E4S: Ecosystem for Science
Release 26.11



Release 26.11 notes

November 16, 2026

High Performance Software Foundation

E4S Team

https://e4s.io

E4S 26.11: What's New?

- E4S, an HPSF project, is the open-source, community-driven *HPC-AI Software Ecosystem for Science*. This curated, Spack based collection of scientific libraries and tools forms the foundation of some of the world's most advanced scientific applications.
- **Apache Guacamole remote desktop** [https://guacamole.apache.org/], providing browser-based access to graphical tools inside E4S containers, including visualization tools such as ParaView and VisIt. See the E4S Guacamole guide [https://e4s.io/guacamole/]
- **Expanded agentic-AI tools**, including the **Hermes Agent** desktop [https://hermes-agent.nousresearch.com/], the **pi coding agent**, **Atlas UI 3**, **OpenCode**, **Ollama,** and the **Orca IDE**, joining the Model Context Protocol (MCP), SGLang, LangChain, LangGraph, Agent2Agent (A2A), OpenAI, Anthropic, and Google Python APIs and Gemini CLI tools introduced in earlier releases
- **GPU communication runtimes NVIDIA Collective Communications Library (NCCL), NVIDIA Inference Xfer Library (NIXL), and NVIDIA NVSHMEM**, which support multi-GPU and multi-node training and high-throughput, disaggregated LLM inference. Other new tools include:
  - NVIDIA BioNeMo Inference Runtime (IR) for high-throughput biomolecular structure prediction inference
  - FFTX with SPIRAL code generation, DIY, Kokkos Tools, Kokkos FFT, TAU Commander, SALT-FM, Chapel
- Adaptive Computing's Heidi AI web-based platform for multi-user, multi-node, ParaTools Pro for E4S™ with Ubuntu 26.04 LTS and Rocky Linux 9.8 images on AWS, Microsoft Azure, Google Cloud, OCI, and IBM Cloud.

PESO – https://adaptivecomputing.com/ and https://paratoolspro.com

E4S: Ecosystem for Science

https://e4s.io

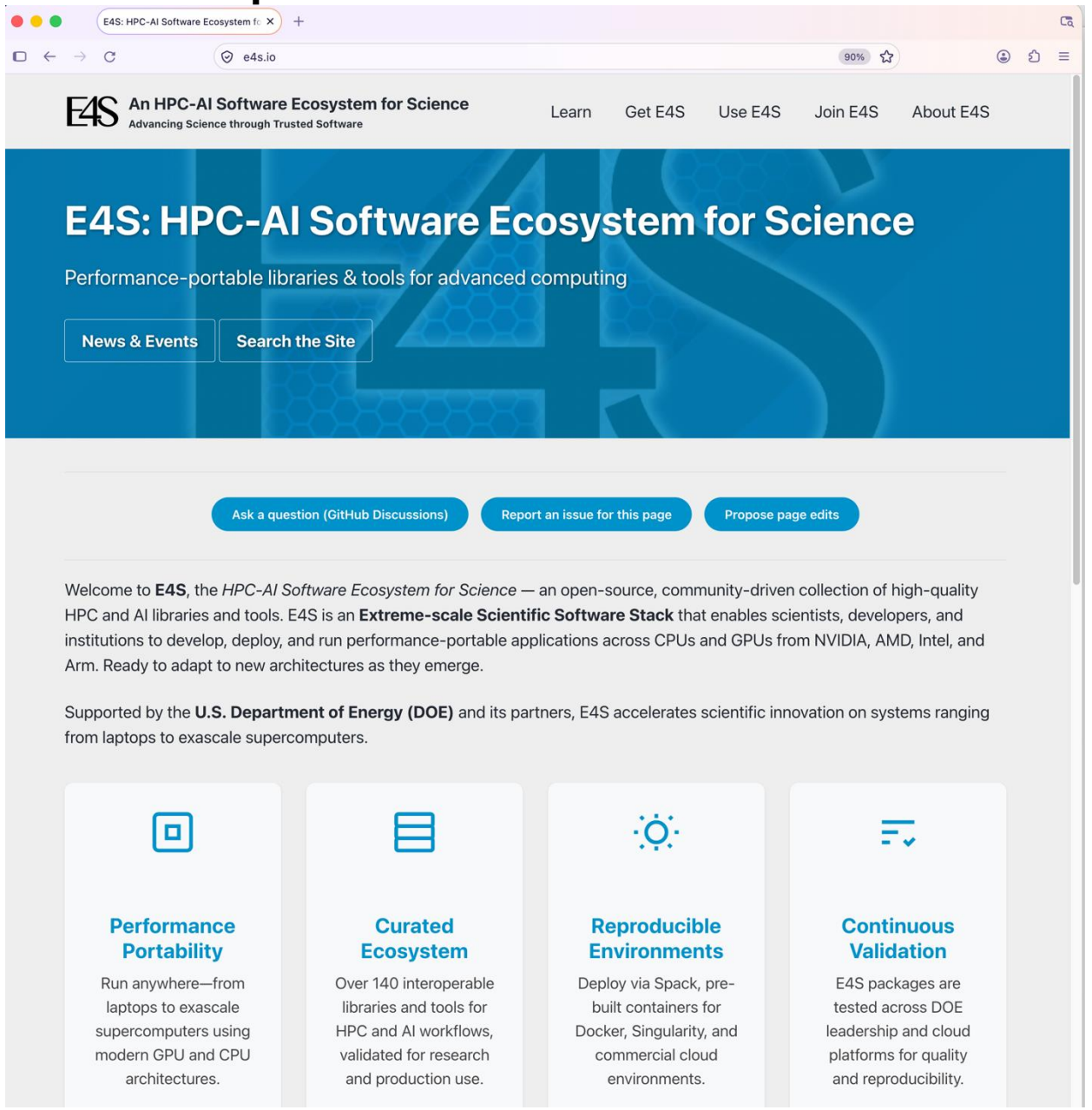
About E4S

- 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. It provides an Extreme-scale Scientific Software Stack.
- 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, CP2K, Quantum Espresso), EDA (e.g., Xyce), and ML packages (e.g., DSPy, Atlas UI 3, Hypothesis, Vllm, HuggingFace CLI, TensorFlow, PyTorch, OpenCV, TorchBraid, Pandas, JAX, LBANN optimized for GPUs where available).
- 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.
- 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, aarch64 (ARM64), and ppc64le (IBM Power 10) 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 26.11 released on November 16, 2026: https://e4s.io/talks/E4S_26.11.pdf

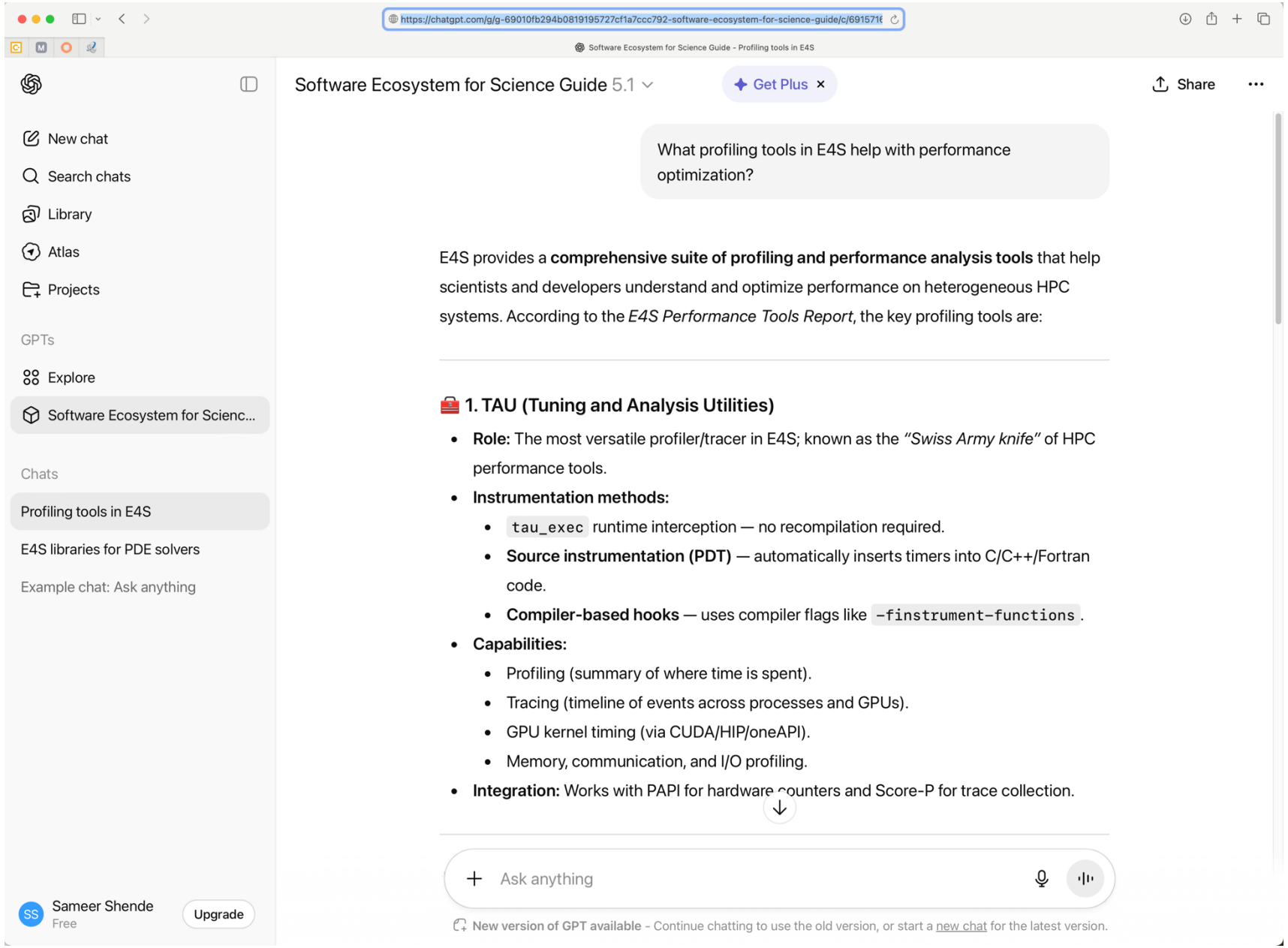
PESO

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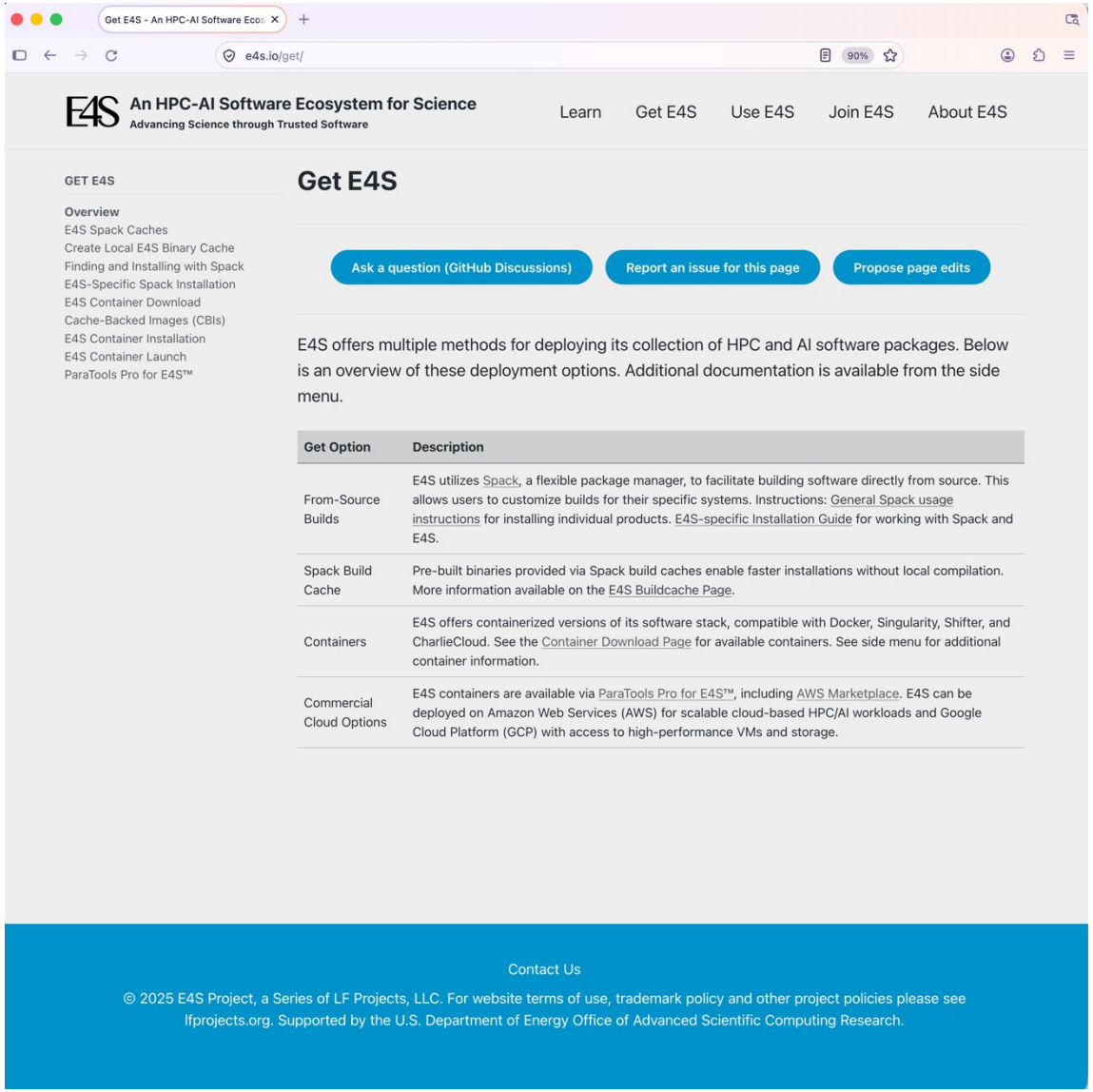
Updated E4S website https://e4s.io

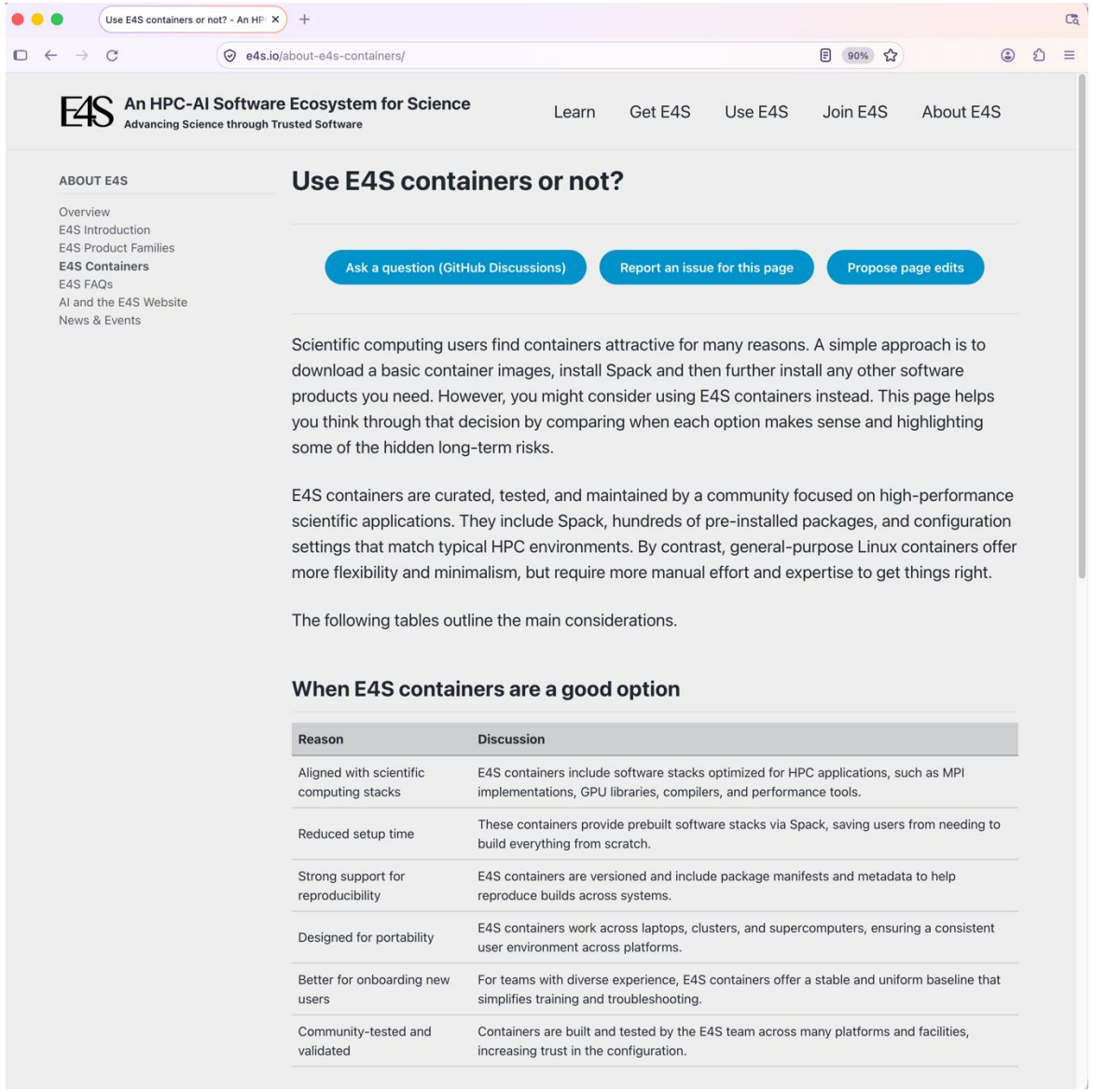


E4S Bot trained on E4S content on OpenAI's ChatGPT

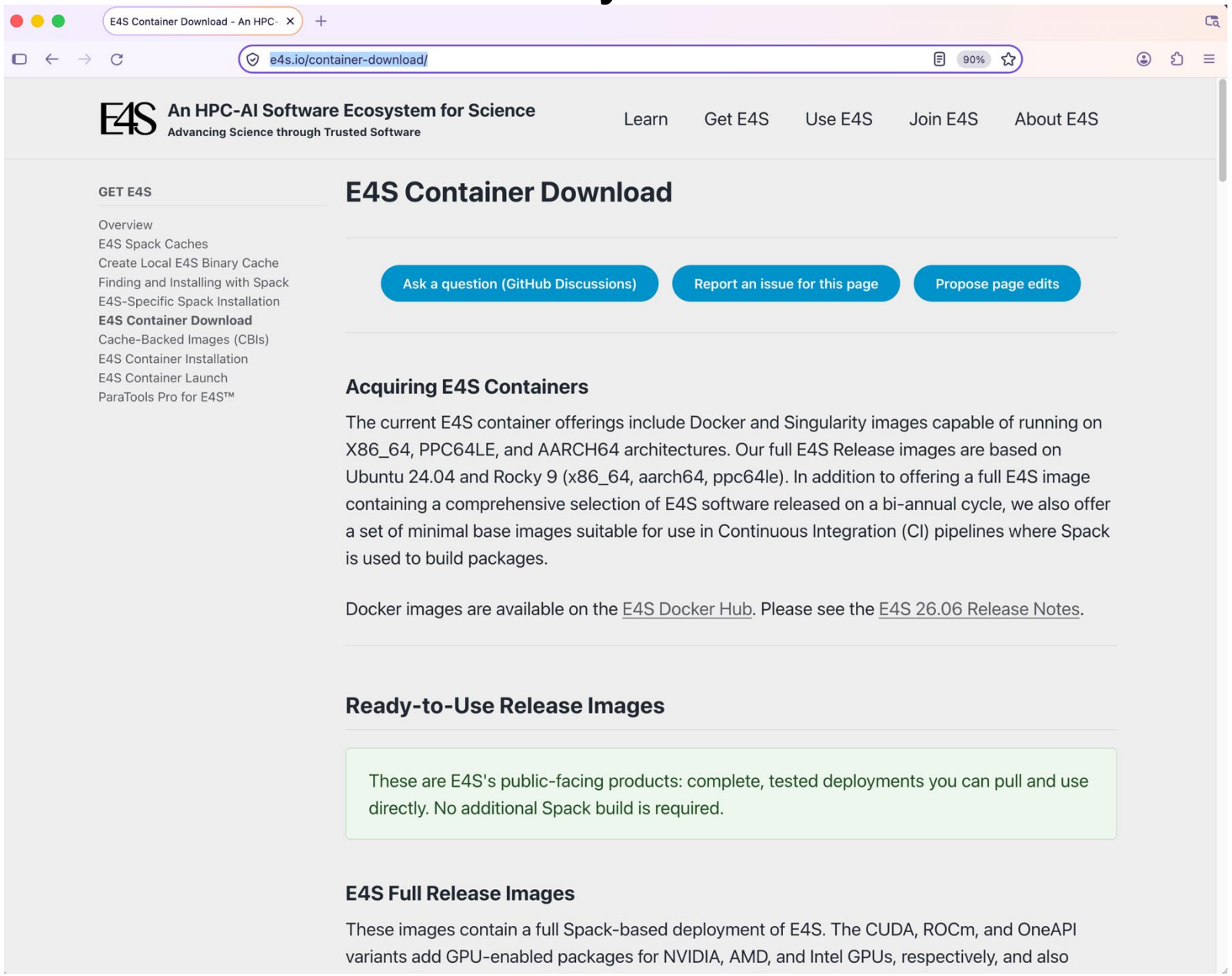


Using E4S


Get E4S - An HPC-AI Software Ecos
e4s.io/get/
90%
An HPC-AI Software Ecosystem for Science
Advancing Science through Trusted Software
Learn
Get E4S
Use E4S
Join E4S
About E4S
GET E4S
Overview
E4S Spack Caches
Create Local E4S Binary Cache
Finding and Installing with Spack
E4S-Specific Spack Installation
E4S Container Download
Cache-Backed Images (CBIs)
E4S Container Installation
E4S Container Launch
ParaTools Pro for E4S™
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E4S offers multiple methods for deploying its collection of HPC and AI software packages. Below is an overview of these deployment options. Additional documentation is available from the side menu.
Get Option
Description
From-Source Builds
E4S utilizes Spack, a flexible package manager, to facilitate building software directly from source. This allows users to customize builds for their specific systems. Instructions: General Spack usage instructions for installing individual products. E4S-specific Installation Guide for working with Spack and E4S.
Spack Build Cache
Pre-built binaries provided via Spack build caches enable faster installations without local compilation. More information available on the E4S Buildcache Page.
Containers
E4S offers containerized versions of its software stack, compatible with Docker, Singularity, Shifter, and CharlieCloud. See the Container Download Page for available containers. See side menu for additional container information.
Commercial Cloud Options
E4S containers are available via ParaTools Pro for E4S™, including AWS Marketplace. E4S can be deployed on Amazon Web Services (AWS) for scalable cloud-based HPC/AI workloads and Google Cloud Platform (GCP) with access to high-performance VMs and storage.
Contact Us
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Use E4S containers or not? - An HP
e4s.io/about-e4s-containers/
90%
An HPC-AI Software Ecosystem for Science
Advancing Science through Trusted Software
Learn
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Use E4S
Join E4S
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Overview
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E4S Product Families
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Use E4S containers or not?
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Scientific computing users find containers attractive for many reasons. A simple approach is to download a basic container images, install Spack and then further install any other software products you need. However, you might consider using E4S containers instead. This page helps you think through that decision by comparing when each option makes sense and highlighting some of the hidden long-term risks.
E4S containers are curated, tested, and maintained by a community focused on high-performance scientific applications. They include Spack, hundreds of pre-installed packages, and configuration settings that match typical HPC environments. By contrast, general-purpose Linux containers offer more flexibility and minimalism, but require more manual effort and expertise to get things right.
The following tables outline the main considerations.
When E4S containers are a good option
Reason
Discussion
Aligned with scientific computing stacks
E4S containers include software stacks optimized for HPC applications, such as MPI implementations, GPU libraries, compilers, and performance tools.
Reduced setup time
These containers provide prebuilt software stacks via Spack, saving users from needing to build everything from scratch.
Strong support for reproducibility
E4S containers are versioned and include package manifests and metadata to help reproduce builds across systems.
Designed for portability
E4S containers work across laptops, clusters, and supercomputers, ensuring a consistent user environment across platforms.
Better for onboarding new users
For teams with diverse experience, E4S containers offer a stable and uniform baseline that simplifies training and troubleshooting.
Community-tested and validated
Containers are built and tested by the E4S team across many platforms and facilities, increasing trust in the configuration.

Download E4S Containers: Rocky Linux 9.8 and Ubuntu 24.04 LTS



Docker and Singularity
ARM64 (aarch64), x86_64, and ppc64le
Support for GPUS:
- NVIDIA
- AMD
- Intel

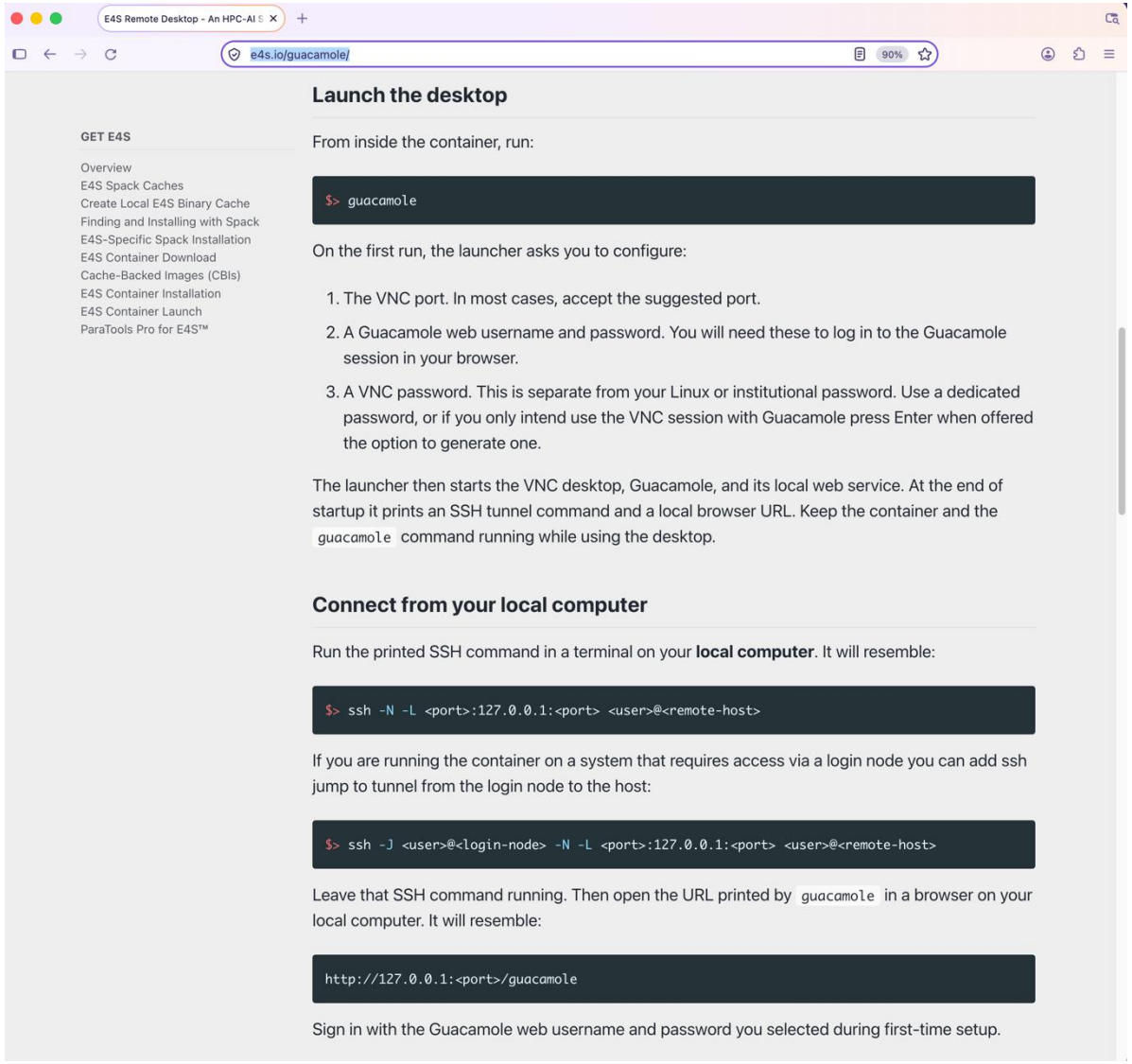
GPU Runtimes:
- CUDA 13.0
- ROCm 7.2.4
- oneAPI 2026.1

Languages:
- C/C++/Fortran
- Python
- Rust
- Julia
- Chapel ...

OSes:
- Rocky Linux 9.8
- Ubuntu 24.04 LTS

PESO

Apache Guacamole® clientless remote desktop in E4S containers




```
Singularity> nvidia-smi -L
GPU 0: NVIDIA RTX PRO 6000 Blackwell Server Edition (UUID: GPU-145d9d72-eeb9-3f6b-a564-053a80968239)
GPU 1: NVIDIA RTX PRO 6000 Blackwell Server Edition (UUID: GPU-b75d856d-95a0-f1d9-3465-15f46b942845)
GPU 2: NVIDIA RTX PRO 6000 Blackwell Server Edition (UUID: GPU-f773511b-2d07-35cb-363d-f021e2072747)
Singularity> grep PRETTY_NAME /etc/os-release
PRETTY_NAME="Rocky Linux 9.8 (Blue Onyx)"
Singularity> which guacamole
/usr/local/bin/guacamole
Singularity> guacamole
-> guacd is not running on 127.0.0.1:4822. Launching it...
-> guacd started (log: /tmp/guacamole-sameer/.guacamole/guacd.log).
================================================
   First-Time Setup: Guacamole & Tomcat Runtime
================================================
State dir: /tmp/guacamole-sameer
VNC mode:  isolated (private config in /tmp/guacamole-sameer/.guacamole/vnc)
Selected free HTTP port: 8081 (shutdown port disabled; stop via signal)
VNC port to use (a free port launches your own session) [5901]:
VNC password file: /tmp/guacamole-sameer/.guacamole/vnc/passwd
Enter desired Guacamole web username [admin]:
Enter password for Guacamole web user (admin):
Confirm password:

IMPORTANT:
  The VNC password is NOT your system login password.
  Guacamole must store the VNC password in plaintext within its
  private configuration so it can automatically connect to the
  VNC server on your behalf. (vncpasswd only stores an obfuscated copy)
  Enter a dedicated password used ONLY for this VNC session or leave empty
  to generate a new random one.
  Do not reuse your Linux, institutional, SSH, or other personal passwords.
  NOTE: VNC authentication only uses the first 8 characters.

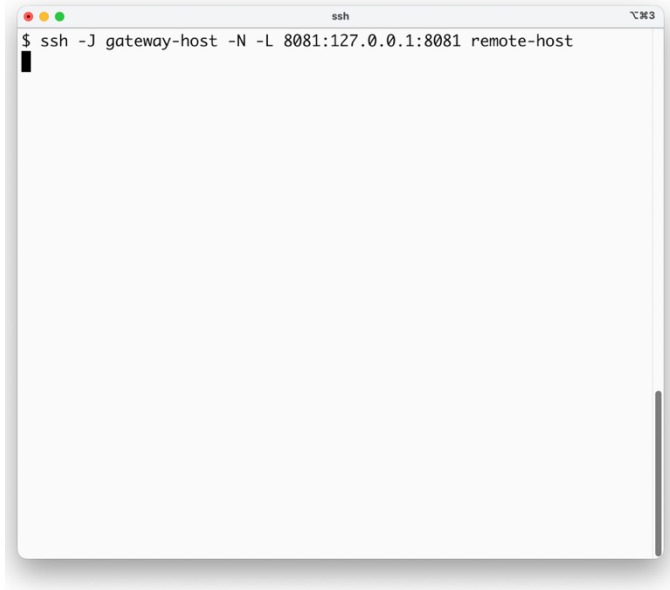
Enter a VNC password for the new session (empty = generate one):
NOTE: VNC authentication only uses the first 8 characters.
Created /tmp/guacamole-sameer/.guacamole/vnc/passwd.
Setup complete!

Resize policy: fixed at 1920x1200 (use --dynamic-resize to follow the browser).
Checking VNC on port 5901...
-> Nothing is listening on port 5901. Launching your own VNC session (isolated mode)...
-> Using VNC password file: /tmp/guacamole-sameer/.guacamole/vnc/passwd
-> Isolated VNC session :1 is up on port 5901 (stopped on exit).
   Logs: /tmp/guacamole-sameer/.guacamole/vnc/xvnc.log, /tmp/guacamole-sameer/.guacamole/vnc/session.log
================================================
 Starting Guacamole Web Interface
================================================
 Local URL: http://127.0.0.1:8081/guacamole

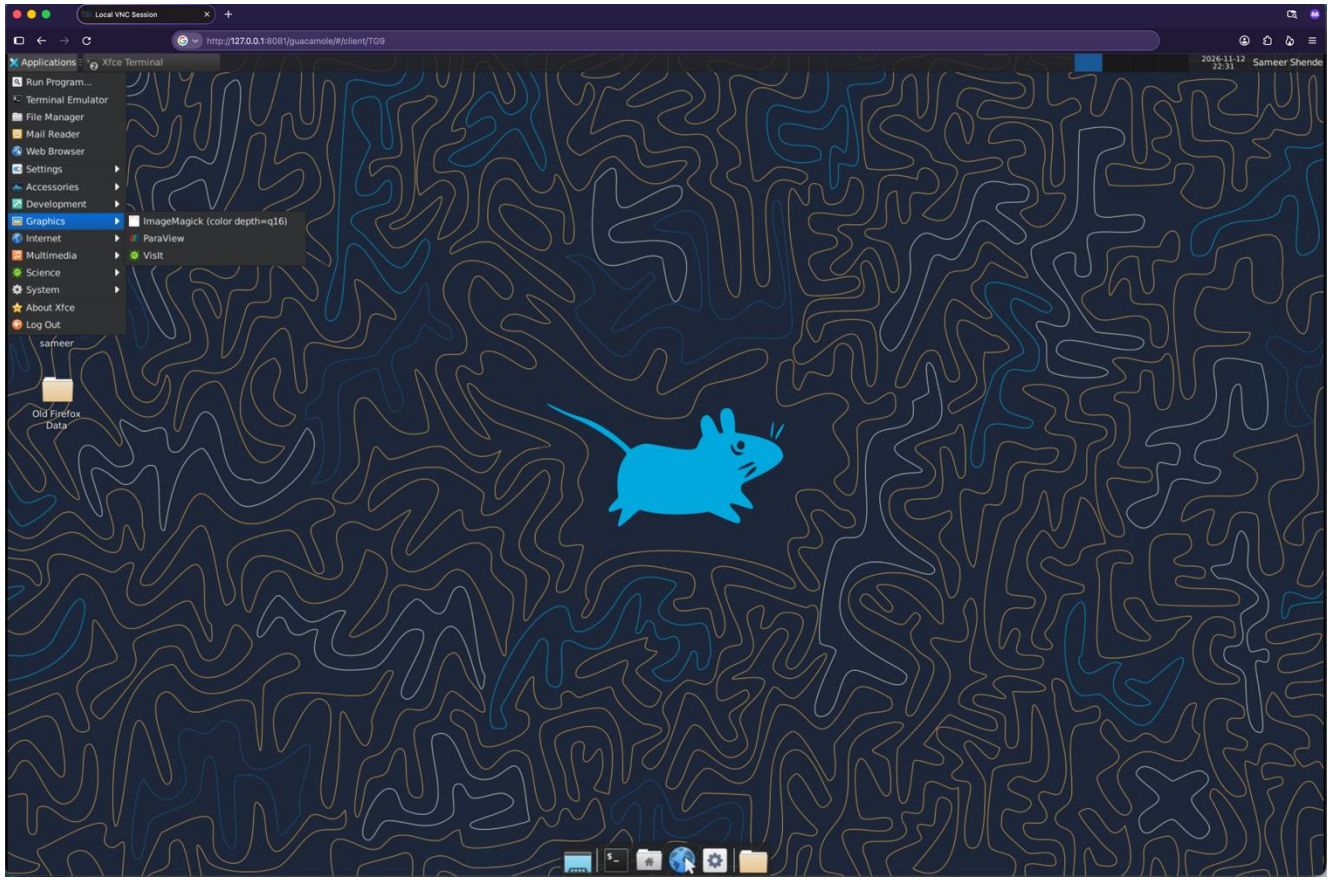
 --- SSH Tunneling Info ---
```

Using Apache Guacamole® with an ssh tunnel and an HTML5 web browser



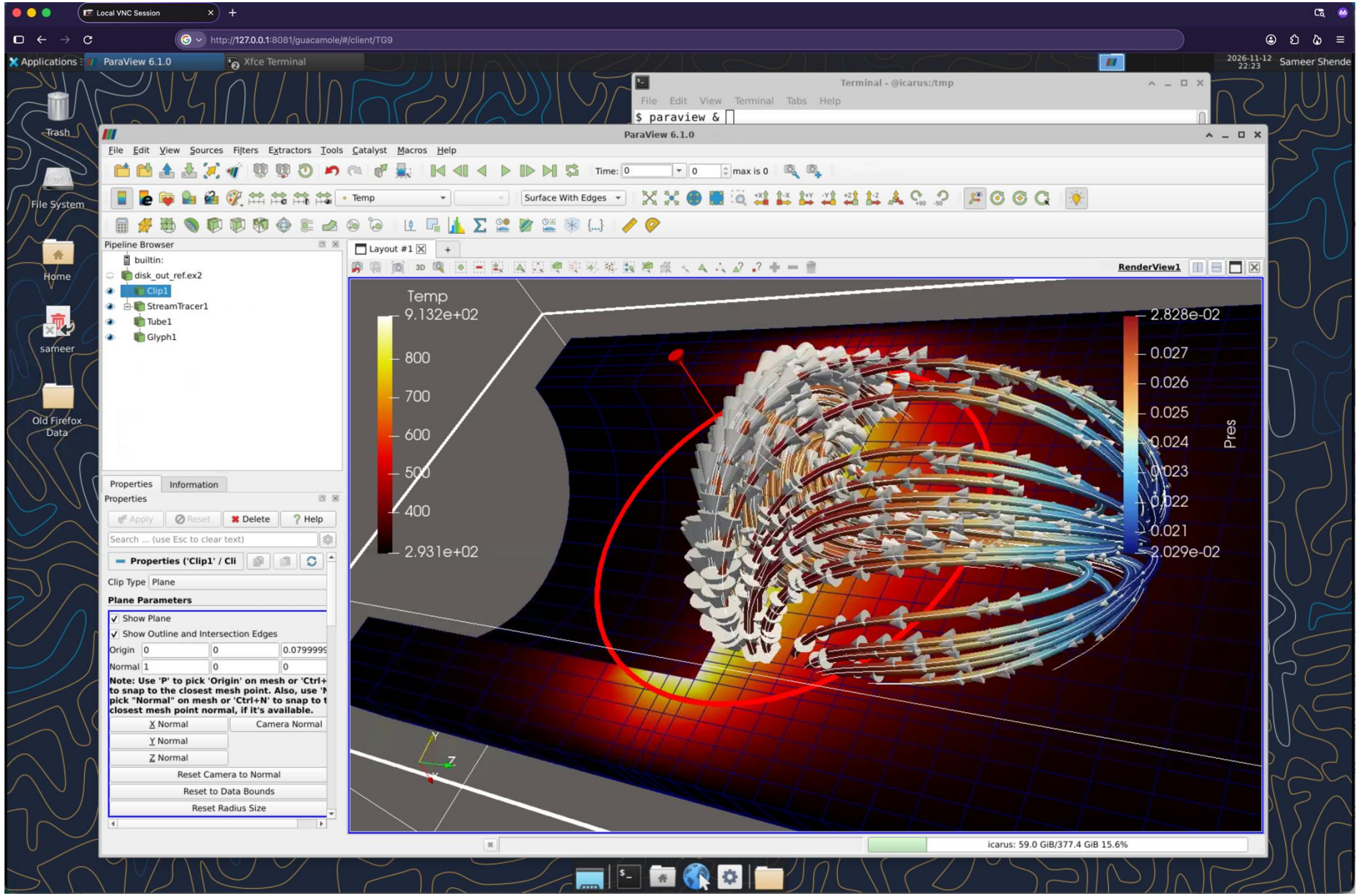




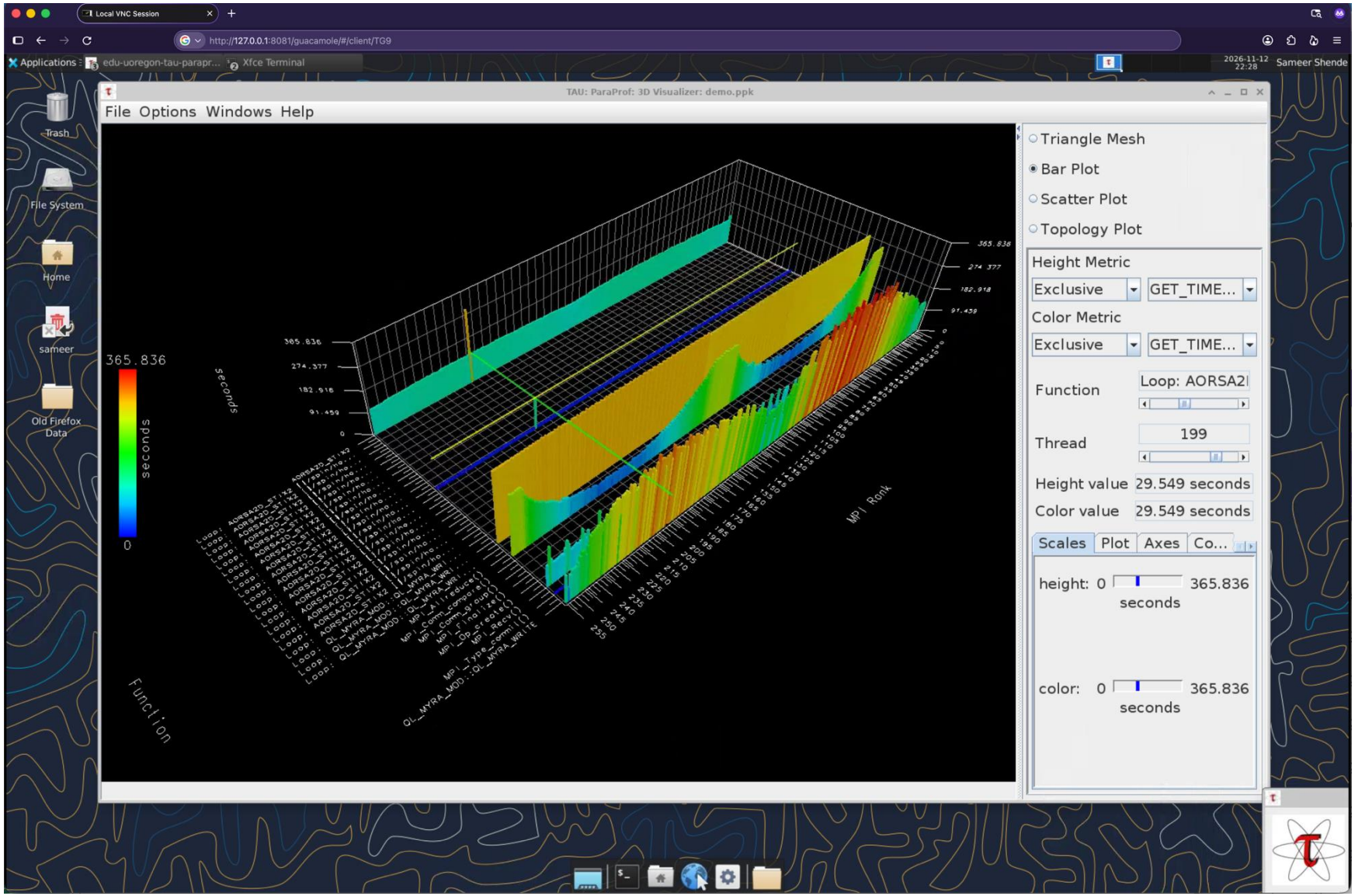


% firefox http://127.0.0.1:8081/guacamole

Visualization tools included in E4S: ParaView

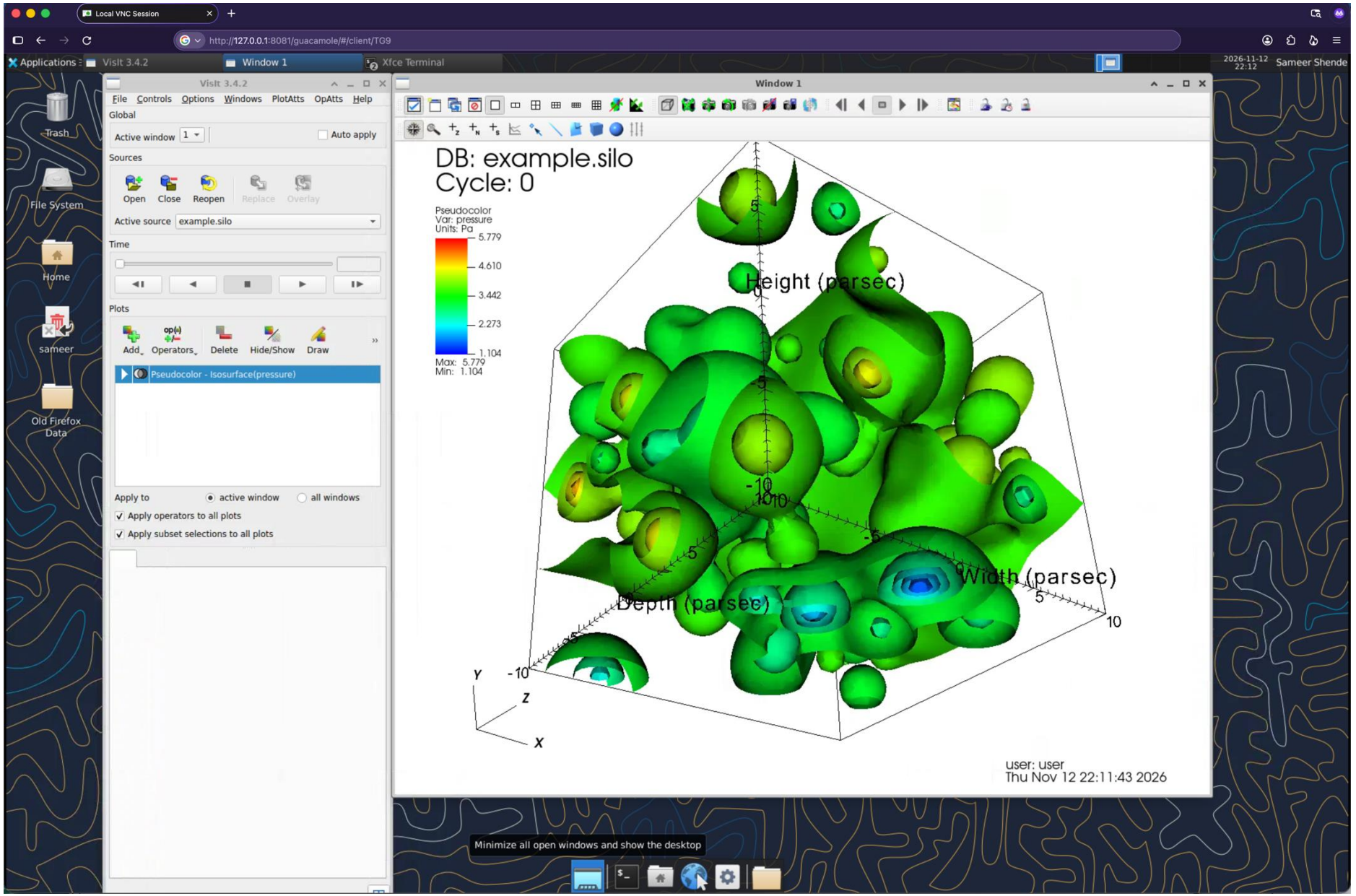


Visualization tools included in E4S: TAU Performance System®

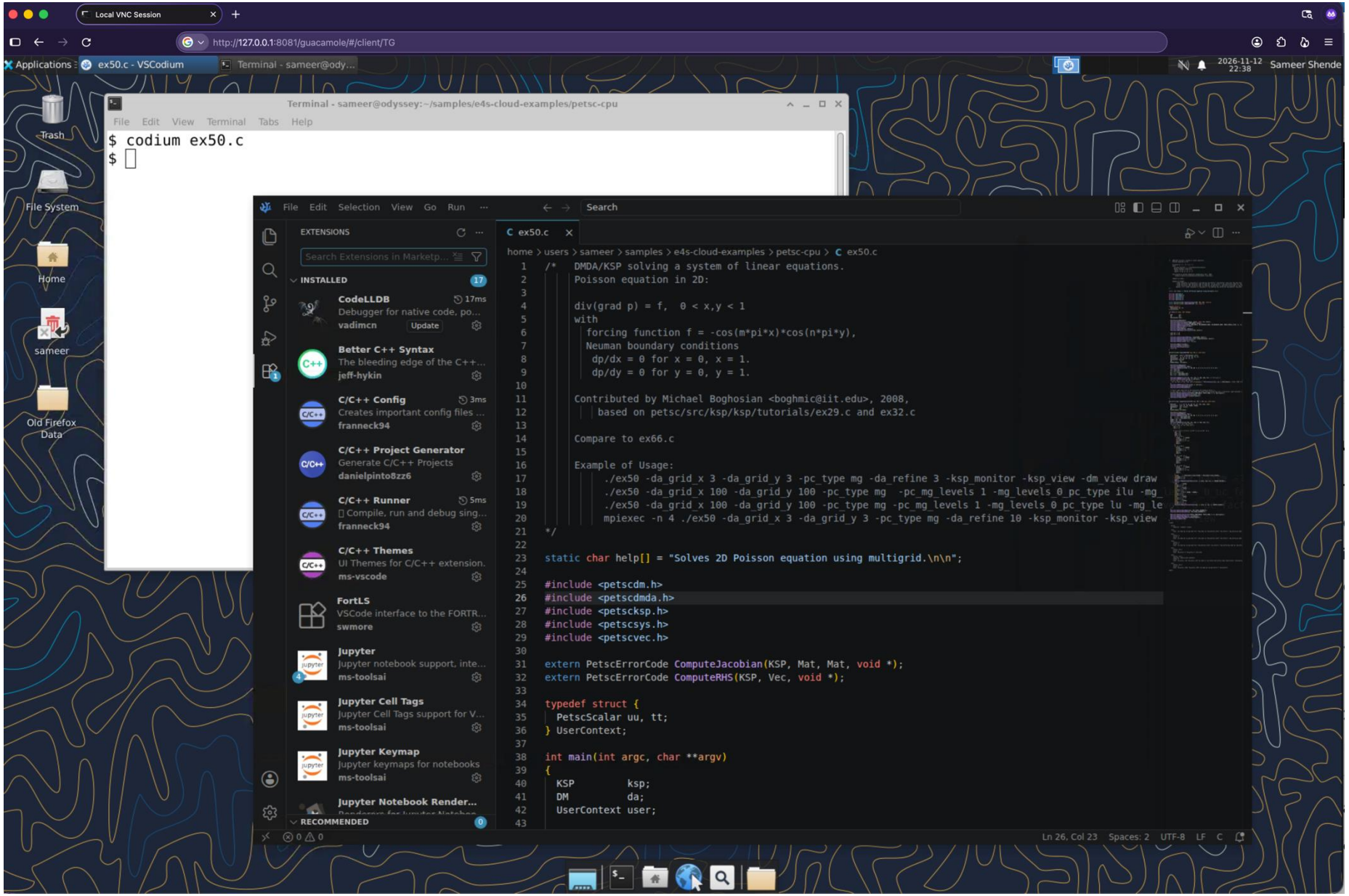


TAU's ParaProf profile browser using Apache Guacamole® remote desktop

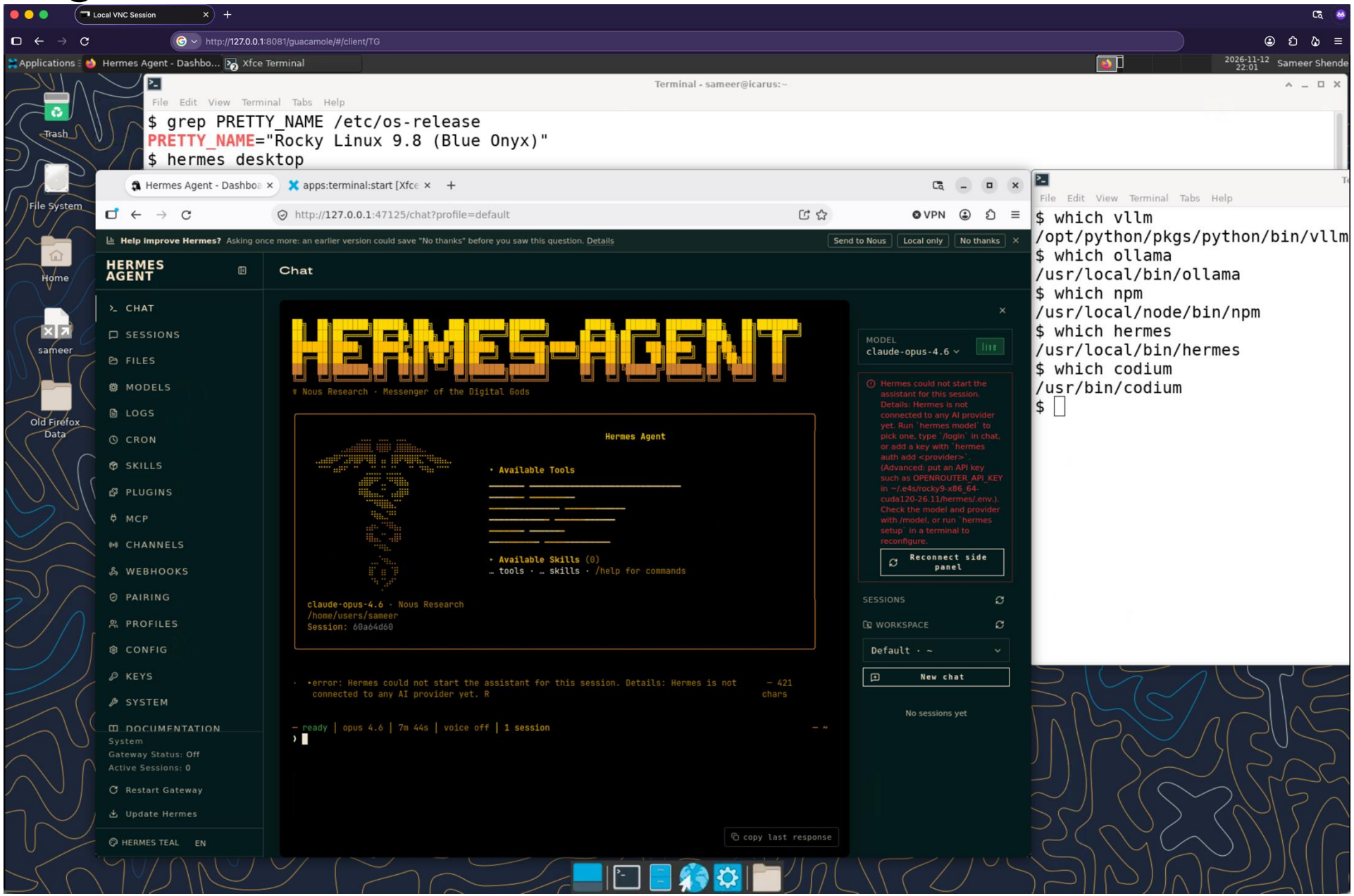
VisIt Visualizer



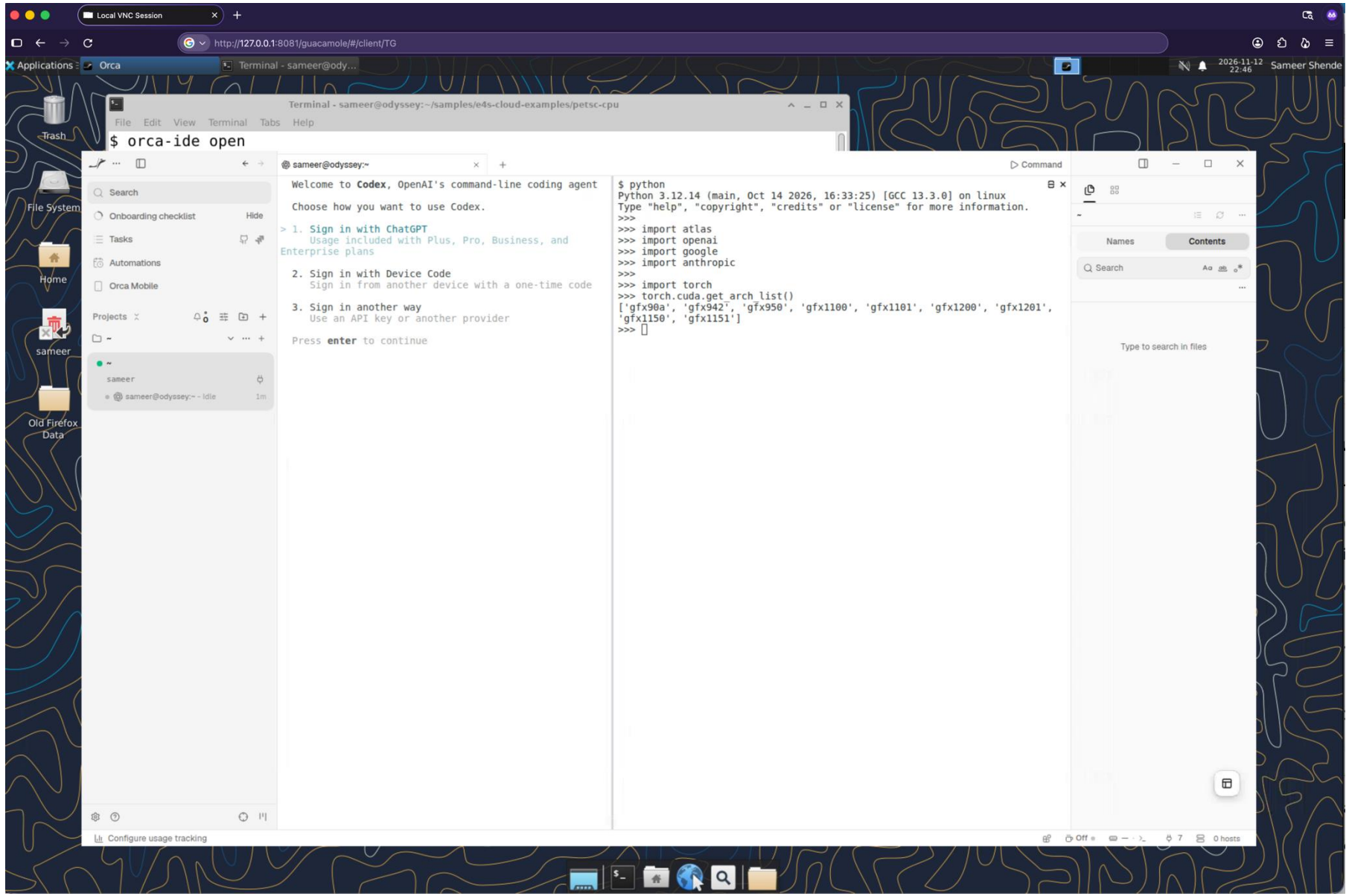
IDE tools included in E4S: Codium



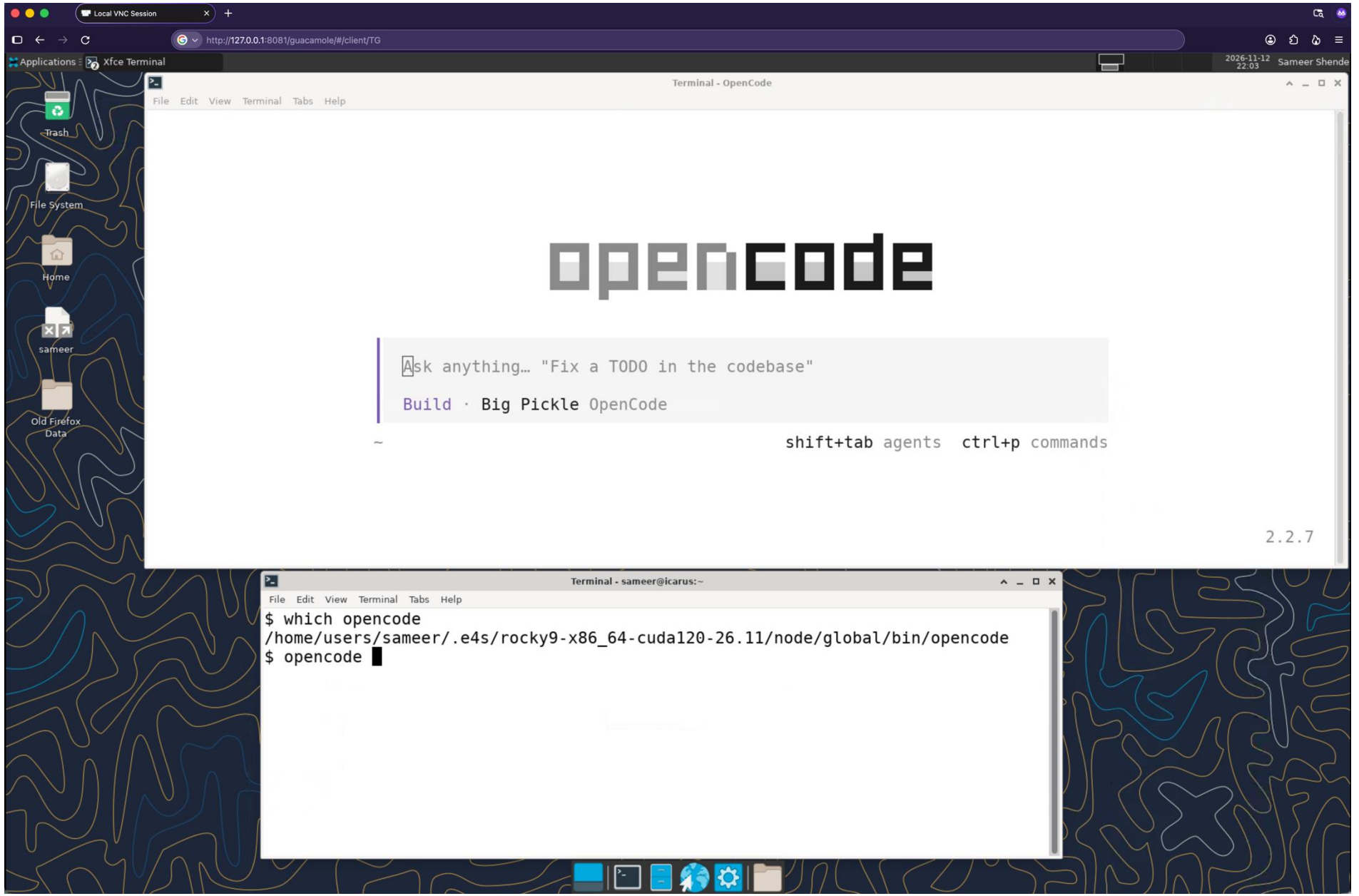
Hermes Agent



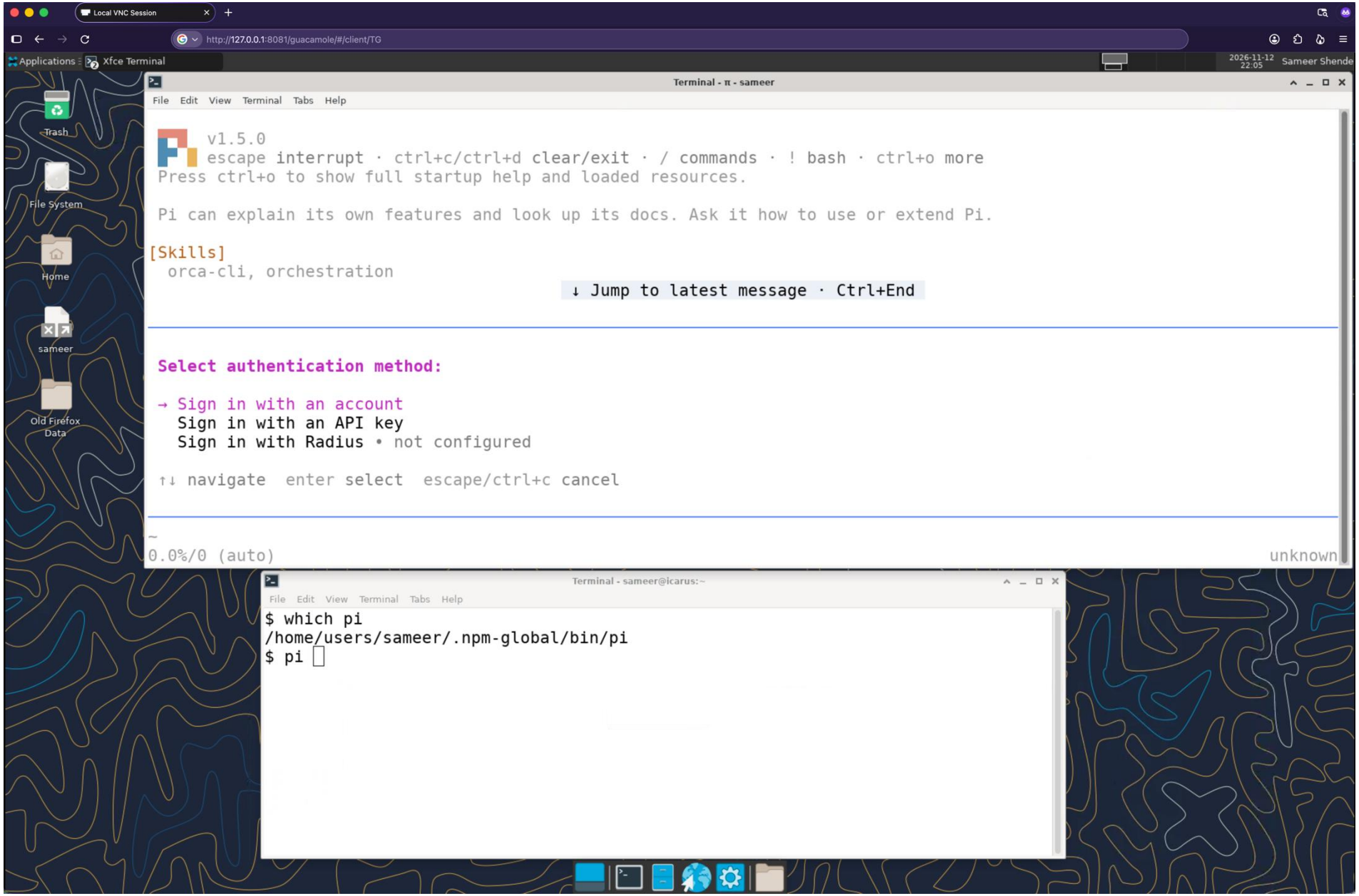
Agentic AI: Orca IDE



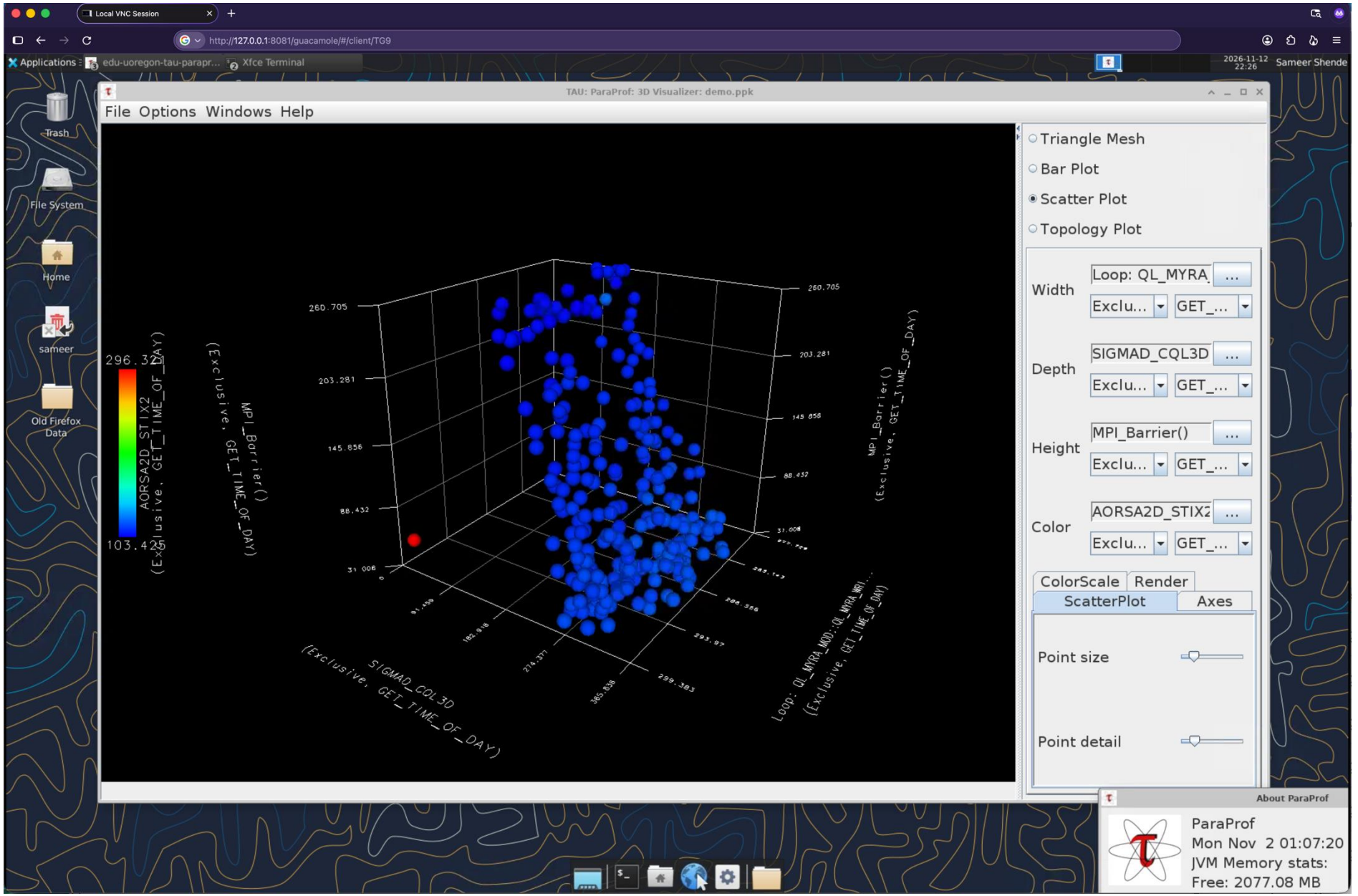
OpenCode: The open source coding agent



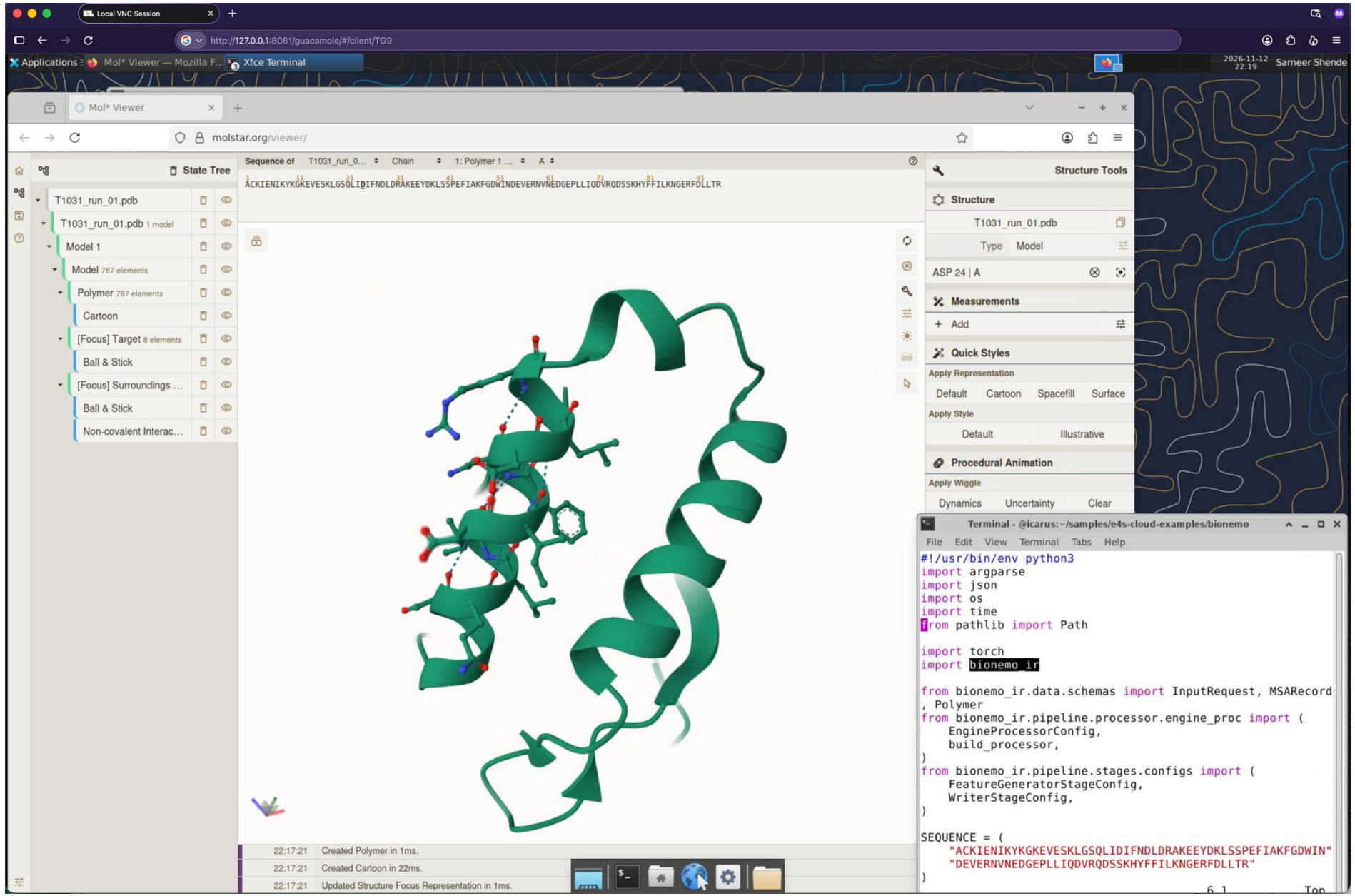
Pi Minimal Agent Harness for coding



Performance Evaluation Tools: TAU Performance System®



NVIDIA BioNeMo Inference Runtime for predicting 3D structure of proteins



Using E4S 26.11 Container Images: Full featured CPU+GPU image

```
$ singularity run --nv e4s-cuda80-full-26.11.1794551293.sif
Singularity> uname -m
x86_64
Singularity> nvidia-smi topo -m | head -5
        GPU0    GPU1    GPU2    GPU3    CPU Affinity    NUMA Affinity   GPU NUMA ID
GPU0     X      NV4     NV4     NV4     32-47   2               N/A
GPU1    NV4      X      NV4     NV4     32-47   2               N/A
GPU2    NV4     NV4      X      NV4     96-111  6               N/A
GPU3    NV4     NV4     NV4      X      96-111  6               N/A
Singularity> grep PRETTY_NAME /etc/os-release
PRETTY_NAME="Ubuntu 24.04.5 LTS"
Singularity> which guacamole
/usr/local/bin/guacamole
Singularity> which openclaw
/home/users/sameer/.e4s/ubuntu2404-x86_64-cuda80-full-26.11/node/global/bin/openclaw
Singularity> which hermes
/usr/local/bin/hermes
Singularity> which opencode
/home/users/sameer/.e4s/ubuntu2404-x86_64-cuda80-full-26.11/node/global/bin/opencode
Singularity> which pi
/home/users/sameer/.e4s/ubuntu2404-x86_64-cuda80-full-26.11/node/global/bin/pi
Singularity> which gemini
/home/users/sameer/.e4s/ubuntu2404-x86_64-cuda80-full-26.11/node/global/bin/gemini
Singularity> which huggingface-cli
/opt/python/pkgs/python/bin/huggingface-cli
Singularity> which ollama
/usr/local/bin/ollama
Singularity> which vllm
/opt/python/pkgs/python/bin/vllm
Singularity> which orca-ide
/usr/local/bin/orca-ide
Singularity> python
Python 3.12.14 (main, Oct 14 2026, 16:33:25) [GCC 13.3.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import torch
>>>
>>> print("CUDA available:", torch.cuda.is_available())
CUDA available: True
>>> print("NCCL initialized/available:", torch.distributed.is_nccl_available())
NCCL initialized/available: True
>>> if torch.distributed.is_nccl_available():
...   print("NCCL version:", torch.cuda.nccl.version())
...
NCCL version: (2, 30, 7)
>>>
Singularity> which spack
/spack/bin/spack
Singularity>
```

Launch container image with singularity --nv argument to use NVIDIA GPUs

E4S 26.11 Linux x86_64 CPU+GPU image Ubuntu 24.04 LTS packages

```
Singularity> spack find -x
-- linux-ubuntu24.04-x86_64_v3 / %c,cxx,fortran=gcc@13.3.0 ------
adios@1.13.1    ascent@0.9.5         cp2k@2026.2            heffte@2.4.1   openmpi@5.0.10          plumed@2.10.1         slate@2025.05.28  sundials@7.9.0      trilinos@17.2.1
adios2@2.12.1   axom@0.15.0          darshan-runtime@3.5.0  heffte@2.4.1   papi@7.2.0              precice@3.4.0         slepc@3.26.0      superlu-dist@9.2.1  variorum@0.8.0
adios2@2.12.1   axom@0.15.0          darshan-util@3.5.0     libceed@1.0.0  papi@7.2.0              quantum-espresso@7.6  slepc@3.26.0      superlu-dist@9.2.1  wps@4.6.0
alquimia@1.1.0  butterflypack@4.1.0  datatransferkit@3.1.1  libceed@1.0.0  parallel-netcdf@1.14.1  rempi@1.1.0           strumpack@8.1.0   tau@2.36            xyce@7.10.0
amrex@26.10     conduit@0.9.8        globalarrays@5.8.2     magma@2.10.0   petsc@3.26.0            scr@3.1.0             strumpack@8.1.0   tau@2.36            zfp@1.0.1
amrex@26.10     cp2k@2025.2          h5bench@1.4            nwchem@7.3.1   phist@1.12.1            slate@2025.05.28      sundials@7.9.0    trilinos@14.4.0     zfp@1.0.1

-- linux-ubuntu24.04-x86_64_v3 / %c,cxx=gcc@13.3.0 --------------
boost@1.90.0       chapel@2.10.0    flecsi@2.4.2     hdf5-vol-cache@v1.1  legion@26.09.1     mpifileutils@0.12      pruners-ninja@1.0.2  turbine@1.3.0     warpx@26.09
bricks@2023.08.25  chapel@2.10.0    gasnet@2025.8.0  hdf5-vol-log@1.4.0   libcatalyst@2.1.0  nccmp@1.11.0.0         pumi@2.2.9           umap@2.1.1
bricks@2023.08.25  cusz@0.14.0      ginkgo@1.11.0    hpctoolkit@2026.0.1  libpressio@0.99.4  nco@5.4.1              qthreads@1.18        umpire@2026.07.1
cabana@0.8.0       diy@3.6.0        ginkgo@1.11.0    hpctoolkit@2026.0.1  libpressio@0.99.4  omega-h@11.2.0-scorec  raja@2026.07.0       umpire@2026.07.1
cabana@0.8.0       dyninst@13.0.0   glvis@4.4        hypre@3.2.0          libunwind@1.8.3    omega-h@11.2.0-scorec  raja@2026.07.0       upcxx@2025.10.0
caliper@2.15.0     faodel@1.2108.1  gmp@6.3.0        lammps@20250722.6    mercury@2.4.1      openfoam@2606          saltfm@0.6.0         upcxx@2025.10.0
caliper@2.15.0     fftx@1.2.0       gotcha@1.0.8     lammps@20250722.6    metall@0.30        openpmd-api@0.17.1     swig@4.0.2-fortran   veloc@1.7
chai@2026.07.0     fftx@1.2.0       gromacs@2026.3   lbann@0.104          mgard@1.6.0        papyrus@1.0.2          sz@2.1.12.5          vtk-m@2.3.0
chai@2026.07.0     flecsi@2.4.2     gromacs@2026.3   legion@26.09.1       mgard@1.6.0        pdt@3.25.2             sz3@3.2.0            vtk-m@2.3.0

-- linux-ubuntu24.04-x86_64_v3 / %c,fortran=gcc@13.3.0 ----------
fpm@0.13.0   libquo@1.4.1  nekbone@17.0          netlib-scalapack@2.2.3  py-libensemble@1.6.1  wannier90@4.0.2
hdf5@1.14.6  nek5000@19.0  netcdf-fortran@4.6.4  plasma@24.8.7           superlu@7.0.1         wrf@4.7.1

-- linux-ubuntu24.04-x86_64_v3 / %c=gcc@13.3.0 ------------------
aml@0.2.1     charliecloud@0.44  flux-core@0.89.0        hdf5-vol-async@1.7  libnrm@0.1.0     parsec@4.0.2411  py-petsc4py@3.26.0
argobots@1.2  flux-core@0.89.0   guacamole-server@1.6.0  hypre@3.2.0         parsec@4.0.2411  py-h5py@3.16.0

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

-- linux-ubuntu24.04-x86_64_v3 / %cxx=gcc@13.3.0 ----------------
arborx@2.1  flit@2.1.0  hpx@1.11.0    kokkos@5.2.2      kokkos-fft@2.0.0      kokkos-kernels@5.2.2  kokkos-tools@5.2.0  loki@0.1.7   mfem@4.10.0
arborx@2.1  hpx@1.11.0  kokkos@5.2.2  kokkos-fft@2.0.0  kokkos-kernels@5.2.2  kokkos-tools@5.2.0    laghos@3.1          mfem@4.10.0  mpark-variant@1.4.0

-- linux-ubuntu24.04-x86_64_v3 / no compilers -------------------
e4s-alc@1.0.3  e4s-cl@1.0.9  guacamole-client@1.6.0  mpich@5.0.1  nrm@0.1.0  py-cinemasci@1.7.9  py-jupyterhub@1.4.1  py-pytuq@1.0.0  tomcat@9.0.96
==> 181 installed packages
Singularity>
```

Full featured NVIDIA A100 GPU x86_64 CPU image

E4S 26.11 Linux x86_64 CPU+GPU image Ubuntu 24.04 LTS packages

```
Singularity> module avail
------------------------------------------------------------ /spack/share/spack/modules/linux-ubuntu24.04-x86_64_v3 -------------------------------------
adios/1.13.1                faodel/1.2108.1                kokkos-tools/5.2.0                omega-h/11.2.0-scorec           strumpack/8.1.0-openmp
adios2/2.12.1               fftx/1.2.0                     kokkos-tools/5.2.0-cuda           omega-h/11.2.0-scorec-cuda80    sundials/7.9.0
adios2/2.12.1-cuda80        fftx/1.2.0-cuda80              kokkos/5.2.2-cuda80               openfoam/2606                   sundials/7.9.0-cuda80
alquimia/1.1.0              flecsi/2.4.2                   kokkos/5.2.2-openmp               openmpi/5.0.10                  superlu-dist/9.2.1
aml/0.2.1                   flecsi/2.4.2-cuda80            laghos/3.1                        openpmd-api/0.17.1              superlu-dist/9.2.1-cuda80
amrex/26.10                 flit/2.1.0                     lammps/20250722.6-cuda80-openmp   papi/7.2.0                      superlu/7.0.1
amrex/26.10-cuda80          flux-core/0.89.0               lammps/20250722.6-openmp          papi/7.2.0-cuda                 swig/4.0.2-fortran
arborx/2.1                  flux-core/0.89.0-cuda          lbann/0.104                       papyrus/1.0.2                   sz/2.1.12.5
arborx/2.1-cuda80           fpm/0.13.0-openmp              legion/26.09.1                    parallel-netcdf/1.14.1          sz3/3.2.0
argobots/1.2                gasnet/2025.8.0                legion/26.09.1-cuda80             parsec/4.0.2411                 tasmanian/8.1
ascent/0.9.5-openmp         ginkgo/1.11.0-cuda80-openmp    libcatalyst/2.1.0                 parsec/4.0.2411-cuda80          tasmanian/8.1-cuda80
axom/0.15.0-cuda80-openmp   ginkgo/1.11.0-openmp           libceed/1.0.0                     pdt/3.25.2                      tau/2.36
axom/0.15.0-openmp          globalarrays/5.8.2             libceed/1.0.0-cuda80              petsc/3.26.0                    tau/2.36-cuda
boost/1.90.0                glvis/4.4                      libnrm/0.1.0                      phist/1.12.1-openmp             tomcat/9.0.96
bricks/2023.08.25           gmp/6.3.0                      libpressio/0.99.4-cuda80-openmp   plasma/24.8.7                   trilinos/14.4.0
bricks/2023.08.25-cuda      gotcha/1.0.8                   libpressio/0.99.4-openmp          plumed/2.10.1                   trilinos/17.2.1-cuda80-cuda
butterflypack/4.1.0-openmp  gromacs/2026.3-cuda80-openmp   libquo/1.4.1                      precice/3.4.0                   turbine/1.3.0
cabana/0.8.0                gromacs/2026.3-openmp          libunwind/1.8.3                   pruners-ninja/1.0.2             umap/2.1.1
cabana/0.8.0-cuda80-cuda    guacamole-client/1.6.0         loki/0.1.7                        pumi/2.2.9                      umpire/2026.07.1
caliper/2.15.0              guacamole-server/1.6.0         magma/2.10.0-cuda80               py-cinemasci/1.7.9              umpire/2026.07.1-cuda80
caliper/2.15.0-cuda80       h5bench/1.4                    mercury/2.4.1                     py-h5py/3.16.0                  upcxx/2025.10.0
chai/2026.07.0              hdf5-vol-async/1.7             metall/0.30                       py-jupyterhub/1.4.1             upcxx/2025.10.0-cuda80
chai/2026.07.0-cuda80       hdf5-vol-cache/v1.1            mfem/4.10.0                       py-libensemble/1.6.1            variorum/0.8.0
chapel/2.10.0               hdf5-vol-log/1.4.0             mfem/4.10.0-cuda80                py-petsc4py/3.26.0              veloc/1.7
chapel/2.10.0-cuda80        hdf5/1.14.6                    mgard/1.6.0-cuda80-openmp         py-pytuq/1.0.0                  vtk-m/2.3.0-cuda80-openmp
charliecloud/0.44           heffte/2.4.1                   mgard/1.6.0-openmp                qthreads/1.18                   vtk-m/2.3.0-openmp
conduit/0.9.8               heffte/2.4.1-cuda80            mpark-variant/1.4.0               quantum-espresso/7.6-openmp     wannier90/4.0.2
cp2k/2025.2-cuda80-openmp   hpctoolkit/2026.0.1            mpich/5.0.1                       raja/2026.07.0                  warpx/26.09
cp2k/2026.2-openmp          hpctoolkit/2026.0.1-cuda       mpifileutils/0.12                 raja/2026.07.0-cuda80           wps/4.6.0
cusz/0.14.0-cuda80          hpx/1.11.0                     nccmp/1.11.0.0                    rempi/1.1.0                     wrf/4.7.1
darshan-runtime/3.5.0       hpx/1.11.0-cuda80              nco/5.4.1-openmp                  saltfm/0.6.0                    xyce/7.10.0
darshan-util/3.5.0          hypre/3.2.0                    nek5000/19.0                      scr/3.1.0                       zfp/1.0.1
datatransferkit/3.1.1       hypre/3.2.0-cuda80             nekbone/17.0                      slate/2025.05.28-cuda80-openmp  zfp/1.0.1-cuda80
diy/3.6.0                   kokkos-fft/2.0.0               netcdf-fortran/4.6.4              slate/2025.05.28-openmp
dyninst/13.0.0-openmp       kokkos-fft/2.0.0-cuda          netlib-scalapack/2.2.3            slepc/3.26.0
e4s-alc/1.0.3               kokkos-kernels/5.2.2-cuda80-cuda nrm/0.1.0                       slepc/3.26.0-cuda80
e4s-cl/1.0.9                kokkos-kernels/5.2.2-openmp    nwchem/7.3.1                      strumpack/8.1.0-cuda80-openmp

Key:
loaded  modulepath
Singularity>
```

Full featured NVIDIA A100 GPU x86_64 CPU image

E4S 26.11 Linux x86_64 CPU image Ubuntu 24.04 LTS packages

```
Singularity> spack find -x
-- linux-ubuntu24.04-x86_64_v3 / %c,cxx,fortran=gcc@13.3.0 ------
adios@1.13.1    axom@0.15.0            darshan-util@3.5.0     libceed@1.0.0          petsc@3.26.0          rempi@1.1.0       sundials@7.9.0      wps@4.6.0
adios2@2.12.1   butterflypack@4.1.0    datatransferkit@3.1.1  nwchem@7.3.1           phist@1.12.1          scr@3.1.0         superlu-dist@9.2.1  xyce@7.10.0
alquimia@1.1.0  conduit@0.9.8          globalarrays@5.8.2     openmpi@5.0.10         plumed@2.10.1         slate@2025.05.28  tau@2.36            zfp@1.0.1
amrex@26.10     cp2k@2026.2            h5bench@1.4            papi@7.2.0             precice@3.4.0         slepc@3.26.0      trilinos@14.4.0
ascent@0.9.5    darshan-runtime@3.5.0  heffte@2.4.1           parallel-netcdf@1.14.1 quantum-espresso@7.6  strumpack@8.1.0   variorum@0.8.0

-- linux-ubuntu24.04-x86_64_v3 / %c,cxx=gcc@13.3.0 --------------
boost@1.90.0       dyninst@13.0.0   gmp@6.3.0            lbann@0.104        mgard@1.6.0            papyrus@1.0.2        swig@4.0.2-fortran  veloc@1.7
bricks@2023.08.25  faodel@1.2108.1  gotcha@1.0.8         legion@26.09.1     mpifileutils@0.12      pdt@3.25.2           sz@2.1.12.5         vtk-m@2.3.0
cabana@0.8.0       fftx@1.2.0       gromacs@2026.3       libcatalyst@2.1.0  nccmp@1.11.0.0         pruners-ninja@1.0.2  sz3@3.2.0           warpx@26.09
caliper@2.15.0     flecsi@2.4.2     hdf5-vol-cache@v1.1  libpressio@0.99.4  nco@5.4.1              pumi@2.2.9           turbine@1.3.0
chai@2026.07.0     gasnet@2025.8.0  hdf5-vol-log@1.4.0   libunwind@1.8.3    omega-h@11.2.0-scorec  qthreads@1.18        umap@2.1.1
chapel@2.10.0      ginkgo@1.11.0    hpctoolkit@2026.0.1  mercury@2.4.1      openfoam@2606          raja@2026.07.0       umpire@2026.07.1
diy@3.6.0          glvis@4.4        lammps@20250722.6    metall@0.30        openpmd-api@0.17.1     saltfm@0.6.0         upcxx@2025.10.0

-- linux-ubuntu24.04-x86_64_v3 / %c,fortran=gcc@13.3.0 ----------
fpm@0.13.0   libquo@1.4.1  nekbone@17.0          netlib-scalapack@2.2.3  py-libensemble@1.6.1  wannier90@4.0.2
hdf5@1.14.6  nek5000@19.0  netcdf-fortran@4.6.4  plasma@24.8.7           superlu@7.0.1         wrf@4.7.1

-- linux-ubuntu24.04-x86_64_v3 / %c=gcc@13.3.0 ------------------
aml@0.2.1     charliecloud@0.44  guacamole-server@1.6.0  hypre@3.2.0   parsec@4.0.2411  py-petsc4py@3.26.0
argobots@1.2  flux-core@0.89.0   hdf5-vol-async@1.7      libnrm@0.1.0  py-h5py@3.16.0

-- 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@2.1  hpx@1.11.0    kokkos-fft@2.0.0      kokkos-tools@5.2.0  loki@0.1.7   mpark-variant@1.4.0
flit@2.1.0  kokkos@5.2.2  kokkos-kernels@5.2.2  laghos@3.1          mfem@4.10.0

-- linux-ubuntu24.04-x86_64_v3 / no compilers -------------------
e4s-alc@1.0.3  e4s-cl@1.0.9  guacamole-client@1.6.0  mpich@5.0.1  nrm@0.1.0  py-cinemasci@1.7.9  py-jupyterhub@1.4.1  py-pytuq@1.0.0  tomcat@9.0.96
==> 134 installed packages
Singularity>
```

E4S 26.11 Linux x86_64 CPU image Ubuntu 24.04 LTS packages

```
Singularity> module avail
---------------------------------------------- /spack/share/spack/modules/linux-ubuntu24.04-x86_64_v3 ----------------------------------------------
adios/1.13.1                 dyninst/13.0.0-openmp   heffte/2.4.1                 mpark-variant/1.4.0     plumed/2.10.1                sz/2.1.12.5
adios2/2.12.1                e4s-alc/1.0.3           hpctoolkit/2026.0.1          mpich/5.0.1             precice/3.4.0                sz3/3.2.0
alquimia/1.1.0               e4s-cl/1.0.9            hpx/1.11.0                   mpifileutils/0.12       pruners-ninja/1.0.2          tasmanian/8.1
aml/0.2.1                    faodel/1.2108.1         hypre/3.2.0                  nccmp/1.11.0.0          pumi/2.2.9                   tau/2.36
amrex/26.10                  fftx/1.2.0              kokkos-fft/2.0.0             nco/5.4.1-openmp        py-cinemasci/1.7.9           tomcat/9.0.96
arborx/2.1                   flecsi/2.4.2            kokkos-kernels/5.2.2-openmp  nek5000/19.0            py-h5py/3.16.0               trilinos/14.4.0
argobots/1.2                 flit/2.1.0              kokkos-tools/5.2.0           nekbone/17.0            py-jupyterhub/1.4.1          turbine/1.3.0
ascent/0.9.5-openmp          flux-core/0.89.0        kokkos/5.2.2-openmp          netcdf-fortran/4.6.4    py-libensemble/1.6.1         umap/2.1.1
axom/0.15.0-openmp           fpm/0.13.0-openmp       laghos/3.1                   netlib-scalapack/2.2.3  py-petsc4py/3.26.0           umpire/2026.07.1
boost/1.90.0                 gasnet/2025.8.0         lammps/20250722.6-openmp     nrm/0.1.0               py-pytuq/1.0.0               upcxx/2025.10.0
bricks/2023.08.25            ginkgo/1.11.0-openmp    lbann/0.104                  nwchem/7.3.1            qthreads/1.18                variorum/0.8.0
butterflypack/4.1.0-openmp   globalarrays/5.8.2      legion/26.09.1               omega-h/11.2.0-scorec   quantum-espresso/7.6-openmp  veloc/1.7
cabana/0.8.0                 glvis/4.4               libcatalyst/2.1.0            openfoam/2606           raja/2026.07.0               vtk-m/2.3.0-openmp
caliper/2.15.0               gmp/6.3.0               libceed/1.0.0                openmpi/5.0.10          rempi/1.1.0                  wannier90/4.0.2
chai/2026.07.0               gotcha/1.0.8            libnrm/0.1.0                 openpmd-api/0.17.1      saltfm/0.6.0                 warpx/26.09
chapel/2.10.0                gromacs/2026.3-openmp   libpressio/0.99.4-openmp     papi/7.2.0              scr/3.1.0                    wps/4.6.0
charliecloud/0.44            guacamole-client/1.6.0  libquo/1.4.1                 papyrus/1.0.2           slate/2025.05.28-openmp      wrf/4.7.1
conduit/0.9.8                guacamole-server/1.6.0  libunwind/1.8.3              parallel-netcdf/1.14.1  slepc/3.26.0                 xyce/7.10.0
cp2k/2026.2-openmp           h5bench/1.4             loki/0.1.7                   parsec/4.0.2411         strumpack/8.1.0-openmp       zfp/1.0.1
darshan-runtime/3.5.0        hdf5-vol-async/1.7      mercury/2.4.1                pdt/3.25.2              sundials/7.9.0
darshan-util/3.5.0           hdf5-vol-cache/v1.1     metall/0.30                  petsc/3.26.0            superlu-dist/9.2.1
datatransferkit/3.1.1        hdf5-vol-log/1.4.0      mfem/4.10.0                  phist/1.12.1-openmp     superlu/7.0.1
diy/3.6.0                    hdf5/1.14.6             mgard/1.6.0-openmp           plasma/24.8.7           swig/4.0.2-fortran

Key:
loaded  modulepath
Singularity>
```

E4S 26.11 Linux x86_64 CPU image Rocky Linux 9.8 packages

```
Singularity> spack find -x
-- linux-rocky9-x86_64_v3 / %c,cxx,fortran=gcc@13.3.1 -----------
adios@1.13.1    axom@0.15.0           darshan-util@3.5.0     libceed@1.0.0          petsc@3.26.0   scr@3.1.0         superlu-dist@9.2.1  xyce@7.10.0
adios2@2.12.1   butterflypack@4.1.0   datatransferkit@3.1.1  nwchem@7.3.1           phist@1.12.1   slate@2025.05.28  tau@2.36            zfp@1.0.1
alquimia@1.1.0  conduit@0.9.8         globalarrays@5.8.2     openmpi@5.0.10         plumed@2.10.1  slepc@3.26.0      trilinos@14.4.0
amrex@26.10     cp2k@2026.2           h5bench@1.4            papi@7.2.0             precice@3.4.0  strumpack@8.1.0   variorum@0.8.0
ascent@0.9.5    darshan-runtime@3.5.0  heffte@2.4.1          parallel-netcdf@1.14.1 rempi@1.1.0    sundials@7.9.0    wps@4.6.0

-- linux-rocky9-x86_64_v3 / %c,cxx=gcc@13.3.1 -------------------
boost@1.90.0       dyninst@13.0.0   gmp@6.3.0           lbann@0.104        mgard@1.6.0           papyrus@1.0.2        swig@4.0.2-fortran  veloc@1.7
bricks@2023.08.25  faodel@1.2108.1  gotcha@1.0.8        legion@26.09.1     mpifileutils@0.12     pdt@3.25.2           sz@2.1.12.5         vtk-m@2.3.0
cabana@0.8.0       fftx@1.2.0       gromacs@2026.3      libcatalyst@2.1.0  nccmp@1.11.0.0        pruners-ninja@1.0.2  sz3@3.2.0           warpx@26.09
caliper@2.15.0     flecsi@2.4.2     hdf5-vol-cache@v1.1 libpressio@0.99.4  nco@5.4.1             pumi@2.2.9           turbine@1.3.0
chai@2026.07.0     gasnet@2025.8.0  hdf5-vol-log@1.4.0  libunwind@1.8.3    omega-h@11.2.0-scorec qthreads@1.18        umap@2.1.1
chapel@2.10.0      ginkgo@1.11.0    hpctoolkit@2026.0.1 mercury@2.4.1      openfoam@2606         raja@2026.07.0       umpire@2026.07.1
diy@3.6.0          glvis@4.4        lammps@20250722.6   metall@0.30        openpmd-api@0.17.1    saltfm@0.6.0         upcxx@2025.10.0

-- linux-rocky9-x86_64_v3 / %c,fortran=gcc@13.3.1 ---------------
fpm@0.13.0   libquo@1.4.1  nekbone@17.0          netlib-scalapack@2.2.3  py-libensemble@1.6.1  wannier90@4.0.2
hdf5@1.14.6  nek5000@19.0  netcdf-fortran@4.6.4  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  guacamole-server@1.6.0  hypre@3.2.0   parsec@4.0.2411  py-petsc4py@3.26.0
argobots@1.2  flux-core@0.89.0   hdf5-vol-async@1.7      libnrm@0.1.0  py-h5py@3.16.0

-- 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@2.1  hpx@1.11.0    kokkos-fft@2.0.0      kokkos-tools@5.2.0  loki@0.1.7   mpark-variant@1.4.0
flit@2.1.0  kokkos@5.2.2  kokkos-kernels@5.2.2  laghos@3.1          mfem@4.10.0

-- linux-rocky9-x86_64_v3 / no compilers ------------------------
e4s-alc@1.0.3  e4s-cl@1.0.9  guacamole-client@1.6.0  mpich@5.0.1  nrm@0.1.0  py-cinemasci@1.7.9  py-jupyterhub@1.4.1  py-pytuq@1.0.0  tomcat@9.0.96
==> 133 installed packages
Singularity>
```

E4S 26.11 Linux x86_64 CPU image Rocky Linux 9.8 packages

```
Singularity> module avail
---------------------------------------------------- /spack/share/spack/modules/linux-rocky9-x86_64_v3 ----------------------------------------------------
adios/1.13.1                dyninst/13.0.0-openmp   heffte/2.4.1                mpark-variant/1.4.0     plumed/2.10.1            sz3/3.2.0
adios2/2.12.1               e4s-alc/1.0.3           hpctoolkit/2026.0.1         mpich/5.0.1             precice/3.4.0            tasmanian/8.1
alquimia/1.1.0              e4s-cl/1.0.9            hpx/1.11.0                  mpifileutils/0.12       pruners-ninja/1.0.2      tau/2.36
aml/0.2.1                   faodel/1.2108.1         hypre/3.2.0                 nccmp/1.11.0.0          pumi/2.2.9               tomcat/9.0.96
amrex/26.10                 fftx/1.2.0              kokkos-fft/2.0.0            nco/5.4.1-openmp        py-cinemasci/1.7.9       trilinos/14.4.0
arborx/2.1                  flecsi/2.4.2            kokkos-kernels/5.2.2-openmp nek5000/19.0            py-h5py/3.16.0           turbine/1.3.0
argobots/1.2                flit/2.1.0              kokkos-tools/5.2.0          nekbone/17.0            py-jupyterhub/1.4.1      umap/2.1.1
ascent/0.9.5-openmp         flux-core/0.89.0        kokkos/5.2.2-openmp         netcdf-fortran/4.6.4    py-libensemble/1.6.1     umpire/2026.07.1
axom/0.15.0-openmp          fpm/0.13.0-openmp       laghos/3.1                  netlib-scalapack/2.2.3  py-petsc4py/3.26.0       upcxx/2025.10.0
boost/1.90.0                gasnet/2025.8.0         lammps/20250722.6-openmp    nrm/0.1.0               py-pytuq/1.0.0           variorum/0.8.0
bricks/2023.08.25           ginkgo/1.11.0-openmp    lbann/0.104                 nwchem/7.3.1            qthreads/1.18            veloc/1.7
butterflypack/4.1.0-openmp  globalarrays/5.8.2      legion/26.09.1              omega-h/11.2.0-scorec   raja/2026.07.0           vtk-m/2.3.0-openmp
cabana/0.8.0                glvis/4.4               libcatalyst/2.1.0           openfoam/2606           rempi/1.1.0              wannier90/4.0.2
caliper/2.15.0              gmp/6.3.0               libceed/1.0.0               openmpi/5.0.10          saltfm/0.6.0             warpx/26.09
chai/2026.07.0              gotcha/1.0.8            libnrm/0.1.0                openpmd-api/0.17.1      scr/3.1.0                wps/4.6.0
chapel/2.10.0               gromacs/2026.3-openmp   libpressio/0.99.4-openmp    papi/7.2.0              slate/2025.05.28-openmp  wrf/4.7.1
charliecloud/0.44           guacamole-client/1.6.0  libquo/1.4.1                papyrus/1.0.2           slepc/3.26.0             xyce/7.10.0
conduit/0.9.8               guacamole-server/1.6.0  libunwind/1.8.3             parallel-netcdf/1.14.1  strumpack/8.1.0-openmp   zfp/1.0.1
cp2k/2026.2-openmp          h5bench/1.4             loki/0.1.7                  parsec/4.0.2411         sundials/7.9.0
darshan-runtime/3.5.0       hdf5-vol-async/1.7      mercury/2.4.1               pdt/3.25.2              superlu-dist/9.2.1
darshan-util/3.5.0          hdf5-vol-cache/v1.1     metall/0.30                 petsc/3.26.0            superlu/7.0.1
datatransferkit/3.1.1       hdf5-vol-log/1.4.0      mfem/4.10.0                 phist/1.12.1-openmp     swig/4.0.2-fortran
diy/3.6.0                   hdf5/1.14.6             mgard/1.6.0-openmp          plasma/24.8.7           sz/2.1.12.5

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

Key:
modulepath
Singularity>
```

E4S 26.11 Linux x86_64 GPU image Ubuntu 24.04 LTS packages

```
Singularity> spack find -x
-- linux-ubuntu24.04-x86_64_v3 / %c,cxx,fortran=gcc@13.3.0 ------
adios2@2.12.1  axom@0.15.0  heffte@2.4.1   magma@2.10.0  petsc@3.26.0      slepc@3.26.0     sundials@7.9.0      tau@2.36         zfp@1.0.1
amrex@26.10    cp2k@2025.2  libceed@1.0.0  papi@7.2.0    slate@2025.05.28  strumpack@8.1.0  superlu-dist@9.2.1  trilinos@17.2.1

-- linux-ubuntu24.04-x86_64_v3 / %c,cxx=gcc@13.3.0 --------------
bricks@2023.08.25  chai@2026.07.0  fftx@1.2.0     gromacs@2026.3       lammps@20250722.6  mgard@1.6.0            umpire@2026.07.1
cabana@0.8.0       chapel@2.10.0   flecsi@2.4.2   hpctoolkit@2026.0.1  legion@26.09.1     omega-h@11.2.0-scorec  upcxx@2025.10.0
caliper@2.15.0     cusz@0.14.0     ginkgo@1.11.0  hypre@3.2.0          libpressio@0.99.4  raja@2026.07.0         vtk-m@2.3.0

-- linux-ubuntu24.04-x86_64_v3 / %c=gcc@13.3.0 ------------------
flux-core@0.89.0  guacamole-server@1.6.0  parsec@4.0.2411

-- 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@2.1  hpx@1.11.0  kokkos@5.2.2  kokkos-fft@2.0.0  kokkos-kernels@5.2.2  kokkos-tools@5.2.0  mfem@4.10.0

-- linux-ubuntu24.04-x86_64_v3 / no compilers -------------------
guacamole-client@1.6.0  mpich@5.0.1  tomcat@9.0.96
==> 52 installed packages
Singularity> module avail
------------------------------------------------- /spack/share/spack/modules/linux-ubuntu24.04-x86_64_v3 -------------------------------------------------
adios2/2.12.1-cuda90        fftx/1.2.0-cuda90             kokkos-fft/2.0.0                mpich/5.0.1                   tasmanian/8.1-cuda90
amrex/26.10-cuda90          flecsi/2.4.2-cuda90           kokkos-kernels/5.2.2-cuda90     omega-h/11.2.0-scorec-cuda90  tau/2.36-cuda
arborx/2.1-cuda90           flux-core/0.89.0-cuda         kokkos-tools/5.2.0              papi/7.2.0-cuda               tomcat/9.0.96
axom/0.15.0-cuda90-openmp   ginkgo/1.11.0-cuda90-openmp   kokkos/5.2.2-cuda90             parsec/4.0.2411-cuda90        trilinos/17.2.1-cuda90
bricks/2023.08.25-cuda      gromacs/2026.3-cuda90-openmp  lammps/20250722.6-cuda90-openmp petsc/3.26.0-cuda90           umpire/2026.07.1-cuda90
cabana/0.8.0-cuda90         guacamole-client/1.6.0        legion/26.09.1-cuda90           raja/2026.07.0-cuda90         upcxx/2025.10.0-cuda90
caliper/2.15.0-cuda90       guacamole-server/1.6.0        libceed/1.0.0-cuda90            slate/2025.05.28-cuda90-openmp vtk-m/2.3.0-cuda90-openmp
chai/2026.07.0-cuda90       heffte/2.4.1-cuda90           libpressio/0.99.4-cuda90-openmp slepc/3.26.0-cuda90            zfp/1.0.1-cuda90
chapel/2.10.0-cuda90        hpctoolkit/2026.0.1-cuda      magma/2.10.0-cuda90             strumpack/8.1.0-cuda90-openmp
cp2k/2025.2-cuda90-openmp   hpx/1.11.0-cuda90             mfem/4.10.0-cuda90              sundials/7.9.0-cuda90
cusz/0.14.0-cuda90          hypre/3.2.0-cuda90            mgard/1.6.0-cuda90-openmp       superlu-dist/9.2.1-cuda90

Key:
loaded  modulepath
Singularity>
```

GPU image optimized for size by GPU type: NVIDIA H200 (cuda90)

E4S Tools: Python and system tools

```
Singularity> python
Python 3.12.14 (main, Oct 14 2026, 16:33:25) [GCC 13.3.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import torch
>>> import transformer_engine
>>> import atlas
>>> import dspy
>>> import nvidia.nvshmem
>>> import nixl
>>> import jax
>>> import flash_attn
>>> import sglang
>>> import langchain
>>> import langgraph
>>> import bionemo_ir
>>> import ray
>>> import a2a
>>> import mcp
>>> import pandas
>>> import hypothesis
>>> import sklearn
>>> import cv2
>>> import ucimlrepo
>>> import transformers
>>> import megatron
>>> import tensorflow
>>> import ray
>>> import huggingface_hub
>>> import triton
>>> import polars
>>> import scipy
>>> import numpy
>>> import seaborn
>>> import leptonai
>>> import tensorboard
>>> import mpi4py
>>> import cupy
>>> import geopandas
>>> import hpc_campaign
>>> import openai
>>> import anthropic
>>> import google
>>>
```

```
Singularity> which hermes
/usr/local/bin/hermes
Singularity> which ollama
/usr/local/bin/ollama
Singularity> which vllm
/opt/python/pkgs/python/bin/vllm
Singularity> which orca-ide
/usr/local/bin/orca-ide
Singularity> which guacamole
/usr/local/bin/guacamole
Singularity> which opencode
/home/users/sameer/.e4s/ubuntu2404-x86_64-cuda90-26.11/node/global/bin/opencode
Singularity> which pi
/home/users/sameer/.e4s/ubuntu2404-x86_64-cuda90-26.11/node/global/bin/pi
Singularity> which paraview
/usr/local/paraview-6.1.0/bin/paraview
Singularity> which visit
/usr/local/visit/bin/visit
Singularity> which codium
/usr/bin/codium
Singularity> which tau
/usr/local/bin/tau
Singularity> which julia
/usr/local/julia/bin/julia
Singularity> which python
/opt/python/pkgs/python/bin/python
Singularity> which valgrind
/usr/bin/valgrind
Singularity> which strace
/usr/bin/strace
Singularity> which ltrace
/usr/bin/ltrace
Singularity> which lsof
/usr/bin/lsof
Singularity> which jupyter
/opt/python/pkgs/python/bin/jupyter
Singularity> which marimo
/opt/python/pkgs/python/bin/marimo
Singularity> which npm
/usr/local/node/bin/npm
Singularity> which uv
/opt/python/pkgs/python/bin/uv
Singularity>
```

E4S 26.11 Linux aarch64 CPU image Ubuntu 24.04 LTS packages

```
Singularity> spack find -x
-- linux-ubuntu24.04-aarch64 / %c,cxx,fortran=gcc@13.3.0 --------
adios@1.13.1    axom@0.15.0           darshan-util@3.5.0     libceed@1.0.0          paraview@6.2.0  quantum-espresso@7.6  strumpack@8.1.0     visit@3.4.1
adios2@2.12.1   butterflypack@4.1.0   datatransferkit@3.1.1  nwchem@7.3.1           petsc@3.26.0    rempi@1.1.0           sundials@7.9.0      wps@4.6.0
alquimia@1.1.0  conduit@0.9.8         globalarrays@5.8.2     openmpi@5.0.10         phist@1.12.1    scr@3.1.0             superlu-dist@9.2.1  zfp@1.0.1
amrex@26.10     cp2k@2026.2           h5bench@1.4            papi@7.2.0             plumed@2.10.1   slate@2025.05.28      tau@2.36
ascent@0.9.5    darshan-runtime@3.5.0  heffte@2.4.1          parallel-netcdf@1.14.1 precice@3.4.0   slepc@3.26.0          trilinos@14.4.0

-- linux-ubuntu24.04-aarch64 / %c,cxx=gcc@13.3.0 ----------------
boost@1.90.0    dyninst@13.0.0   gmp@6.3.0           lammps@20250722.6  mercury@2.4.1      omega-h@11.2.0-scorec  pumi@2.2.9          sz3@3.2.0         vtk-m@2.3.0
cabana@0.8.0    faodel@1.2108.1  gotcha@1.0.8        lbann@0.104        metall@0.30        openfoam@2606          qthreads@1.18       turbine@1.3.0     warpx@26.09
caliper@2.15.0  fftx@1.2.0       gromacs@2026.3      legion@26.09.1     mgard@1.6.0        openpmd-api@0.17.1     raja@2026.07.0      umap@2.1.1
chai@2026.07.0  flecsi@2.4.2     hdf5-vol-cache@v1.1 libcatalyst@2.1.0  mpifileutils@0.12  papyrus@1.0.2          saltfm@0.6.0        umpire@2026.07.1
chapel@2.10.0   gasnet@2025.8.0  hdf5-vol-log@1.4.0  libpressio@0.99.4  nccmp@1.11.0.0     pdt@3.25.2             swig@4.0.2-fortran  upcxx@2025.10.0
diy@3.6.0       ginkgo@1.11.0    hpctoolkit@2026.0.1 libunwind@1.8.3    nco@5.4.1          pruners-ninja@1.0.2    sz@2.1.12.5         veloc@1.7

-- linux-ubuntu24.04-aarch64 / %c,fortran=gcc@13.3.0 ------------
fpm@0.13.0   libquo@1.4.1  nekbone@17.0          netlib-scalapack@2.2.3  py-libensemble@1.6.1  wannier90@4.0.2
hdf5@1.14.6  nek5000@19.0  netcdf-fortran@4.6.4  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  guacamole-server@1.6.0  hypre@3.2.0   parsec@4.0.2411  py-petsc4py@3.26.0
argobots@1.2  flux-core@0.89.0   hdf5-vol-async@1.7      libnrm@0.1.0  py-h5py@3.16.0

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

-- linux-ubuntu24.04-aarch64 / %cxx=gcc@13.3.0 ------------------
arborx@2.1  flit@2.1.0  hpx@1.11.0  kokkos@5.2.2  kokkos-fft@2.0.0  kokkos-kernels@5.2.2  kokkos-tools@5.2.0  laghos@3.1  loki@0.1.7  mfem@4.10.0  mpark-variant@1.4.0

-- linux-ubuntu24.04-aarch64 / no compilers ---------------------
e4s-alc@1.0.3  e4s-cl@1.0.9  guacamole-client@1.6.0  mpich@5.0.1  nrm@0.1.0  py-cinemasci@1.7.9  py-jupyterhub@1.4.1  py-pytuq@1.0.0  tomcat@9.0.96
==> 132 installed packages
Singularity>
```

E4S 26.11 Linux aarch64 CPU image Ubuntu 24.04 LTS packages

```
Singularity> module avail
------------------------------------------------------------ /spack/share/spack/modules/linux-ubuntu24.04-aarch64 ------------------------------------------------------------
adios/1.13.1                darshan-util/3.5.0      guacamole-server/1.6.0      libceed/1.0.0              nrm/0.1.0              py-cinemasci/1.7.9          sz/2.1.12.5
adios2/2.12.1               datatransferkit/3.1.1   h5bench/1.4                 libnrm/0.1.0               nwchem/7.3.1           py-h5py/3.16.0              sz3/3.2.0
alquimia/1.1.0              diy/3.6.0               hdf5-vol-async/1.7          libpressio/0.99.4-openmp   omega-h/11.2.0-scorec  py-jupyterhub/1.4.1         tasmanian/8.1
aml/0.2.1                   dyninst/13.0.0-openmp   hdf5-vol-cache/v1.1         libquo/1.4.1               openfoam/2606          py-libensemble/1.6.1        tau/2.36
amrex/26.10                 e4s-alc/1.0.3           hdf5-vol-log/1.4.0          libunwind/1.8.3            openmpi/5.0.10         py-petsc4py/3.26.0          tomcat/9.0.96
arborx/2.1                  e4s-cl/1.0.9            hdf5/1.14.6                 loki/0.1.7                 openpmd-api/0.17.1     py-pytuq/1.0.0              trilinos/14.4.0
argobots/1.2                faodel/1.2108.1         heffte/2.4.1                mercury/2.4.1              papi/7.2.0             qthreads/1.18               turbine/1.3.0
ascent/0.9.5-openmp         fftx/1.2.0              hpctoolkit/2026.0.1         metall/0.30                papyrus/1.0.2          quantum-espresso/7.6-openmp umap/2.1.1
axom/0.15.0-openmp          flecsi/2.4.2            hpx/1.11.0                  mfem/4.10.0                parallel-netcdf/1.14.1 raja/2026.07.0              umpire/2026.07.1
boost/1.90.0                flit/2.1.0              hypre/3.2.0                 mgard/1.6.0-openmp         paraview/6.2.0         rempi/1.1.0                 upcxx/2025.10.0
butterflypack/4.1.0-openmp  flux-core/0.89.0        kokkos-fft/2.0.0            mpark-variant/1.4.0        parsec/4.0.2411        saltfm/0.6.0                veloc/1.7
cabana/0.8.0                fpm/0.13.0-openmp       kokkos-kernels/5.2.2-openmp mpich/5.0.1                pdt/3.25.2             scr/3.1.0                   visit/3.4.1
caliper/2.15.0              gasnet/2025.8.0         kokkos-tools/5.2.0          mpifileutils/0.12          petsc/3.26.0           slate/2025.05.28-openmp     vtk-m/2.3.0-openmp
chai/2026.07.0              ginkgo/1.11.0-openmp    kokkos/5.2.2-openmp         nccmp/1.11.0.0             phist/1.12.1-openmp    slepc/3.26.0                wannier90/4.0.2
chapel/2.10.0               globalarrays/5.8.2      laghos/3.1                  nco/5.4.1-openmp           plasma/24.8.7          strumpack/8.1.0-openmp      warpx/26.09
charliecloud/0.44           gmp/6.3.0               lammps/20250722.6-openmp    nek5000/19.0               plumed/2.10.1          sundials/7.9.0              wps/4.6.0
conduit/0.9.8               gotcha/1.0.8            lbann/0.104                 nekbone/17.0               precice/3.4.0          superlu-dist/9.2.1          wrf/4.7.1
cp2k/2026.2-openmp          gromacs/2026.3-openmp   legion/26.09.1              netcdf-fortran/4.6.4       pruners-ninja/1.0.2    superlu/7.0.1               zfp/1.0.1
darshan-runtime/3.5.0       guacamole-client/1.6.0  libcatalyst/2.1.0           netlib-scalapack/2.2.3     pumi/2.2.9             swig/4.0.2-fortran

Key:
modulepath
Singularity>
```

E4S 26.11 Linux aarch64 CPU image Rocky Linux 9.8 packages

```
Singularity> spack find -x
-- linux-rocky9-aarch64 / %c,cxx,fortran=gcc@13.3.1 -------------
adios@1.13.1    ascent@0.9.5         cp2k@2026.2            globalarrays@5.8.2  nwchem@7.3.1           petsc@3.26.0   rempi@1.1.0       strumpack@8.1.0     trilinos@14.4.0
adios2@2.12.1   axom@0.15.0          darshan-runtime@3.5.0  h5bench@1.4         openmpi@5.0.10         phist@1.12.1   scr@3.1.0         sundials@7.9.0      visit@3.4.1
alquimia@1.1.0  butterflypack@4.1.0  darshan-util@3.5.0     heffte@2.4.1        papi@7.2.0             plumed@2.10.1  slate@2025.05.28  superlu-dist@9.2.1  wps@4.6.0
amrex@26.10     conduit@0.9.8        datatransferkit@3.1.1  libceed@1.0.0       parallel-netcdf@1.14.1 precice@3.4.0  slepc@3.26.0      tau@2.36            zfp@1.0.1

-- linux-rocky9-aarch64 / %c,cxx=gcc@13.3.1 ---------------------
boost@1.90.0    dyninst@13.0.0   gmp@6.3.0           lammps@20250722.6  mercury@2.4.1      omega-h@11.2.0-scorec  pumi@2.2.9         sz3@3.2.0         vtk-m@2.3.0
cabana@0.8.0    faodel@1.2108.1  gotcha@1.0.8        lbann@0.104        metall@0.30        openfoam@2606          qthreads@1.18      turbine@1.3.0     warpx@26.09
caliper@2.15.0  fftx@1.2.0       gromacs@2026.3      legion@26.09.1     mgard@1.6.0        openpmd-api@0.17.1     raja@2026.07.0     umap@2.1.1
chai@2026.07.0  flecsi@2.4.2     hdf5-vol-cache@v1.1  libcatalyst@2.1.0  mpifileutils@0.12  papyrus@1.0.2          saltfm@0.6.0       umpire@2026.07.1
chapel@2.10.0   gasnet@2025.8.0  hdf5-vol-log@1.4.0   libpressio@0.99.4  nccmp@1.11.0.0     pdt@3.25.2             swig@4.0.2-fortran  upcxx@2025.10.0
diy@3.6.0       ginkgo@1.11.0    hpctoolkit@2026.0.1  libunwind@1.8.3    nco@5.4.1          pruners-ninja@1.0.2    sz@2.1.12.5        veloc@1.7

-- linux-rocky9-aarch64 / %c,fortran=gcc@13.3.1 -----------------
fpm@0.13.0   libquo@1.4.1  nekbone@17.0          netlib-scalapack@2.2.3  py-libensemble@1.6.1  wannier90@4.0.2
hdf5@1.14.6  nek5000@19.0  netcdf-fortran@4.6.4  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  guacamole-server@1.6.0  hypre@3.2.0   parsec@4.0.2411  py-petsc4py@3.26.0
argobots@1.2  flux-core@0.89.0   hdf5-vol-async@1.7      libnrm@0.1.0  py-h5py@3.16.0

-- 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@5.2.2  kokkos-fft@2.0.0  kokkos-kernels@5.2.2  kokkos-tools@5.2.0  laghos@3.1  loki@0.1.7  mfem@4.10.0  mpark-variant@1.4.0

-- linux-rocky9-aarch64 / no compilers --------------------------
e4s-alc@1.0.3  e4s-cl@1.0.9  guacamole-client@1.6.0  mpich@5.0.1  nrm@0.1.0  py-cinemasci@1.7.9  py-jupyterhub@1.4.1  py-pytuq@1.0.0  tomcat@9.0.96
==> 130 installed packages
Singularity>
```

E4S 26.11 Linux aarch64 CPU image Rocky Linux 9.8 packages

```
Singularity> module avail
------------------------------------------------------------------ /spack/share/spack/modules/linux-rocky9-aarch64 -------------------------------------------------------------------
adios/1.13.1                darshan-util/3.5.0      guacamole-server/1.6.0      libceed/1.0.0             nrm/0.1.0              py-h5py/3.16.0          tasmanian/8.1
adios2/2.12.1               datatransferkit/3.1.1   h5bench/1.4                 libnrm/0.1.0              nwchem/7.3.1           py-jupyterhub/1.4.1     tau/2.36
alquimia/1.1.0              diy/3.6.0               hdf5-vol-async/1.7          libpressio/0.99.4-openmp  omega-h/11.2.0-scorec  py-libensemble/1.6.1    tomcat/9.0.96
aml/0.2.1                   dyninst/13.0.0-openmp   hdf5-vol-cache/v1.1         libquo/1.4.1              openfoam/2606          py-petsc4py/3.26.0      trilinos/14.4.0
amrex/26.10                 e4s-alc/1.0.3           hdf5-vol-log/1.4.0          libunwind/1.8.3           openmpi/5.0.10         py-pytuq/1.0.0          turbine/1.3.0
arborx/2.1                  e4s-cl/1.0.9            hdf5/1.14.6                 loki/0.1.7                openpmd-api/0.17.1     qthreads/1.18           umap/2.1.1
argobots/1.2                faodel/1.2108.1         heffte/2.4.1                mercury/2.4.1             papi/7.2.0             raja/2026.07.0          umpire/2026.07.1
ascent/0.9.5-openmp         fftx/1.2.0              hpctoolkit/2026.0.1         metall/0.30               papyrus/1.0.2          rempi/1.1.0             upcxx/2025.10.0
axom/0.15.0-openmp          flecsi/2.4.2            hpx/1.11.0                  mfem/4.10.0               parallel-netcdf/1.14.1 saltfm/0.6.0            veloc/1.7
boost/1.90.0                flit/2.1.0              hypre/3.2.0                 mgard/1.6.0-openmp        parsec/4.0.2411        scr/3.1.0               visit/3.4.1
butterflypack/4.1.0-openmp  flux-core/0.89.0        kokkos-fft/2.0.0            mpark-variant/1.4.0       pdt/3.25.2             slate/2025.05.28-openmp vtk-m/2.3.0-openmp
cabana/0.8.0                fpm/0.13.0-openmp       kokkos-kernels/5.2.2-openmp mpich/5.0.1               petsc/3.26.0           slepc/3.26.0            wannier90/4.0.2
caliper/2.15.0              gasnet/2025.8.0         kokkos-tools/5.2.0          mpifileutils/0.12         phist/1.12.1-openmp    strumpack/8.1.0-openmp  warpx/26.09
chai/2026.07.0              ginkgo/1.11.0-openmp    kokkos/5.2.2-openmp         nccmp/1.11.0.0            plasma/24.8.7          sundials/7.9.0          wps/4.6.0
chapel/2.10.0               globalarrays/5.8.2      laghos/3.1                  nco/5.4.1-openmp          plumed/2.10.1          superlu-dist/9.2.1      wrf/4.7.1
charliecloud/0.44           gmp/6.3.0               lammps/20250722.6-openmp    nek5000/19.0              precice/3.4.0          superlu/7.0.1           zfp/1.0.1
conduit/0.9.8               gotcha/1.0.8            lbann/0.104                 nekbone/17.0              pruners-ninja/1.0.2    swig/4.0.2-fortran
cp2k/2026.2-openmp          gromacs/2026.3-openmp   legion/26.09.1              netcdf-fortran/4.6.4      pumi/2.2.9             sz/2.1.12.5
darshan-runtime/3.5.0       guacamole-client/1.6.0  libcatalyst/2.1.0           netlib-scalapack/2.2.3    py-cinemasci/1.7.9     sz3/3.2.0

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

Key:
modulepath
Singularity>
```

E4S 26.11 GPU image aarch64 Python packages

```
Singularity> python
Python 3.12.14 (main, Oct 14 2026, 23:40:21) [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 transformer_engine
>>> import atlas
>>> import dspy
>>> import nvidia.nvshmem
>>> import nixl
>>> import jax
>>> import flash_attn
>>> import sglang
>>> import langchain
>>> import langgraph
>>> import bionemo_ir
>>> import ray
>>> import a2a
>>> import mcp
>>> import pandas
>>> import hypothesis
>>> import sklearn
>>> import cv2
>>> import ucimlrepo
>>> import transformers
>>> import megatron
>>> import tensorflow
>>> import ray
>>> import huggingface_hub
>>> import triton
>>> import polars
>>> import scipy
>>> import numpy
>>> import seaborn
>>> import leptonai
>>> import tensorboard
>>> import mpi4py
>>> import cupy
>>> import geopandas
>>> import hpc_campaign
>>> import openai
>>> import anthropic
>>> import google
>>> cap = torch.cuda.get_device_capability(0); print(f'sm_{cap[0]}{cap[1]}')
sm_90
>>>
```

NVIDIA Grace Hopper

```
Singularity> python
Python 3.12.14 (main, Oct 14 2026, 23:40:21) [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 transformer_engine
>>> import atlas
>>> import dspy
>>> import nvidia.nvshmem
>>> import nixl
>>> import jax
>>> import flash_attn
>>> import sglang
>>> import langchain
>>> import langgraph
>>> import bionemo_ir
>>> import ray
>>> import a2a
>>> import mcp
>>> import pandas
>>> import hypothesis
>>> import sklearn
>>> import ucimlrepo
>>> import transformers
>>> import megatron
>>> import tensorflow
>>> import ray
>>> import huggingface_hub
>>> import triton
>>> import polars
>>> import scipy
>>> import numpy
>>> import seaborn
>>> import leptonai
>>> import tensorboard
>>> import mpi4py
>>> import cupy
>>> import geopandas
>>> import hpc_campaign
>>> import openai
>>> import anthropic
>>> import google
>>> cap = torch.cuda.get_device_capability(0); print(f'sm_{cap[0]}{cap[1]}')
sm_121
>>>
Singularity> grep PRETTY_NAME /etc/os-release
PRETTY_NAME="Rocky Linux 9.8 (Blue Onyx)"
Singularity> uname -m
aarch64
Singularity>
```

NVIDIA Grace Blackwell

E4S 26.11 Intel oneAPI GPU image Ubuntu 24.04 LTS packages

```
Singularity> clinfo -l | grep GPU
 `-- Device #0: Intel(R) Data Center GPU Max 1100
Singularity> grep PRETTY_NAME /etc/os-release
PRETTY_NAME="Ubuntu 24.04.5 LTS"
Singularity> spack find -x
-- linux-ubuntu24.04-x86_64_v3 / %c,cxx,fortran=gcc@13.3.0 ------
adios2@2.12.1  openmpi@5.0.10  scr@3.1.0

-- linux-ubuntu24.04-x86_64_v3 / %c,cxx,fortran=oneapi@2026.1.1 -
adios@1.13.1  axom@0.15.0            darshan-util@3.5.0     heffte@2.4.1            phist@1.12.1          slate@2025.05.28    tau@2.36         variorum@0.8.0
amrex@26.10   butterflypack@4.1.0    datatransferkit@3.1.1  libceed@1.0.0           plumed@2.10.1         strumpack@8.1.0     tau@2.36         zfp@1.0.1
amrex@26.10   conduit@0.9.8          globalarrays@5.8.2     papi@7.2.0              quantum-espresso@7.6  sundials@7.9.0      trilinos@14.4.0
ascent@0.9.5  darshan-runtime@3.5.0  h5bench@1.4            parallel-netcdf@1.14.1  rempi@1.1.0           superlu-dist@9.2.1  unifyfs@2.0

-- linux-ubuntu24.04-x86_64_v3 / %c,cxx=gcc@13.3.0 --------------
cabana@0.8.0  openfoam@2606  openpmd-api@0.17.1  swig@4.0.2-fortran  turbine@1.3.0

-- linux-ubuntu24.04-x86_64_v3 / %c,cxx=oneapi@2026.1.1 ---------
bolt@2.0           faodel@1.2108.1  gromacs@2026.3       libcatalyst@2.1.0  mpifileutils@0.12      pruners-ninja@1.0.2  sz@2.1.12.5       upcxx@2025.10.0
boost@1.90.0       gasnet@2025.8.0  hdf5-vol-log@1.4.0   libunwind@1.8.3    nccmp@1.11.0.0         pumi@2.2.9           sz3@3.2.0         veloc@1.7
bricks@2023.08.25  ginkgo@1.11.0    hpctoolkit@2026.0.1  mercury@2.4.1      omega-h@11.2.0-scorec  qthreads@1.18        umap@2.1.1        vtk-m@2.3.0
caliper@2.15.0     gmp@6.3.0        hpctoolkit@2026.0.1  metall@0.30        papyrus@1.0.2          raja@2026.07.0       umpire@2026.07.1
chai@2026.07.0     gotcha@1.0.8     legion@26.09.1       mgard@1.6.0        pdt@3.25.2             saltfm@0.6.0         upcxx@2025.10.0

-- linux-ubuntu24.04-x86_64_v3 / %c,fortran=gcc@13.3.0 ----------
py-libensemble@1.6.1

-- linux-ubuntu24.04-x86_64_v3 / %c,fortran=oneapi@2026.1.1 -----
hdf5@1.14.6  libquo@1.4.1  nekbone@17.0  netcdf-fortran@4.6.4  netlib-scalapack@2.2.3  superlu@7.0.1  wannier90@4.0.2

-- linux-ubuntu24.04-x86_64_v3 / %c=gcc@13.3.0 ------------------
charliecloud@0.44  guacamole-server@1.6.0  parsec@4.0.2411

-- linux-ubuntu24.04-x86_64_v3 / %c=oneapi@2026.1.1 -------------
aml@0.2.1  aml@0.2.1  argobots@1.2  flux-core@0.89.0  hdf5-vol-async@1.7  hypre@3.2.0  libnrm@0.1.0

-- linux-ubuntu24.04-x86_64_v3 / %cxx,fortran=oneapi@2026.1.1 ---
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@2026.1.1 -----------
arborx@2.1  arborx@2.1  flit@2.1.0  kokkos@5.2.2  kokkos@5.2.2  kokkos-kernels@5.2.2  laghos@3.1  loki@0.1.7  mfem@4.10.0  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  guacamole-client@1.6.0  intel-oneapi-mpi@2021.18.0  nrm@0.1.0  py-jupyterhub@1.4.1  stc@0.9.0  tomcat@9.0.96
==> 116 installed packages
Singularity>
```

E4S 26.11 Intel oneAPI GPU image Ubuntu 24.04 LTS packages

```
Singularity> module avail
---------------------------------------------------------- /spack/share/spack/modules/linux-ubuntu24.04-x86_64_v3 ----------------------------------------------
adios/1.13.1                darshan-runtime/3.5.0   hdf5-vol-log/1.4.0              metall/0.30             plumed/2.10.1                 tasmanian/8.1
adios2/2.12.1               darshan-util/3.5.0      hdf5/1.14.6                     mfem/4.10.0             pruners-ninja/1.0.2           tau/2.36
aml/0.2.1                   datatransferkit/3.1.1   heffte/2.4.1                    mgard/1.6.0-openmp      pumi/2.2.9                    tau/2.36-level-zero
aml/0.2.1-level-zero        e4s-alc/1.0.3           hpctoolkit/2026.0.1             mpark-variant/1.4.0     py-jupyterhub/1.4.1           tomcat/9.0.96
amrex/26.10                 e4s-cl/1.0.9            hpctoolkit/2026.0.1-level-zero  mpifileutils/0.12       py-libensemble/1.6.1          trilinos/14.4.0
amrex/26.10-sycl            exaworks/0.1.0          hpx/1.11.0                      nccmp/1.11.0.0          qthreads/1.18                 turbine/1.3.0
arborx/2.1                  faodel/1.2108.1         hypre/3.2.0                     nekbone/17.0            quantum-espresso/7.6-openmp   umap/2.1.1
arborx/2.1-sycl             flit/2.1.0              intel-oneapi-mpi/2021.18.0      netcdf-fortran/4.6.4    raja/2026.07.0                umpire/2026.07.1
argobots/1.2                flux-core/0.89.0        kokkos-kernels/5.2.2-openmp     netlib-scalapack/2.2.3  rempi/1.1.0                   unifyfs/2.0
ascent/0.9.5-openmp         fortrilinos/2.3.0       kokkos/5.2.2-openmp             nrm/0.1.0               saltfm/0.6.0                  upcxx/2025.10.0
axom/0.15.0-openmp          gasnet/2025.8.0         kokkos/5.2.2-openmp-sycl        omega-h/11.2.0-scorec   scr/3.1.0                     upcxx/2025.10.0-level-zero
bolt/2.0                    ginkgo/1.11.0-openmp    laghos/3.1                      openfoam/2606           slate/2025.05.28-openmp       variorum/0.8.0
boost/1.90.0                globalarrays/5.8.2      legion/26.09.1                  openmpi/5.0.10          stc/0.9.0                     veloc/1.7
bricks/2023.08.25           gmp/6.3.0               libcatalyst/2.1.0               openpmd-api/0.17.1      strumpack/8.1.0-openmp        vtk-m/2.3.0
butterflypack/4.1.0-openmp  gotcha/1.0.8            libceed/1.0.0                   papi/7.2.0              sundials/7.9.0                wannier90/4.0.2
cabana/0.8.0                gromacs/2026.3-openmp   libnrm/0.1.0                    papyrus/1.0.2           superlu-dist/9.2.1            zfp/1.0.1
caliper/2.15.0              guacamole-client/1.6.0  libquo/1.4.1                    parallel-netcdf/1.14.1  superlu/7.0.1
chai/2026.07.0              guacamole-server/1.6.0  libunwind/1.8.3                 parsec/4.0.2411         swig/4.0.2-fortran
charliecloud/0.44           h5bench/1.4             loki/0.1.7                      pdt/3.25.2              sz/2.1.12.5
conduit/0.9.8               hdf5-vol-async/1.7      mercury/2.4.1                   phist/1.12.1-openmp     sz3/3.2.0

------------------------------------------------------------------------ /opt/intel/oneapi/modulefiles ------------------------------------------------------------------------
ccl/2022.1.0                  compiler-rt/2026.1.1  debugger/2026.1.0       dnnl/3.11.4  intel_ipp_intel64/2026.0    mkl/2026.1   tbb/2023.1  umf/1.1.0
ccl/latest                    compiler-rt/latest    debugger/latest         dnnl/latest  intel_ipp_intel64/latest    mkl/latest   tbb/latest  umf/latest
compiler-intel-llvm/2026.1.1  compiler/2026.1.1     dev-utilities/2025.3.0  dpl/2022.13  intel_ippcp_intel64/2026.0  mpi/2021.18  tcm/1.5     vtune/2026.4
compiler-intel-llvm/latest    compiler/latest       dev-utilities/latest    dpl/latest   intel_ippcp_intel64/latest  mpi/latest   tcm/latest  vtune/latest

Key:
loaded  modulepath
Singularity>
```

E4S 26.11 AMD ROCm 7.2.4 GPU image Ubuntu 24.04 LTS

```
Singularity> ls /opt/rocm-7.2.4/bin/hipcc
/opt/rocm-7.2.4/bin/hipcc
Singularity> spack find -x
-- linux-ubuntu24.04-x86_64_v3 / %c,cxx,fortran=gcc@13.3.0 ------
amrex@26.10   libceed@1.0.0  papi@7.2.0    slate@2025.05.28  strumpack@8.1.0  superlu-dist@9.2.1
heffte@2.4.1  magma@2.10.0   petsc@3.26.0  slepc@3.26.0      sundials@7.9.0   tau@2.36

-- linux-ubuntu24.04-x86_64_v3 / %c,cxx=gcc@13.3.0 --------------
cabana@0.8.0    chai@2026.07.0   hpctoolkit@2026.0.1  legion@26.09.1  umpire@2026.07.1  vtk-m@2.3.0
caliper@2.15.0  gasnet@2025.8.0  hypre@3.2.0          raja@2026.07.0  upcxx@2025.10.0

-- linux-ubuntu24.04-x86_64_v3 / %c=gcc@13.3.0 ------------------
guacamole-server@1.6.0

-- 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@2.1  kokkos@5.2.2  kokkos-fft@2.0.0  kokkos-tools@5.2.0  mfem@4.10.0

-- linux-ubuntu24.04-x86_64_v3 / no compilers -------------------
guacamole-client@1.6.0  mpich@5.0.1  tomcat@9.0.96
==> 33 installed packages
Singularity> module avail
------------------------------------------ /spack/share/spack/modules/linux-ubuntu24.04-x86_64_v3 -------------------------------
amrex/26.10-gfx942         guacamole-server/1.6.0    legion/26.09.1-gfx942  raja/2026.07.0-gfx942           tau/2.36-rocm
arborx/2.1-gfx942          heffte/2.4.1-gfx942       libceed/1.0.0-gfx942   slate/2025.05.28-gfx942-openmp  tomcat/9.0.96
cabana/0.8.0-gfx942-rocm   hpctoolkit/2026.0.1-rocm  magma/2.10.0-gfx942    slepc/3.26.0-gfx942             umpire/2026.07.1-gfx942
caliper/2.15.0-gfx942      hypre/3.2.0-gfx942        mfem/4.10.0-gfx942     strumpack/8.1.0-gfx942-openmp   upcxx/2025.10.0-gfx942
chai/2026.07.0-gfx942      kokkos-fft/2.0.0          mpich/5.0.1            sundials/7.9.0-gfx942           vtk-m/2.3.0-gfx942
gasnet/2025.8.0-gfx942     kokkos-tools/5.2.0        papi/7.2.0-gfx942      superlu-dist/9.2.1-gfx942
guacamole-client/1.6.0     kokkos/5.2.2-gfx942       petsc/3.26.0-gfx942    tasmanian/8.1-gfx942

Key:
loaded  modulepath
Singularity>
```

E4S 26.11 ppc64le CPU Ubuntu image

```
Singularity> lscpu  | grep name
Model name:                          POWER10 (architected), altivec supported
Singularity> spack find -x
-- linux-ubuntu20.04-ppc64le / %c,cxx,fortran=gcc@9.4.0 ---------
adios@1.13.1    butterflypack@4.1.0    globalarrays@5.8.2  openmpi@5.0.10          plumed@2.10.1         slepc@3.26.0        trilinos@14.4.0
adios2@2.12.1   conduit@0.9.8          h5bench@1.4         papi@7.2.0              quantum-espresso@7.6  strumpack@8.1.0     unifyfs@2.0
alquimia@1.1.0  darshan-runtime@3.5.0  heffte@2.4.1        parallel-netcdf@1.14.1  rempi@1.1.0           sundials@7.9.0      wps@4.6.0
amrex@25.05     darshan-util@3.5.0     libceed@1.0.0       petsc@3.26.0            scr@3.1.0             superlu-dist@9.2.1  zfp@1.0.1
ascent@0.9.5    datatransferkit@3.1.1  nwchem@7.3.1        phist@1.12.1            slate@2025.05.28      tau@2.36

-- linux-ubuntu20.04-ppc64le / %c,cxx=gcc@9.4.0 -----------------
bolt@2.0           faodel@1.2108.1  hdf5-vol-cache@v1.1  libunwind@1.7.2    omega-h@11.2.0-scorec  qthreads@1.18       veloc@1.7
boost@1.90.0       fftx@1.2.0       hdf5-vol-log@1.4.0   mercury@2.4.1      openfoam@2606          swig@4.0.2-fortran  vtk-m@2.3.0
bricks@2023.08.25  gasnet@2025.8.0  lammps@20250722.6    metall@0.30        openpmd-api@0.17.1     sz@2.1.12.5
cabana@0.8.0       ginkgo@1.11.0    lbann@0.104          mgard@1.6.0        papyrus@1.0.2          sz3@3.2.0
caliper@2.15.0     glvis@4.4        legion@26.09.1       mpifileutils@0.12  pdt@3.25.2             turbine@1.3.0
diy@3.6.0          gmp@6.3.0        libcatalyst@2.1.0    nccmp@1.11.0.0     pruners-ninja@1.0.2    umap@2.1.1
dyninst@13.0.0     gotcha@1.0.8     libpressio@0.99.4    nco@5.4.1          pumi@2.2.9             upcxx@2025.10.0

-- linux-ubuntu20.04-ppc64le / %c,fortran=gcc@9.4.0 -------------
fpm@0.13.0   libquo@1.4.1  nekbone@17.0          netlib-scalapack@2.2.3  py-libensemble@1.6.1  wannier90@4.0.2
hdf5@1.14.6  nek5000@19.0  netcdf-fortran@4.6.4  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  argobots@1.2  flux-core@0.89.0  hdf5-vol-async@1.7  hypre@3.2.0  libnrm@0.1.0  parsec@4.0.2411  py-h5py@3.16.0  py-petsc4py@3.26.0

-- 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@4.10.0  mpark-variant@1.4.0

-- linux-ubuntu20.04-ppc64le / no compilers ---------------------
e4s-alc@1.0.3  e4s-cl@1.0.9  mpich@5.0.1  py-jupyterhub@1.4.1
==> 114 installed packages
Singularity>
```

E4S 26.11 ppc64le CPU Ubuntu image

```
Singularity> module avail
------------------------------------------ /spack/share/spack/modules/linux-ubuntu20.04-ppc64le ------------------------------------------
adios/1.13.1                fftx/1.2.0                  lbann/0.104               omega-h/11.2.0-scorec       slate/2025.05.28-openmp
adios2/2.12.1               flit/2.1.0                  legion/26.09.1            openfoam/2606               slepc/3.26.0
alquimia/1.1.0              flux-core/0.89.0            libcatalyst/2.1.0         openmpi/5.0.10              strumpack/8.1.0-openmp
aml/0.2.1                   fortrilinos/2.3.0           libceed/1.0.0             openpmd-api/0.17.1          sundials/7.9.0
amrex/25.05                 fpm/0.13.0-openmp           libnrm/0.1.0              papi/7.2.0                  superlu-dist/9.2.1
arborx/2.1                  gasnet/2025.8.0             libpressio/0.99.4-openmp  papyrus/1.0.2               superlu/7.0.1
argobots/1.2                ginkgo/1.11.0-openmp        libquo/1.4.1              parallel-netcdf/1.14.1      swig/4.0.2-fortran
ascent/0.9.5-openmp         globalarrays/5.8.2          libunwind/1.7.2           parsec/4.0.2411             sz/2.1.12.5
bolt/2.0                    glvis/4.4                   loki/0.1.7                pdt/3.25.2                  sz3/3.2.0
boost/1.90.0                gmp/6.3.0                   mercury/2.4.1             petsc/3.26.0                tasmanian/8.1
bricks/2023.08.25           gotcha/1.0.8                metall/0.30               phist/1.12.1-openmp         tau/2.36
butterflypack/4.1.0-openmp  h5bench/1.4                 mfem/4.10.0               plasma/24.8.7               trilinos/14.4.0
cabana/0.8.0                hdf5-vol-async/1.7          mgard/1.6.0-openmp        plumed/2.10.1               turbine/1.3.0
caliper/2.15.0              hdf5-vol-cache/v1.1         mpark-variant/1.4.0       pruners-ninja/1.0.2         umap/2.1.1
conduit/0.9.8               hdf5-vol-log/1.4.0          mpich/5.0.1               pumi/2.2.9                  unifyfs/2.0
darshan-runtime/3.5.0       hdf5/1.14.6                 mpifileutils/0.12         py-h5py/3.16.0              upcxx/2025.10.0
darshan-util/3.5.0          heffte/2.4.1                nccmp/1.11.0.0            py-jupyterhub/1.4.1         veloc/1.7
datatransferkit/3.1.1       hpx/1.11.0                  nco/5.4.1-openmp          py-libensemble/1.6.1        vtk-m/2.3.0-openmp
diy/3.6.0                   hypre/3.2.0                 nek5000/19.0              py-petsc4py/3.26.0          wannier90/4.0.2
dyninst/13.0.0-openmp       kokkos-kernels/4.7.04-openmp nekbone/17.0             qthreads/1.18               wps/4.6.0
e4s-alc/1.0.3               kokkos/4.7.04-openmp        netcdf-fortran/4.6.4      quantum-espresso/7.6-openmp wrf/4.7.1
e4s-cl/1.0.9                laghos/3.1                  netlib-scalapack/2.2.3    rempi/1.1.0                 zfp/1.0.1
faodel/1.2108.1             lammps/20250722.6-openmp    nwchem/7.3.1              scr/3.1.0

Key:
loaded  modulepath
Singularity>
```

E4S 26.11 ppc64le GPU Ubuntu image

```
Singularity> lscpu | grep name
Model name:                          POWER9, altivec supported
Singularity> uname -m
ppc64le
Singularity> spack find
-- linux-ubuntu20.04-ppc64le / %c,cxx,fortran=gcc@9.4.0 ---------
adiak@0.5.0    arpack-ng@3.9.1      heffte@2.4.1     papi@7.2.0    slepc@3.26.0     superlu-dist@9.2.1  zfp@0.5.5
adios2@2.12.1  butterflypack@4.1.0  magma@2.10.0     petsc@3.26.0  strumpack@8.1.0  superlu-dist@9.2.1  zfp@1.0.1
amrex@25.05    conduit@0.9.8        openblas@0.3.34  petsc@3.26.0  sundials@7.9.0   tau@2.36            zfp@1.0.1

-- linux-ubuntu20.04-ppc64le / %c,cxx=gcc@9.4.0 -----------------
asio@1.32.0        dyninst@13.0.0   hwloc@2.13.0       libpng@1.6.58        nvcomp@2.2.0          python@3.14.5             yaml-cpp@0.9.0
binutils@2.47      eigen@3.4.1      icu4c@76.1         libunwind@1.7.2      omega-h@11.2.0-scorec snappy@1.2.1              yaml-cpp@0.9.0
boost@1.86.0       elfutils@0.194   intel-tbb@2022.3.0 libzmq@4.3.5         opencl-clhpp@2.0.16   spiral-package-fftx@1.3.0 zlib-ng@2.3.3
boost@1.86.0       expat@2.9.0      jansson@2.14       lz4@1.10.0           openssl@3.6.1         spiral-software@8.6.0     zlib-ng@2.3.3
bricks@2023.08.25  fftx@1.2.0       lammps@20250722.6  metis@5.1.0          openssl@3.6.1         sz@2.1.12.5               zstd@1.5.7
cabana@0.8.0       gasnet@2025.8.0  libarchive@3.8.5   metis@5.1.0          parmetis@4.0.3        sz3@3.2.0
caliper@2.15.0     gettext@1.0      libcatalyst@2.1.0  mgard@1.6.0          parmetis@4.0.3        upcxx@2025.10.0
cmake@3.31.12      ginkgo@1.11.0    libdwarf@2.3.0     ncurses@6.6          pdt@3.25.2            voropp@0.4.6
curl@8.22.0        gperftools@2.15  libffi@3.5.2       nghttp2@1.67.1       protobuf@21.12        vtk-m@2.3.0
curl@8.22.0        hwloc@2.13.0     libiberty@2.46.0   nlohmann-json@3.12.0 pugixml@1.15          xrootd@5.9.6

-- linux-ubuntu20.04-ppc64le / %c,fortran=gcc@9.4.0 -------------
fftw@3.3.11  hdf5@1.8.23  hdf5@1.14.6  hypre@3.2.0  netlib-scalapack@2.2.3

-- linux-ubuntu20.04-ppc64le / %c=gcc@9.4.0 ----------------------
bzip2@1.0.8       gsl@2.8          libiconv@1.18      libxcrypt@4.5.2  lua@5.4.8          pkgconf@2.5.1     sqlite@3.53.1
c-blosc2@2.15.1   hypre@3.2.0      libmd@1.1.0        libxml2@2.15.3   lua-luaposix@36.3  py-cffi@2.1.1     tar@1.35
flux-core@0.89.0  isa-l@2.32.1     libpciaccess@0.17  libxml2@2.15.3   lzo@2.10           py-pycparser@3.0  unzip@6.0
gdbm@1.26         libbsd@0.12.2    libsodium@1.0.22   libyaml@0.2.5    parsec@4.0.2411    py-pyyaml@6.0.3   util-linux-uuid@2.41
gmake@4.4.1       libfabric@2.7.0  libxcrypt@4.5.2    lizard@2.1       pigz@2.8           readline@8.3      xz@5.8.3

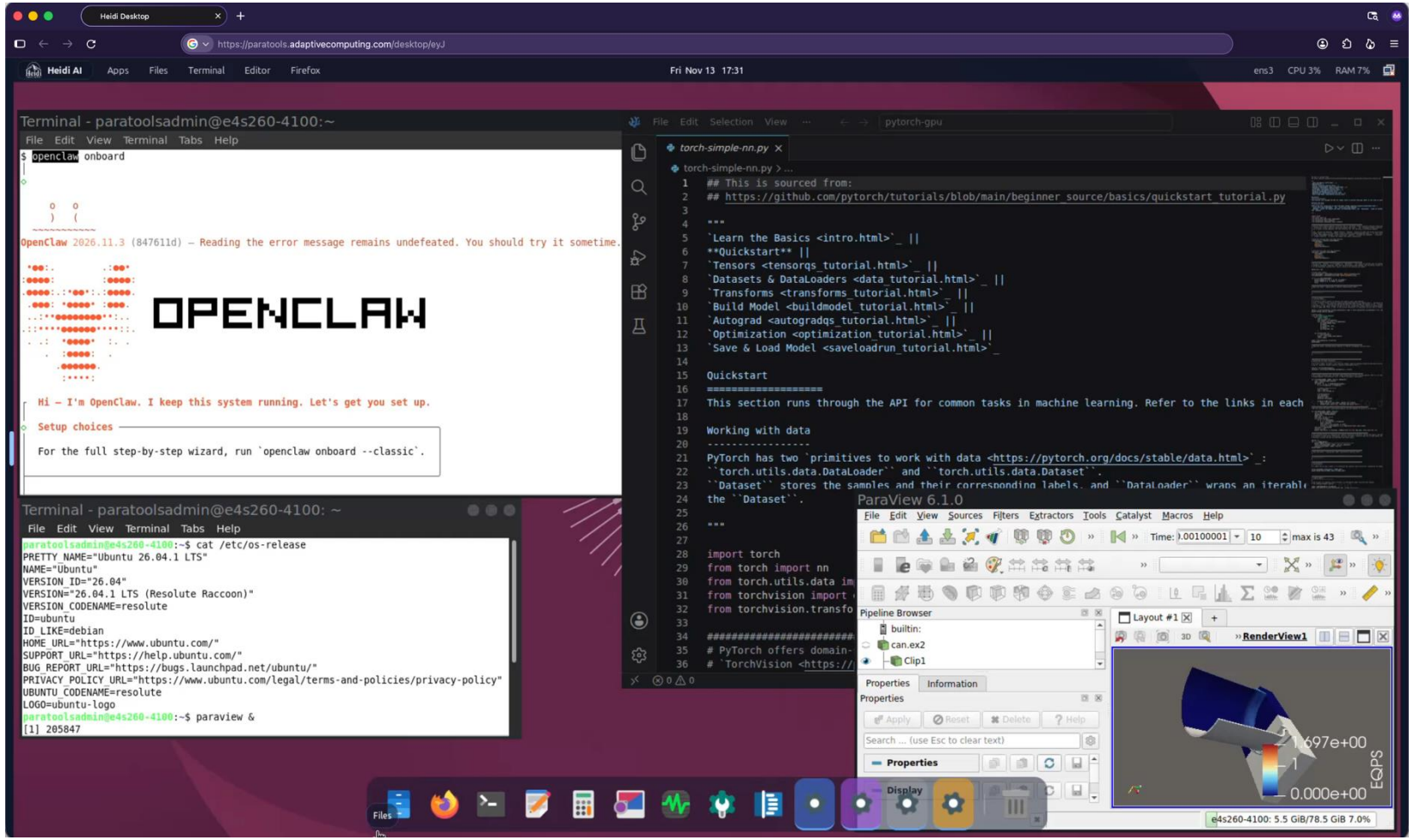
-- linux-ubuntu20.04-ppc64le / %cxx,fortran=gcc@9.4.0 -----------
tasmanian@8.1

-- linux-ubuntu20.04-ppc64le / %cxx=gcc@9.4.0 -------------------
hpx@1.11.0  kokkos@4.6.02  kokkos@4.7.04  kokkos@4.7.04  kokkos-kernels@4.7.04  kokkos-nvcc-wrapper@5.2.2  mfem@4.10.0

-- linux-ubuntu20.04-ppc64le / no compilers ----------------------
cuda@11.4.4  gcc@9.4.0          glibc@2.31   openjdk@17.0.4.1_1  py-ply@3.11           python-venv@1.0          spiral-package-mpi@1.1.0
cuda@11.4.4  gcc-runtime@9.4.0  mpich@5.0.1  py-packaging@26.2   py-setuptools@83.0.0  spiral-package-jit@1.1.0  spiral-package-simt@1.1.0
==> 148 installed packages
Singularity> nvidia-smi -L
GPU 0: Tesla V100-SXM2-32GB (UUID: GPU-764f3003-0721-0d82-6732-1c74c2d344d5)
GPU 1: Tesla V100-SXM2-32GB (UUID: GPU-2745d3bf-1037-2f3f-59c3-844427393b75)
GPU 2: Tesla V100-SXM2-32GB (UUID: GPU-b4f479d1-480f-a425-ebee-175d6064117e)
GPU 3: Tesla V100-SXM2-32GB (UUID: GPU-e7ad0bf6-5183-5cc0-1024-e1430abb65a1)
Singularity>
```

PESO

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



Adaptive Computing's Heidi AI web-based platform for multi-user, multi-node, ParaTools Pro for E4S™ image with Ubuntu 26.04 LTS and Rocky Linux 9.8 images on AWS, Microsoft Azure, Google Cloud, OCI, and IBM Cloud.

https://adaptivecomputing.com/ and https://paratoolspro.com

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