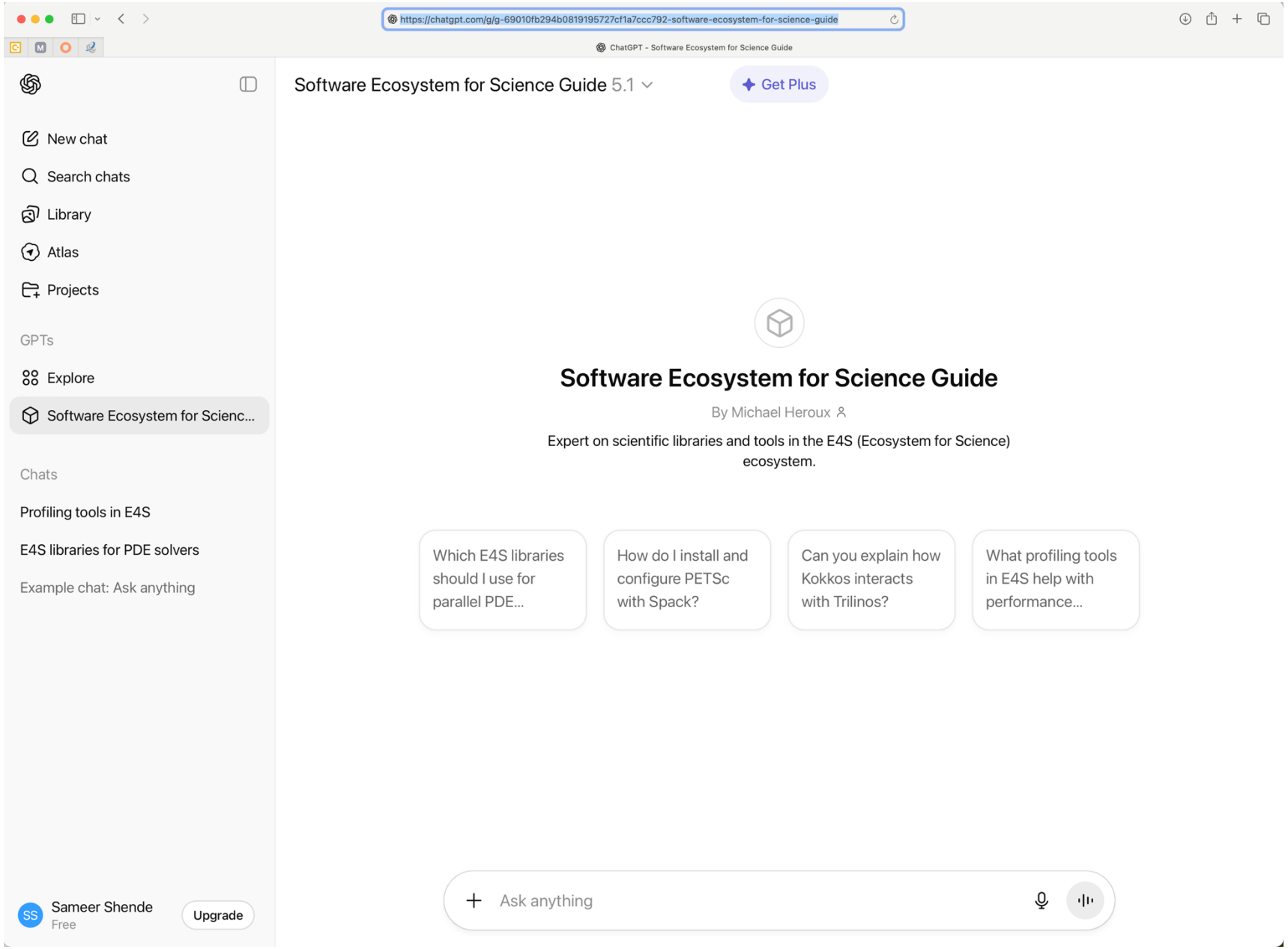
Updated E4S website https://e4s.io

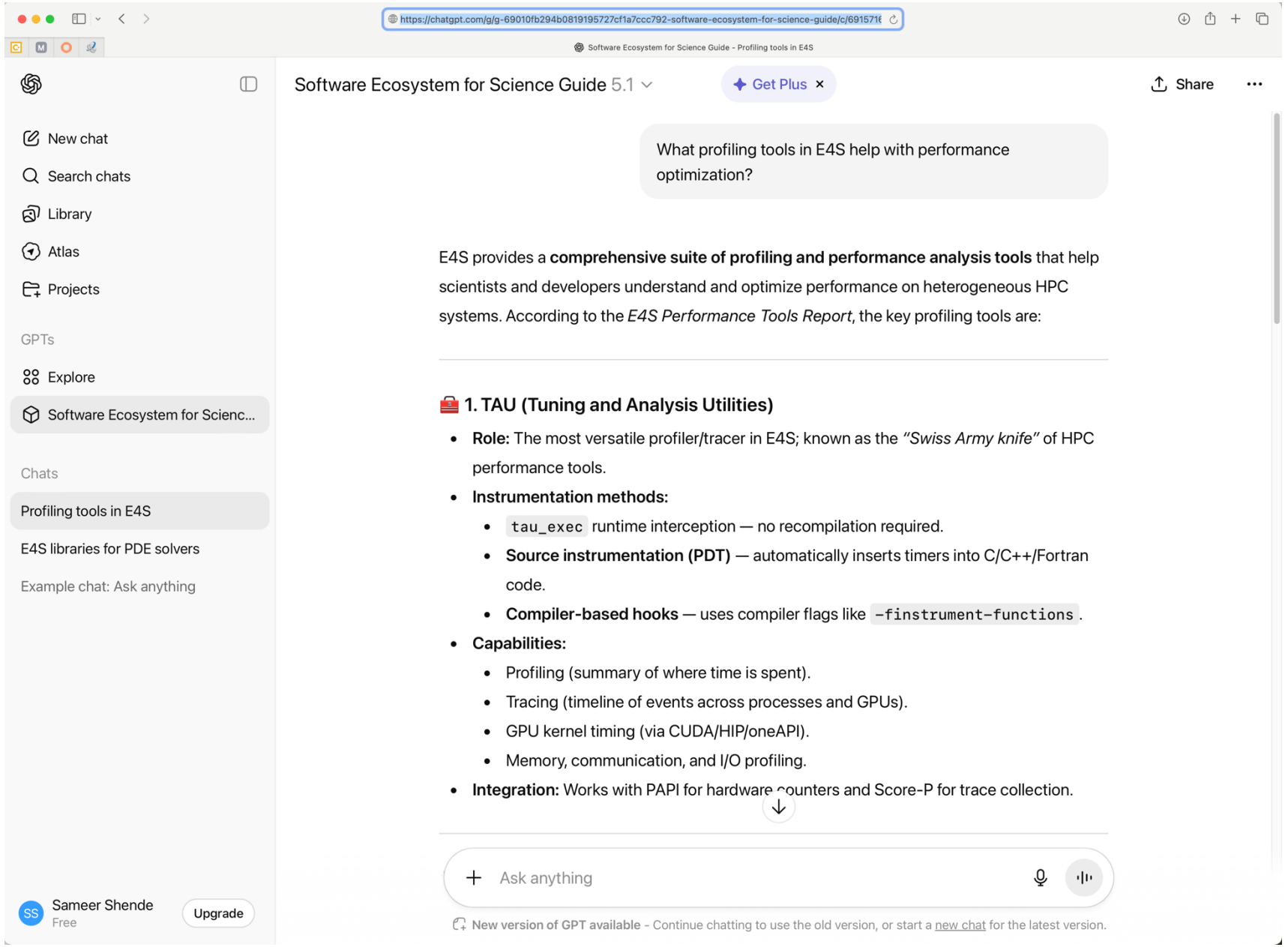


Chatbot integration in E4S Website

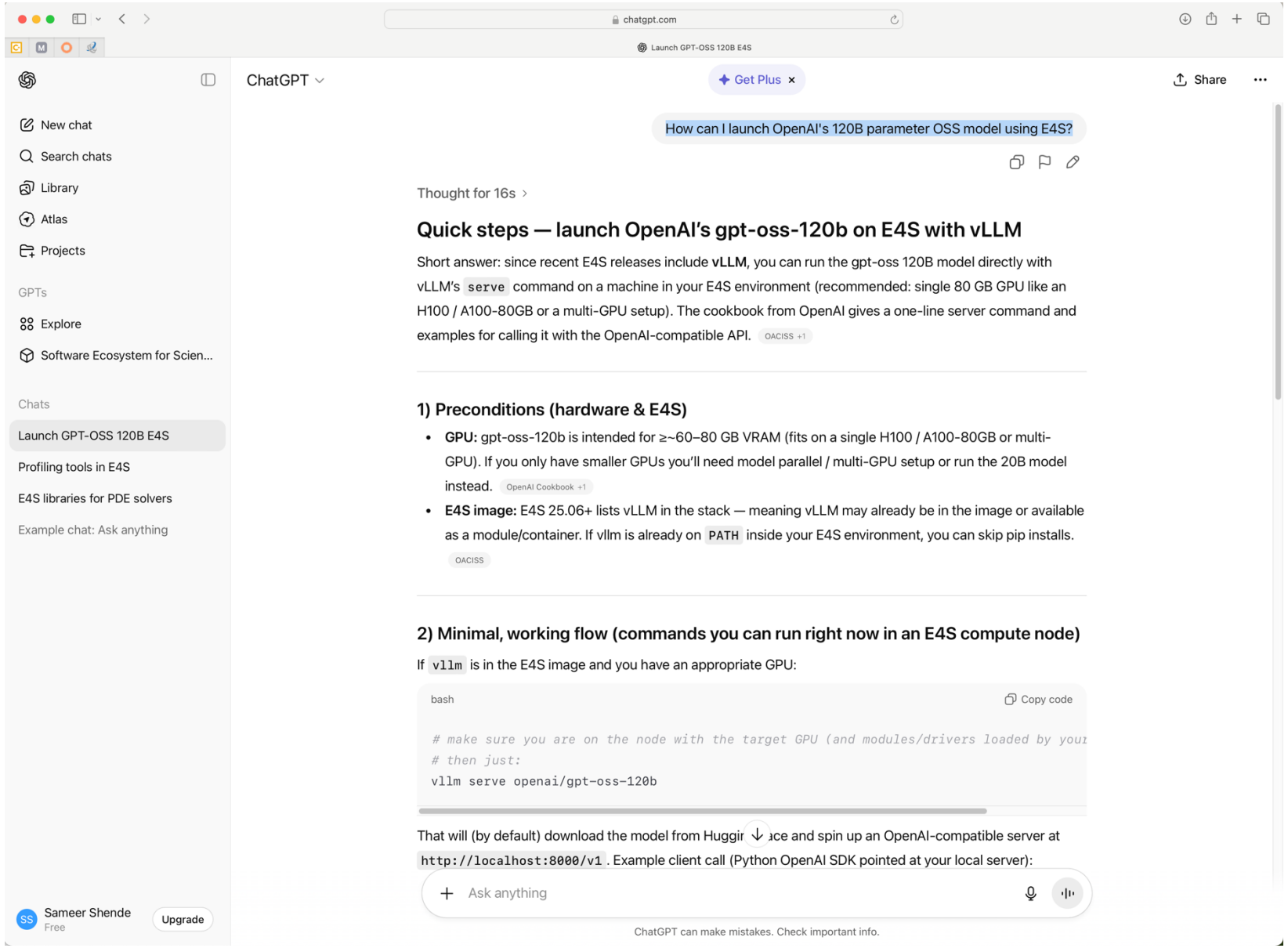
Chatbot integration in E4S Website



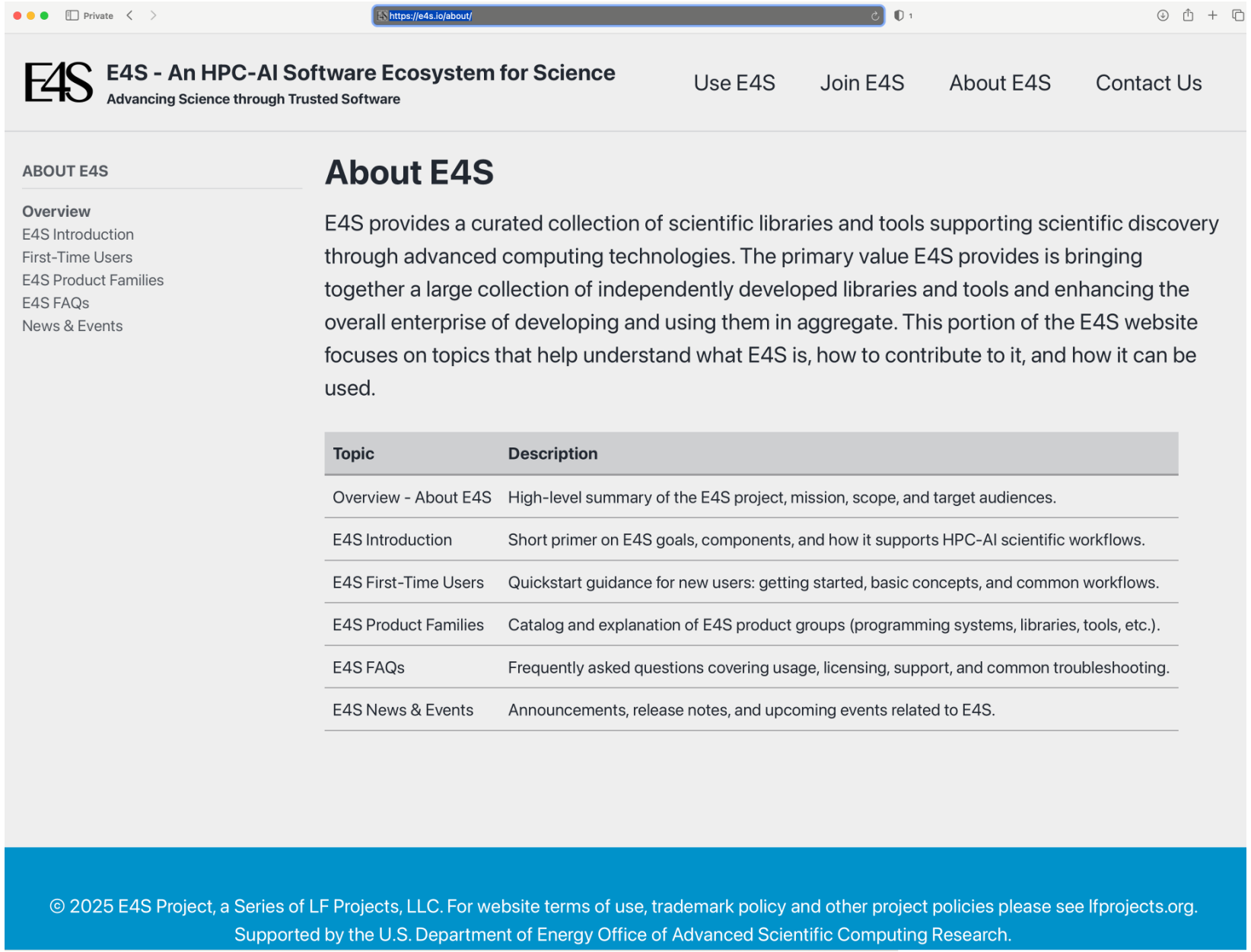
E4S Bot trained on E4S content on OpenAI's ChatGPT



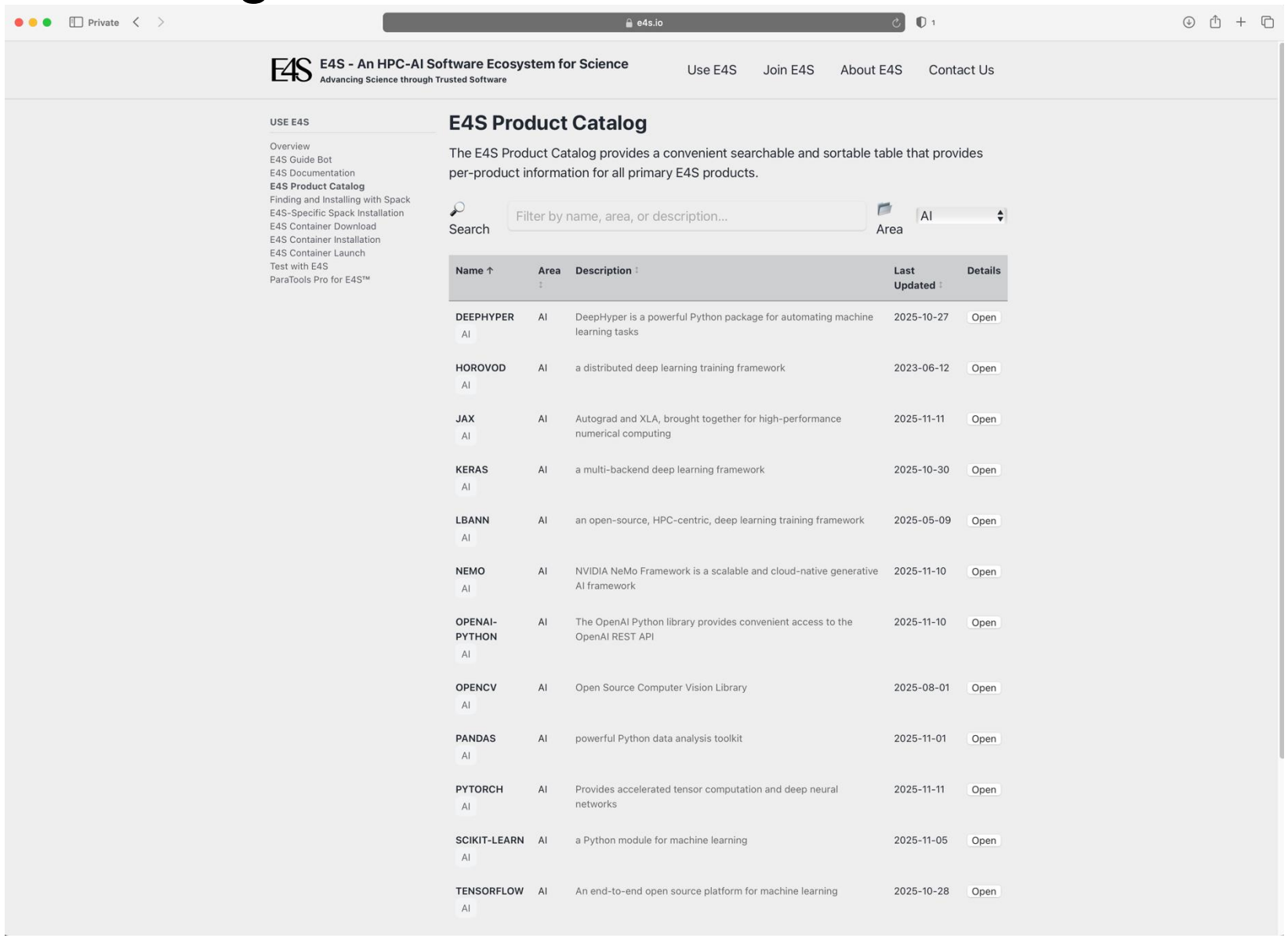
E4S Bot


chatgpt.com
Launch GPT-OSS 120B E4S
ChatGPT
Get Plus
Share
New chat
Search chats
Library
Atlas
Projects
GPTs
Explore
Software Ecosystem for Scien...
Chats
Launch GPT-OSS 120B E4S
Profiling tools in E4S
E4S libraries for PDE solvers
Example chat: Ask anything
Sameer Shende
Free
Upgrade
How can I launch OpenAI's 120B parameter OSS model using E4S?
Thought for 16s
Quick steps — launch OpenAI's gpt-oss-120b on E4S with vLLM
Short answer: since recent E4S releases include vLLM, you can run the gpt-oss 120B model directly with vLLM's serve command on a machine in your E4S environment (recommended: single 80 GB GPU like an H100 / A100-80GB or a multi-GPU setup). The cookbook from OpenAI gives a one-line server command and examples for calling it with the OpenAI-compatible API.
OACISS +1
1) Preconditions (hardware & E4S)
GPU: gpt-oss-120b is intended for ≥~60–80 GB VRAM (fits on a single H100 / A100-80GB or multi-GPU). If you only have smaller GPUs you'll need model parallel / multi-GPU setup or run the 20B model instead.
OpenAI Cookbook +1
E4S image: E4S 25.06+ lists vLLM in the stack — meaning vLLM may already be in the image or available as a module/container. If vllm is already on PATH inside your E4S environment, you can skip pip installs.
OACISS
2) Minimal, working flow (commands you can run right now in an E4S compute node)
If vllm is in the E4S image and you have an appropriate GPU:
bash
Copy code
make sure you are on the node with the target GPU (and modules/drivers loaded by your
then just:
vllm serve openai/gpt-oss-120b
That will (by default) download the model from Huggi ce and spin up an OpenAI-compatible server at http://localhost:8000/v1. Example client call (Python OpenAI SDK pointed at your local server):
Ask anything
ChatGPT can make mistakes. Check important info.

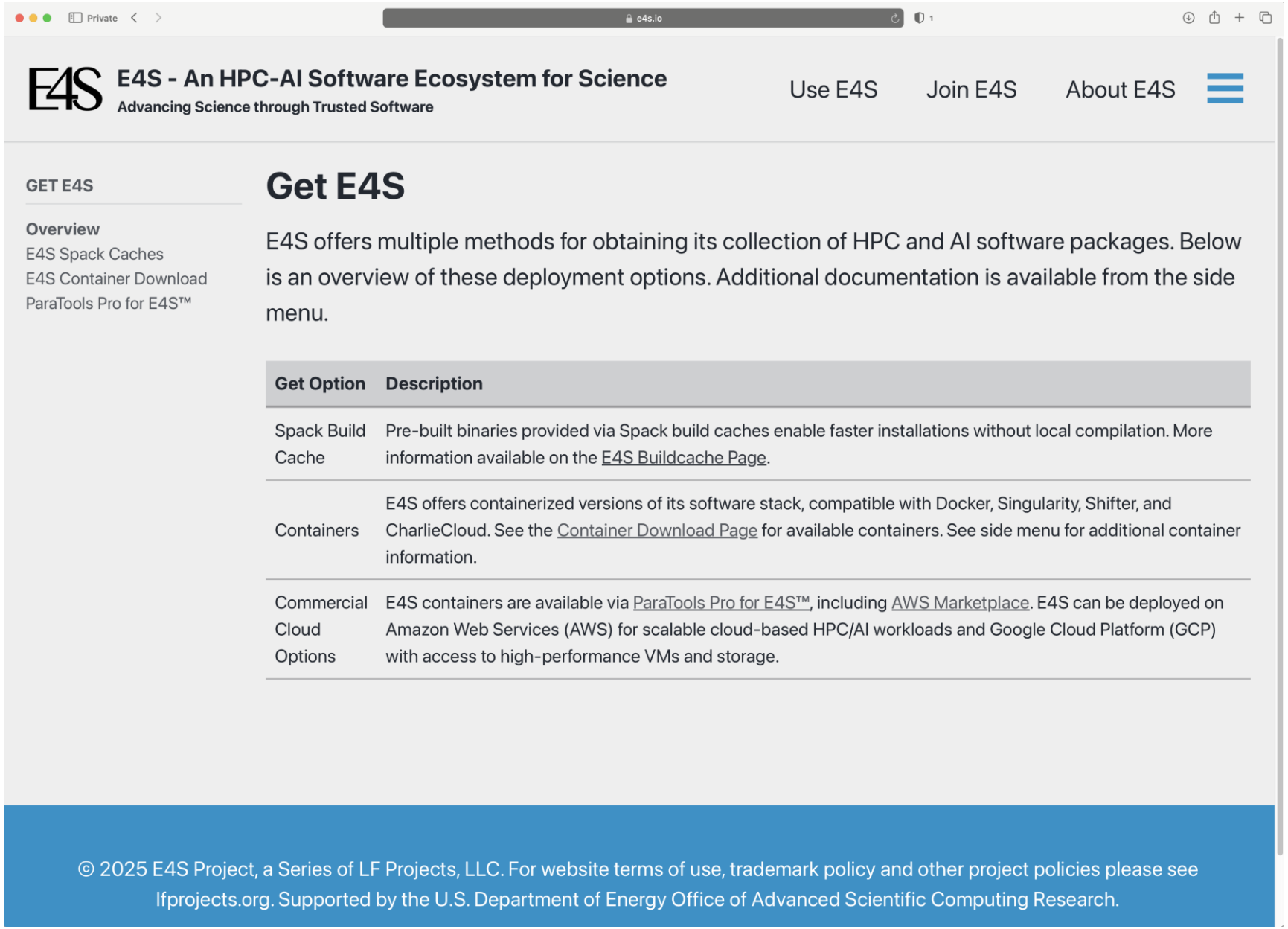
E4S Documentation



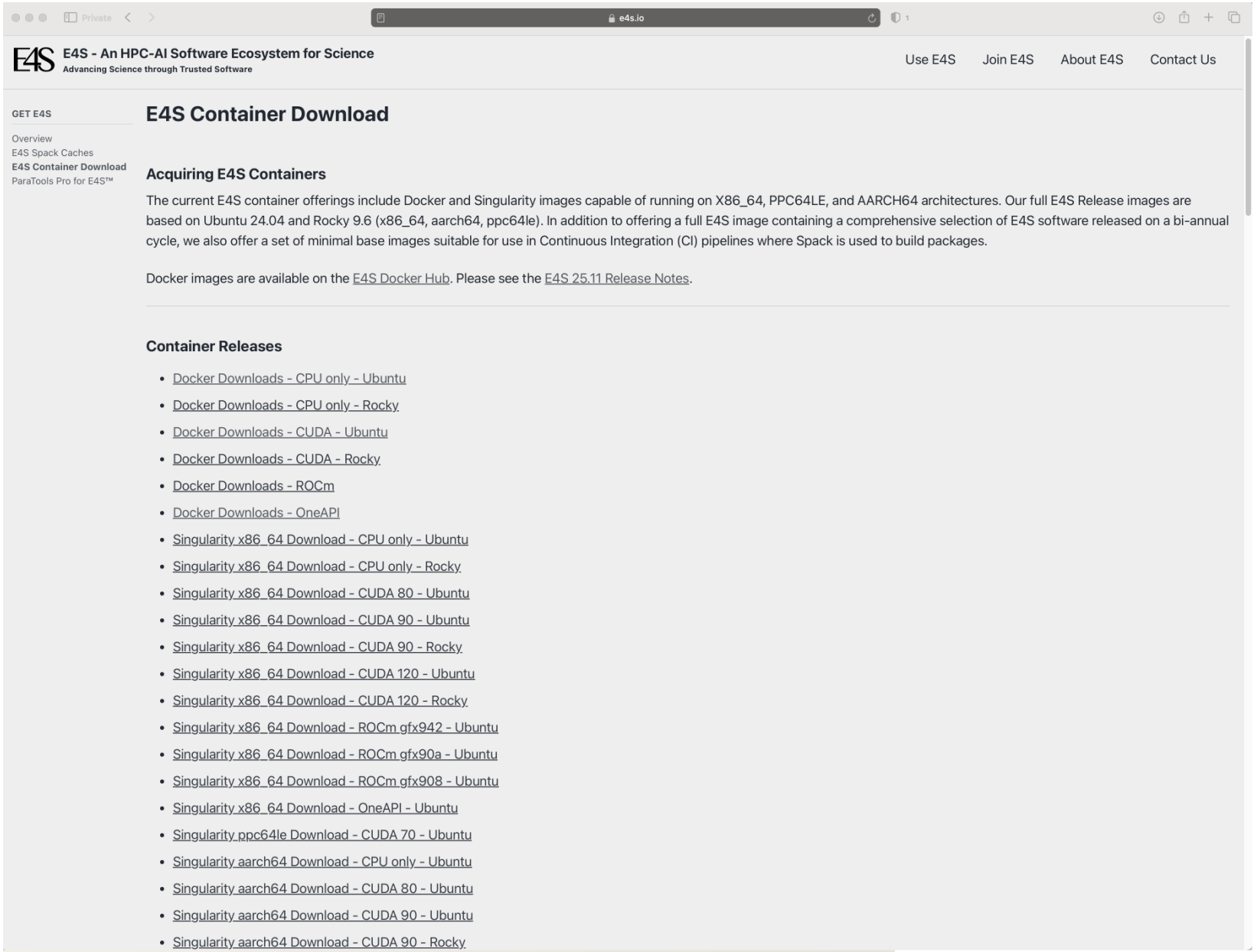
E4S Product Catalog



E4S: Bare-metal installation, Containers, and Cloud images



Download E4S Containers: Rocky Linux 9.6 and Ubuntu 24.04 LTS



- Docker and Singularity
- ARM64 (aarch64), x86_64, and ppc64le
- Support for GPUS:
  - NVIDIA
  - AMD
  - Intel
- GPU Runtimes:
  - CUDA 12.9
  - ROCm 6.4.3
  - oneAPI 2025.2
- Languages:
  - C/C++/Fortran
  - Python
  - Rust
  - Julia
  - Chapel ...
- OSes:
  - Rocky Linux 9.6
  - Ubuntu 24.04 LTS

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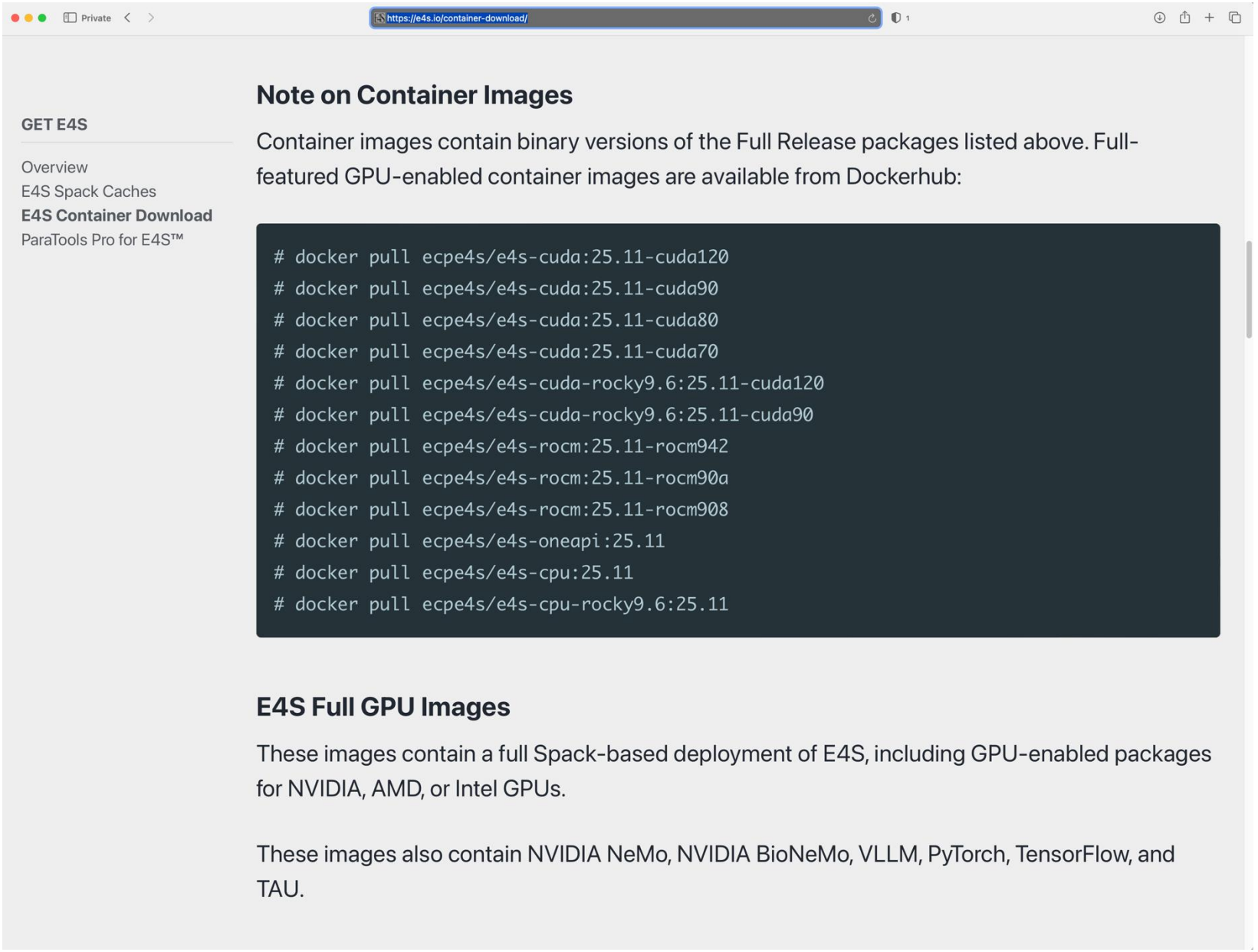
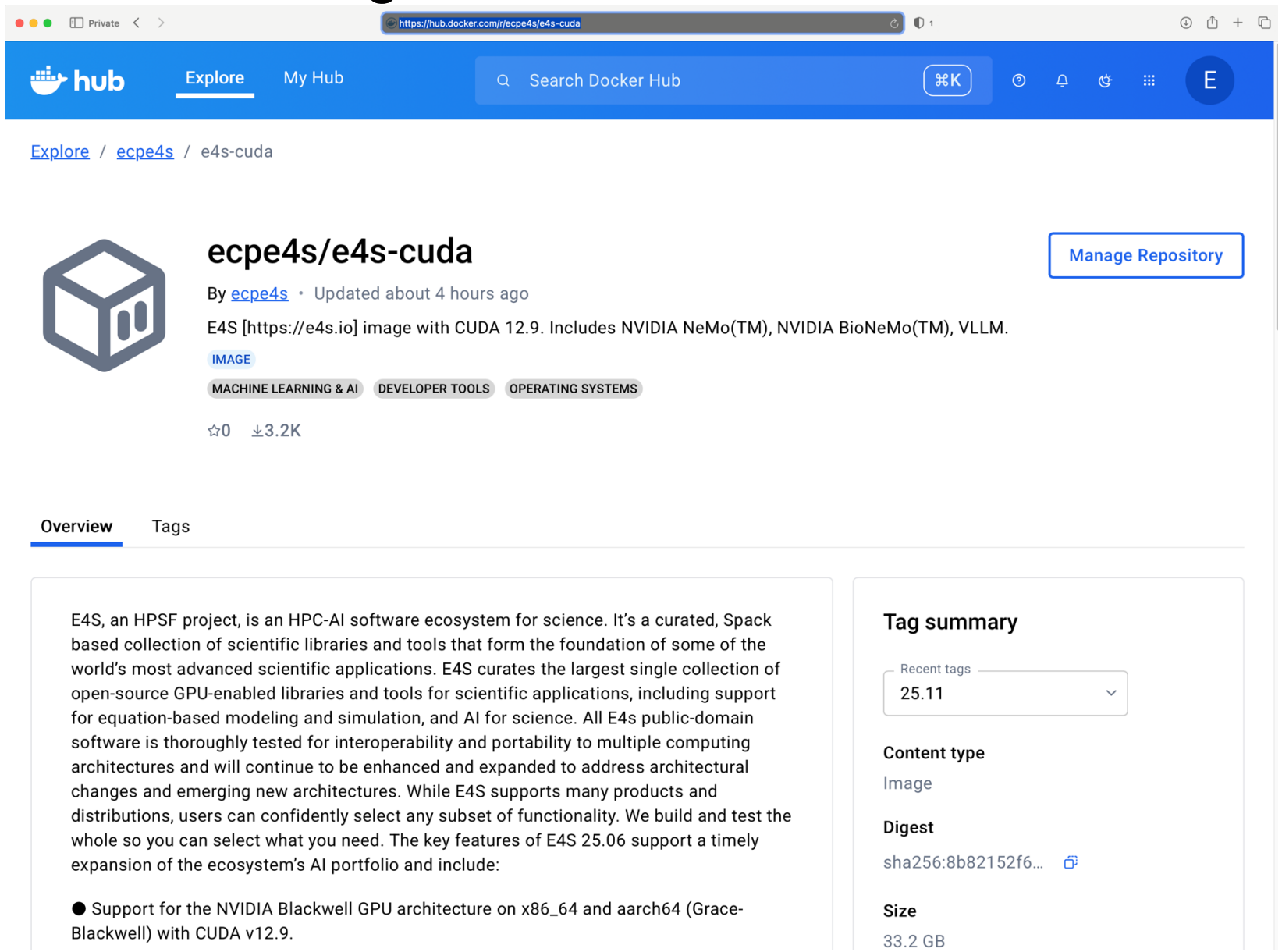
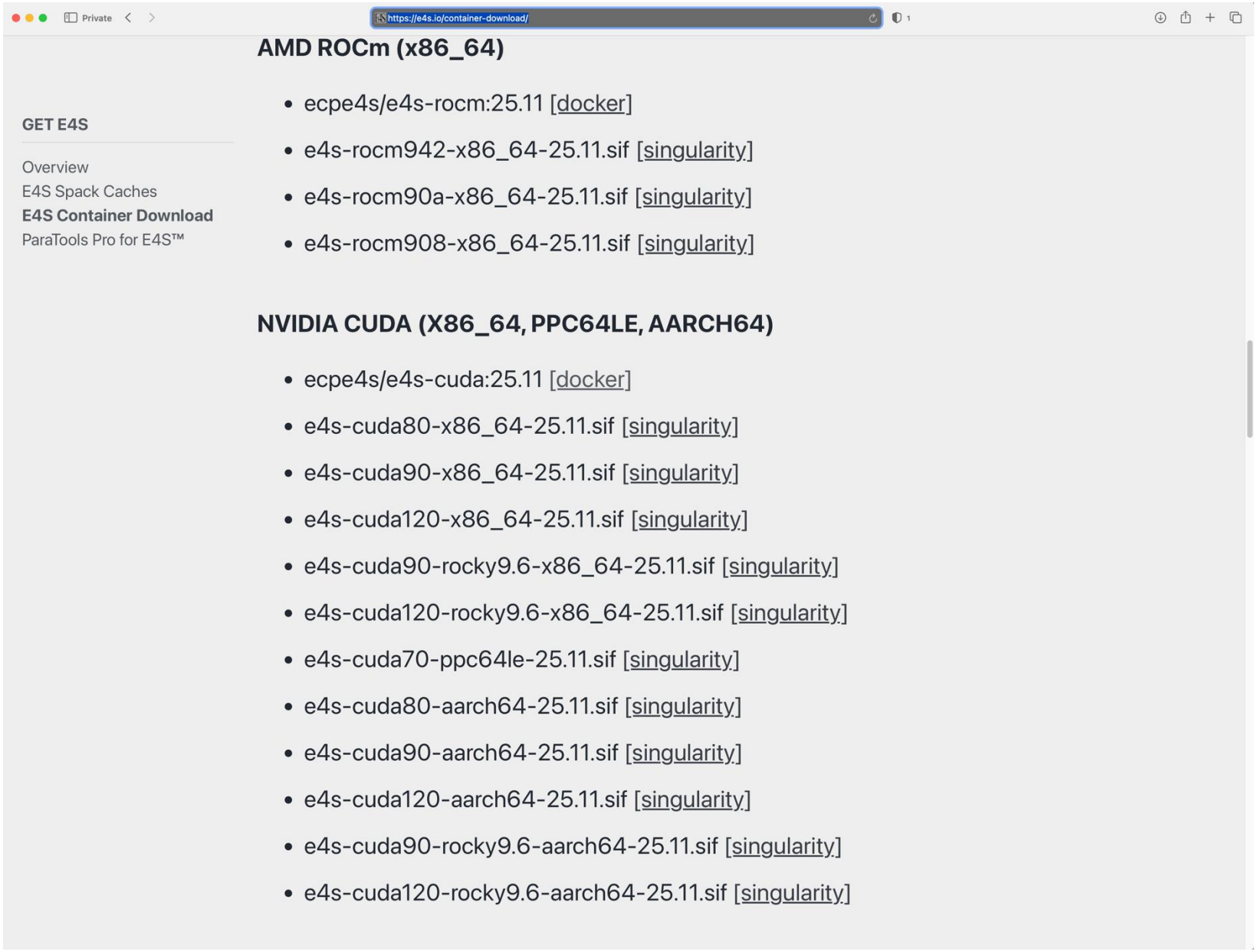
E4S container images available on DockerHub



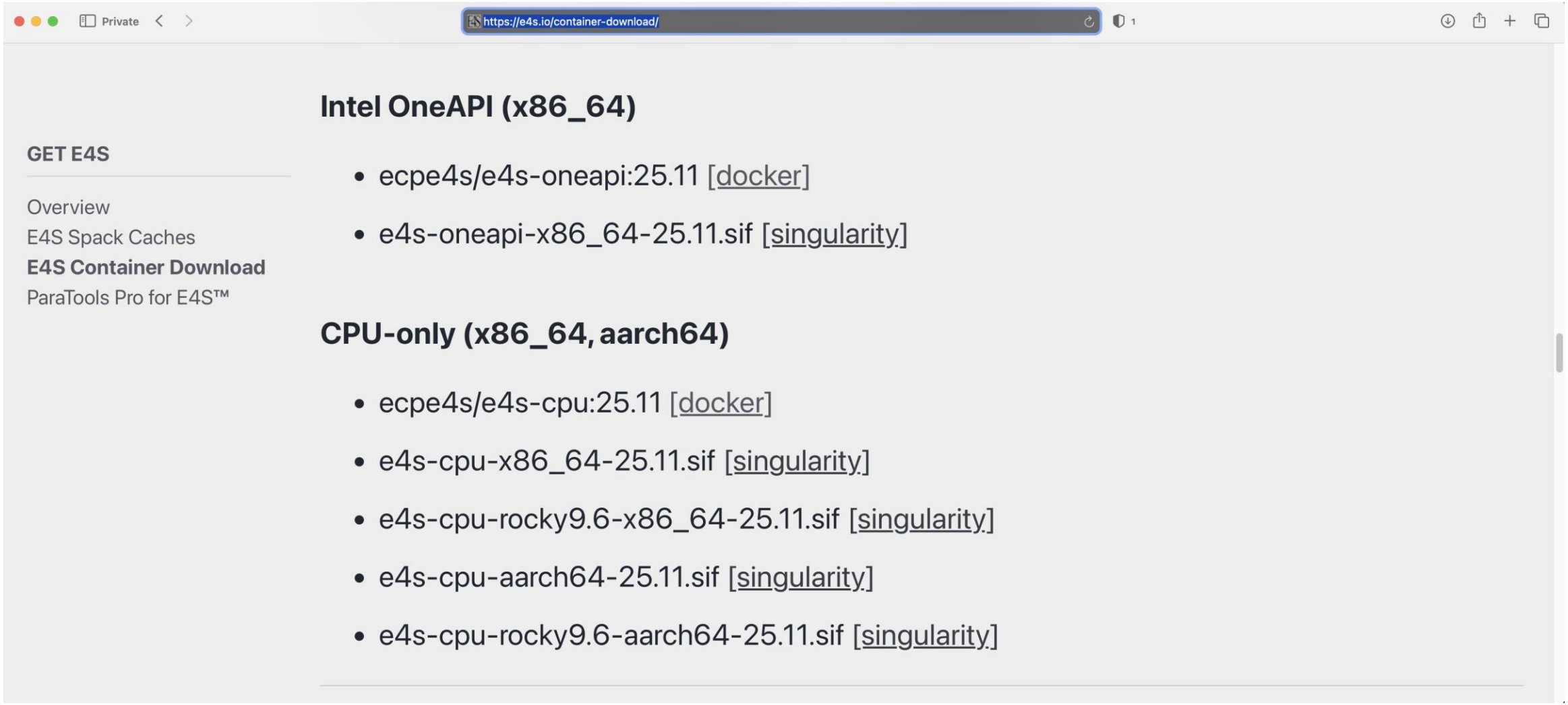
E4S 25.11 container images available on DockerHub



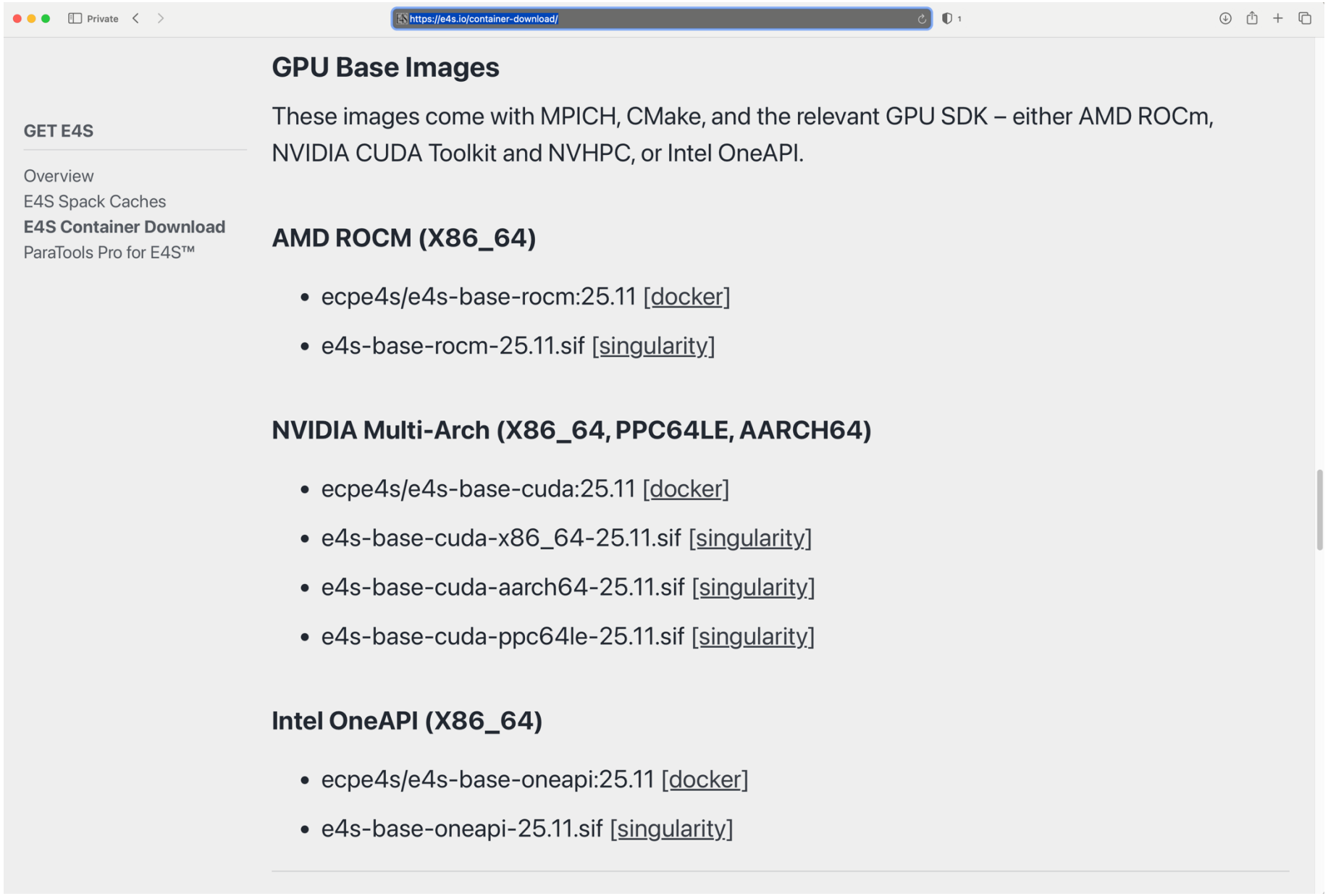
Download E4S containers: NVIDIA and AMD GPUs



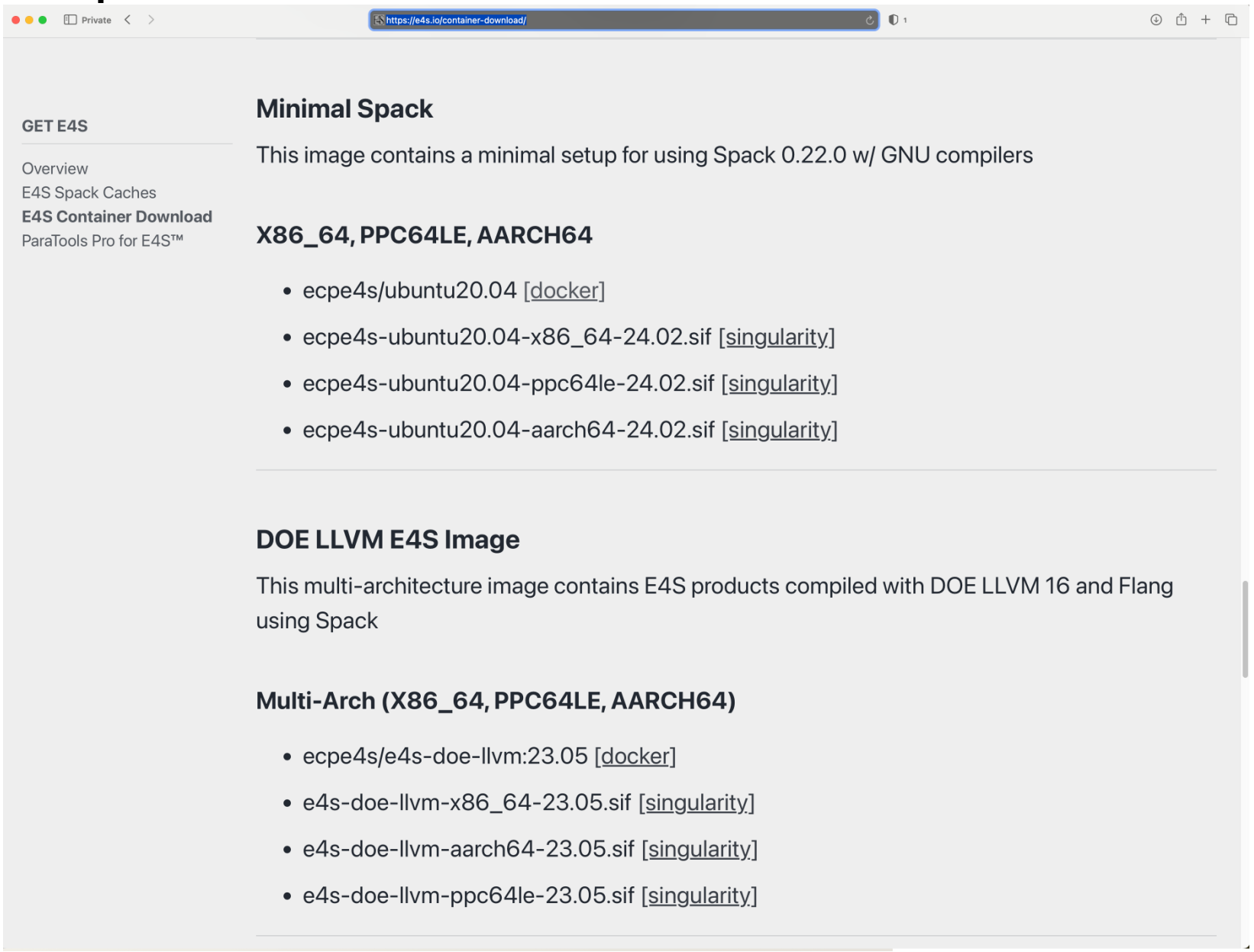
E4S Containers: Intel oneAPI (CPU/GPU) and CPU only



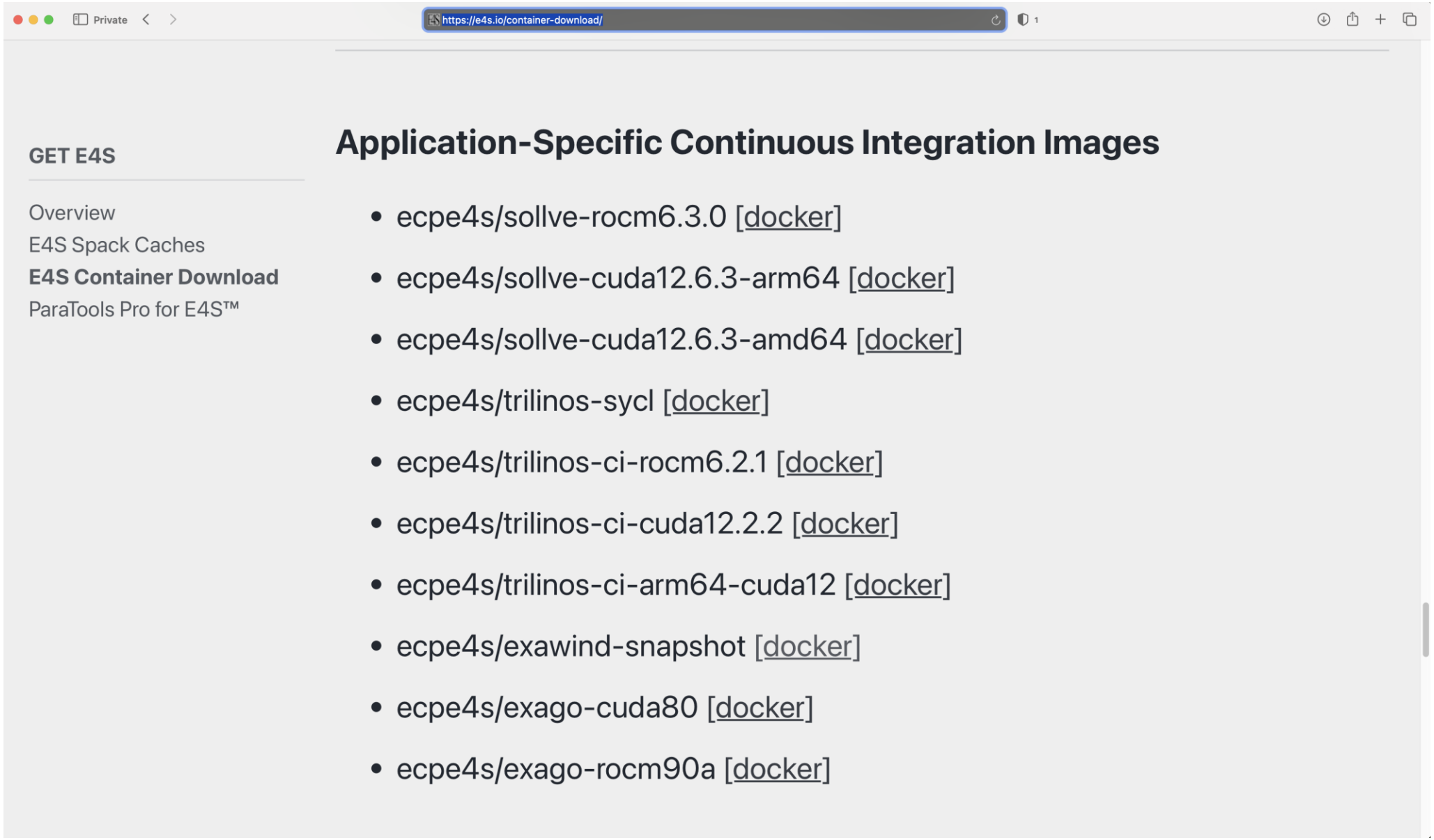
E4S Base Containers with GPU runtimes and MPI



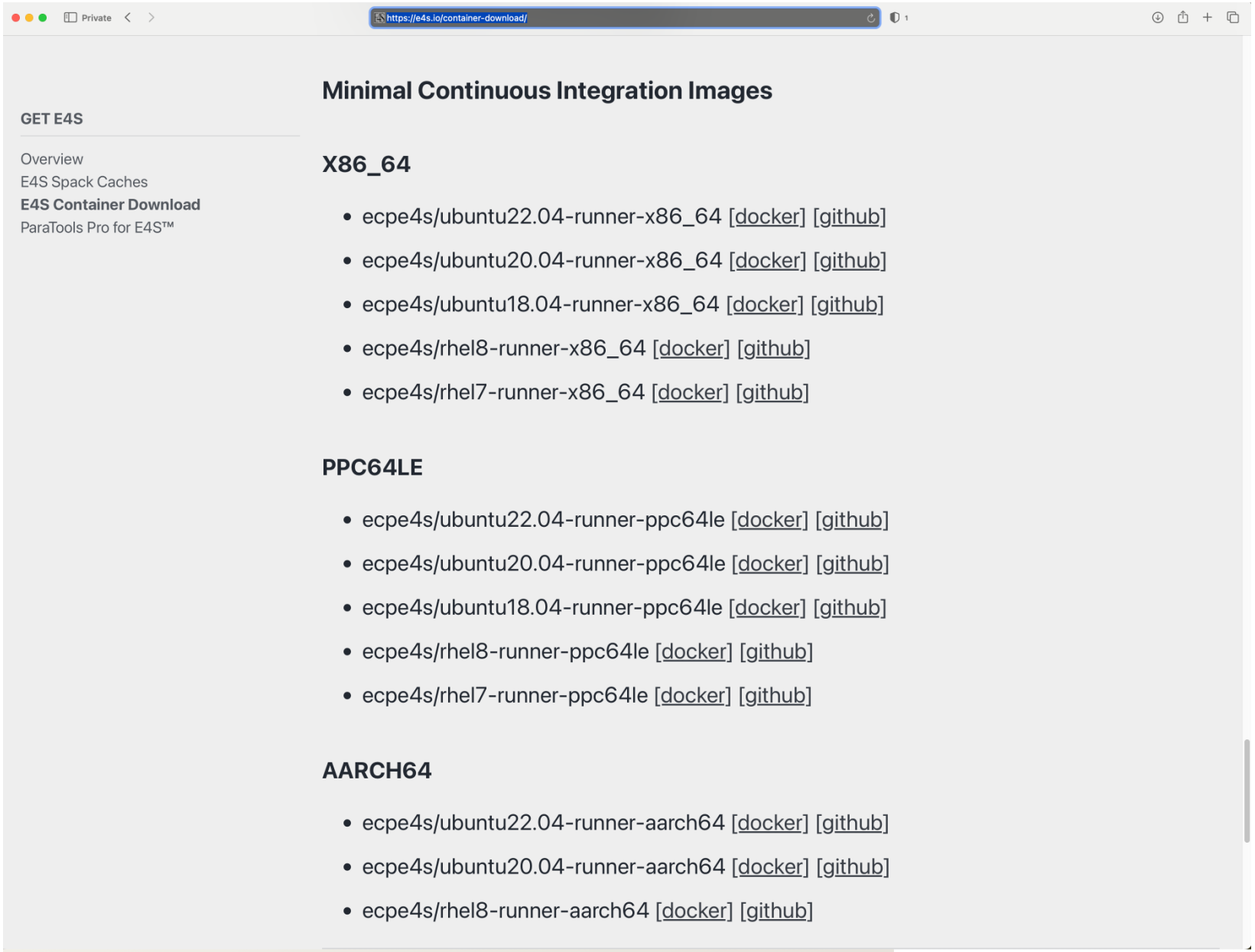
Minimal E4S Spack containers



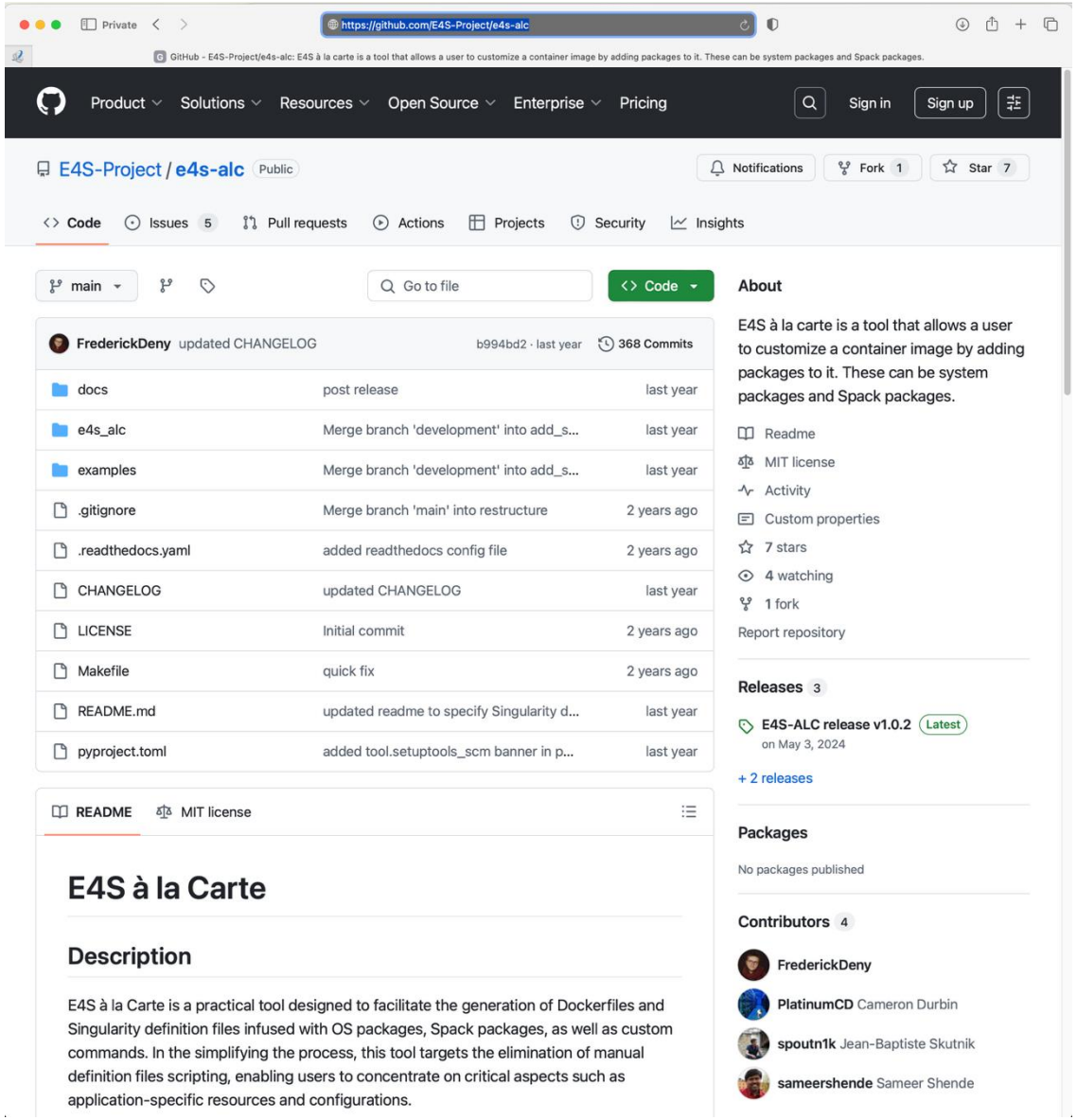
E4S Application Specific Container Images for CI: Customization



E4S Container Images for CI: Gitlab Runners



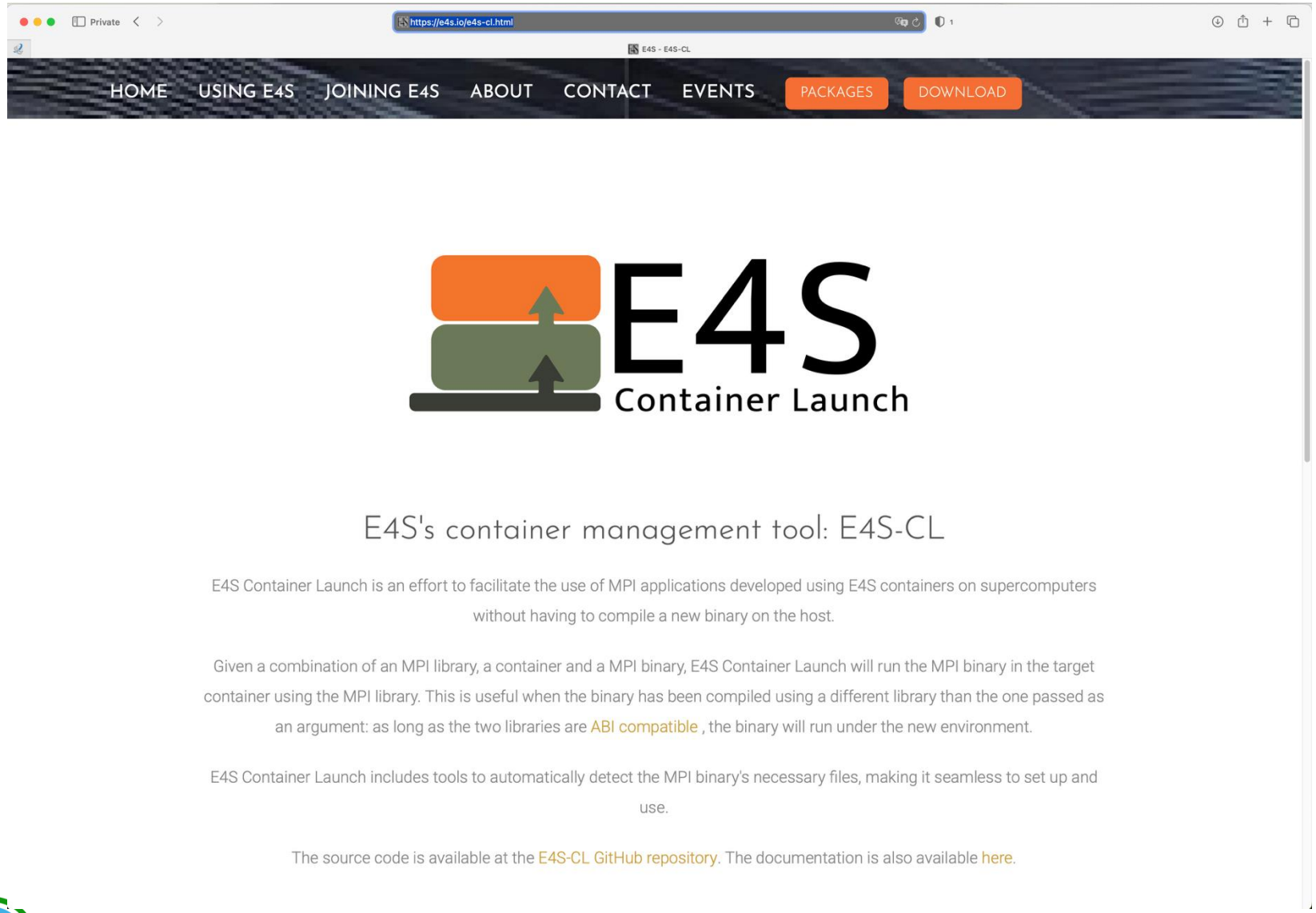
E4S Tools: E4S à la carte or e4s-alc: Customize container images



- Add new system packages
- Add new Spack packages
- Add new tarballs
- Customize the container image
- Start with a base image
- Add packages
- Create a new container image!

https://github.com/E4s-Project/e4s-alc

E4S Tools: e4s-cl: Container Launch tool for MPI applications



- Distribute your MPI application as a binary with an E4S image
- While deploying on a system substitute the embedded containerized MPI in application with the system/vendor MPI
- Use inter-node network interfaces efficiently for near native performance!

https://e4s.io/e4s-cl.html

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 srun -n <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
% e4s-cl srun -n 4 ./a.out
```

E4S Container Launch

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

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E4S Tools: e4s-chain-spack.sh to customize software stack

```
sameer@mothra:~$ ls ~/images
e4s-cuda80-x86_64-25.06.sif
sameer@mothra:~$ singularity run --nv ~/images/e4s-cuda80-x86_64-25.06.sif
Singularity> /etc/e4s/e4s-chain-spack.sh ~/spack
Cloning into '/home/sameer/spack'...
remote: Enumerating objects: 686113, done.
remote: Counting objects: 100% (976/976), done.
remote: Compressing objects: 100% (463/463), done.
remote: Total 686113 (delta 772), reused 518 (delta 510), pack-reused 685137 (from 3)
Receiving objects: 100% (686113/686113), 230.82 MiB | 37.06 MiB/s, done.
Resolving deltas: 100% (326280/326280), done.

------
Configuration SUCCESS!

Downstream: /home/sameer/spack
Upstream: /spack

To use the downstream Spack instance, run the following command in your shell:
. /home/sameer/spack/share/spack/setup-env.sh
------

Singularity> . /home/sameer/spack/share/spack/setup-env.sh
Singularity> spack find valgrind
==> Error: No package matches the query: valgrind
Singularity> spack install valgrind
[+] /usr/local/mpich/install/mpich (external mpich-4.2.3-47excoypwhfmhx57rfs6reouvninugcf)
[+] /usr (external glibc-2.35-a7drdl4tlx4bu3mzhor75pskvd3pdot6)
[+] /spack/opt/spack/linux-ubuntu22.04-x86_64_v3/gcc-11.4.0/gcc-runtime-11.4.0-f63c77kavzjtpmnhucd2oyfaxagwjzla
[+] /spack/opt/spack/linux-ubuntu22.04-x86_64_v3/gcc-11.4.0/boost-1.86.0-6qkv24gbidwxhllgah6jrkym5ev2cng5
[+] /spack/opt/spack/linux-ubuntu22.04-x86_64_v3/gcc-11.4.0/gmake-4.4.1-qp5blvcyuzgzhqsrp2ew6gq2nlos34b2
==> Installing valgrind-3.23.0-feuxx36lsqp7quzmhmo4opbiadwpsars [6/6]
==> No binary for valgrind-3.23.0-feuxx36lsqp7quzmhmo4opbiadwpsars found: installing from source
==> Fetching https://mirror.spack.io/_source-cache/archive/c5/c5c34a3380457b9b75606df890102e7df2c702b9420c2ebef9540f8b5d56264d.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-3.23.0-feuxx36lsqp7quzmhmo4opbiadwpsars
  Stage: 3.78s.  Autoreconf: 0.01s.  Configure: 48.56s.  Build: 37.71s.  Install: 2.97s.  Post-install: 0.60s.  Total: 1m 33.97s
[+] /home/sameer/spack/opt/spack/linux-ubuntu22.04-x86_64_v3/gcc-11.4.0/valgrind-3.23.0-feuxx36lsqp7quzmhmo4opbiadwpsars
Singularity> spack load valgrind
Singularity> which valgrind
/home/sameer/spack/opt/spack/linux-ubuntu22.04-x86_64_v3/gcc-11.4.0/valgrind-3.23.0-feuxx36lsqp7quzmhmo4opbiadwpsars/bin/valgrind
```

Specify location of downstream Spack installation directory

Source downstream Spack's setup-env.sh

Install a new Spack package in downstream Spack directory

Load new package (valgrind) using spack load

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https://e4s.io

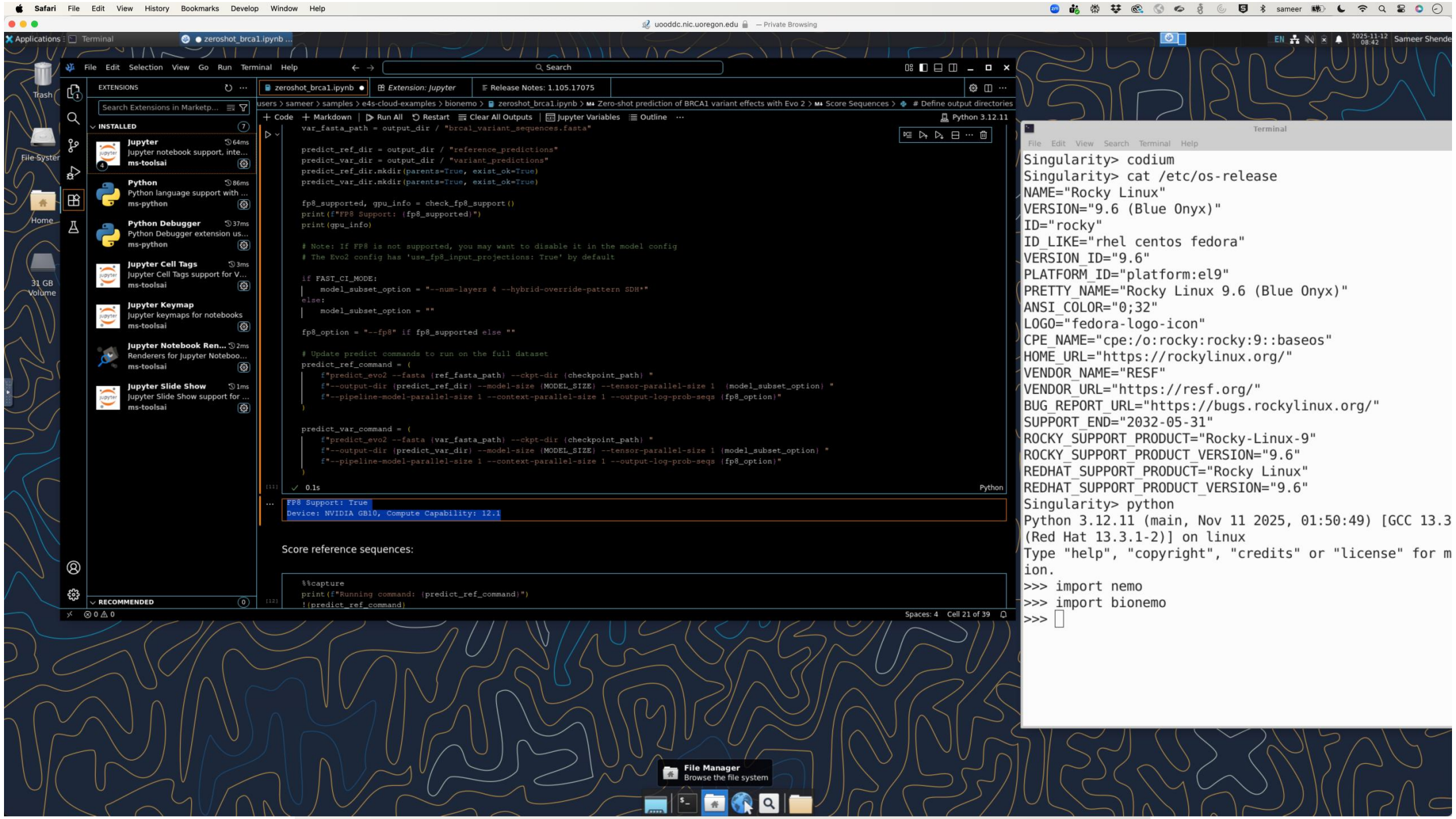
E4S Tools: e4s-chain-spack.sh to customize software stack

```
Singularity> which valgrind
/home/sameer/spack/opt/spack/linux-ubuntu22.04-x86_64_v3/gcc-11.4.0/valgrind-3.23.0-feuxx36lsqp7quzmhmo4opbiadwpsars/bin/valgrind
Singularity> valgrind --help
usage: valgrind [options] prog-and-args

  tool-selection option, with default in [ ]:
    --tool=<name>             use the Valgrind tool named <name> [memcheck]
                              available tools are:
                              memcheck cachegrind callgrind helgrind drd
                              massif dhat lackey none exp-bbv

  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
    -q --quiet                run silently; only print error msgs
    -v --verbose              be more verbose -- show misc extra info
    --trace-children=no|yes   Valgrind-ise child processes (follow execve)? [no]
    --trace-children-skip=patt1,patt2,...    specifies a list of executables
                              that --trace-children=yes should not trace into
    --trace-children-skip-by-arg=patt1,patt2,...   same as --trace-children-skip=
                              but check the argv[] entries for children, rather
                              than the exe name, to make a follow/no-follow decision
    --child-silent-after-fork=no|yes omit child output between fork & exec? [no]
    --vgdb=no|yes|full        activate gdbserver? [yes]
                              full is slower but provides precise watchpoint/step
    --vgdb-error=<number>     invoke gdbserver after <number> errors [999999999]
                              to get started quickly, use --vgdb-error=0
                              and follow the on-screen directions
    --vgdb-stop-at=event1,event2,... invoke gdbserver for given events [none]
         where event is one of:
           startup exit abexit valgrindabexit all none
    --track-fds=no|yes|all    track open file descriptors? [no]
                              all includes reporting stdin, stdout and stderr
    --time-stamp=no|yes       add timestamps to log messages? [no]
    --log-fd=<number>         log messages to file descriptor [2=stderr]
    --log-file=<file>         log messages to <file>
    --log-socket=ipaddr:port  log messages to socket ipaddr:port
    --enable-debuginfod=no|yes query debuginfod servers for missing
                              debuginfo [yes]

  user options for Valgrind tools that report errors:
    --xml=yes                 emit error output in XML (some tools only)
    --xml-fd=<number>         XML output to file descriptor
    --xml-file=<file>         XML output to <file>
    --xml-socket=ipaddr:port  XML output to socket ipaddr:port
    --xml-user-comment=STR    copy STR verbatim into XML output
    --demangle=no|yes         automatically demangle C++ names? [yes]
    --num-callers=<number>    show <number> callers in stack traces [12]
    --error-limit=no|yes      stop showing new errors if too many? [yes]
    --exit-on-first-error=no|yes exit code on the first error found? [no]
    --error-exitcode=<number> exit code to return if errors found [0=disable]
    --error-markers=<begin>,<end> add lines with begin/end markers before/after
                              each error output in plain text mode [none]
    --show-error-list=no|yes|all  show detected errors list and
                              suppression counts at exit [no].
                              all means to also print suppressed errors.
    -s                        same as --show-error-list=yes
```

Downstream Spack's package is loaded in your environment

e4s-chain-spack.sh helps customize the software stack using upstream /spack (read-only in the container) for package dependencies while installing a new package in the downstream Spack in your writable home directory.

E4S: NVIDIA BioNeMo™ on NVIDIA Grace-Blackwell architecture



E4S: NVIDIA Grace-Blackwell CUDA 120 Rocky Linux 9.6 image

```
$ singularity run --nv e4s-cuda120-rocky9.6-aarch64-25.11.sif
Singularity>
Singularity> nvidia-smi -L
GPU 0: NVIDIA GB10 (UUID: GPU-233b4e95-c45e-17bd-40d5-daa39dbbd475)
Singularity> spack find -x
-- linux-rocky9-aarch64 / %c,cxx,fortran=gcc@13.3.1 -------------
adios2@2.10.2  caliper@2.12.1  hypre@2.33.0    magma@2.9.0      petsc@3.24.0      slepc@3.24.0     sundials@7.5.0      tau@2.35         umpire@2025.03.0
amrex@25.10    heffte@2.4.1    libceed@0.12.0  paraview@5.13.3  slate@2025.05.28  strumpack@8.0.0  superlu-dist@9.1.0  trilinos@16.1.0  zfp@1.0.1

-- linux-rocky9-aarch64 / %c,cxx=gcc@13.3.1 ----------------------
cabana@0.7.0    chapel@2.6.0  flecsi@2.4.1   gromacs@2025.3       lammps@20250722  libpressio@0.99.4        omega-h@10.8.6-scorec  vtk-m@2.3.0
chai@2025.03.0  fftx@1.2.0    ginkgo@1.10.0  hpctoolkit@2025.0.1  legion@25.03.0   mgard@compat-2023-12-09  upcxx@2023.9.0

-- linux-rocky9-aarch64 / %c=gcc@13.3.1 -------------------------
parsec@4.0.2411

-- linux-rocky9-aarch64 / %cxx,fortran=gcc@13.3.1 ---------------
tasmanian@8.1

-- linux-rocky9-aarch64 / %cxx=gcc@13.3.1 -----------------------
arborx@1.5  hpx@1.11.0  kokkos@4.7.01  kokkos-kernels@4.7.01

-- linux-rocky9-aarch64 / no compilers --------------------------
e4s-alc@1.0.3  e4s-cl@1.0.5  mpich@4.3.1
==> 42 installed packages
Singularity> module avail
---------------------------------------------------------------------------- /spack/share/spack/modules/linux-rocky9-aarch64 -----------------------------------------------------------------------------
adios2/2.10.2-cuda120   e4s-alc/1.0.3                hpctoolkit/2025.0.1-cuda        libceed/0.12.0-cuda120                  parsec/4.0.2411-cuda120          tasmanian/8.1-cuda120
amrex/25.10-cuda120     e4s-cl/1.0.5                 hpx/1.11.0-cuda120              libpressio/0.99.4-cuda120-openmp        petsc/3.24.0-cuda120             tau/2.35-cuda
arborx/1.5-cuda120      fftx/1.2.0-cuda120           hypre/2.33.0-cuda120            magma/2.9.0-cuda120                     slate/2025.05.28-cuda120-openmp  trilinos/16.1.0-cuda120
cabana/0.7.0-cuda120    flecsi/2.4.1-cuda120         kokkos-kernels/4.7.01-cuda120   mgard/compat-2023-12-09-cuda120-openmp  slepc/3.24.0-cuda120             umpire/2025.03.0-cuda120
caliper/2.12.1-cuda120  ginkgo/1.10.0-cuda120-openmp kokkos/4.7.01-cuda120          mpich/4.3.1                             strumpack/8.0.0-cuda120-openmp   upcxx/2023.9.0-cuda120
chai/2025.03.0-cuda120  gromacs/2025.3-cuda120-openmp lammps/20250722-cuda120-openmp omega-h/10.8.6-scorec-cuda120       sundials/7.5.0-cuda120           vtk-m/2.3.0-cuda120-openmp
chapel/2.6.0-cuda120    heffte/2.4.1-cuda120         legion/25.03.0-cuda70           paraview/5.13.3                         superlu-dist/9.1.0-cuda120       zfp/1.0.1-cuda120

Key:
loaded  modulepath
Singularity> cat /etc/os-release | grep PRETTY_NAME
PRETTY_NAME="Rocky Linux 9.6 (Blue Onyx)"
Singularity> uname -m
aarch64
Singularity>
```

E4S: NVIDIA x86_64-Blackwell (CUDA 120) Rocky Linux 9.6 image

```
$ singularity run --nv e4s-cuda120-rocky9.6-x86_64-25.11.sif
Singularity>
Singularity> nvidia-smi -L
GPU 0: NVIDIA RTX PRO 6000 Blackwell Server Edition (UUID: GPU-0a3e5316-2d97-bf04-1ed7-011560029cf3)
Singularity> spack find -x
-- linux-rocky9-x86_64_v3 / %c,cxx,fortran=gcc@13.3.1 -----------
adios2@2.10.2   heffte@2.4.1  libceed@0.12.0  papi@7.2.0        strumpack@8.0.0  superlu-dist@9.1.0  umpire@2025.03.0
caliper@2.12.1  hypre@2.33.0  magma@2.9.0     slate@2025.05.28  sundials@7.5.0   tau@2.35            zfp@1.0.1

-- linux-rocky9-x86_64_v3 / %c,cxx=gcc@13.3.1 -------------------
bricks@2023.08.25  cabana@0.7.0  chai@2025.03.0  chapel@2.6.0  cusz@0.14.0  fftx@1.2.0  flecsi@2.4.1  ginkgo@1.10.0  hpctoolkit@2025.0.1  legion@25.03.0  mgard@compat-2023-12-09  vtk-m@2.3.0

-- linux-rocky9-x86_64_v3 / %c=gcc@13.3.1 -----------------------
parsec@4.0.2411

-- linux-rocky9-x86_64_v3 / %cxx,fortran=gcc@13.3.1 -------------
tasmanian@8.1

-- linux-rocky9-x86_64_v3 / %cxx=gcc@13.3.1 ---------------------
arborx@1.5  hpx@1.11.0  kokkos@4.7.01  kokkos-kernels@4.7.01

-- linux-rocky9-x86_64_v3 / no compilers ------------------------
e4s-alc@1.0.3  e4s-cl@1.0.5  mpich@4.3.1
==> 35 installed packages
Singularity> module avail
------------------------------------------------------------------------------ /spack/share/spack/modules/linux-rocky9-x86_64_v3 ------------------------------------------------------------------------------
adios2/2.10.2-cuda120   chapel/2.6.0-cuda120  ginkgo/1.10.0-cuda120-openmp   kokkos/4.7.01-cuda120                   papi/7.2.0-cuda                 tasmanian/8.1-cuda120
arborx/1.5-cuda120      cusz/0.14.0-cuda120   heffte/2.4.1-cuda120           legion/25.03.0-cuda70                   parsec/4.0.2411-cuda120         tau/2.35-cuda
bricks/2023.08.25-cuda  e4s-alc/1.0.3         hpctoolkit/2025.0.1-cuda       libceed/0.12.0-cuda120                  slate/2025.05.28-cuda120-openmp umpire/2025.03.0-cuda120
cabana/0.7.0-cuda120    e4s-cl/1.0.5          hpx/1.11.0-cuda120             magma/2.9.0-cuda120                     strumpack/8.0.0-cuda120-openmp  vtk-m/2.3.0-cuda120-openmp
caliper/2.12.1-cuda120  fftx/1.2.0-cuda120    hypre/2.33.0-cuda120           mgard/compat-2023-12-09-cuda120-openmp  sundials/7.5.0-cuda120          zfp/1.0.1-cuda120
chai/2.03.0-cuda120     flecsi/2.4.1-cuda120  kokkos-kernels/4.7.01-cuda120  mpich/4.3.1                             superlu-dist/9.1.0-cuda120

------------------------------------------------------------------------------ /usr/share/Modules/modulefiles ------------------------------------------------------------------------------
dot  module-git  module-info  modules  null  use.own

Key:
loaded  modulepath
Singularity> cat /etc/os-release | grep PRETTY_NAME
PRETTY_NAME="Rocky Linux 9.6 (Blue Onyx)"
Singularity> uname -m
x86_64
Singularity>
```

E4S: NVIDIA x86_64-Blackwell (CUDA 120) Rocky Linux 9.6 image

```
Singularity> module avail
------------------------------------------------------------------------------ /spack/share/spack/modules/linux-rocky9-x86_64_v3 ------------------------------------------------------------------------------
adios2/2.10.2-cuda120   chapel/2.6.0-cuda120  ginkgo/1.10.0-cuda120-openmp   kokkos/4.7.01-cuda120                 papi/7.2.0-cuda                  tasmanian/8.1-cuda120
arborx/1.5-cuda120      cusz/0.14.0-cuda120   heffte/2.4.1-cuda120           legion/25.03.0-cuda70                 parsec/4.0.2411-cuda120          tau/2.35-cuda
bricks/2023.08.25-cuda  e4s-alc/1.0.3         hpctoolkit/2025.0.1-cuda       libceed/0.12.0-cuda120                slate/2025.05.28-cuda120-openmp  umpire/2025.03.0-cuda120
cabana/0.7.0-cuda120    e4s-cl/1.0.5          hpx/1.11.0-cuda120             magma/2.9.0-cuda120                   strumpack/8.0.0-cuda120-openmp   vtk-m/2.3.0-cuda120-openmp
caliper/2.12.1-cuda120  fftx/1.2.0-cuda120    hypre/2.33.0-cuda120           mgard/compat-2023-12-09-cuda120-openmp sundials/7.5.0-cuda120           zfp/1.0.1-cuda120
chai/2025.03.0-cuda120  flecsi/2.4.1-cuda120  kokkos-kernels/4.7.01-cuda120  mpich/4.3.1                           superlu-dist/9.1.0-cuda120

------------------------------------------------------------------------------ /usr/share/Modules/modulefiles ------------------------------------------------------------------------------
dot  module-git  module-info  modules  null  use.own

Key:
loaded  modulepath
Singularity> spack find -x
-- linux-rocky9-x86_64_v3 / %c,cxx,fortran=gcc@13.3.1 -----------
adios2@2.10.2   heffte@2.4.1  libceed@0.12.0  papi@7.2.0        strumpack@8.0.0  superlu-dist@9.1.0  umpire@2025.03.0
caliper@2.12.1  hypre@2.33.0  magma@2.9.0     slate@2025.05.28  sundials@7.5.0   tau@2.35            zfp@1.0.1

-- linux-rocky9-x86_64_v3 / %c,cxx=gcc@13.3.1 -------------------
bricks@2023.08.25  cabana@0.7.0  chai@2025.03.0  chapel@2.6.0  cusz@0.14.0  fftx@1.2.0  flecsi@2.4.1  ginkgo@1.10.0  hpctoolkit@2025.0.1  legion@25.03.0  mgard@compat-2023-12-09  vtk-m@2.3.0

-- linux-rocky9-x86_64_v3 / %c=gcc@13.3.1 -----------------------
parsec@4.0.2411

-- linux-rocky9-x86_64_v3 / %cxx,fortran=gcc@13.3.1 -------------
tasmanian@8.1

-- linux-rocky9-x86_64_v3 / %cxx=gcc@13.3.1 ---------------------
arborx@1.5  hpx@1.11.0  kokkos@4.7.01  kokkos-kernels@4.7.01

-- linux-rocky9-x86_64_v3 / no compilers ------------------------
e4s-alc@1.0.3  e4s-cl@1.0.5  mpich@4.3.1
==> 35 installed packages
Singularity>
```

E4S NVIDIA Blackwell x86_64 Rocky Linux 9.6 Python Packages

```
$ singularity run --nv e4s-cuda120-rocky9.6-x86_64-25.11.sif
Singularity> nvidia-smi -L
GPU 0: NVIDIA RTX PRO 6000 Blackwell Server Edition (UUID: GPU-0a3e5316-2d97-bf04-1ed7-011560029cf3)
Singularity> uname -m
x86_64
Singularity> which python
/opt/python/pkgs/python-3.12.11/bin/python
Singularity> ls /opt/python/pkgs/python-3.12.11/lib/python3.12/
abc.py               compileall.py                ensurepip      imaplib.py      ntpath.py       _py_abc.py      signal.py                                  sysconfig.py        unittest
aifc.py              _compression.py              enum.py        imghdr.py       nturl2path.py   __pycache__     _sitebuiltins.py                           tabnanny.py         urllib
_aix_support.py      concurrent                   filecmp.py     importlib       numbers.py      pyclbr.py       site-packages                              tarfile.py          uuid.py
antigravity.py       config-3.12-x86_64-linux-gnu fileinput.py   inspect.py      opcode.py       py_compile.py   site.py                                    telnetlib.py        uu.py
argparse.py          configparser.py              fnmatch.py     io.py           operator.py     _pydatetime.py  smtplib.py                                 tempfile.py         venv
ast.py               contextlib.py                fractions.py   ipaddress.py    optparse.py     _pydecimal.py   sndhdr.py                                  test                warnings.py
asyncio              contextvars.py               ftplib.py      json            os.py           pydoc_data      socket.py                                  textwrap.py         wave.py
base64.py            copy.py                      functools.py   keyword.py      _osx_support.py pydoc.py        socketserver.py                            this.py             weakref.py
bdb.py               copyreg.py                   __future__.py  lib2to3         pathlib.py      _pyio.py        sqlite3                                    _threading_local.py _weakrefset.py
bisect.py            cProfile.py                  genericpath.py lib-dynload     pdb.py          _pylong.py      sre_compile.py                             threading.py        webbrowser.py
bz2.py               crypt.py                     getopt.py      LICENSE.txt     __phello__      queue.py        sre_constants.py                           timeit.py           wsgiref
calendar.py          csv.py                       getpass.py     linecache.py    pickle.py       quopri.py       sre_parse.py                               tkinter             xdrlib.py
cgi.py               ctypes                       gettext.py     locale.py       pickletools.py  random.py       ssl.py                                     tokenize.py         xml
cgitb.py             curses                       glob.py        logging         pipes.py        re              statistics.py                              token.py            xmlrpc
chunk.py             dataclasses.py               graphlib.py    lzma.py         pkgutil.py      reprlib.py      stat.py                                    tomllib             zipapp.py
cmd.py               datetime.py                  gzip.py        mailbox.py      platform.py     rlcompleter.py  stringprep.py                              traceback.py        zipfile
codecs.py            dbm                          hashlib.py     mailcap.py      plistlib.py     runpy.py        string.py                                  tracemalloc.py      zipimport.py
codeop.py            decimal.py                   heapq.py       _markupbase.py  poplib.py       sched.py        _strptime.py                               trace.py            zoneinfo
code.py              difflib.py                   __hello__.py   mimetypes.py    posixpath.py    secrets.py      struct.py                                  tty.py
collections          dis.py                       hmac.py        modulefinder.py pprint.py       selectors.py    subprocess.py                              turtledemo
_collections_abc.py  doctest.py                   html           multiprocessing profile.py      shelve.py       sunau.py                                   turtle.py
colorsys.py          email                        http           netrc.py        pstats.py       shlex.py        symtable.py                                types.py
_compat_pickle.py    encodings                    idlelib        nntplib.py      pty.py          shutil.py       _sysconfigdata__linux_x86_64-linux-gnu.py  typing.py
Singularity> ls -l /opt/python/pkgs/python-3.12.11/lib/python3.12/site-packages/ | wc -l
1337
```

PESO

E4S NVIDIA Blackwell x86_64 Rocky Linux 9.6 Python Packages

```
GPU 0: NVIDIA RTX PRO 6000 Blackwell Server Edition (UUID: GPU-0a3e5316-2d97-bf04-1ed7-011560029cf3)
Singularity> which adk
/opt/python/pkgs/python-3.12.11/bin/adk
Singularity> which jupyter
/opt/python/pkgs/python-3.12.11/bin/jupyter
Singularity> which vllm
/opt/python/pkgs/python-3.12.11/bin/vllm
Singularity> which marimo
/opt/python/pkgs/python-3.12.11/bin/marimo
Singularity>
Singularity> python
Python 3.12.11 (main, Nov  4 2025, 19:11:59) [GCC 13.3.1 20240611 (Red Hat 13.3.1-2)] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import torch
>>> import nemo
>>> import bionemo
>>> import jax
>>> import openai
>>> import google.genai
>>> import huggingface_hub
>>> import polars
>>> import tensorflow
>>> import pandas
>>> import sklearn
>>> import cv2
>>> import dsi
>>> import zarr
>>>
>>> import matplotlib
>>> import plotly
>>> import seaborn
>>> import mpi4py
>>> import numpy
>>> import scipy
>>> import polars
>>>
>>> torch.cuda.get_arch_list()
['sm_70', 'sm_75', 'sm_80', 'sm_86', 'sm_90', 'sm_100', 'sm_120', 'compute_120']
>>> torch.cuda.is_available()
True
>>>
Singularity> which nvcc
/usr/local/cuda/bin/nvcc
Singularity> nvcc --version
nvcc: NVIDIA (R) Cuda compiler driver
Copyright (c) 2005-2025 NVIDIA Corporation
Built on Tue_May_27_02:21:03_PDT_2025
Cuda compilation tools, release 12.9, V12.9.86
Build cuda_12.9.r12.9/compiler.36037853_0
Singularity> which codium
/usr/bin/codium
```

E4S: NVIDIA Grace-Hopper (CUDA 90) Ubuntu 24.04 LTS image

```
$ singularity run --nv e4s-cuda90-aarch64-25.11.sif
Singularity> spack find -x
-- linux-ubuntu24.04-aarch64 / %c,cxx,fortran=gcc@13.3.0 --------
adios2@2.10.2  axom@0.10.1     heffte@2.4.1  libceed@0.12.0  paraview@5.13.3  slate@2025.05.28  strumpack@8.0.0  superlu-dist@9.1.0  trilinos@16.1.0   zfp@1.0.1
amrex@25.10    caliper@2.12.1  hypre@2.33.0  magma@2.9.0     petsc@3.24.0     slepc@3.24.0      sundials@7.5.0   tau@2.35            umpire@2025.03.0

-- linux-ubuntu24.04-aarch64 / %c,cxx=gcc@13.3.0 ----------------
cabana@0.7.0    chapel@2.6.0  fftx@1.2.0    ginkgo@1.10.0   hpctoolkit@2025.0.1  legion@25.03.0     mgard@compat-2023-12-09  raja@2025.03.0  vtk-m@2.3.0
chai@2025.03.0  cusz@0.14.0   flecsi@2.4.1  gromacs@2025.3  lammps@20250722      libpressio@0.99.4  omega-h@10.8.6-scorec    upcxx@2023.9.0

-- linux-ubuntu24.04-aarch64 / %c=gcc@13.3.0 --------------------
parsec@4.0.2411

-- linux-ubuntu24.04-aarch64 / %cxx,fortran=gcc@13.3.0 ----------
tasmanian@8.1

-- linux-ubuntu24.04-aarch64 / %cxx=gcc@13.3.0 ------------------
arborx@1.5  hpx@1.11.0  kokkos@4.7.01  kokkos-kernels@4.7.01  mfem@4.8.0

-- linux-ubuntu24.04-aarch64 / no compilers ---------------------
e4s-alc@1.0.3  e4s-cl@1.0.5  mpich@4.3.1
==> 46 installed packages
Singularity>
exit
$ singularity run --nv e4s-cpu-aarch64-25.11.sif
Singularity> spack find -x
-- linux-ubuntu24.04-aarch64 / %c,cxx,fortran=gcc@13.3.0 --------
adios@1.13.1    axom@0.10.1           darshan-util@3.4.7    h5bench@1.4       papi@7.2.0             plumed@2.9.2          slate@2025.05.28    tau@2.35          zfp@1.0.1
adios2@2.10.2   butterflypack@3.2.0   datatransferkit@3.1.1 heffte@2.4.1      parallel-netcdf@1.14.1 precice@3.3.0         slepc@3.24.0        trilinos@16.1.0
alquimia@1.1.0  caliper@2.12.1        exago@1.6.0           libcatalyst@2.0.0 paraview@5.13.3        quantum-espresso@7.5  strumpack@8.0.0     umpire@2025.03.0
amrex@25.10     conduit@0.9.5         globalarrays@5.8.2    libceed@0.12.0    petsc@3.24.0           rempi@1.1.0           sundials@7.5.0      wps@4.5
ascent@0.9.5    darshan-runtime@3.4.7 gptune@4.0.0          openmpi@5.0.8     phist@1.12.1           scr@3.1.0             superlu-dist@9.1.0  xyce@7.10.0

-- linux-ubuntu24.04-aarch64 / %c,cxx=gcc@13.3.0 ----------------
boost@1.88.0    faodel@1.2108.1  glvis@4.4           hdf5-vol-log@1.4.0   libunwind@1.7.2         nco@5.3.4             pdt@3.25.2          swig@4.0.2-fortran  upcxx@2023.9.0
cabana@0.7.0    fftx@1.2.0       gmp@6.3.0           hpctoolkit@2025.0.1  metall@0.30             omega-h@10.8.6-scorec pruners-ninja@1.0.1 sz@2.1.12.5         veloc@1.7
chai@2025.03.0  flecsi@2.4.1     gotcha@1.0.8        lammps@20250722      mgard@compat-2023-12-09 openfoam@2412         pumi@2.2.9          sz3@3.2.0           vtk-m@2.3.0
chapel@2.6.0    gasnet@2025.8.0  gromacs@2025.3      lbann@0.104          mpifileutils@0.12       openpmd-api@0.16.1    qthreads@1.18       turbine@1.3.0       warpx@25.04
dyninst@13.0.0  ginkgo@1.10.0    hdf5-vol-cache@v1.1  legion@25.03.0       nccmp@1.9.1.0           papyrus@1.0.2         raja@2025.03.0      umap@2.1.1

-- linux-ubuntu24.04-aarch64 / %c,fortran=gcc@13.3.0 ------------
fpm@0.10.0   hypre@2.33.0  nek5000@19.0  netcdf-fortran@4.6.2   plasma@24.8.7        py-petsc4py@3.24.0  wannier90@3.1.0
hdf5@1.14.6  libquo@1.4    nekbone@17.0  netlib-scalapack@2.2.2  py-libensemble@1.5.0  superlu@7.0.0       wrf@4.6.1

-- linux-ubuntu24.04-aarch64 / %c=gcc@13.3.0 --------------------
aml@0.2.1  argobots@1.2  charliecloud@0.40  hdf5-vol-async@1.7  libnrm@0.1.0  parsec@4.0.2411  py-h5py@3.14.0

-- linux-ubuntu24.04-aarch64 / %cxx,fortran=gcc@13.3.0 ----------
tasmanian@8.1

-- linux-ubuntu24.04-aarch64 / %cxx=gcc@13.3.0 ------------------
arborx@2.0.1  flit@2.1.0  hpx@1.11.0  kokkos@4.7.01  kokkos-kernels@4.7.01  laghos@3.1  loki@0.1.7  mfem@4.8.0  mpark-variant@1.4.0

-- linux-ubuntu24.04-aarch64 / no compilers ---------------------
e4s-alc@1.0.3  e4s-cl@1.0.5  mpich@4.3.1  nrm@0.1.0  py-cinemasci@1.7.0  py-jupyterhub@1.4.1  stc@0.9.0
==> 123 installed packages
Singularity>
```

E4S: Rocky Linux 9.6 x86_64 CPU image

```
$ singularity run e4s-cpu-rocky9.6-x86_64-25.11.sif
Singularity>
Singularity> cat /etc/os-release | grep PRETTY_NAME
PRETTY_NAME="Rocky Linux 9.6 (Blue Onyx)"
Singularity>
Singularity> spack find -x
-- linux-rocky9-x86_64_v3 / %c,cxx,fortran=gcc@13.3.1 -----------
adios@1.13.1    axom@0.10.1          darshan-runtime@3.4.7  gptune@4.0.0       openmpi@5.0.8           plumed@2.9.2          slate@2025.05.28    tau@2.35          xyce@7.10.0
adios2@2.10.2   butterflypack@3.2.0  darshan-util@3.4.7     h5bench@1.4        papi@7.2.0              precice@3.3.0         slepc@3.24.0        trilinos@16.1.0   zfp@1.0.1
alquimia@1.1.0  caliper@2.12.1       datatransferkit@3.1.1  heffte@2.4.1       parallel-netcdf@1.14.1  quantum-espresso@7.5  strumpack@8.0.0     umpire@2025.03.0
amrex@25.10     conduit@0.9.5        exago@1.6.0            libcatalyst@2.0.0  petsc@3.24.0            rempi@1.1.0           sundials@7.5.0      variorum@0.8.0
ascent@0.9.5    cp2k@2025.2          globalarrays@5.8.2     libceed@0.12.0     phist@1.12.1            scr@3.1.0             superlu-dist@9.1.0  wps@4.5

-- linux-rocky9-x86_64_v3 / %c,cxx=gcc@13.3.1 --------------------
boost@1.88.0       dyninst@13.0.0   ginkgo@1.10.0   hdf5-vol-cache@v1.1  legion@25.03.0          nccmp@1.9.1.0          papyrus@1.0.2       raja@2025.03.0      umap@2.1.1
bricks@2023.08.25  faodel@1.2108.1  glvis@4.4       hdf5-vol-log@1.4.0   libunwind@1.8.3         nco@5.3.4              pdt@3.25.2          swig@4.0.2-fortran  upcxx@2023.9.0
cabana@0.7.0       fftx@1.2.0       gmp@6.3.0       hpctoolkit@2025.0.1  metall@0.30             omega-h@10.8.6-scorec  pruners-ninja@1.0.1 sz@2.1.12.5         veloc@1.7
chai@2025.03.0     flecsi@2.4.1     gotcha@1.0.8    lammps@20250722      mgard@compat-2023-12-09 openfoam@2412          pumi@2.2.9          sz3@3.2.0           vtk-m@2.3.0
chapel@2.6.0       gasnet@2025.8.0  gromacs@2025.3  lbann@0.104          mpifileutils@0.12       openpmd-api@0.16.1     qthreads@1.18       turbine@1.3.0       warpx@25.04

-- linux-rocky9-x86_64_v3 / %c,fortran=gcc@13.3.1 ---------------
fpm@0.10.0   hypre@2.33.0  nek5000@19.0  netcdf-fortran@4.6.2    plasma@24.8.7         py-petsc4py@3.24.0  wannier90@3.1.0
hdf5@1.14.6  libquo@1.4    nekbone@17.0  netlib-scalapack@2.2.2  py-libensemble@1.5.0  superlu@7.0.0       wrf@4.6.1

-- linux-rocky9-x86_64_v3 / %c=gcc@13.3.1 ------------------------
aml@0.2.1  argobots@1.2  charliecloud@0.40  hdf5-vol-async@1.7  libnrm@0.1.0  parsec@4.0.2411  py-h5py@3.14.0

-- linux-rocky9-x86_64_v3 / %cxx,fortran=gcc@13.3.1 -------------
tasmanian@8.1

-- linux-rocky9-x86_64_v3 / %cxx=gcc@13.3.1 ----------------------
arborx@2.0.1  flit@2.1.0  hpx@1.11.0  kokkos@4.7.01  kokkos-kernels@4.7.01  laghos@3.1  loki@0.1.7  mfem@4.8.0  mpark-variant@1.4.0

-- linux-rocky9-x86_64_v3 / no compilers ------------------------
e4s-alc@1.0.3  e4s-cl@1.0.5  mpich@4.3.1  nrm@0.1.0  py-cinemasci@1.7.0  py-jupyterhub@1.4.1  stc@0.9.0
==> 125 installed packages
Singularity>
```

E4S: Rocky Linux 9.6 x86_64 CPU image

```
Singularity> module avail
-------------------------------------------------------------------------- /spack/share/spack/modules/linux-rocky9-x86_64_v3 ---------------------------------------------------------------
adios/1.13.1                cp2k/2025.2-openmp     gotcha/1.0.8                libcatalyst/2.0.0              nrm/0.1.0              py-h5py/3.14.0              sz3/3.2.0
adios2/2.10.2               darshan-runtime/3.4.7  gptune/4.0.0                libceed/0.12.0                 omega-h/10.8.6-scorec  py-jupyterhub/1.4.1         tasmanian/8.1
alquimia/1.1.0              darshan-util/3.4.7     gromacs/2025.3-openmp       libnrm/0.1.0                   openfoam/2412          py-libensemble/1.5.0        tau/2.35
aml/0.2.1                   datatransferkit/3.1.1  h5bench/1.4                 libquo/1.4                     openmpi/5.0.8          py-petsc4py/3.24.0          trilinos/16.1.0
amrex/25.10                 dyninst/13.0.0-openmp  hdf5-vol-async/1.7          libunwind/1.8.3                openpmd-api/0.16.1     qthreads/1.18               turbine/1.3.0
arborx/2.0.1                e4s-alc/1.0.3          hdf5-vol-cache/v1.1         loki/0.1.7                     papi/7.2.0             quantum-espresso/7.5-openmp umap/2.1.1
argobots/1.2                e4s-cl/1.0.5           hdf5-vol-log/1.4.0          metall/0.30                    papyrus/1.0.2          raja/2025.03.0              umpire/2025.03.0
ascent/0.9.5-openmp         exago/1.6.0            hdf5/1.14.6                 mfem/4.8.0                     parallel-netcdf/1.14.1 rempi/1.1.0                 upcxx/2023.9.0
axom/0.10.1-openmp          faodel/1.2108.1        heffte/2.4.1                mgard/compat-2023-12-09-openmp parsec/4.0.2411        scr/3.1.0                   variorum/0.8.0
boost/1.88.0                fftx/1.2.0             hpctoolkit/2025.0.1         mpark-variant/1.4.0            pdt/3.25.2             slate/2025.05.28-openmp     veloc/1.7
bricks/2023.08.25           flecsi/2.4.1           hpx/1.11.0                  mpich/4.3.1                    petsc/3.24.0           slepc/3.24.0                vtk-m/2.3.0-openmp
butterflypack/3.2.0-openmp  flit/2.1.0             hypre/2.33.0                mpifileutils/0.12              phist/1.12.1-openmp    stc/0.9.0                   wannier90/3.1.0
cabana/0.7.0                fpm/0.10.0-openmp      kokkos-kernels/4.7.01-openmp nccmp/1.9.1.0                  plasma/24.8.7          strumpack/8.0.0-openmp      warpx/25.04
caliper/2.12.1              gasnet/2025.8.0        kokkos/4.7.01-openmp        nco/5.3.4-openmp               plumed/2.9.2           sundials/7.5.0              wps/4.5
chai/2025.03.0              ginkgo/1.10.0-openmp   laghos/3.1                  nek5000/19.0                   precice/3.3.0          superlu-dist/9.1.0          wrf/4.6.1
chapel/2.6.0                globalarrays/5.8.2     lammps/20250722-openmp      nekbone/17.0                   pruners-ninja/1.0.1    superlu/7.0.0               xyce/7.10.0
charliecloud/0.40           glvis/4.4              lbann/0.104                 netcdf-fortran/4.6.2           pumi/2.2.9             swig/4.0.2-fortran          zfp/1.0.1
conduit/0.9.5               gmp/6.3.0              legion/25.03.0              netlib-scalapack/2.2.2         py-cinemasci/1.7.0     sz/2.1.12.5

Key:
loaded  modulepath
Singularity>
```

E4S Intel oneAPI Ubuntu 24.04 LTS CPU/GPU image

```
$ singularity run e4s-oneapi-x86_64-25.11.sif
Singularity> spack find -x
-- linux-ubuntu24.04-x86_64_v3 / %c,cxx,fortran=gcc@13.3.0 ------
adios@1.13.1    axom@0.10.1          darshan-runtime@3.4.7  gptune@4.0.0       openmpi@5.0.8          plumed@2.9.2          slate@2025.05.28    tau@2.35          xyce@7.10.0
adios2@2.10.2   butterflypack@3.2.0  darshan-util@3.4.7     h5bench@1.4        papi@7.2.0             precice@3.3.0         slepc@3.24.0        trilinos@16.1.0   zfp@1.0.1
alquimia@1.1.0  caliper@2.12.1       datatransferkit@3.1.1  heffte@2.4.1       parallel-netcdf@1.14.1 quantum-espresso@7.5  strumpack@8.0.0     umpire@2025.03.0
amrex@25.10     conduit@0.9.5        exago@1.6.0            libcatalyst@2.0.0  petsc@3.24.0           rempi@1.1.0           sundials@7.5.0      variorum@0.8.0
ascent@0.9.5    cp2k@2025.2          globalarrays@5.8.2     libceed@0.12.0     phist@1.12.1           scr@3.1.0             superlu-dist@9.1.0  wps@4.5

-- linux-ubuntu24.04-x86_64_v3 / %c,cxx,fortran=oneapi@2025.2.1 -
amrex@25.10  heffte@2.4.1  petsc@3.24.0  sundials@7.5.0  tau@2.35  tau@2.35

-- linux-ubuntu24.04-x86_64_v3 / %c,cxx=gcc@13.3.0 --------------
boost@1.88.0       dyninst@13.0.0   ginkgo@1.10.0   hdf5-vol-cache@v1.1  legion@25.03.0          nccmp@1.9.1.0          papyrus@1.0.2        raja@2025.03.0      umap@2.1.1
bricks@2023.08.25  faodel@1.2108.1  glvis@4.4       hdf5-vol-log@1.4.0   libunwind@1.8.3         nco@5.3.4              pdt@3.25.2           swig@4.0.2-fortran  upcxx@2023.9.0
cabana@0.7.0       fftx@1.2.0       gmp@6.3.0       hpctoolkit@2025.0.1  metall@0.30             omega-h@10.8.6-scorec  pruners-ninja@1.0.1  sz@2.1.12.5         veloc@1.7
chai@2025.03.0     flecsi@2.4.1     gotcha@1.0.8    lammps@20250722      mgard@compat-2023-12-09 openfoam@2412          pumi@2.2.9           sz3@3.2.0           vtk-m@2.3.0
chapel@2.6.0       gasnet@2025.8.0  gromacs@2025.3  lbann@0.104          mpifileutils@0.12       openpmd-api@0.16.1     qthreads@1.18        turbine@1.3.0       warpx@25.04

-- linux-ubuntu24.04-x86_64_v3 / %c,cxx=oneapi@2025.2.1 ---------
cabana@0.7.0  ginkgo@1.10.0  hpctoolkit@2025.0.1  upcxx@2023.9.0

-- linux-ubuntu24.04-x86_64_v3 / %c,fortran=gcc@13.3.0 ----------
fpm@0.10.0   hypre@2.33.0  nek5000@19.0  netcdf-fortran@4.6.2    plasma@24.8.7         py-petsc4py@3.24.0  wannier90@3.1.0
hdf5@1.14.6  libquo@1.4    nekbone@17.0  netlib-scalapack@2.2.2  py-libensemble@1.5.0  superlu@7.0.0       wrf@4.6.1

-- linux-ubuntu24.04-x86_64_v3 / %c=gcc@13.3.0 ------------------
aml@0.2.1  argobots@1.2  charliecloud@0.40  hdf5-vol-async@1.7  libnrm@0.1.0  parsec@4.0.2411  py-h5py@3.14.0

-- linux-ubuntu24.04-x86_64_v3 / %c=oneapi@2025.2.1 -------------
aml@0.2.1

-- linux-ubuntu24.04-x86_64_v3 / %cxx,fortran=gcc@13.3.0 --------
tasmanian@8.1

-- linux-ubuntu24.04-x86_64_v3 / %cxx=gcc@13.3.0 ----------------
arborx@2.0.1  flit@2.1.0  hpx@1.11.0  kokkos@4.7.01  kokkos-kernels@4.7.01  laghos@3.1  loki@0.1.7  mfem@4.8.0  mpark-variant@1.4.0

-- linux-ubuntu24.04-x86_64_v3 / %cxx=oneapi@2025.2.1 -----------
arborx@2.0.1  kokkos@4.7.01  kokkos-kernels@4.7.01

-- linux-ubuntu24.04-x86_64_v3 / no compilers -------------------
e4s-alc@1.0.3  e4s-cl@1.0.5  intel-oneapi-mpi@2021.16.0  nrm@0.1.0  py-cinemasci@1.7.0  py-jupyterhub@1.4.1  stc@0.9.0
==> 139 installed packages
Singularity>
```

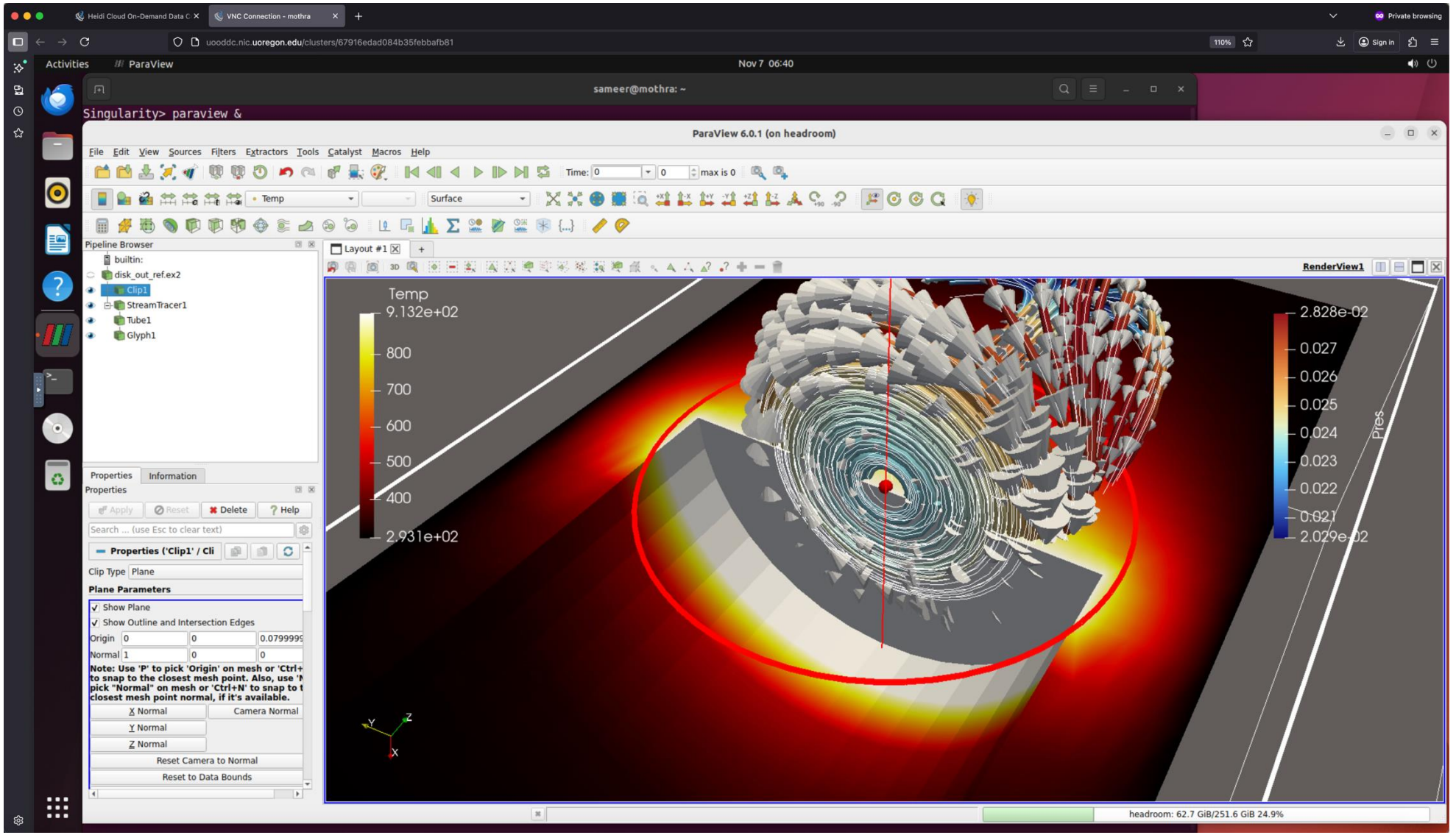
E4S IBM ppc64le Power image with GPU

```
$ singularity run e4s-cuda70-ppc64le-25.11.sif
Singularity> lscpu | grep POWER
Model name:                      POWER10 (architected), altivec supported
Singularity> spack find +cuda
-- linux-ubuntu20.04-ppc64le / %c,cxx,fortran=gcc@9.4.0 ---------
amrex@25.10  caliper@2.12.1  heffte@2.4.1  hypre@2.33.0  paraview@5.13.3  petsc@3.24.0      slepc@3.24.0     sundials@7.5.0      tau@2.35      umpire@2025.03.0  umpire@2025.03.0
axom@0.10.1  exago@1.6.0     hiop@1.0.0    magma@2.9.0   petsc@3.24.0     slate@2025.05.28  strumpack@8.0.0  superlu-dist@9.1.0  umpire@6.0.0  umpire@2025.03.0  zfp@1.0.1

-- linux-ubuntu20.04-ppc64le / %c,cxx=gcc@9.4.0 -----------------
bricks@2023.08.25  camp@0.2.3      camp@2025.03.0  fftx@1.2.0    ginkgo@1.10.0         hwloc@2.12.2     mgard@compat-2023-12-09  omega-h@10.8.6-scorec  raja@2025.03.0  upcxx@2023.9.0
cabana@0.7.0       camp@2025.03.0  chai@2025.03.0  flecsi@2.4.1  hpctoolkit@2024.01.1  lammps@20250722  nvcomp@2.2.0             raja@0.14.0            raja@2025.03.0  vtk-m@2.3.0

-- linux-ubuntu20.04-ppc64le / %c=gcc@9.4.0 ----------------------
flux-core@0.73.0  parsec@4.0.2411

-- linux-ubuntu20.04-ppc64le / %cxx,fortran=gcc@9.4.0 -----------
tasmanian@8.1

-- linux-ubuntu20.04-ppc64le / %cxx=gcc@9.4.0 -------------------
blaspp@2025.05.28  hpx@1.11.0  kokkos@4.6.02  kokkos@4.7.01  kokkos@4.7.01  kokkos-kernels@4.7.01  lapackpp@2025.05.28  mfem@4.8.0
==> 53 installed packages
Singularity> spack find -x
-- linux-ubuntu20.04-ppc64le / %c,cxx,fortran=gcc@9.4.0 ---------
adios@1.13.1    axom@0.10.1           darshan-util@3.4.7    h5bench@1.4        nwchem@7.2.3           petsc@3.24.0         slate@2025.05.28  sundials@7.5.0      trilinos@16.1.0   zfp@1.0.1
alquimia@1.1.0  butterflypack@3.2.0    datatransferkit@3.1.1  heffte@2.4.1       openmpi@5.0.8          petsc@3.24.0         slate@2025.05.28  sundials@7.5.0      umpire@2025.03.0
amrex@25.10     caliper@2.12.1         exago@1.6.0            heffte@2.4.1       papi@7.2.0             plumed@2.9.2         slepc@3.24.0      superlu-dist@9.1.0  umpire@2025.03.0
amrex@25.10     caliper@2.12.1         exago@1.6.0            hypre@2.33.0       parallel-netcdf@1.14.1 quantum-espresso@7.5 slepc@3.24.0      superlu-dist@9.1.0  wps@4.5
ascent@0.9.5    conduit@0.9.5          globalarrays@5.8.2     libcatalyst@2.0.0  paraview@5.13.3        rempi@1.1.0          strumpack@8.0.0   tau@2.35            xyce@7.10.0
axom@0.10.1     darshan-runtime@3.4.7  gptune@4.0.0           magma@2.9.0        paraview@5.13.3        scr@3.1.0            strumpack@8.0.0   tau@2.35            zfp@1.0.1

-- linux-ubuntu20.04-ppc64le / %c,cxx=gcc@9.4.0 -----------------
bolt@2.0           chai@2025.03.0   fftx@1.2.0       gmp@6.3.0            lammps@20250722    metall@0.30             omega-h@10.8.6-scorec  qthreads@1.18       turbine@1.3.0   vtk-m@2.3.0
boost@1.88.0       chai@2025.03.0   flecsi@2.4.1     gotcha@1.0.8         lammps@20250722    mgard@compat-2023-12-09 omega-h@10.8.6-scorec  raja@2025.03.0      umap@2.1.1
bricks@2023.08.25  chapel@2.6.0     gasnet@2025.8.0  hdf5-vol-cache@v1.1  lbann@0.104        mgard@compat-2023-12-09 papyrus@1.0.2          raja@2025.03.0      upcxx@2023.9.0
bricks@2023.08.25  dyninst@13.0.0   ginkgo@1.10.0    hdf5-vol-log@1.4.0   legion@25.03.0     mpifileutils@0.12       pdt@3.25.2             swig@4.0.2-fortran  upcxx@2023.9.0
cabana@0.7.0       faodel@1.2108.1  ginkgo@1.10.0    hpctoolkit@2024.01.1 libpressio@0.99.4  nccmp@1.9.1.0           pruners-ninja@1.0.1    sz@2.1.12.5         veloc@1.7
cabana@0.7.0       fftx@1.2.0       glvis@4.4        hpctoolkit@2024.01.1 libunwind@1.7.2    nco@5.3.4               pumi@2.2.9             sz3@3.2.0           vtk-m@2.3.0

-- linux-ubuntu20.04-ppc64le / %c,fortran=gcc@9.4.0 -------------
fpm@0.10.0   hypre@2.33.0  nek5000@19.0  netcdf-fortran@4.6.2  plasma@24.8.7        py-petsc4py@3.24.0  wannier90@3.1.0
hdf5@1.14.6  libquo@1.4    nekbone@17.0  netlib-scalapack@2.2.2  py-libensemble@1.5.0  superlu@7.0.0       wrf@4.6.1

-- linux-ubuntu20.04-ppc64le / %c=gcc@9.4.0 ----------------------
aml@0.2.1  argobots@1.2  charliecloud@0.40  flux-core@0.73.0  flux-core@0.73.0  hdf5-vol-async@1.7  libnrm@0.1.0  parsec@4.0.2411  parsec@4.0.2411  py-h5py@3.14.0

-- linux-ubuntu20.04-ppc64le / %cxx,fortran=gcc@9.4.0 -----------
fortrilinos@2.3.0  tasmanian@8.1  tasmanian@8.1

-- linux-ubuntu20.04-ppc64le / %cxx=gcc@9.4.0 -------------------
arborx@2.0.1  flit@2.1.0  hpx@1.11.0  hpx@1.11.0  kokkos@4.7.01  kokkos@4.7.01  kokkos-kernels@4.7.01  kokkos-kernels@4.7.01  laghos@3.1  loki@0.1.7  mfem@4.8.0  mfem@4.8.0  mpark-variant@1.4.0

-- linux-ubuntu20.04-ppc64le / no compilers ----------------------
e4s-alc@1.0.3  e4s-cl@1.0.5  exaworks@0.1.0  mpich@4.3.1  nrm@0.1.0  py-cinemasci@1.7.0  py-jupyterhub@1.4.1  stc@0.9.0
==> 158 installed packages
Singularity>
```

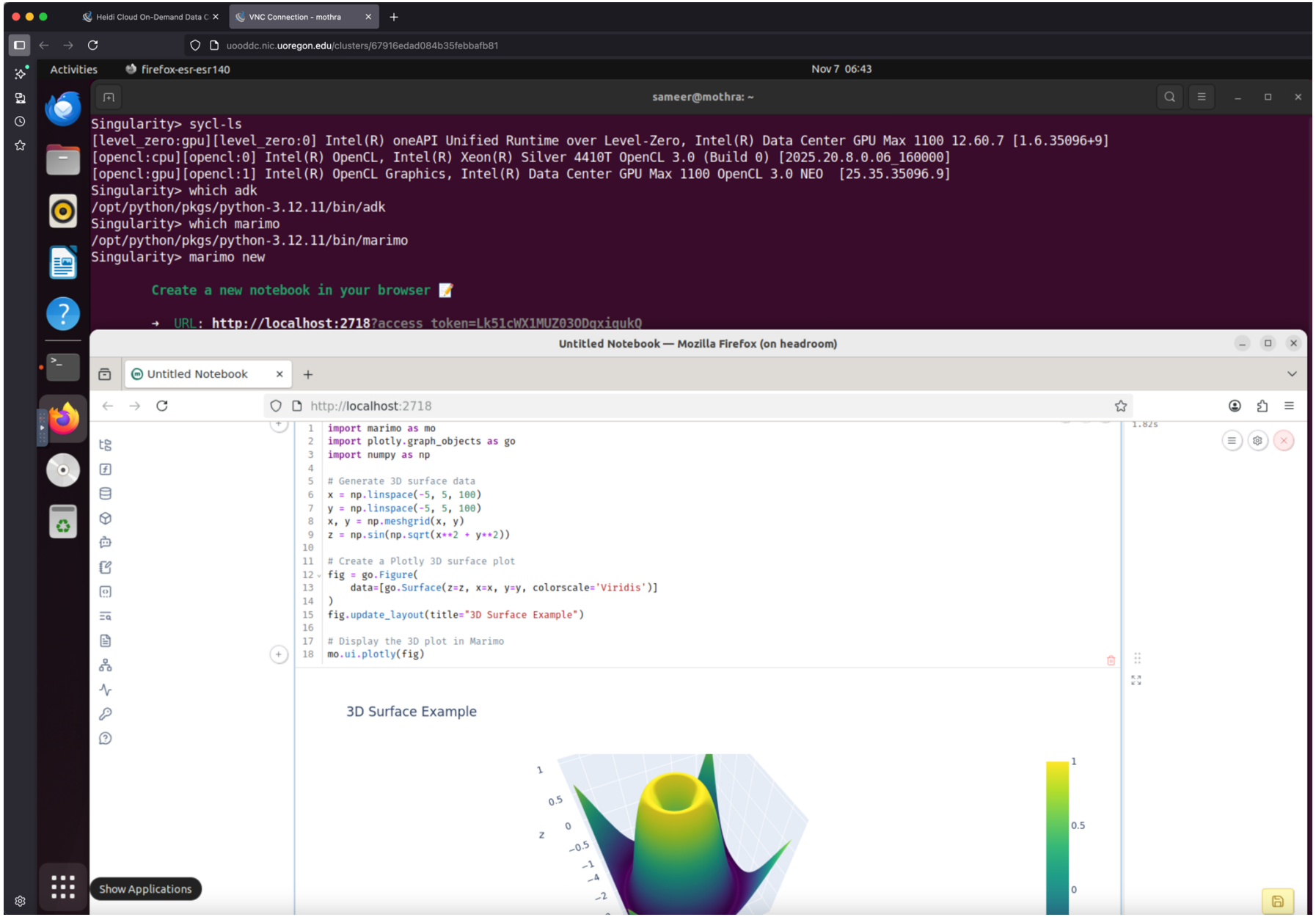
E4S: AMD MI300A GPU support with ROCm 6.4.3

```
$ singularity run e4s-rocm942-x86_64-25.11.sif
Singularity> which hipcc
/opt/rocm/bin/hipcc
Singularity> hipcc --version
HIP version: 6.4.43484-123eb5128
AMD clang version 19.0.0git (https://github.com/RadeonOpenCompute/llvm-project roc-6.4.3 25224 d366fa84f3fdcbd4b10847ebd5db572ae12a34fb)
Target: x86_64-unknown-linux-gnu
Thread model: posix
InstalledDir: /opt/rocm-6.4.3/lib/llvm/bin
Configuration file: /opt/rocm-6.4.3/lib/llvm/bin/clang++.cfg
Singularity> which adk
/opt/python/pkgs/python-3.12.11/bin/adk
Singularity> which codium
/usr/bin/codium
Singularity> which python
/opt/python/pkgs/python-3.12.11/bin/python
Singularity>
Singularity> module avail
------------------------------------------------------------------------ /spack/share/spack/modules/linux-ubuntu24.04-x86_64_v3 ------------------------------------------------------------
amrex/25.10-gfx942        e4s-alc/1.0.3               heffte/2.4.1-gfx942       libceed/0.12.0-gfx942  petsc/3.24.0-gfx942            superlu-dist/9.1.0-gfx942  upcxx/2023.9.0-gfx942
arborx/2.0.1-gfx942       e4s-cl/1.0.5                hpctoolkit/2025.0.1-rocm  magma/2.9.0-gfx942     raja/2025.03.0-gfx942          tasmanian/8.1-gfx942       vtk-m/2.3.0-gfx942
cabana/0.7.0-gfx942-rocm  fftx/1.2.0-gfx942           hypre/2.33.0-gfx942       mfem/4.8.0-gfx942      slepc/3.24.0-gfx942            tau/2.35-rocm
caliper/2.12.1-gfx942     gasnet/2025.8.0-gfx942      kokkos/4.7.01-gfx942      mpich/4.3.1            strumpack/8.0.0-gfx942-openmp  trilinos/16.1.0-gfx942
chai/2025.03.0-gfx942     ginkgo/1.10.0-gfx942-openmp legion/25.03.0-gfx942     papi/7.2.0-gfx942      sundials/7.5.0-gfx942          umpire/2025.03.0-gfx942

Key:
loaded  modulepath
Singularity> spack find -x
-- linux-ubuntu24.04-x86_64_v3 / %c,cxx,fortran=gcc@13.3.0 ------
amrex@25.10     heffte@2.4.1  libceed@0.12.0  papi@7.2.0    slepc@3.24.0     sundials@7.5.0      tau@2.35         umpire@2025.03.0
caliper@2.12.1  hypre@2.33.0  magma@2.9.0     petsc@3.24.0  strumpack@8.0.0  superlu-dist@9.1.0  trilinos@16.1.0

-- linux-ubuntu24.04-x86_64_v3 / %c,cxx=gcc@13.3.0 --------------
cabana@0.7.0  chai@2025.03.0  fftx@1.2.0  gasnet@2025.8.0  ginkgo@1.10.0  hpctoolkit@2025.0.1  legion@25.03.0  raja@2025.03.0  upcxx@2023.9.0  vtk-m@2.3.0

-- linux-ubuntu24.04-x86_64_v3 / %cxx,fortran=gcc@13.3.0 --------
tasmanian@8.1

-- linux-ubuntu24.04-x86_64_v3 / %cxx=gcc@13.3.0 ----------------
arborx@2.0.1  kokkos@4.7.01  mfem@4.8.0

-- linux-ubuntu24.04-x86_64_v3 / no compilers -------------------
e4s-alc@1.0.3  e4s-cl@1.0.5  mpich@4.3.1
==> 32 installed packages
Singularity> rocminfo | grep "gfx942:"
      Name:                    amdgcn-amd-amdhsa--gfx942:sramecc+:xnack-
      Name:                    amdgcn-amd-amdhsa--gfx942:sramecc+:xnack-
      Name:                    amdgcn-amd-amdhsa--gfx942:sramecc+:xnack-
      Name:                    amdgcn-amd-amdhsa--gfx942:sramecc+:xnack-
Singularity>
```

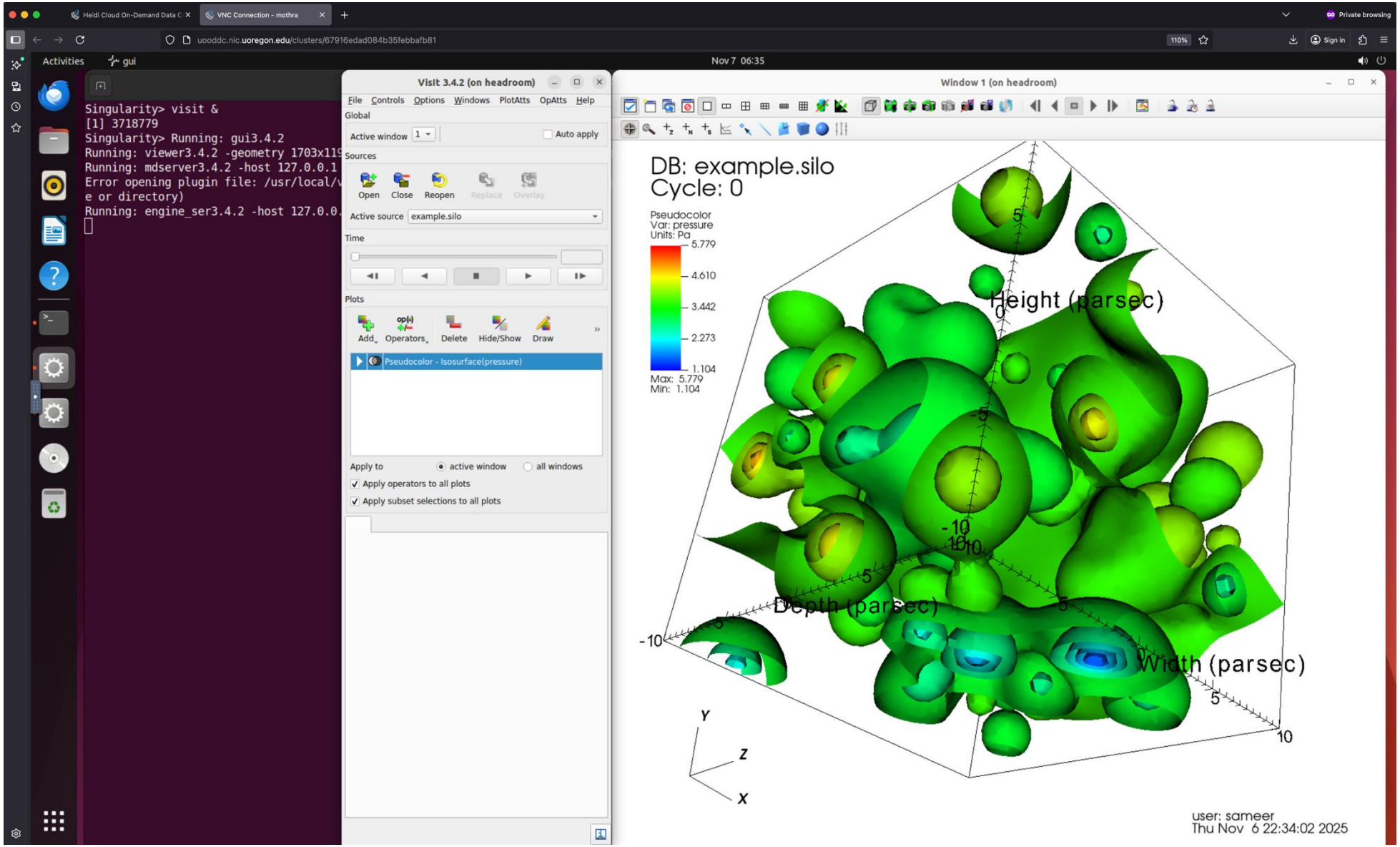
E4S: Visualization Tools: ParaView



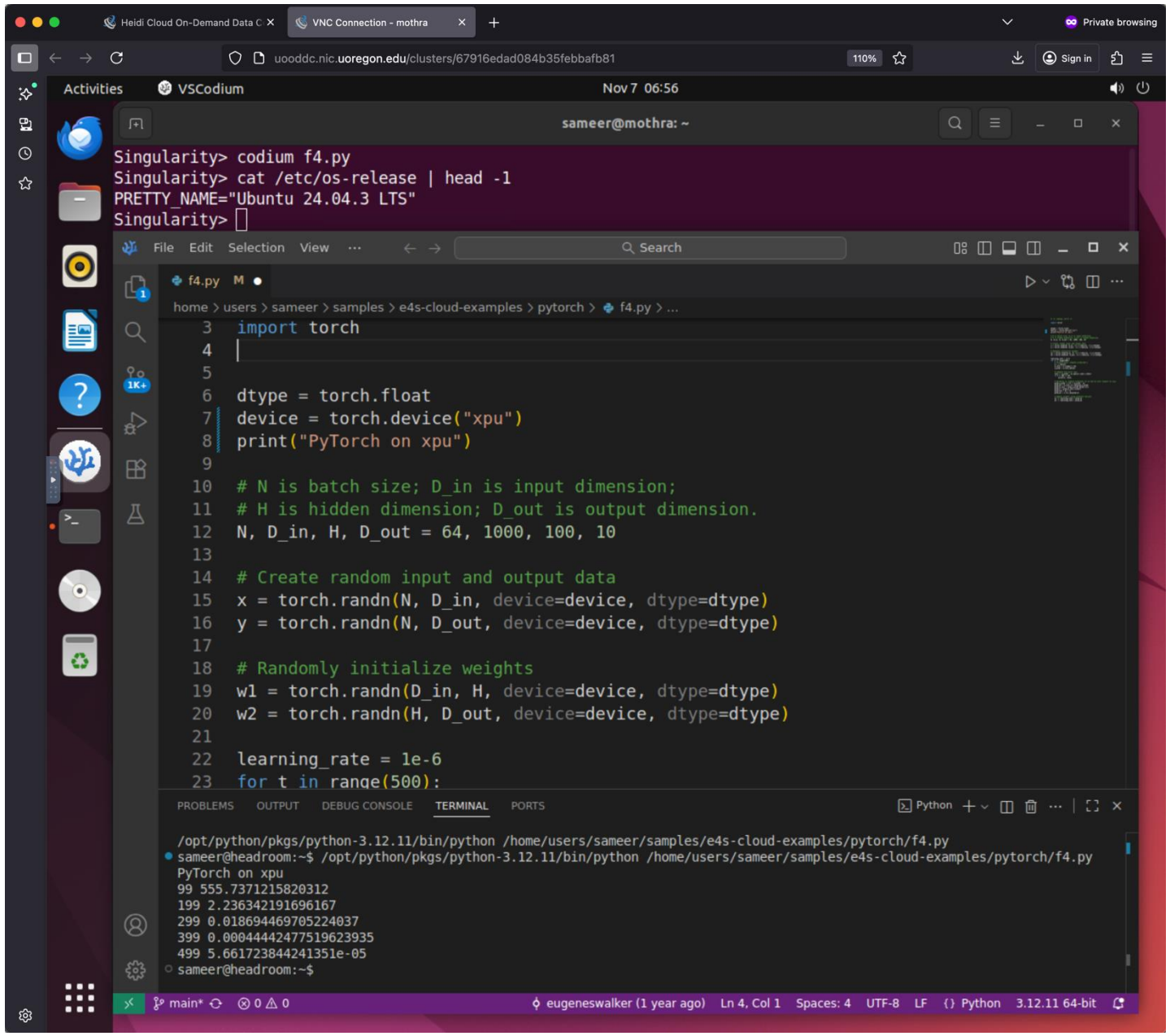
E4S: Marimo Reactive Notebooks



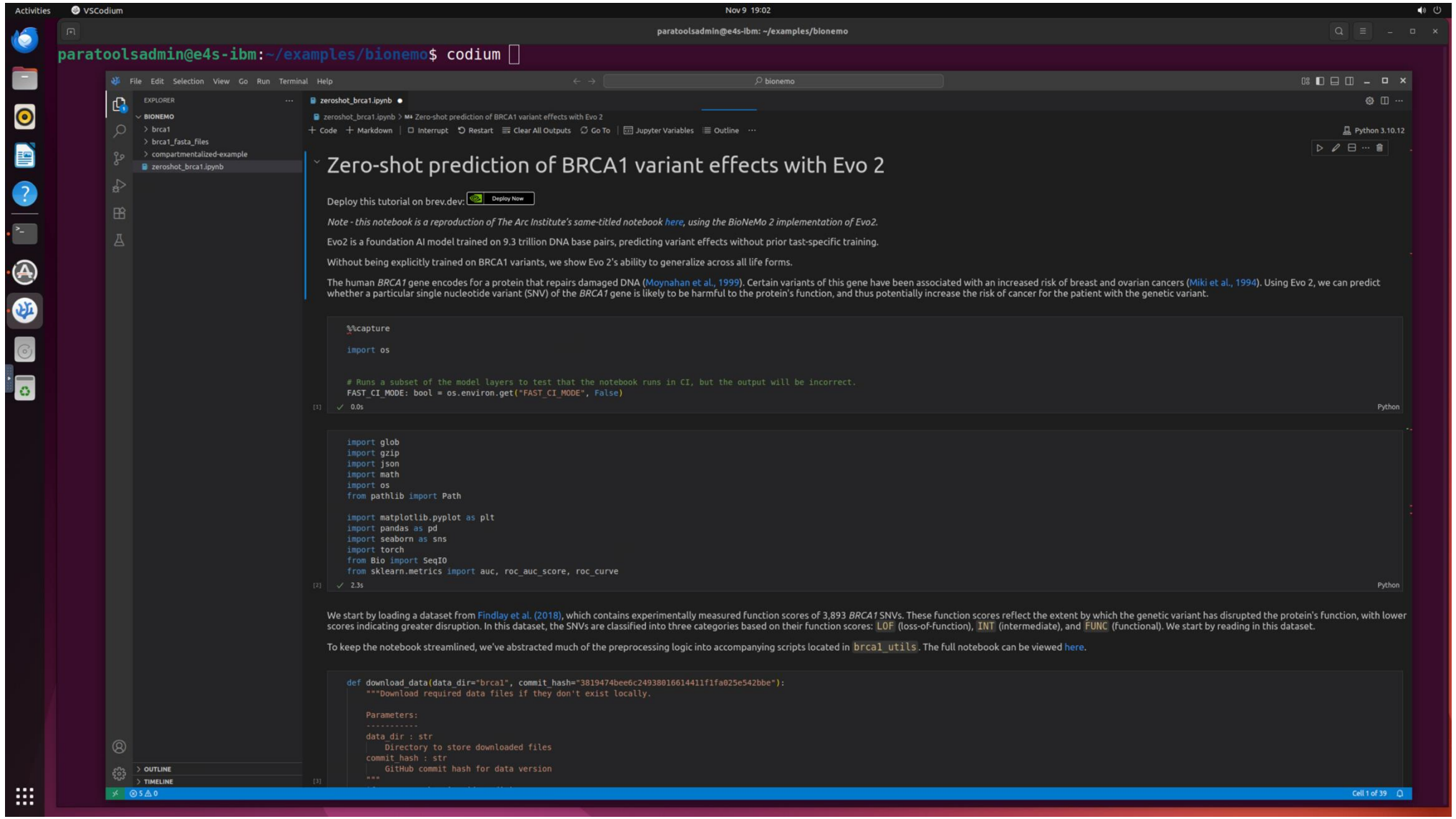
E4S: VisIt


Activities
gui
Nov 7 06:35
Singularity> visit &
[1] 3718779
Singularity> Running: gui3.4.2
Running: viewer3.4.2 -geometry 1703x119
Running: mdserver3.4.2 -host 127.0.0.1
Error opening plugin file: /usr/local/v
e or directory)
Running: engine_ser3.4.2 -host 127.0.0.
VisIt 3.4.2 (on headroom)
File Controls Options Windows PlotAtts OpAtts Help
Global
Active window 1
Auto apply
Sources
Open Close Reopen Replace Overlay
Active source example.silo
Time
Plots
Add Operators Delete Hide/Show Draw
Pseudocolor - Isosurface(pressure)
Apply to active window all windows
Apply operators to all plots
Apply subset selections to all plots
Window 1 (on headroom)
DB: example.silo
Cycle: 0
Pseudocolor
Var: pressure
Units: Pa
5.779
4.610
3.442
2.273
1.104
Max: 5.779
Min: 1.104
Height (parsec)
Depth (parsec)
Width (parsec)
Y
Z
X
user: sameer
Thu Nov 6 22:34:02 2025

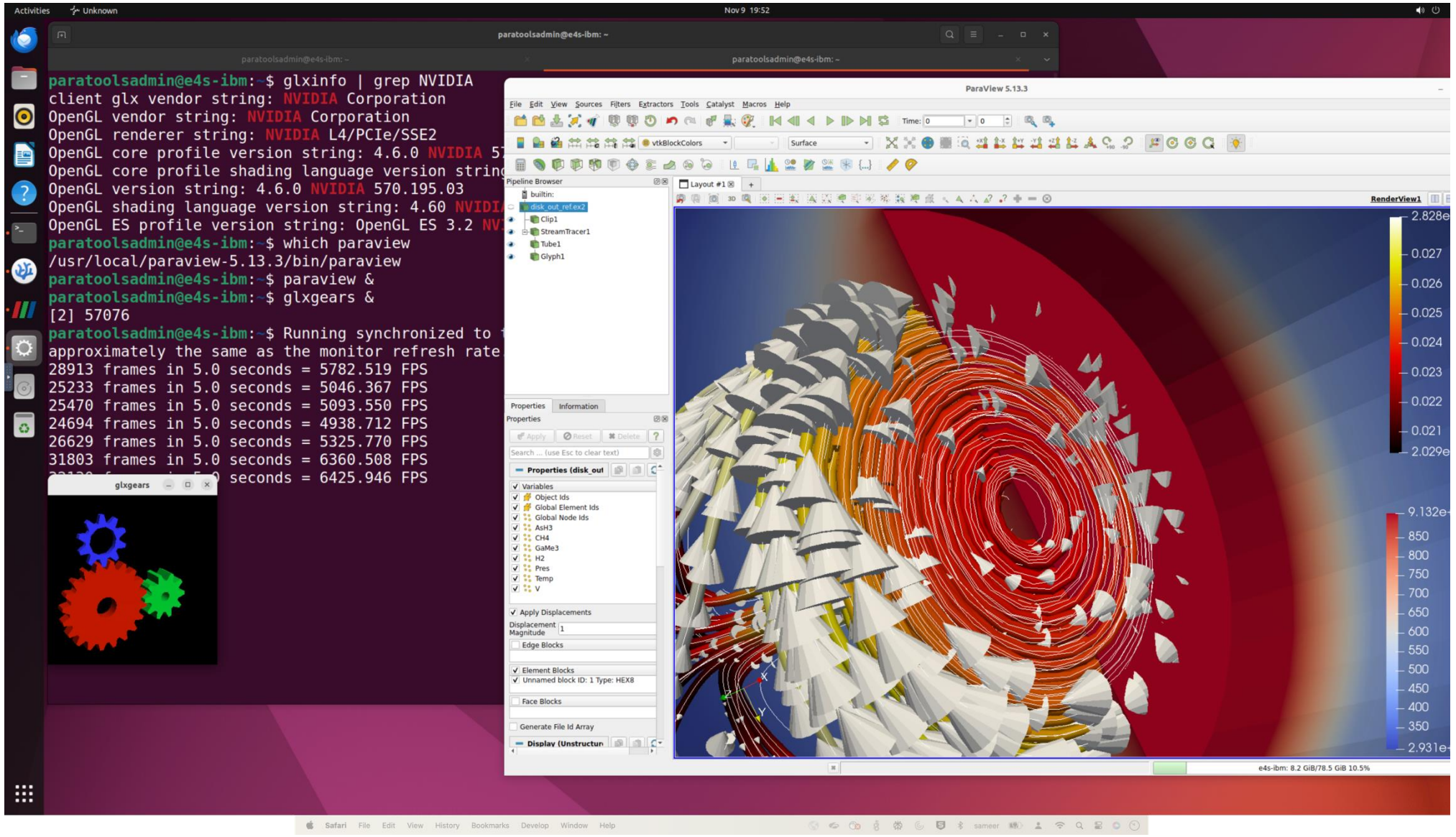
E4S: VS Codium Integrated Development Environment



ParaTools Pro for E4S™: NVIDIA BioNeMo™ on IBM Cloud



ParaTools Pro for E4S™: HPC-AI Software Ecosystem on Clouds



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Thank you

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