E4S: The Extreme-scale Scientific Software Stack Release 26.06

Release 26.06 notes

June 22, 2026

High Performance Software Foundation

E4S Team

https://e4s.io

E4S 26.06: What's New?

https://e4s.io

- E4S is a curated Spack based distribution of 125+ HPC-AI packages.
- Compared with 25.11, E4S 26.06 adds a much richer agentic AI layer, deeper LLM inference optimization, and more workflow tooling around fine-tuning, serving, and domain-specific AI
  - Sglang, MCP, langchain, langgraph, a2a, flash_attr
  - Coding agent pi, NVIDIA NemoClaw, OpenClaw, NVIDIA NeMo, NVIDIA BioNeMo, Megatron, transformers, cupy
  - Ray, peft, triton
  - API: openai, google, anthropic
  - Chemistry: rdkit
- Support for updated Rocky Linux 9.8 with Hopper and Blackwell, Ubuntu 24.04 LTS.
- Spack 1.1.1 integration [https://github.com/spack/spack/releases/tag/v1.1.1].
- HPC Applications include: CP2K, DealII, FFTX, GROMACS, LAMMPS, Nek5000, Nekbone, NWChem, OpenFOAM, WarpX, WRF, Quantum Espresso, and Xyce with GPU support where available.
- CUDA upgraded to 13.2 (aarch64, x86_64), ROCm upgraded to 7.2.3, oneAPI upgraded to 2026.0.
- Adaptive Computing's Heidi web-based platform for multi-user, multi-node, ParaTools Pro for E4S™ with Ubuntu 26.04 LTS and Rocky Linux 9.7 cloud images on AWS, Microsoft Azure, Google Cloud, OCI, and IBM Cloud.
  - https://adaptivecomputing.com/ and https://paratoolspro.com

E4S: Extreme-scale Scientific Software Stack

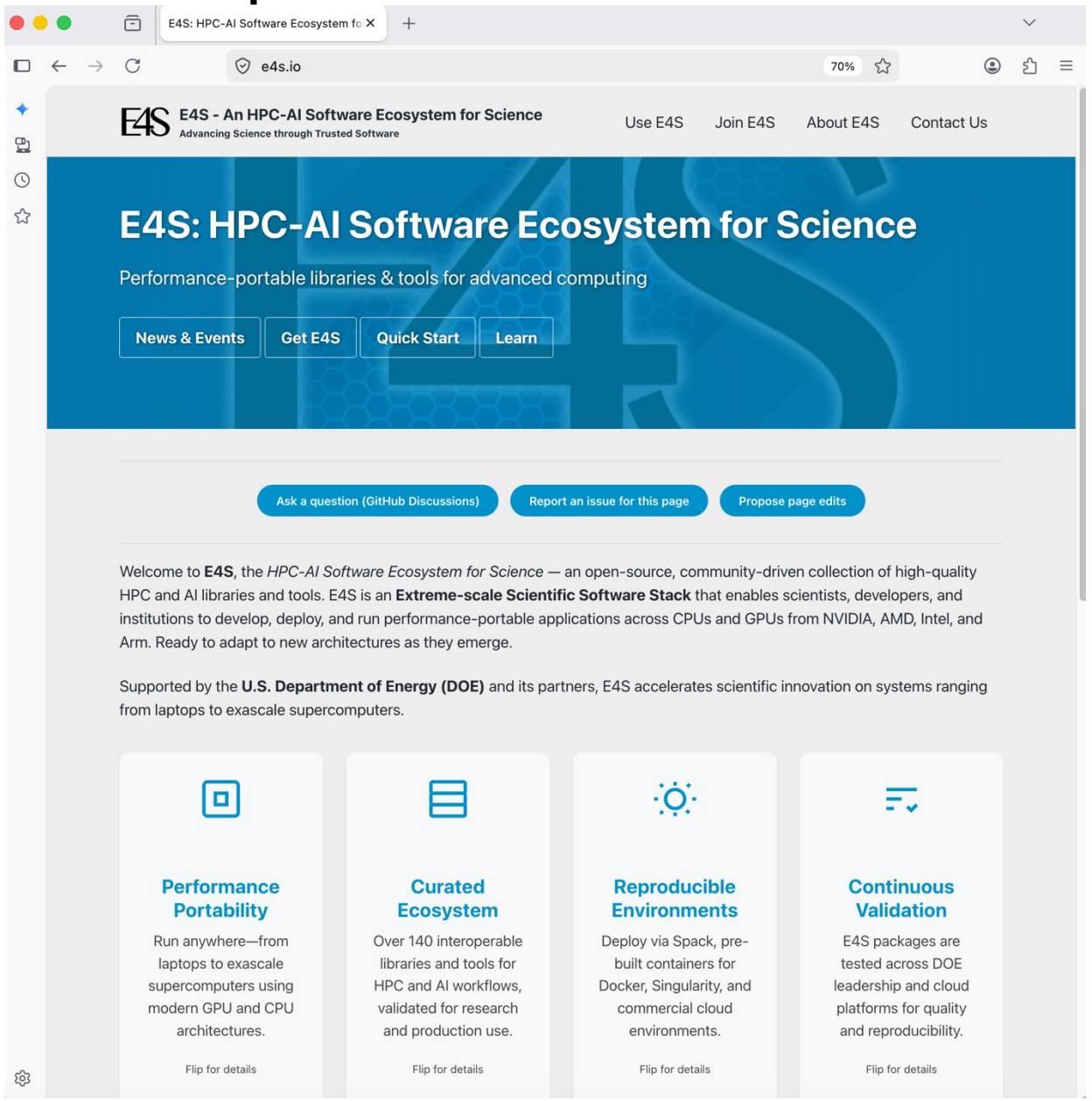
https://e4s.io

About E4S

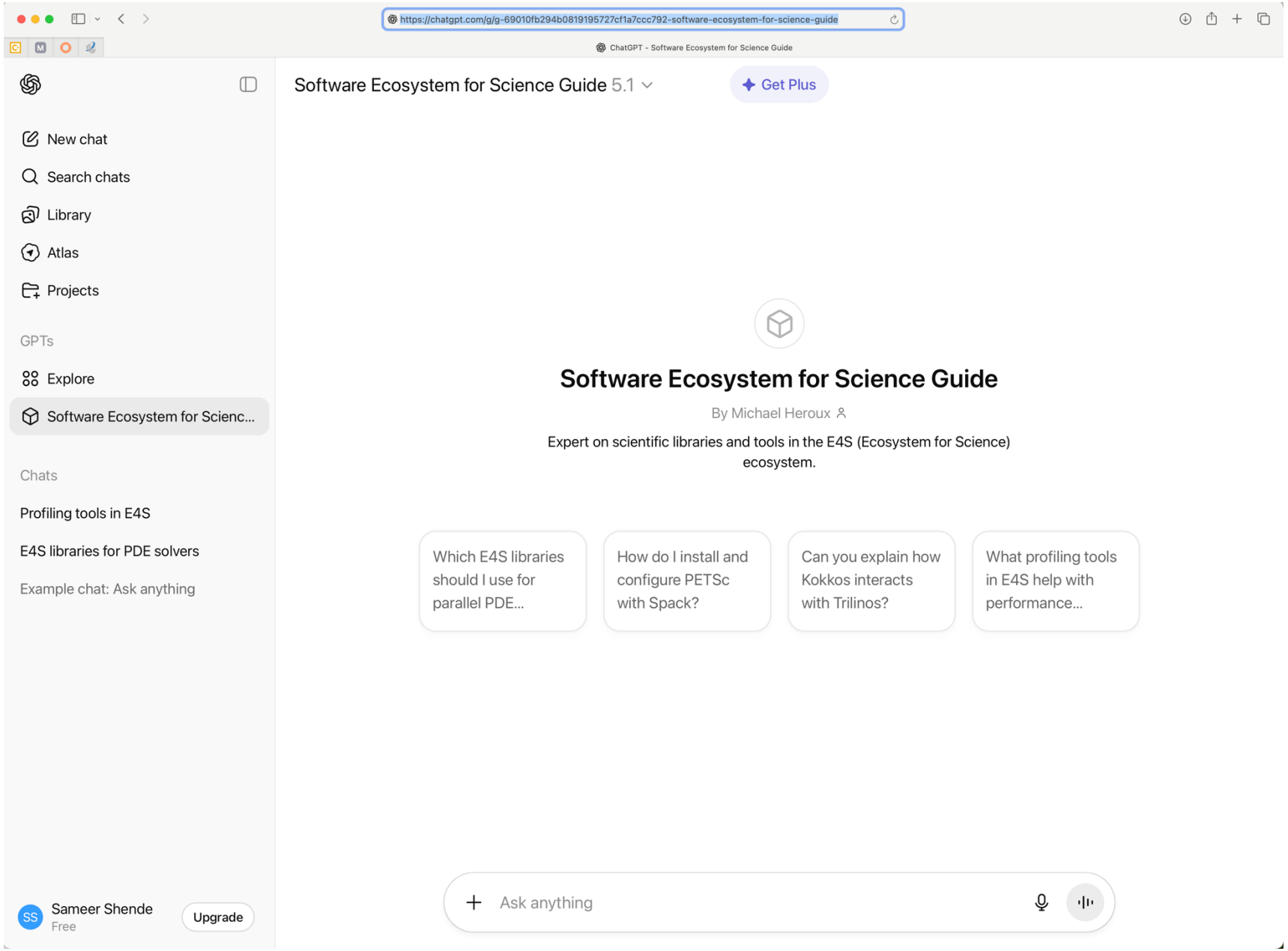
- E4S is an **ecosystem for science** and a community effort to provide open-source software packages for developing, deploying and running scientific applications on HPC platforms.
- E4S has built a comprehensive, coherent software stack that enables application developers to productively develop highly 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 26.06 released on June 22, 2026: https://e4s.io/talks/E4S_26.06.pdf

PESO Argonne BERKELEY LAB Brookhaven National Laboratory kitware Los Alamos OAK RIDGE National Laboratory ParaTools Sandia National Laboratories SUSTAINABLE HORIZONS INSTITUTE

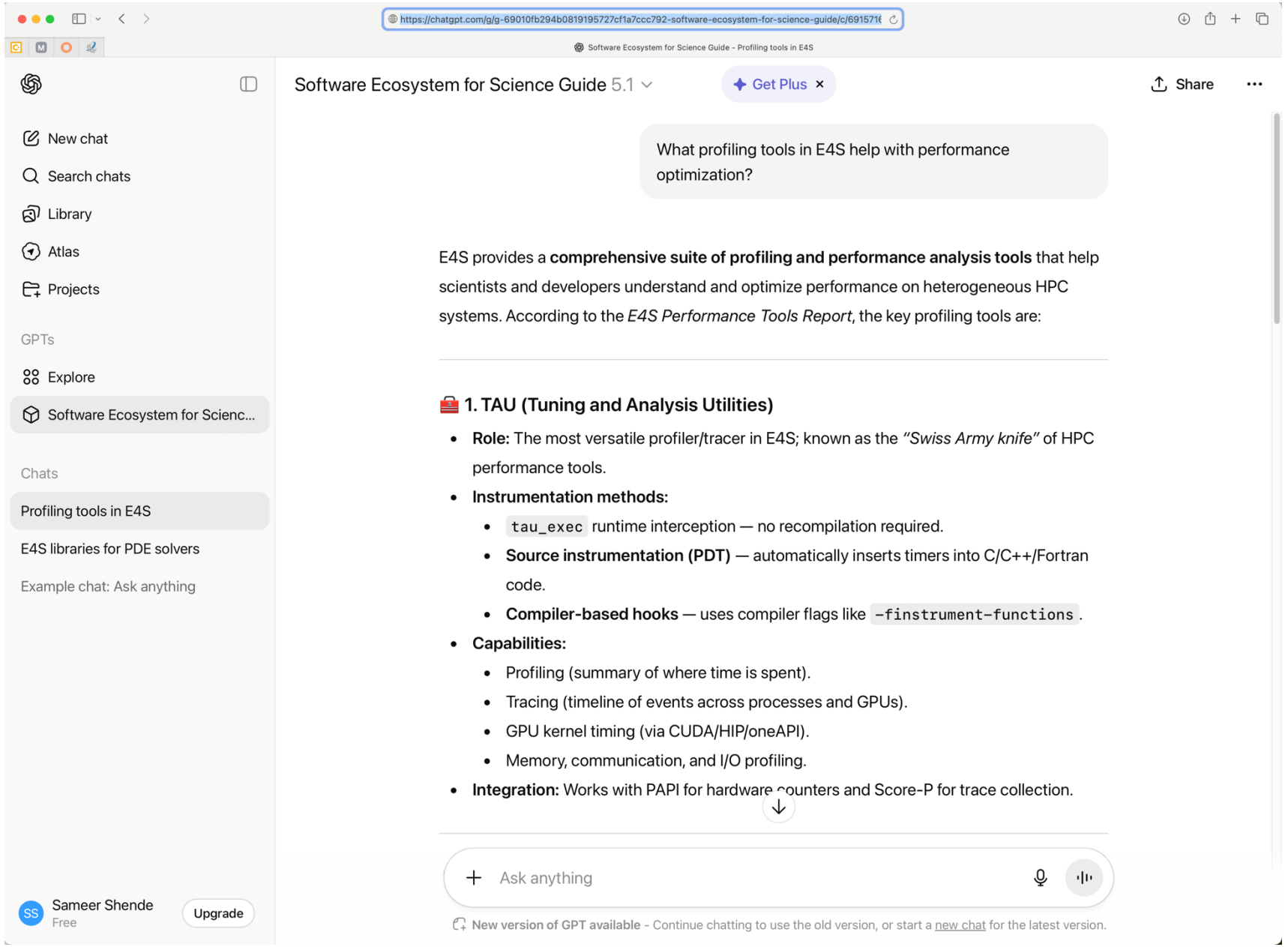
Updated E4S website https://e4s.io



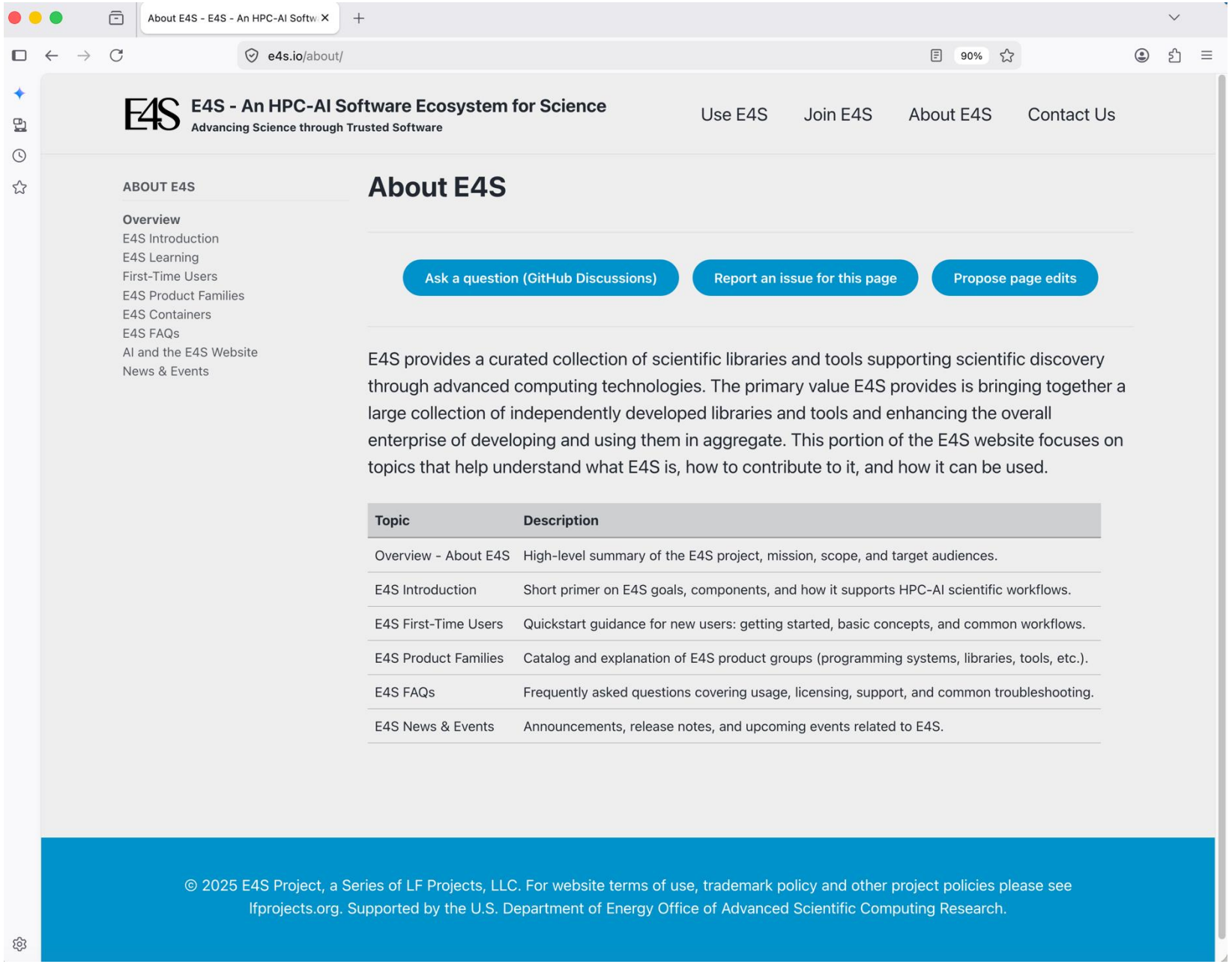
Chatbot integration in E4S Website



E4S Bot trained on E4S content on OpenAI's ChatGPT



E4S Documentation



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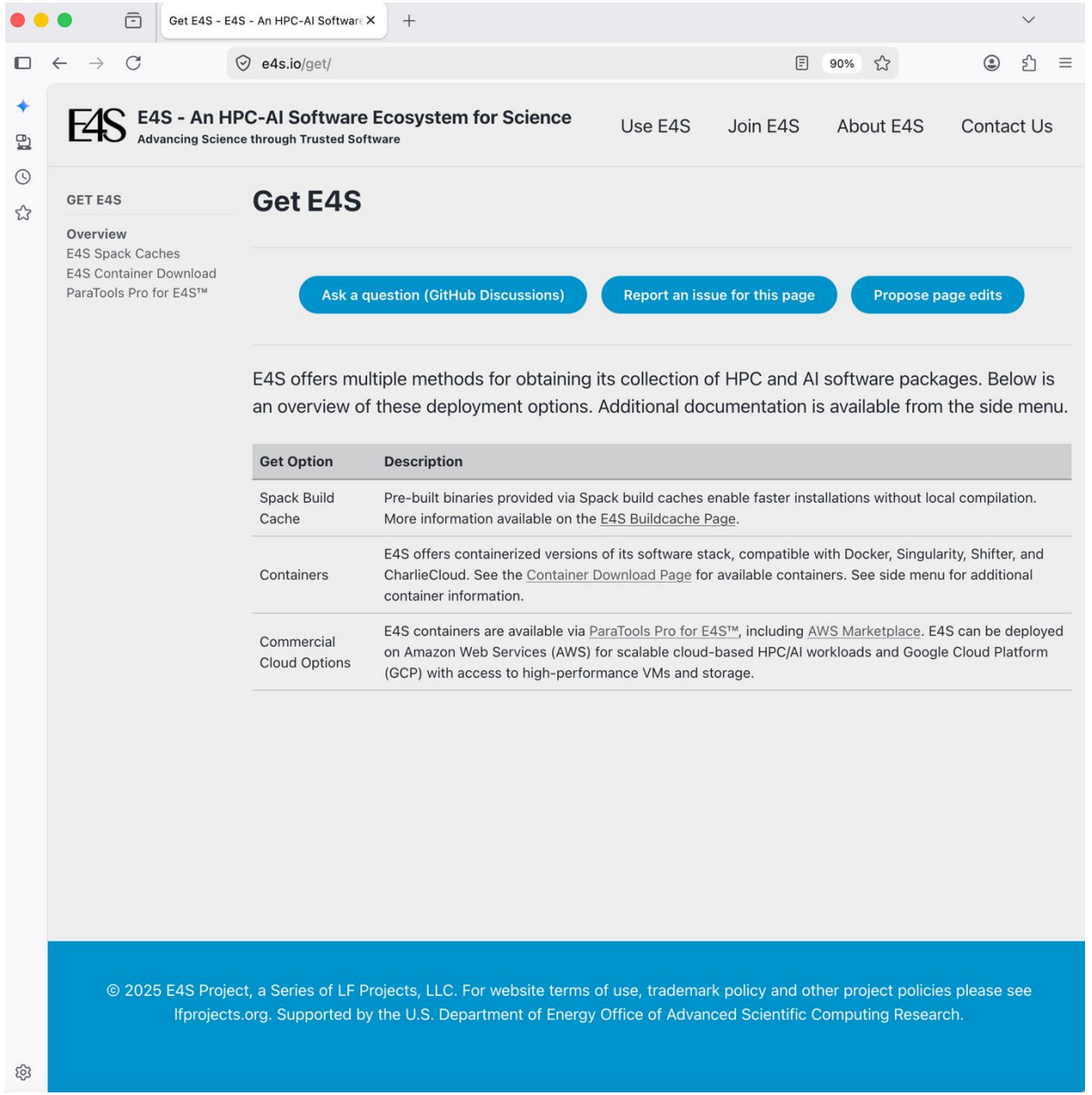
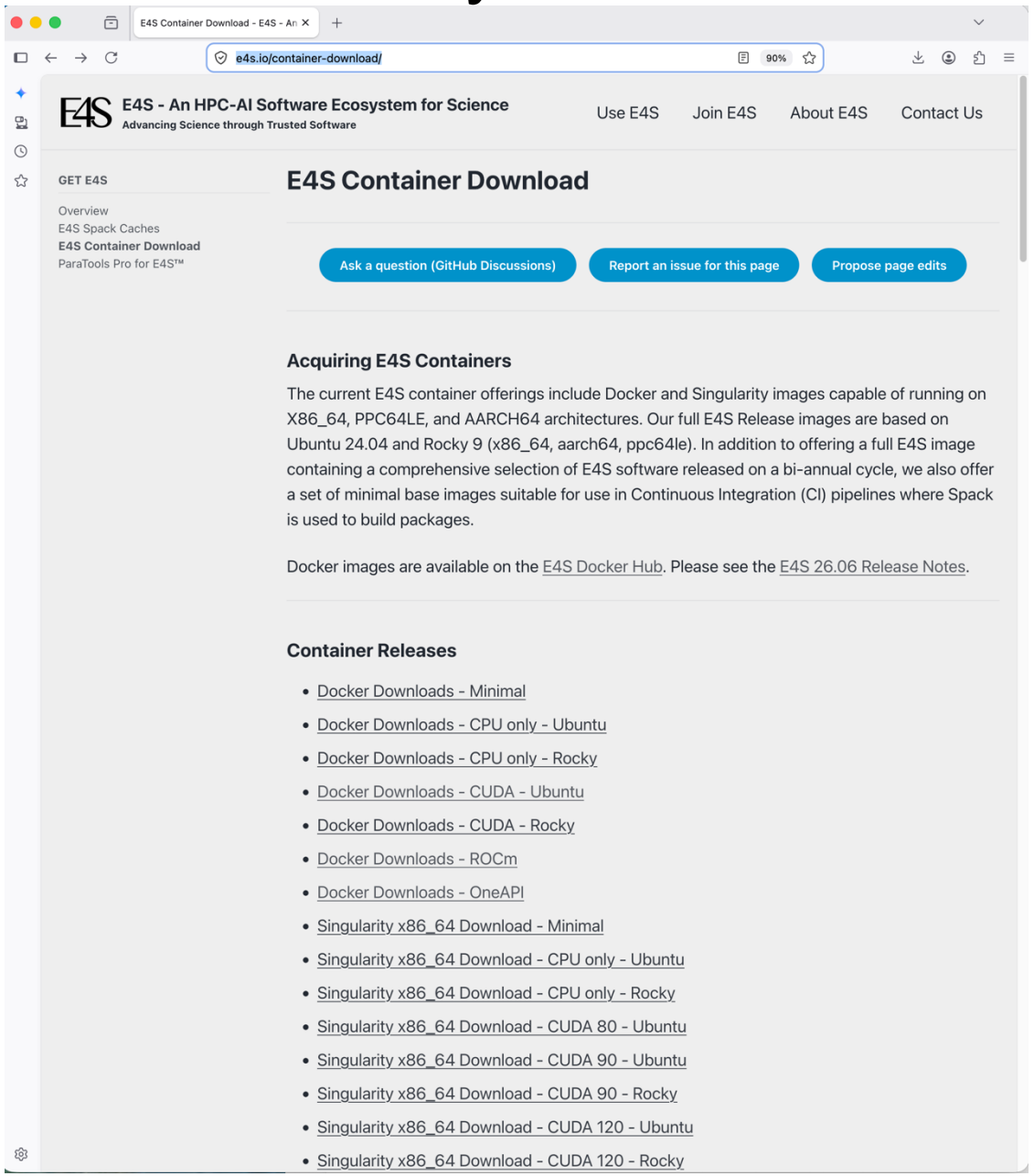
E4S: Bare-metal installation, Containers, and Cloud images



Download E4S Containers: Rocky Linux 9.7 and Ubuntu 24.04 LTS



- Docker and Singularity
- ARM64 (aarch64), x86_64, and ppc64le
- Support for GPUS:
  - NVIDIA
  - AMD
  - Intel
- GPU Runtimes:
  - CUDA 13.2
  - ROCm 7.2.3
  - oneAPI 2026.0
- Languages:
  - C/C++/Fortran
  - Python
  - Rust
  - Julia
  - Chapel ...
- OSes:
  - Rocky Linux 9.7
  - Ubuntu 24.04 LTS

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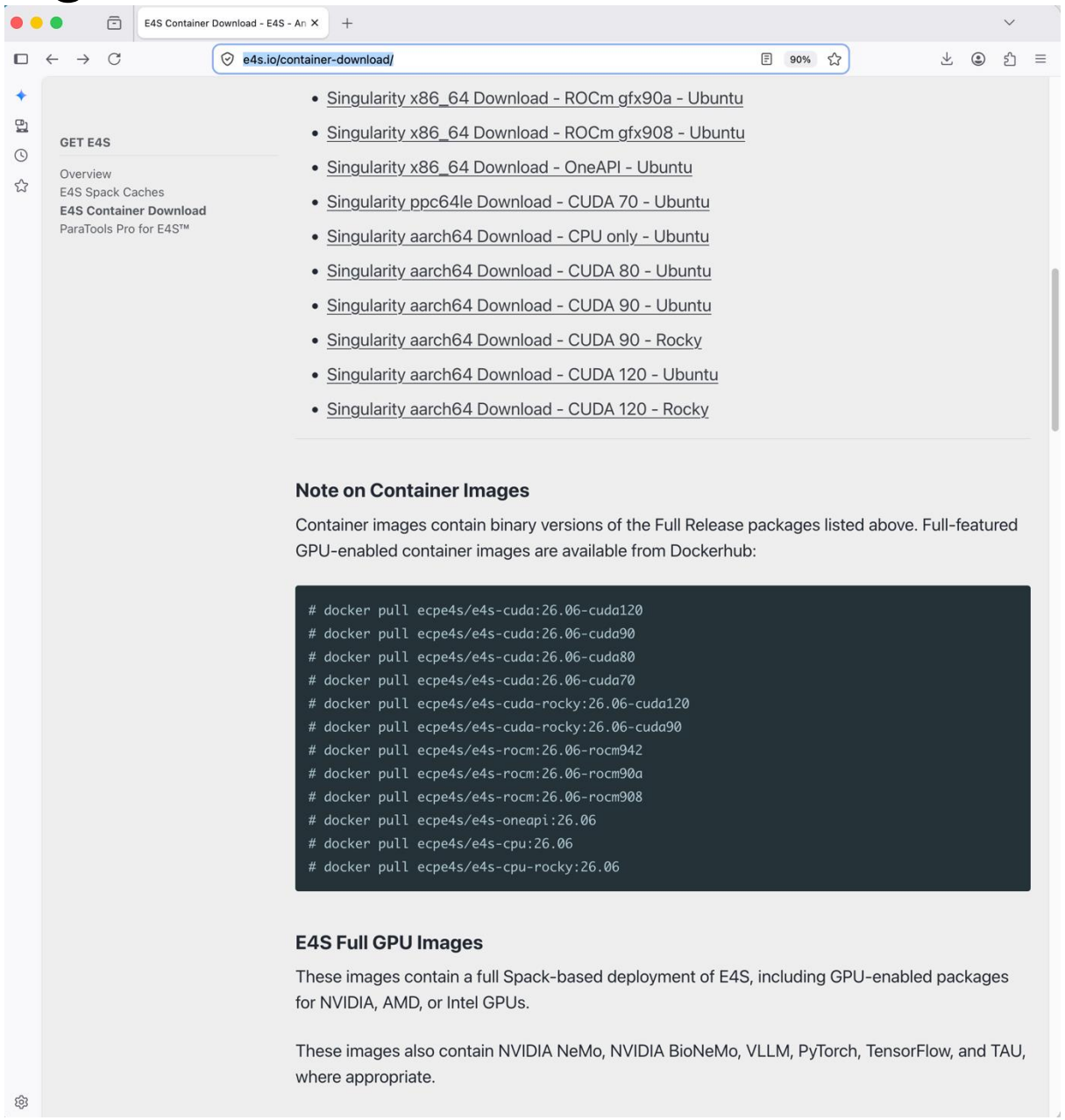
E4S container images available on DockerHub



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E4S: CPU Rocky Linux 9.8 x86_64 Singularity image

```
Singularity> spack find -x
-- linux-rocky9-x86_64_v3 / %c,cxx,fortran=gcc@13.3.1 -----------
adios@1.13.1          cp2k@2026.1            libceed@0.12.0          quantum-espresso@7.5  tau@2.35.2
adios2@2.12.1         darshan-runtime@3.4.7  openmpi@5.0.10          rempi@1.1.0           trilinos@16.2.0
alquimia@1.1.0        darshan-util@3.4.7     papi@7.2.0              scr@3.1.0             variorum@0.8.0
amrex@26.05           datatransferkit@3.1.1  parallel-netcdf@1.14.1  slate@2025.05.28      wps@4.5
ascent@0.9.5          globalarrays@5.8.2     petsc@3.25.1            slepc@3.25.1          xyce@7.10.0
axom@0.14.0           gptune@5.0.0           phist@1.12.1            strumpack@8.0.0       zfp@1.0.1
butterflypack@3.2.0   h5bench@1.4            plumed@2.10.0           sundials@7.7.0
conduit@0.9.6         heffte@2.4.1           precice@3.4.0           superlu-dist@9.2.1

-- linux-rocky9-x86_64_v3 / %c,cxx=gcc@13.3.1 -------------------
boost@1.90.0       ginkgo@1.11.0        legion@26.03.0     omega-h@11.0.0-scorec  sz@2.1.12.5
bricks@2023.08.25  glvis@4.4            libcatalyst@2.1.0  openfoam@2512          sz3@3.2.0
cabana@0.7.0       gmp@6.3.0            libpressio@0.99.4  openpmd-api@0.17.0     turbine@1.3.0
caliper@2.14.0     gotcha@1.0.8         libunwind@1.8.3    papyrus@1.0.2          umap@2.1.1
chai@2025.12.0     gromacs@2026.1       mercury@2.4.1      pdt@3.25.2             umpire@2025.12.0
chapel@2.8.0       hdf5-vol-cache@v1.1  metall@0.30        pruners-ninja@1.0.2    upcxx@2025.10.0
dyninst@13.0.1     hdf5-vol-log@1.4.0   mgard@1.6.0        pumi@2.2.9             veloc@1.7
faodel@1.2108.1    hpctoolkit@2026.0.1  mpifileutils@0.12  qthreads@1.18          vtk-m@2.3.0
fftx@1.2.0         lammps@20250722.3    nccmp@1.9.1.0      raja@2025.12.2         warpx@26.04
gasnet@2025.8.0    lbann@0.104          nco@5.3.4          swig@4.0.2-fortran

-- linux-rocky9-x86_64_v3 / %c,fortran=gcc@13.3.1 ---------------
fpm@0.13.0   libquo@1.4    nekbone@17.0          netlib-scalapack@2.2.3  py-libensemble@1.5.0  wannier90@3.1.0
hdf5@1.14.6  nek5000@19.0  netcdf-fortran@4.6.2  plasma@24.8.7           superlu@7.0.1         wrf@4.7.1

-- linux-rocky9-x86_64_v3 / %c=gcc@13.3.1 -----------------------
aml@0.2.1     charliecloud@0.44  hdf5-vol-async@1.7  libnrm@0.1.0     py-h5py@3.16.0
argobots@1.2  flux-core@0.81.0   hypre@3.1.0         parsec@4.0.2411  py-petsc4py@3.25.1

-- 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@2.1  hpx@1.11.0    kokkos-kernels@5.1.1  loki@0.1.7  mpark-variant@1.4.0
flit@2.1.0  kokkos@5.1.1  laghos@3.1            mfem@4.9.0

-- linux-rocky9-x86_64_v3 / no compilers ------------------------
e4s-alc@1.0.3  exaworks@0.1.0  nrm@0.1.0           py-jupyterhub@1.4.1
e4s-cl@1.0.9   mpich@4.3.2     py-cinemasci@1.7.9  stc@0.9.0
==> 127 installed packages
```

E4S: CUDA Rocky Linux 9.8 x86_64 Singularity image

```
Singularity> spack find -x
-- linux-rocky9-x86_64_v3 / %c,cxx,fortran=gcc@13.3.1 -----------
adios2@2.12.1  cp2k@2025.2     magma@2.10.0  slate@2025.05.28  sundials@7.7.0      trilinos@16.2.0
amrex@26.05    heffte@2.4.1    papi@7.2.0    slepc@3.25.1      superlu-dist@9.2.1  zfp@1.0.1
axom@0.14.0    libceed@0.12.0  petsc@3.25.1  strumpack@8.0.0   tau@2.35.2

-- linux-rocky9-x86_64_v3 / %c,cxx=gcc@13.3.1 -------------------
bricks@2023.08.25  chapel@2.8.0   gromacs@2026.1       legion@26.03.0         raja@2025.12.2
cabana@0.7.0       cusz@0.14.0    hpctoolkit@2026.0.1  libpressio@0.99.4      umpire@2025.12.0
caliper@2.14.0     fftx@1.2.0     hypre@3.1.0          mgard@1.6.0            upcxx@2025.10.0
chai@2025.12.0     ginkgo@1.11.0  lammps@20250722.3    omega-h@11.0.0-scorec  vtk-m@2.3.0

-- linux-rocky9-x86_64_v3 / %c=gcc@13.3.1 -----------------------
flux-core@0.81.0  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@2.1  hpx@1.11.0  kokkos@5.1.1  kokkos-kernels@5.1.1  mfem@4.9.0

-- linux-rocky9-x86_64_v3 / no compilers ------------------------
mpich@4.3.2
==> 46 installed packages
Singularity>
```

E4S: Expanded, curated collection of Python based tools for AI

```
Singularity> python
Python 3.12.12 (main, Mar  2 2026, 16:39:05) [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 transformers
>>> import vllm
>>> import jax
>>> import cupy
>>> import triton
>>> import flash_attn
>>> import transformer_engine
>>> import accelerate
>>> import peft
>>> import sglang
>>> import ray
>>> import nemo_run
>>> import langchain
>>> import langgraph
>>> import bionemo
>>> import a2a
>>> import mcp
>>> import pandas
>>> import mlflow
>>> import openai
>>> import anthropic
>>> import google
>>> import huggingface_hub
>>> import tokenizers
>>> import mpi4py
>>> import s3fs
>>> import jupyter
>>> import marimo
>>> import tritonclient
```

```
>>> import ray
>>> import megatron
>>> import nemo_run
>>> import datasets
>>> import gradio
>>> import geopandas
>>> import polars
>>> import numpy
>>> import scipy
>>> import seaborn
>>> import leptonai
>>> import lightning
>>> import tensorboard
>>> import outlines
```

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E4S: Intel oneAPI 2026.0 Singularity image supports Intel GPUs

```
$ singularity run --nv e4s-oneapi-x86_64-26-06-1781565945.sif
Singularity> spack find -x
-- linux-ubuntu24.04-x86_64_v3 / %c,cxx,fortran=gcc@13.3.0 ------
adios2@2.12.1  gptune@5.0.0  openmpi@5.0.10  scr@3.1.0

-- linux-ubuntu24.04-x86_64_v3 / %c,cxx,fortran=oneapi@2026.0.0 -
adios@1.13.1  axom@0.14.0            darshan-util@3.4.7     heffte@2.4.1           phist@1.12.1      strumpack@8.0.0     tau@2.35.2       zfp@1.0.1
amrex@26.05   butterflypack@3.2.0    datatransferkit@3.1.1  libceed@0.12.0         plumed@2.10.0     sundials@7.7.0      trilinos@16.2.0
amrex@26.05   conduit@0.9.6          globalarrays@5.8.2     papi@7.2.0             rempi@1.1.0       superlu-dist@9.2.1  unifyfs@2.0
ascent@0.9.5  darshan-runtime@3.4.7  h5bench@1.4            parallel-netcdf@1.14.1 slate@2025.05.28  tau@2.35.2          variorum@0.8.0

-- linux-ubuntu24.04-x86_64_v3 / %c,cxx=gcc@13.3.0 %fortran=oneapi@2026.0.0
quantum-espresso@7.5

-- linux-ubuntu24.04-x86_64_v3 / %c,cxx=gcc@13.3.0 --------------
openfoam@2512  openpmd-api@0.17.0  swig@4.0.2-fortran

-- linux-ubuntu24.04-x86_64_v3 / %c,cxx=oneapi@2026.0.0 ---------
bolt@2.0           cabana@0.7.0     gasnet@2025.8.0  gromacs@2026.1       legion@26.03.0     metall@0.30        omega-h@11.0.0-scorec  pumi@2.2.9      sz3@3.2.0         upcxx@2025.10.0
boost@1.90.0       caliper@2.14.0   ginkgo@1.11.0    hdf5-vol-log@1.4.0   libcatalyst@2.1.0  mgard@1.6.0        papyrus@1.0.2          qthreads@1.18   turbine@1.3.0     upcxx@2025.10.0
bricks@2023.08.25  chai@2025.12.0   gmp@6.3.0        hpctoolkit@2026.0.1  libunwind@1.8.3    mpifileutils@0.12  pdt@3.25.2             raja@2025.12.2  umap@2.1.1        veloc@1.7
cabana@0.7.0       faodel@1.2108.1  gotcha@1.0.8     hpctoolkit@2026.0.1  mercury@2.4.1      nccmp@1.9.1.0      pruners-ninja@1.0.2    sz@2.1.12.5     umpire@2025.12.0  vtk-m@2.3.0

-- linux-ubuntu24.04-x86_64_v3 / %c,fortran=gcc@13.3.0 ----------
py-libensemble@1.5.0

-- linux-ubuntu24.04-x86_64_v3 / %c,fortran=oneapi@2026.0.0 -----
hdf5@1.14.6  libquo@1.4  nekbone@17.0  netcdf-fortran@4.6.2  netlib-scalapack@2.2.3  superlu@7.0.1  wannier90@3.1.0

-- linux-ubuntu24.04-x86_64_v3 / %c=gcc@13.3.0 ------------------
charliecloud@0.44  parsec@4.0.2411

-- linux-ubuntu24.04-x86_64_v3 / %c=oneapi@2026.0.0 -------------
aml@0.2.1  aml@0.2.1  argobots@1.2  flux-core@0.81.0  hdf5-vol-async@1.7  hypre@3.1.0  libnrm@0.1.0

-- linux-ubuntu24.04-x86_64_v3 / %cxx,fortran=oneapi@2026.0.0 ---
fortrilinos@2.3.0  tasmanian@8.1

-- linux-ubuntu24.04-x86_64_v3 / %cxx=gcc@13.3.0 ----------------
hpx@1.11.0

-- linux-ubuntu24.04-x86_64_v3 / %cxx=oneapi@2026.0.0 -----------
arborx@2.1  arborx@2.1  flit@2.1.0  kokkos@5.1.1  kokkos@5.1.1  kokkos-kernels@5.1.1  laghos@3.1  loki@0.1.7  mfem@4.9.0  mpark-variant@1.4.0

-- linux-ubuntu24.04-x86_64_v3 / no compilers -------------------
e4s-alc@1.0.3  e4s-cl@1.0.9  exaworks@0.1.0  intel-oneapi-mpi@2021.18.0  nrm@0.1.0  py-jupyterhub@1.4.1  stc@0.9.0
==> 114 installed packages
Singularity>
```

E4S: AMD ROCm 7.2.3 Singularity image

```
Singularity> ls /opt/rocm-7.2.3/bin/hipcc
/opt/rocm-7.2.3/bin/hipcc
Singularity> spack find -x +rocm
-- linux-ubuntu24.04-x86_64_v3 / %c,cxx,fortran=gcc@13.3.0 ------
amrex@26.05   libceed@0.12.0  papi@7.2.0    slate@2025.05.28  sundials@7.7.0      tau@2.35.2
heffte@2.4.1  magma@2.10.0    petsc@3.25.1  slepc@3.25.1      superlu-dist@9.2.1  trilinos@16.2.0

-- linux-ubuntu24.04-x86_64_v3 / %c,cxx=gcc@13.3.0 --------------
caliper@2.14.0  gasnet@2025.8.0      hypre@3.1.0     raja@2025.12.2    upcxx@2025.10.0
chai@2025.12.0  hpctoolkit@2026.0.1  legion@26.03.0  umpire@2025.12.0  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 ----------------
kokkos@5.1.1  mfem@4.9.0
==> 25 installed packages
```

E4S: CPU aarch64 Singularity image (macOS M-series, NVIDIA Grace)

```
Singularity> spack find -x
-- linux-ubuntu24.04-aarch64 / %c,cxx,fortran=gcc@13.3.0 --------
adios@1.13.1    axom@0.14.0           darshan-util@3.4.7     heffte@2.4.1           paraview@6.1.0  quantum-espresso@7.5  strumpack@8.0.0     wps@4.5
adios2@2.12.1   butterflypack@3.2.0   datatransferkit@3.1.1  libceed@0.12.0         petsc@3.25.1    rempi@1.1.0           sundials@7.7.0      zfp@1.0.1
alquimia@1.1.0  conduit@0.9.6         globalarrays@5.8.2     openmpi@5.0.10         phist@1.12.1    scr@3.1.0             superlu-dist@9.2.1
amrex@26.05     cp2k@2026.1           gptune@5.0.0           papi@7.2.0             plumed@2.10.0   slate@2025.05.28      tau@2.35.2
ascent@0.9.5    darshan-runtime@3.4.7 h5bench@1.4            parallel-netcdf@1.14.1 precice@3.4.0   slepc@3.25.1          trilinos@16.2.0

-- linux-ubuntu24.04-aarch64 / %c,cxx=gcc@13.3.0 ----------------
boost@1.90.0    faodel@1.2108.1  gotcha@1.0.8         lbann@0.104        metall@0.30           openfoam@2512        qthreads@1.18       umap@2.1.1
cabana@0.7.0    fftx@1.2.0       gromacs@2026.1       legion@26.03.0     mgard@1.6.0           openpmd-api@0.17.0   raja@2025.12.2      umpire@2025.12.0
caliper@2.14.0  gasnet@2025.8.0  hdf5-vol-cache@v1.1  libcatalyst@2.1.0  mpifileutils@0.12     papyrus@1.0.2        swig@4.0.2-fortran  upcxx@2025.10.0
chai@2025.12.0  ginkgo@1.11.0    hdf5-vol-log@1.4.0   libpressio@0.99.4  nccmp@1.9.1.0         pdt@3.25.2           sz@2.1.12.5         veloc@1.7
chapel@2.8.0    glvis@4.4        hpctoolkit@2026.0.1  libunwind@1.7.2    nco@5.3.4             pruners-ninja@1.0.2  sz3@3.2.0           vtk-m@2.3.0
dyninst@13.0.1  gmp@6.3.0        lammps@20250722.3    mercury@2.4.1      omega-h@11.0.0-scorec pumi@2.2.9           turbine@1.3.0       warpx@26.04

-- linux-ubuntu24.04-aarch64 / %c,fortran=gcc@13.3.0 ------------
fpm@0.13.0   libquo@1.4    nekbone@17.0          netlib-scalapack@2.2.3  py-libensemble@1.5.0  wannier90@3.1.0
hdf5@1.14.6  nek5000@19.0  netcdf-fortran@4.6.2  plasma@24.8.7           superlu@7.0.1         wrf@4.7.1

-- linux-ubuntu24.04-aarch64 / %c=gcc@13.3.0 --------------------
aml@0.2.1     charliecloud@0.44  hdf5-vol-async@1.7  libnrm@0.1.0     py-h5py@3.16.0
argobots@1.2  flux-core@0.81.0   hypre@3.1.0         parsec@4.0.2411  py-petsc4py@3.25.1

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

-- linux-ubuntu24.04-aarch64 / %cxx=gcc@13.3.0 ------------------
arborx@2.1  flit@2.1.0  hpx@1.11.0  kokkos@5.1.1  kokkos-kernels@5.1.1  laghos@3.1  loki@0.1.7  mfem@4.9.0  mpark-variant@1.4.0

-- linux-ubuntu24.04-aarch64 / no compilers ---------------------
e4s-alc@1.0.3  e4s-cl@1.0.9  exaworks@0.1.0  mpich@4.3.2  nrm@0.1.0  py-cinemasci@1.7.9  py-jupyterhub@1.4.1  stc@0.9.0
==> 125 installed packages
```

E4S: CUDA aarch64 Ubuntu Singularity image

```
Singularity> spack find -x
-- linux-ubuntu24.04-aarch64 / %c,cxx,fortran=gcc@13.3.0 --------
adios2@2.12.1  axom@0.14.0  heffte@2.4.1    magma@2.10.0    petsc@3.25.1      slepc@3.25.1     sundials@7.7.0      tau@2.35.2       zfp@1.0.1
amrex@26.05    cp2k@2025.2  libceed@0.12.0  paraview@6.1.0  slate@2025.05.28  strumpack@8.0.0  superlu-dist@9.2.1  trilinos@16.2.0

-- linux-ubuntu24.04-aarch64 / %c,cxx=gcc@13.3.0 ----------------
cabana@0.7.0    cusz@0.14.0    gromacs@2026.1       lammps@20250722.3  mgard@1.6.0            umpire@2025.12.0
caliper@2.14.0  fftx@1.2.0     hpctoolkit@2026.0.1  legion@26.03.0     omega-h@11.0.0-scorec  upcxx@2025.10.0
chai@2025.12.0  ginkgo@1.11.0  hypre@3.1.0          libpressio@0.99.4  raja@2025.12.2         vtk-m@2.3.0

-- linux-ubuntu24.04-aarch64 / %c=gcc@13.3.0 --------------------
flux-core@0.81.0  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@2.1  hpx@1.11.0  kokkos@5.1.1  kokkos-kernels@5.1.1  mfem@4.9.0

-- linux-ubuntu24.04-aarch64 / no compilers ---------------------
mpich@4.3.2
==> 44 installed packages
```

E4S: CPU aarch64 Rocky Linux 9.7 Singularity image

```
Singularity> spack find -x
-- linux-rocky9-aarch64 / %c,cxx,fortran=gcc@13.3.1 -------------
adios@1.13.1    butterflypack@3.2.0    globalarrays@5.8.2  papi@7.2.0             quantum-espresso@7.5  sundials@7.7.0
adios2@2.12.1   conduit@0.9.6          gptune@5.0.0        parallel-netcdf@1.14.1 rempi@1.1.0           superlu-dist@9.2.1
alquimia@1.1.0  cp2k@2026.1            h5bench@1.4         petsc@3.25.1           scr@3.1.0             tau@2.35.2
amrex@26.05     darshan-runtime@3.4.7  heffte@2.4.1        phist@1.12.1           slate@2025.05.28      trilinos@16.2.0
ascent@0.9.5    darshan-util@3.4.7     libceed@0.12.0      plumed@2.10.0          slepc@3.25.1          wps@4.5
axom@0.14.0     datatransferkit@3.1.1  openmpi@5.0.10      precice@3.4.0          strumpack@8.0.0       zfp@1.0.1

-- linux-rocky9-aarch64 / %c,cxx=gcc@13.3.1 ----------------------
boost@1.90.0    faodel@1.2108.1  gotcha@1.0.8         lbann@0.104        metall@0.30           openfoam@2512        qthreads@1.18       umap@2.1.1
cabana@0.7.0    fftx@1.2.0       gromacs@2026.1       legion@26.03.0     mgard@1.6.0           openpmd-api@0.17.0   raja@2025.12.2      umpire@2025.12.0
caliper@2.14.0  gasnet@2025.8.0  hdf5-vol-cache@v1.1  libcatalyst@2.1.0  mpifileutils@0.12     papyrus@1.0.2        swig@4.0.2-fortran  upcxx@2025.10.0
chai@2025.12.0  ginkgo@1.11.0    hdf5-vol-log@1.4.0   libpressio@0.99.4  nccmp@1.9.1.0         pdt@3.25.2           sz@2.1.12.5         veloc@1.7
chapel@2.8.0    glvis@4.4        hpctoolkit@2026.0.1  libunwind@1.7.2    nco@5.3.4             pruners-ninja@1.0.2  sz3@3.2.0           vtk-m@2.3.0
dyninst@13.0.1  gmp@6.3.0        lammps@20250722.3    mercury@2.4.1      omega-h@11.0.0-scorec pumi@2.2.9           turbine@1.3.0       warpx@26.04

-- linux-rocky9-aarch64 / %c,fortran=gcc@13.3.1 -----------------
fpm@0.13.0   libquo@1.4    nekbone@17.0          netlib-scalapack@2.2.3  py-libensemble@1.5.0  wannier90@3.1.0
hdf5@1.14.6  nek5000@19.0  netcdf-fortran@4.6.2  plasma@24.8.7           superlu@7.0.1         wrf@4.7.1

-- linux-rocky9-aarch64 / %c=gcc@13.3.1 -------------------------
aml@0.2.1     charliecloud@0.44  hdf5-vol-async@1.7  libnrm@0.1.0     py-h5py@3.16.0
argobots@1.2  flux-core@0.81.0   hypre@3.1.0         parsec@4.0.2411  py-petsc4py@3.25.1

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

-- linux-rocky9-aarch64 / %cxx=gcc@13.3.1 -----------------------
arborx@2.1  flit@2.1.0  hpx@1.11.0  kokkos@5.1.1  kokkos-kernels@5.1.1  laghos@3.1  loki@0.1.7  mfem@4.9.0  mpark-variant@1.4.0

-- linux-rocky9-aarch64 / no compilers --------------------------
e4s-alc@1.0.3  e4s-cl@1.0.9  exaworks@0.1.0  mpich@4.3.2  nrm@0.1.0  py-cinemasci@1.7.9  py-jupyterhub@1.4.1  stc@0.9.0
==> 124 installed packages
```

E4S: CUDA aarch64 Rocky Linux 9.7 Singularity image

```
Singularity> spack find -x
-- linux-rocky9-aarch64 / %c,cxx,fortran=gcc@13.3.1 -------------
adios2@2.12.1  axom@0.14.0  heffte@2.4.1    magma@2.10.0  slate@2025.05.28  strumpack@8.0.0  superlu-dist@9.2.1  trilinos@16.2.0
amrex@26.05    cp2k@2025.2  libceed@0.12.0  petsc@3.25.1  slepc@3.25.1      sundials@7.7.0   tau@2.35.2          zfp@1.0.1

-- linux-rocky9-aarch64 / %c,cxx=gcc@13.3.1 ----------------------
cabana@0.7.0    cusz@0.14.0    gromacs@2026.1       lammps@20250722.3  mgard@1.6.0            umpire@2025.12.0
caliper@2.14.0  fftx@1.2.0     hpctoolkit@2026.0.1  legion@26.03.0     omega-h@11.0.0-scorec  upcxx@2025.10.0
chai@2025.12.0  ginkgo@1.11.0  hypre@3.1.0          libpressio@0.99.4  raja@2025.12.2         vtk-m@2.3.0

-- linux-rocky9-aarch64 / %c=gcc@13.3.1 -------------------------
flux-core@0.81.0  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@2.1  hpx@1.11.0  kokkos@5.1.1  kokkos-kernels@5.1.1  mfem@4.9.0

-- linux-rocky9-aarch64 / no compilers --------------------------
mpich@4.3.2
==> 43 installed packages
```

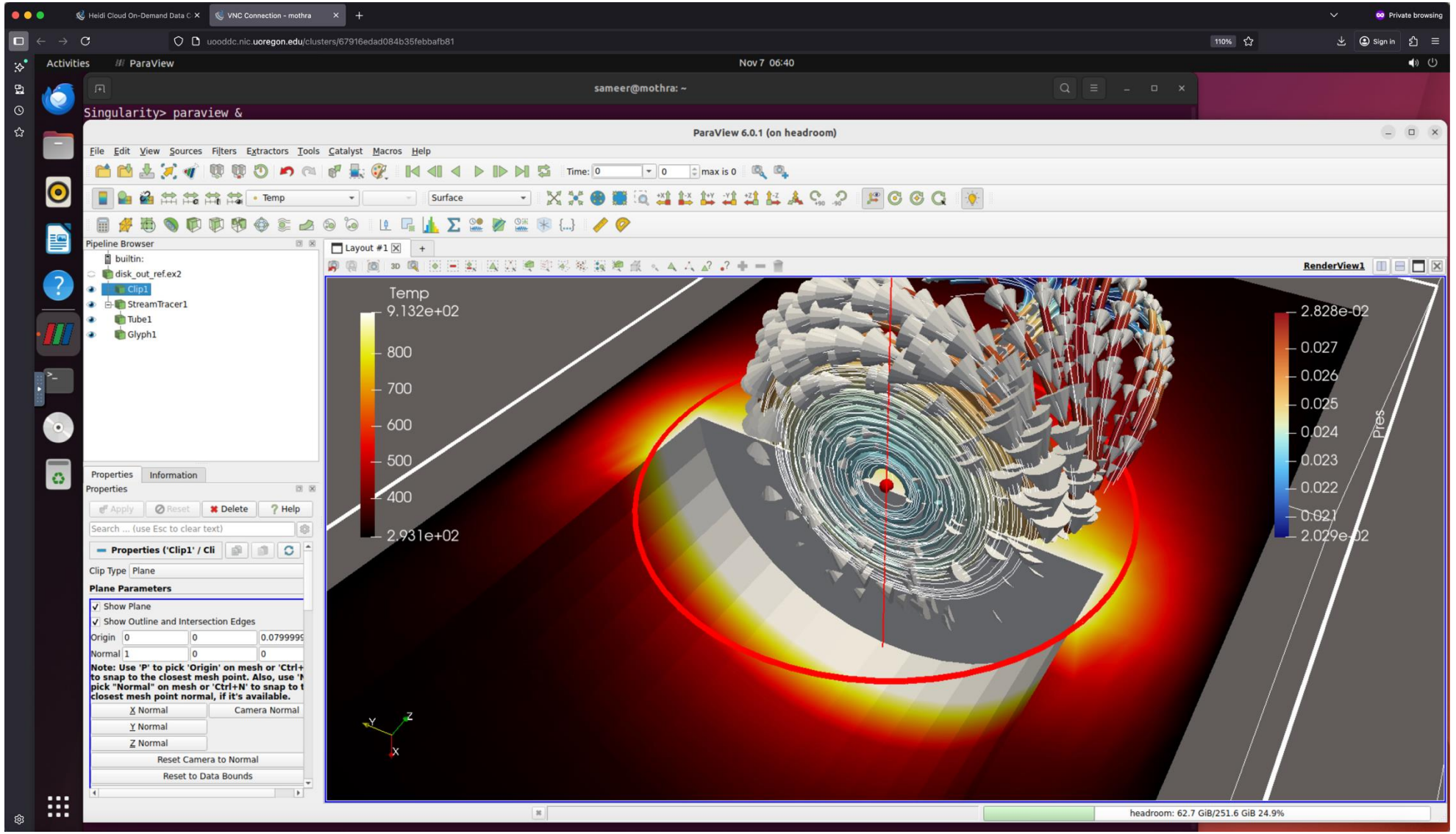
E4S: CPU IBM ppc64le Ubuntu Singularity image

```
Singularity> spack find -x
-- linux-ubuntu20.04-ppc64le / %c,cxx,fortran=gcc@9.4.0 ---------
adios@1.13.1    axom@0.14.0           datatransferkit@3.1.1  nwchem@7.3.1          phist@1.12.1          slate@2025.05.28    tau@2.35.2
adios2@2.12.1   butterflypack@3.2.0   globalarrays@5.8.2     openmpi@5.0.10        plumed@2.10.0         slepc@3.25.1        trilinos@16.2.0
alquimia@1.1.0  conduit@0.9.6         h5bench@1.4            papi@7.2.0            quantum-espresso@7.5  strumpack@8.0.0     unifyfs@2.0
amrex@25.05     darshan-runtime@3.4.7 heffte@2.4.1           parallel-netcdf@1.14.1 rempi@1.1.0          sundials@7.7.0      wps@4.5
ascent@0.9.5    darshan-util@3.4.7    libceed@0.12.0         petsc@3.25.1          scr@3.1.0             superlu-dist@9.2.1  zfp@1.0.1

-- linux-ubuntu20.04-ppc64le / %c,cxx=gcc@9.4.0 -----------------
bolt@2.0           faodel@1.2108.1  hdf5-vol-cache@v1.1  libpressio@0.99.4  nco@5.3.4              pumi@2.2.9          umap@2.1.1
boost@1.90.0       fftx@1.2.0       hdf5-vol-log@1.4.0   libunwind@1.7.2    omega-h@11.0.0-scorec  qthreads@1.18       umpire@2025.12.0
bricks@2023.08.25  gasnet@2025.8.0  hpctoolkit@2024.01.1 mercury@2.4.1      openfoam@2512          raja@2025.12.2      upcxx@2025.10.0
cabana@0.7.0       ginkgo@1.11.0    lammps@20250722.3    metall@0.30        openpmd-api@0.17.0     swig@4.0.2-fortran  veloc@1.7
caliper@2.14.0     glvis@4.4        lbann@0.104          mgard@1.6.0        papyrus@1.0.2          sz@2.1.12.5         vtk-m@2.3.0
chai@2025.12.0     gmp@6.3.0        legion@26.03.0       mpifileutils@0.12  pdt@3.25.2             sz3@3.2.0           warpx@25.04
dyninst@13.0.1     gotcha@1.0.8     libcatalyst@2.1.0    nccmp@1.9.1.0      pruners-ninja@1.0.2    turbine@1.3.0

-- linux-ubuntu20.04-ppc64le / %c,fortran=gcc@9.4.0 -------------
fpm@0.13.0   libquo@1.4    nekbone@17.0          netlib-scalapack@2.2.3  py-libensemble@1.5.0  wannier90@3.1.0
hdf5@1.14.6  nek5000@19.0  netcdf-fortran@4.6.2  plasma@24.8.7           superlu@7.0.1         wrf@4.7.1

-- linux-ubuntu20.04-ppc64le / %c=gcc@9.4.0 ---------------------
aml@0.2.1     charliecloud@0.44  hdf5-vol-async@1.7  libnrm@0.1.0     py-h5py@3.16.0
argobots@1.2  flux-core@0.81.0   hypre@3.1.0         parsec@4.0.2411  py-petsc4py@3.25.1

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

-- linux-ubuntu20.04-ppc64le / %cxx=gcc@9.4.0 -------------------
arborx@2.1  flit@2.1.0  hpx@1.11.0  kokkos@4.7.04  kokkos-kernels@4.7.04  laghos@3.1  loki@0.1.7  mfem@4.9.0  mpark-variant@1.4.0

-- linux-ubuntu20.04-ppc64le / no compilers ---------------------
e4s-alc@1.0.3  e4s-cl@1.0.9  exaworks@0.1.0  mpich@4.3.2  nrm@0.1.0  py-jupyterhub@1.4.1  stc@0.9.0
==> 123 installed packages
```

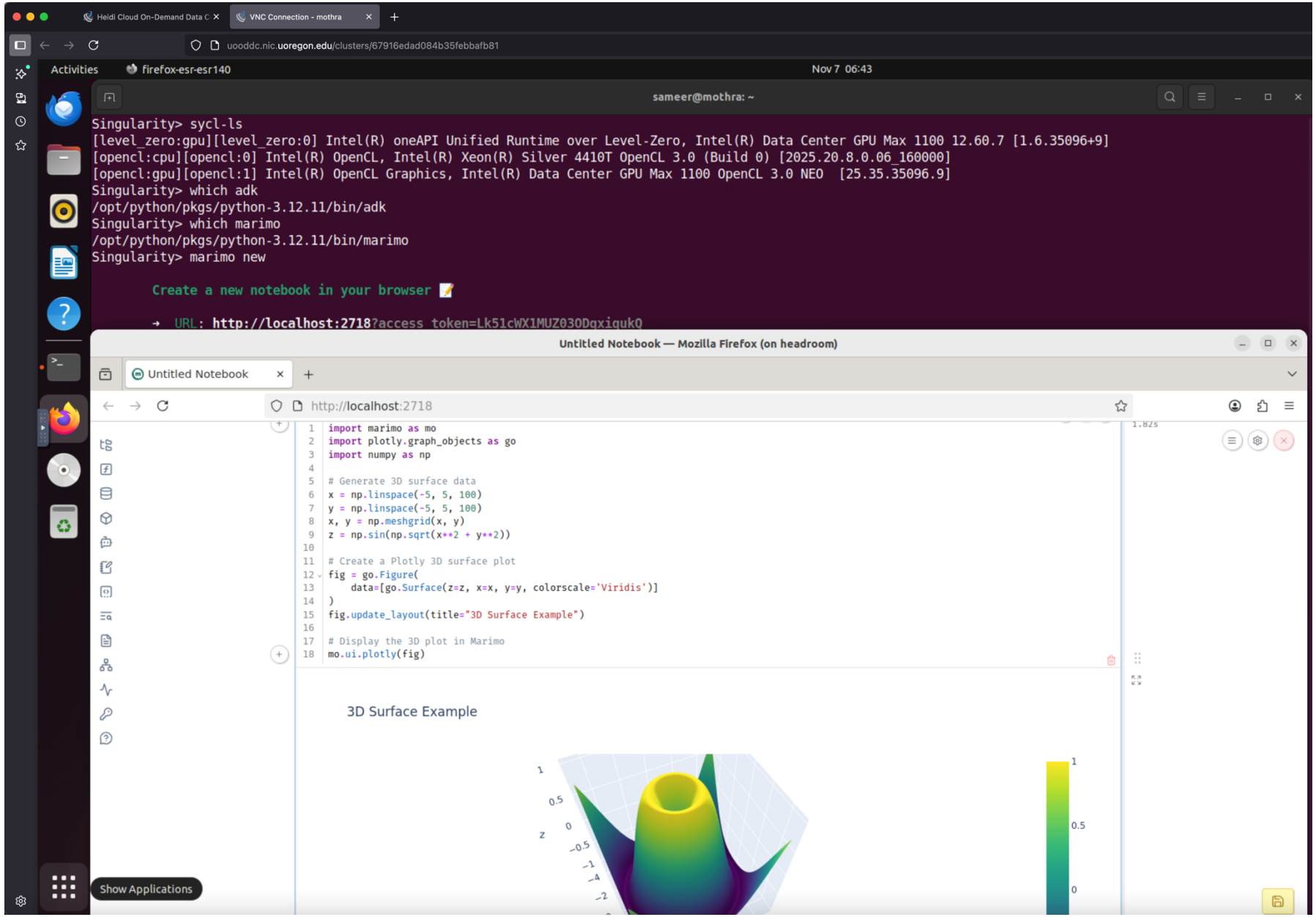
E4S: CUDA IBM ppc64le Ubuntu Singularity image

```
Singularity> spack find -x
-- linux-ubuntu20.04-ppc64le / %c,cxx,fortran=gcc@9.4.0 ---------
adios2@2.12.1  heffte@2.4.1    magma@2.10.0  slepc@3.25.1     sundials@7.7.0      tau@2.35.2
amrex@25.05    libceed@0.12.0  petsc@3.25.1  strumpack@8.0.0  superlu-dist@9.2.1  zfp@1.0.1

-- linux-ubuntu20.04-ppc64le / %c,cxx=gcc@9.4.0 -----------------
bricks@2023.08.25  caliper@2.14.0  fftx@1.2.0     hpctoolkit@2024.01.1  lammps@20250722.3  omega-h@11.0.0-scorec  upcxx@2025.10.0
cabana@0.7.0       chai@2025.12.0  ginkgo@1.11.0  hypre@3.1.0           mgard@1.6.0        umpire@2025.12.0       vtk-m@2.3.0

-- linux-ubuntu20.04-ppc64le / %c=gcc@9.4.0 ---------------------
flux-core@0.81.0  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 -------------------
hpx@1.11.0  kokkos@4.7.04  kokkos-kernels@4.7.04  mfem@4.9.0

-- linux-ubuntu20.04-ppc64le / no compilers ---------------------
mpich@4.3.2
==> 34 installed packages
Singularity>
```

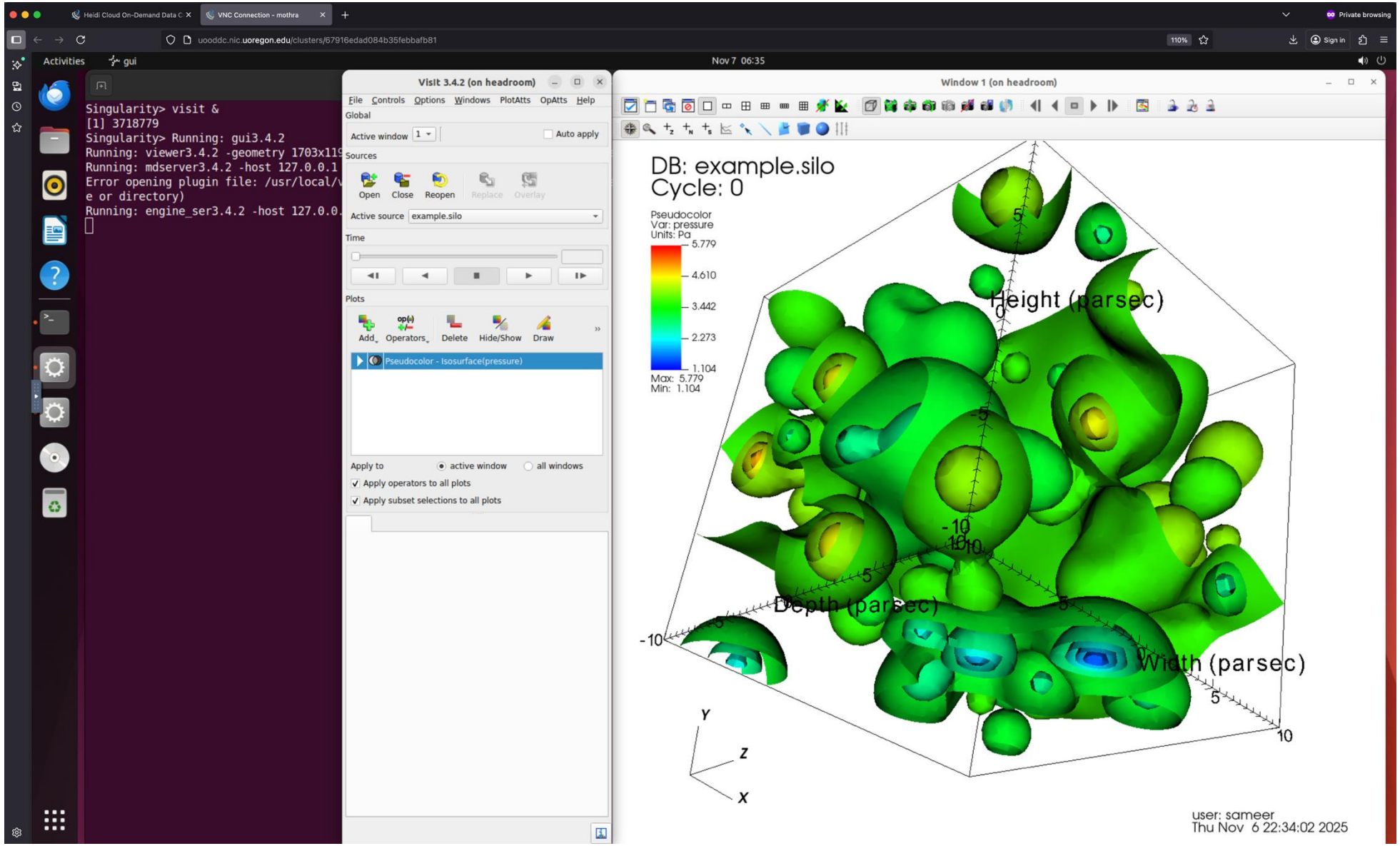
E4S: Visualization Tools: ParaView



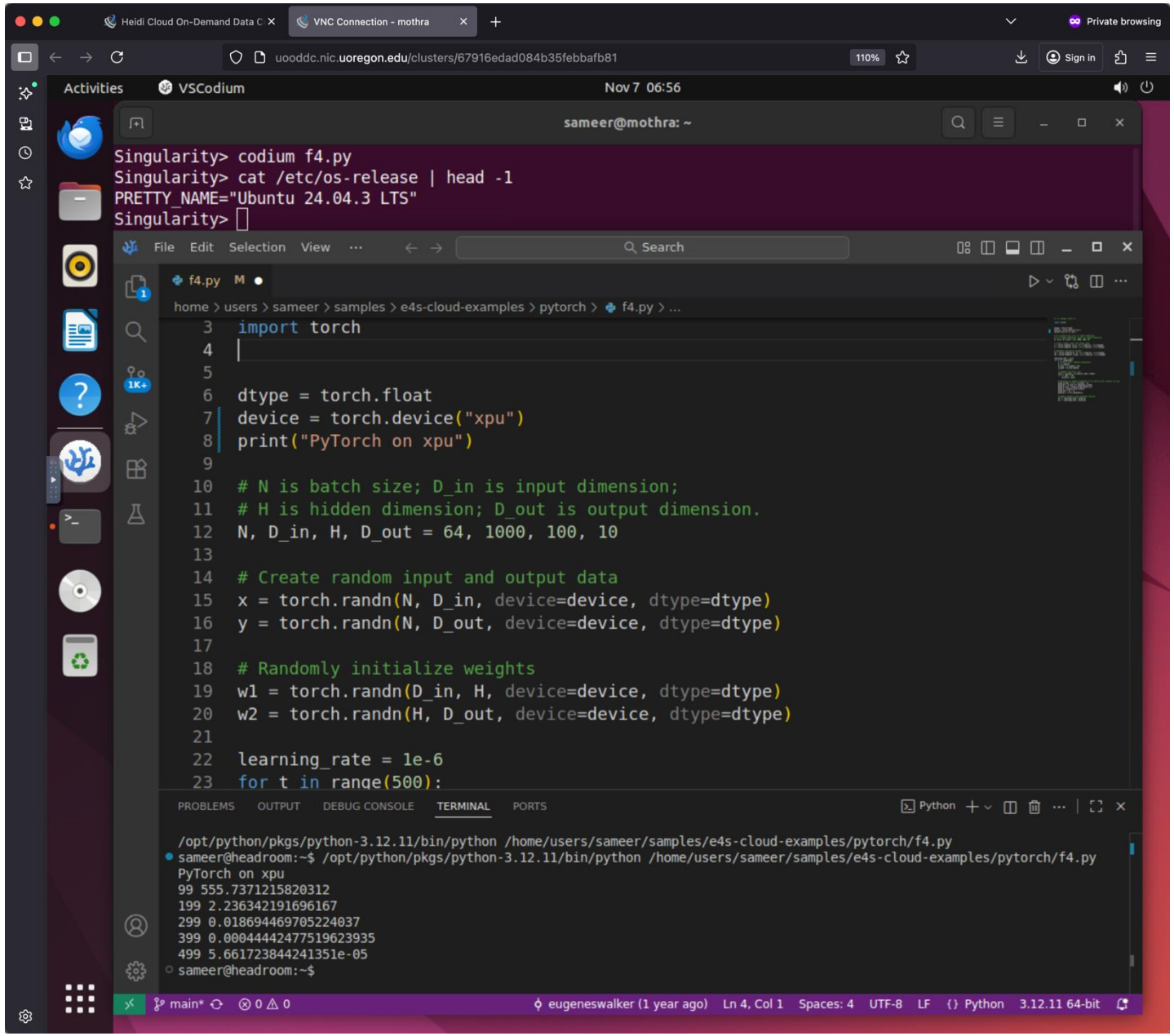
E4S: Marimo Reactive Notebooks



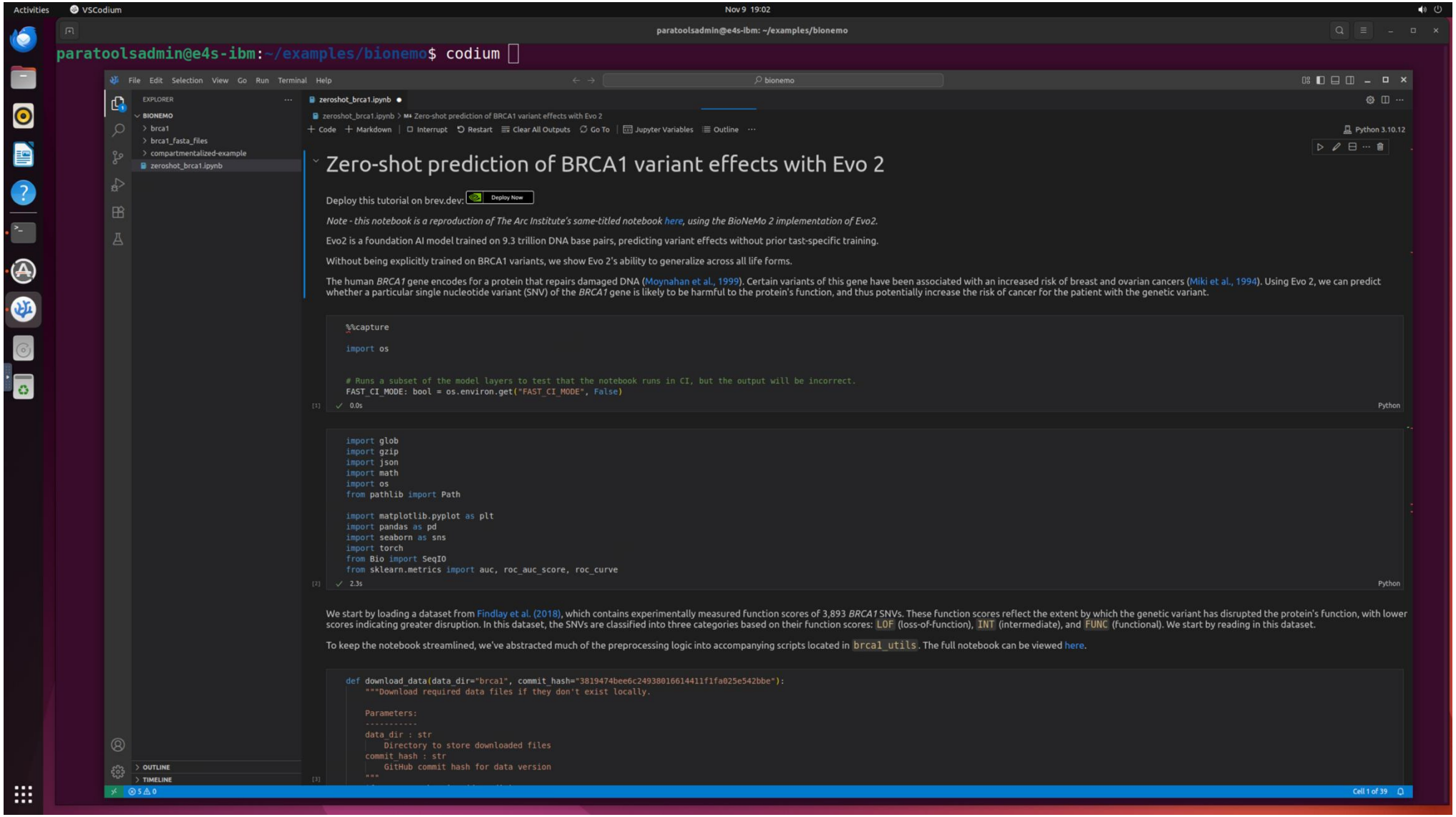
E4S: VisIt


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

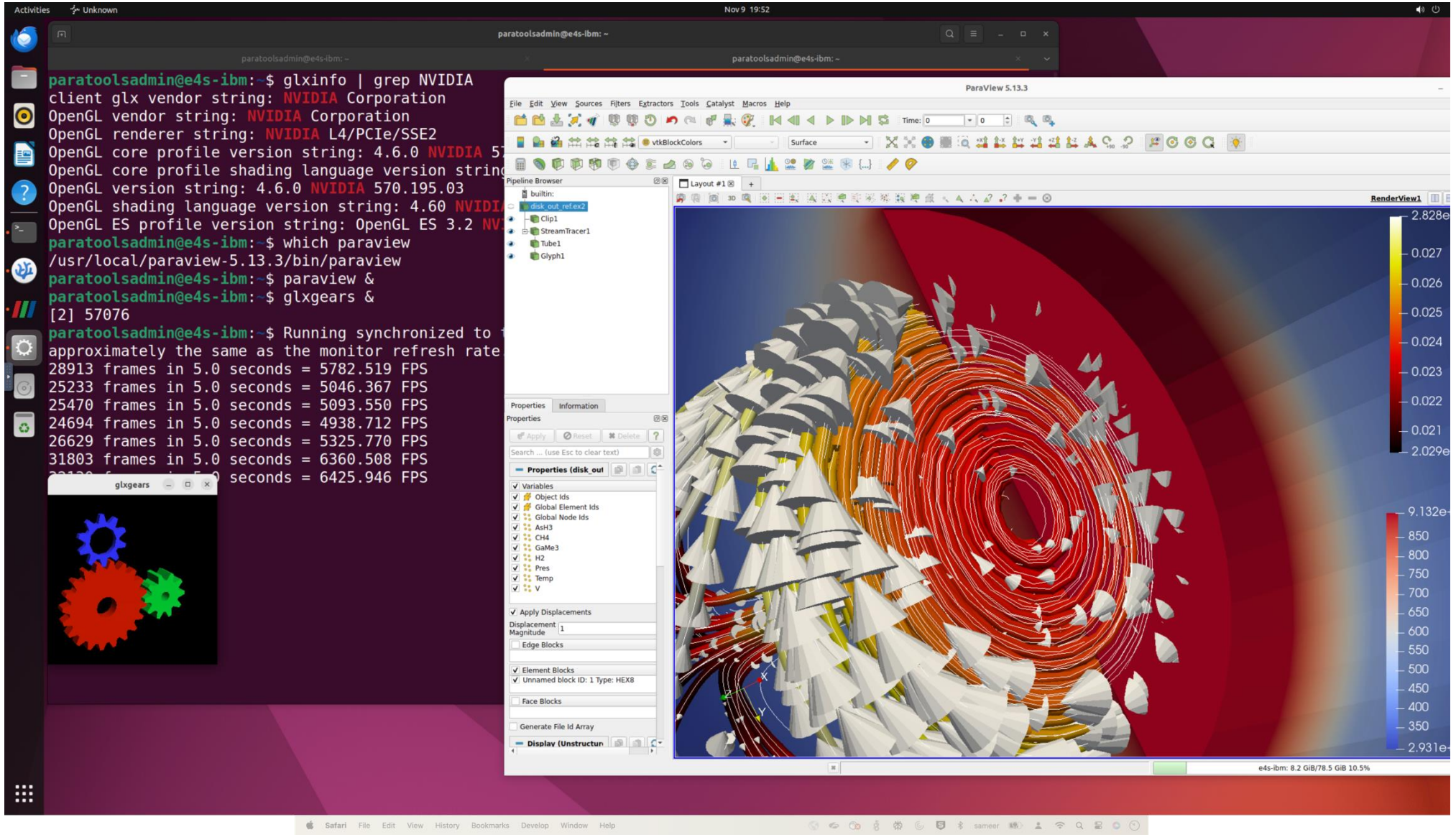
E4S: VS Codium Integrated Development Environment



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



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



Acknowledgment

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

PESO