

E4S: The Extreme-scale Scientific Software Stack Release 26.06

Release 26.06 notes

June 22, 2026



HPSF

HIGH PERFORMANCE
SOFTWARE FOUNDATION

High Performance Software Foundation

E4S Team

<https://e4s.io>



U.S. DEPARTMENT OF
ENERGY

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Science

E4S 26.06: What's New?



- 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, DeaIII, 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



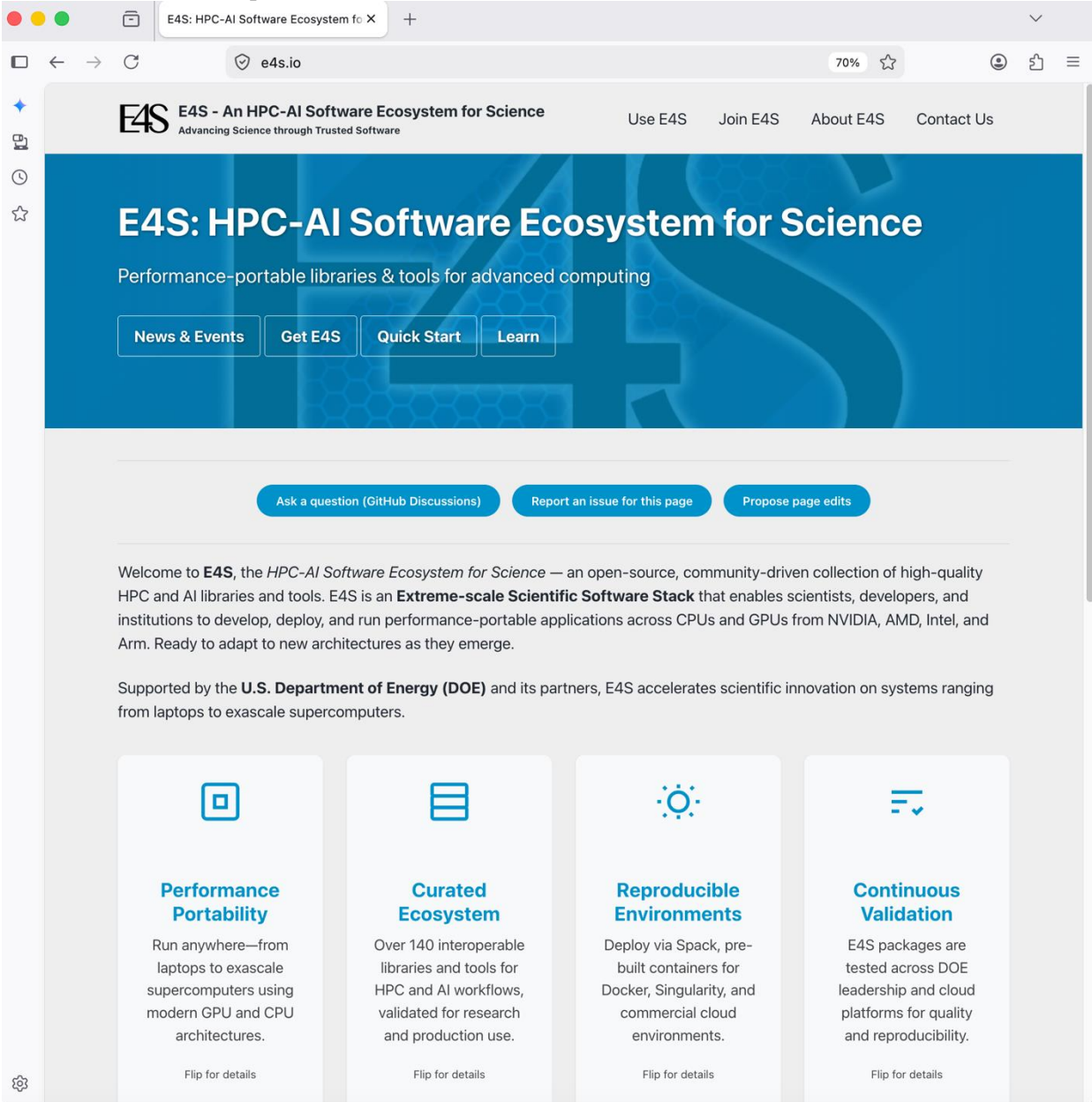
<https://e4s.io>

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



Updated E4S website <https://e4s.io>



The screenshot shows the E4S website homepage. At the top, there is a navigation bar with the E4S logo and the text "E4S - An HPC-AI Software Ecosystem for Science" and "Advancing Science through Trusted Software". To the right of the logo are links for "Use E4S", "Join E4S", "About E4S", and "Contact Us". Below the navigation bar is a large blue banner with the title "E4S: HPC-AI Software Ecosystem for Science" and the subtitle "Performance-portable libraries & tools for advanced computing". Underneath the banner are four buttons: "News & Events", "Get E4S", "Quick Start", and "Learn". Below the banner are three buttons: "Ask a question (GitHub Discussions)", "Report an issue for this page", and "Propose page edits". The main content area starts with a paragraph: "Welcome to **E4S**, the *HPC-AI Software Ecosystem for Science* — an open-source, community-driven collection of high-quality HPC and AI libraries and tools. E4S is an **Extreme-scale Scientific Software Stack** that enables scientists, developers, and institutions to develop, deploy, and run performance-portable applications across CPUs and GPUs from NVIDIA, AMD, Intel, and Arm. Ready to adapt to new architectures as they emerge." Below this is another paragraph: "Supported by the **U.S. Department of Energy (DOE)** and its partners, E4S accelerates scientific innovation on systems ranging from laptops to exascale supercomputers." At the bottom, there are four feature cards: "Performance Portability" (Run anywhere—from laptops to exascale supercomputers using modern GPU and CPU architectures.), "Curated Ecosystem" (Over 140 interoperable libraries and tools for HPC and AI workflows, validated for research and production use.), "Reproducible Environments" (Deploy via Spack, pre-built containers for Docker, Singularity, and commercial cloud environments.), and "Continuous Validation" (E4S packages are tested across DOE leadership and cloud platforms for quality and reproducibility.). Each card has a "Flip for details" link at the bottom.

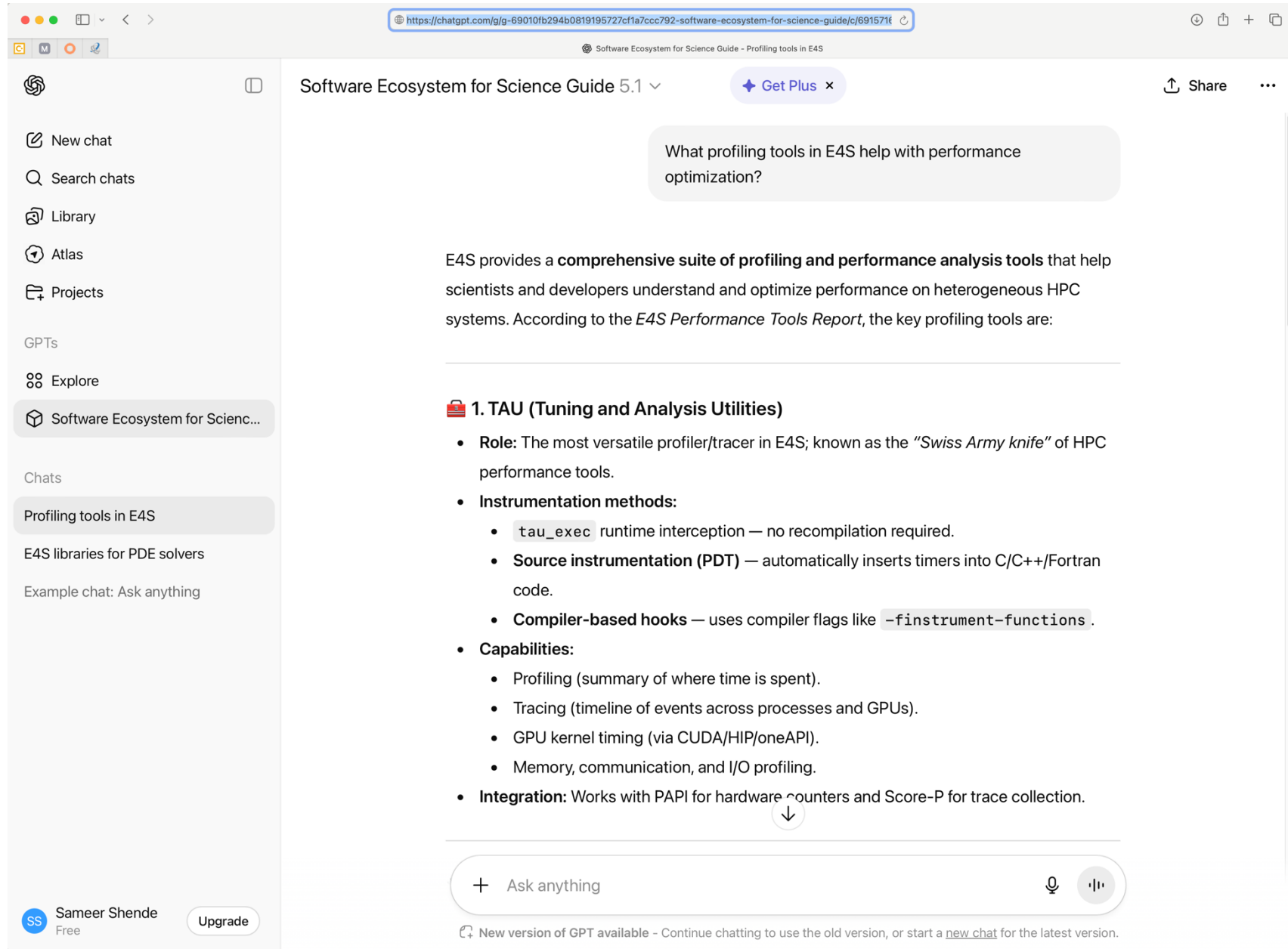


Chatbot integration in E4S Website

The screenshot shows a web browser window with the URL `https://chatgpt.com/g/g-69010fb294b0819195727cf1a7ccc792-software-ecosystem-for-science-guide`. The page title is "Software Ecosystem for Science Guide 5.1" with a "Get Plus" button. The left sidebar contains navigation options: "New chat", "Search chats", "Library", "Atlas", "Projects", "GPTs", "Explore", and "Software Ecosystem for Scienc...". Under "Chats", there are entries for "Profiling tools in E4S", "E4S libraries for PDE solvers", and "Example chat: Ask anything". The main content area features a cube icon, the title "Software Ecosystem for Science Guide", the author "By Michael Heroux", and a description: "Expert on scientific libraries and tools in the E4S (Ecosystem for Science) ecosystem." Below this are four question cards: "Which E4S libraries should I use for parallel PDE...", "How do I install and configure PETSc with Spack?", "Can you explain how Kokkos interacts with Trilinos?", and "What profiling tools in E4S help with performance...". At the bottom, there is a text input field with a plus sign and the text "Ask anything", a microphone icon, and a voice icon. The bottom left corner of the interface shows the user "Sameer Shende" with a "Free" status and an "Upgrade" button.



E4S Bot trained on E4S content on OpenAI's ChatGPT



The screenshot shows a web browser window with the URL <https://chatgpt.com/g/g-69010fb294b081919572cf1a7ccc792-software-ecosystem-for-science-guide/c/691571f>. The page title is "Software Ecosystem for Science Guide 5.1". The chat history on the left includes "New chat", "Search chats", "Library", "Atlas", "Projects", "GPTs", "Explore", and "Software Ecosystem for Scienc...". The current chat is titled "Profiling tools in E4S".

The user's question is: "What profiling tools in E4S help with performance optimization?"

The AI's response is:

E4S provides a **comprehensive suite of profiling and performance analysis tools** that help scientists and developers understand and optimize performance on heterogeneous HPC systems. According to the *E4S Performance Tools Report*, the key profiling tools are:

1. TAU (Tuning and Analysis Utilities)

- **Role:** The most versatile profiler/tracer in E4S; known as the "Swiss Army knife" of HPC performance tools.
- **Instrumentation methods:**
 - `tau_exec` runtime interception — no recompilation required.
 - **Source instrumentation (PDT)** — automatically inserts timers into C/C++/Fortran code.
 - **Compiler-based hooks** — uses compiler flags like `-finstrument-functions`.
- **Capabilities:**
 - Profiling (summary of where time is spent).
 - Tracing (timeline of events across processes and GPUs).
 - GPU kernel timing (via CUDA/HIP/oneAPI).
 - Memory, communication, and I/O profiling.
- **Integration:** Works with PAPI for hardware counters and Score-P for trace collection.

At the bottom of the chat, there is a text input field with the placeholder "Ask anything" and a microphone icon. A small downward arrow icon is visible below the "Integration" bullet point.

At the bottom left, there is a logo for "Sameer Shende Free" with an "Upgrade" button. At the bottom right, there is a note: "New version of GPT available - Continue chatting to use the old version, or start a [new chat](#) for the latest version."

E4S Documentation

E4S - An HPC-AI Software Ecosystem for Science
Advancing Science through Trusted Software

Use E4S | Join E4S | About E4S | Contact Us

ABOUT E4S

- Overview
- E4S Introduction
- E4S Learning
- First-Time Users
- E4S Product Families
- E4S Containers
- E4S FAQs
- AI and the E4S Website
- News & Events

About E4S

[Ask a question \(GitHub Discussions\)](#) | [Report an issue for this page](#) | [Propose page edits](#)

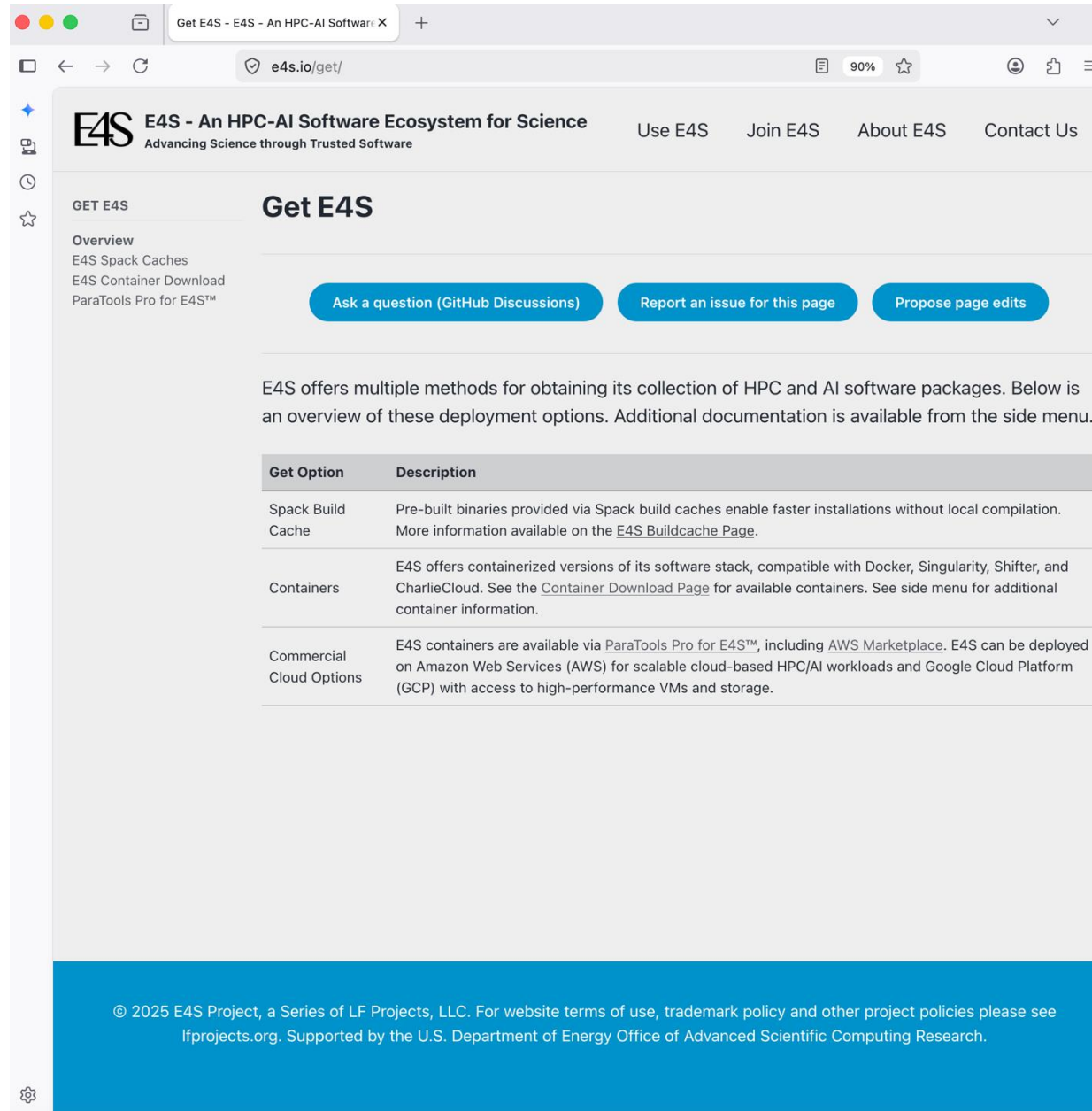
E4S provides a curated collection of scientific libraries and tools supporting scientific discovery through advanced computing technologies. The primary value E4S provides is bringing together a large collection of independently developed libraries and tools and enhancing the overall enterprise of developing and using them in aggregate. This portion of the E4S website focuses on topics that help understand what E4S is, how to contribute to it, and how it can be used.

Topic	Description
Overview - About E4S	High-level summary of the E4S project, mission, scope, and target audiences.
E4S Introduction	Short primer on E4S goals, components, and how it supports HPC-AI scientific workflows.
E4S First-Time Users	Quickstart guidance for new users: getting started, basic concepts, and common workflows.
E4S Product Families	Catalog and explanation of E4S product groups (programming systems, libraries, tools, etc.).
E4S FAQs	Frequently asked questions covering usage, licensing, support, and common troubleshooting.
E4S News & Events	Announcements, release notes, and upcoming events related to E4S.

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



The screenshot shows a web browser window displaying the E4S website. The browser's address bar shows 'e4s.io/get/'. The website header includes the E4S logo and the tagline 'E4S - An HPC-AI Software Ecosystem for Science' with the subtitle 'Advancing Science through Trusted Software'. Navigation links for 'Use E4S', 'Join E4S', 'About E4S', and 'Contact Us' are present. The main content area is titled 'Get E4S' and features three buttons: 'Ask a question (GitHub Discussions)', 'Report an issue for this page', and 'Propose page edits'. Below these buttons, a paragraph states: 'E4S offers multiple methods for obtaining its collection of HPC and AI software packages. Below is an overview of these deployment options. Additional documentation is available from the side menu.' A table follows, detailing the deployment options:

Get Option	Description
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.

At the bottom of the page, a blue footer contains the copyright notice: '© 2025 E4S Project, a Series of LF Projects, LLC. For website terms of use, trademark policy and other project policies please see [lfprojects.org](#). Supported by the U.S. Department of Energy Office of Advanced Scientific Computing Research.'

Download E4S Containers: Rocky Linux 9.7 and Ubuntu 24.04 LTS

E4S E4S - An HPC-AI Software Ecosystem for Science
Advancing Science through Trusted Software

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GET E4S

Overview
E4S Spack Caches
E4S Container Download
ParaTools Pro for E4S™

E4S Container Download

Ask a question (GitHub Discussions) Report an issue for this page Propose page edits

Acquiring E4S Containers

The current E4S container offerings include Docker and Singularity images capable of running on X86_64, PPC64LE, and AARCH64 architectures. Our full E4S Release images are based on Ubuntu 24.04 and Rocky 9 (x86_64, aarch64, ppc64le). In addition to offering a full E4S image containing a comprehensive selection of E4S software released on a bi-annual cycle, we also offer a set of minimal base images suitable for use in Continuous Integration (CI) pipelines where Spack is used to build packages.

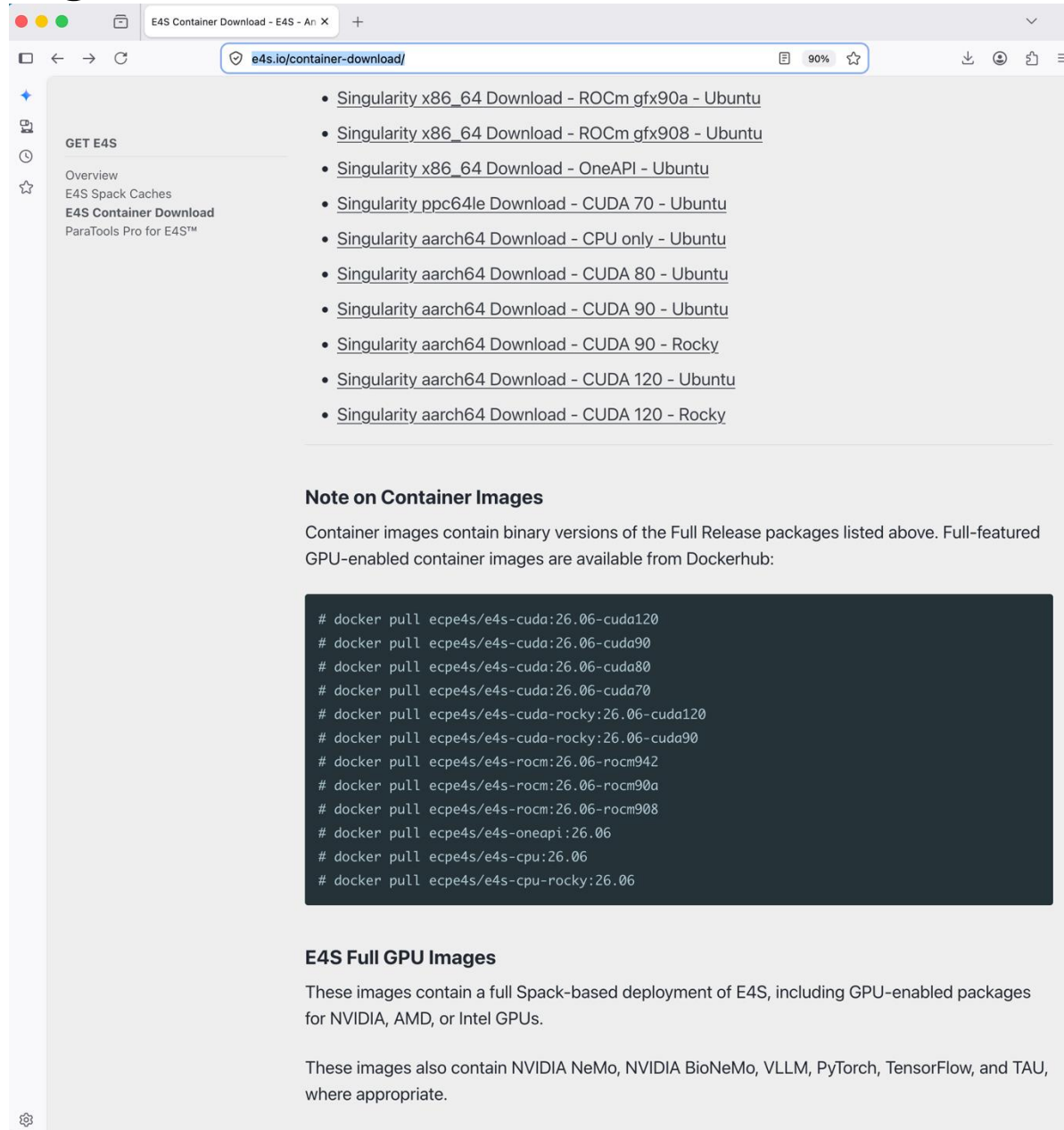
Docker images are available on the [E4S Docker Hub](#). Please see the [E4S 26.06 Release Notes](#).

Container Releases

- [Docker Downloads - Minimal](#)
- [Docker Downloads - CPU only - Ubuntu](#)
- [Docker Downloads - CPU only - Rocky](#)
- [Docker Downloads - CUDA - Ubuntu](#)
- [Docker Downloads - CUDA - Rocky](#)
- [Docker Downloads - ROCm](#)
- [Docker Downloads - OneAPI](#)
- [Singularity x86_64 Download - Minimal](#)
- [Singularity x86_64 Download - CPU only - Ubuntu](#)
- [Singularity x86_64 Download - CPU only - Rocky](#)
- [Singularity x86_64 Download - CUDA 80 - Ubuntu](#)
- [Singularity x86_64 Download - CUDA 90 - Ubuntu](#)
- [Singularity x86_64 Download - CUDA 90 - Rocky](#)
- [Singularity x86_64 Download - CUDA 120 - Ubuntu](#)
- [Singularity x86_64 Download - CUDA 120 - Rocky](#)

- 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

E4S container images available on DockerHub



The screenshot shows a web browser window with the URL e4s.io/container-download/. The page is titled "E4S Container Download" and features a sidebar with navigation links: "GET E4S", "Overview", "E4S Spack Caches", "E4S Container Download", and "ParaTools Pro for E4S™". The main content area lists ten download links for Singularity containers, categorized by architecture (x86_64 and aarch64) and GPU/CUDA configuration (ROCm, CUDA, CPU only, and Rocky Linux).

- [Singularity x86_64 Download - ROCm gfx90a - Ubuntu](#)
- [Singularity x86_64 Download - ROCm gfx908 - Ubuntu](#)
- [Singularity x86_64 Download - OneAPI - Ubuntu](#)
- [Singularity ppc64le Download - CUDA 70 - Ubuntu](#)
- [Singularity aarch64 Download - CPU only - Ubuntu](#)
- [Singularity aarch64 Download - CUDA 80 - Ubuntu](#)
- [Singularity aarch64 Download - CUDA 90 - Ubuntu](#)
- [Singularity aarch64 Download - CUDA 90 - Rocky](#)
- [Singularity aarch64 Download - CUDA 120 - Ubuntu](#)
- [Singularity aarch64 Download - CUDA 120 - Rocky](#)

Note on Container Images

Container images contain binary versions of the Full Release packages listed above. Full-featured GPU-enabled container images are available from Dockerhub:

```
# docker pull ecpe4s/e4s-cuda:26.06-cuda120
# docker pull ecpe4s/e4s-cuda:26.06-cuda90
# docker pull ecpe4s/e4s-cuda:26.06-cuda80
# docker pull ecpe4s/e4s-cuda:26.06-cuda70
# docker pull ecpe4s/e4s-cuda-rocky:26.06-cuda120
# docker pull ecpe4s/e4s-cuda-rocky:26.06-cuda90
# docker pull ecpe4s/e4s-rocm:26.06-rocm942
# docker pull ecpe4s/e4s-rocm:26.06-rocm90a
# docker pull ecpe4s/e4s-rocm:26.06-rocm908
# docker pull ecpe4s/e4s-oneapi:26.06
# docker pull ecpe4s/e4s-cpu:26.06
# docker pull ecpe4s/e4s-cpu-rocky:26.06
```

E4S Full GPU Images

These images contain a full Spack-based deployment of E4S, including GPU-enabled packages for NVIDIA, AMD, or Intel GPUs.

These images also contain NVIDIA NeMo, NVIDIA BioNeMo, VLLM, PyTorch, TensorFlow, and TAU, where appropriate.

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    lammers@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
```

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 -----
adios@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  libcatylist@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  libnm@0.1.0

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

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

-- linux-ubuntu24.04-x86_64_v3 / %c,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   mpiutils@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 / %c,cxx,fortran=gcc@9.4.0 -----
fortrilinos@2.3.0  tasmanian@8.1

-- linux-ubuntu20.04-ppc64le / %c,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  lammmps@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

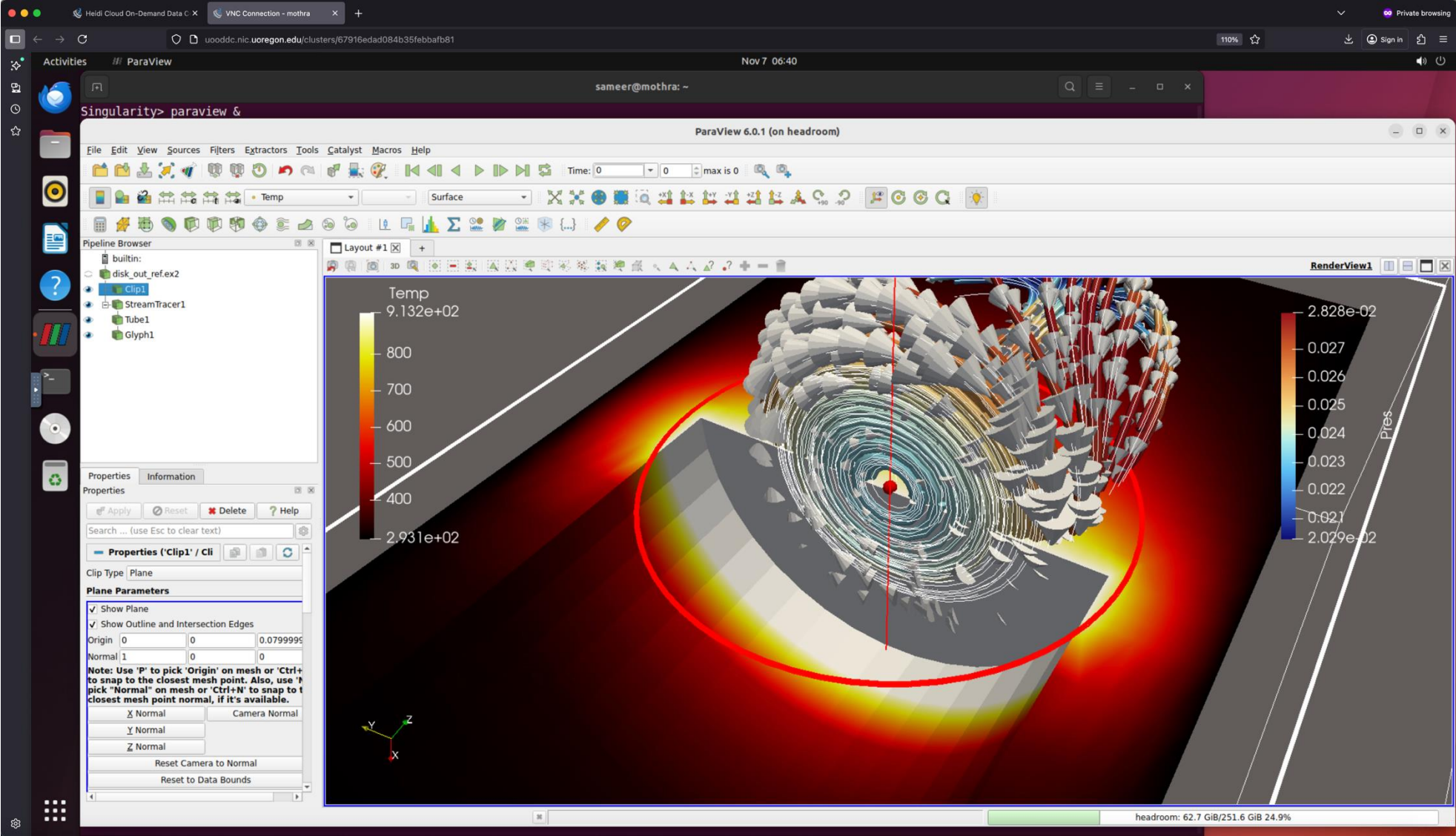
-- linux-ubuntu20.04-ppc64le / %c=gcc@9.4.0 -----
flux-core@0.81.0  parsec@4.0.2411

-- 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

The screenshot shows a terminal window on the left and a web browser window on the right. The terminal window displays the following commands and output:

```
Singularity> sycl-ls
[level_zero:gpu][level_zero:0] Intel(R) oneAPI Unified Runtime over Level-Zero, Intel(R) Data Center GPU Max 1100 12.60.7 [1.6.35096+9]
[opencl:cpu][opencl:0] Intel(R) OpenCL, Intel(R) Xeon(R) Silver 4410T OpenCL 3.0 (Build 0) [2025.20.8.0.06 160000]
[opencl:gpu][opencl:1] Intel(R) OpenCL Graphics, Intel(R) Data Center GPU Max 1100 OpenCL 3.0 NEO [25.35.35096.9]
Singularity> which adk
/opt/python/pkgs/python-3.12.11/bin/adk
Singularity> which marimo
/opt/python/pkgs/python-3.12.11/bin/marimo
Singularity> marimo new
```

The web browser window shows a Marimo notebook titled "Untitled Notebook" running on `http://localhost:2718`. The notebook code is as follows:

```
1 import marimo as mo
2 import plotly.graph_objects as go
3 import numpy as np
4
5 # Generate 3D surface data
6 x = np.linspace(-5, 5, 100)
7 y = np.linspace(-5, 5, 100)
8 x, y = np.meshgrid(x, y)
9 z = np.sin(np.sqrt(x**2 + y**2))
10
11 # Create a Plotly 3D surface plot
12 fig = go.Figure(
13     data=[go.Surface(z=z, x=x, y=y, colorscale='Viridis')]
14 )
15 fig.update_layout(title="3D Surface Example")
16
17 # Display the 3D plot in Marimo
18 mo.ui.plotly(fig)
```

The notebook output displays a 3D surface plot titled "3D Surface Example". The plot shows a bell-shaped surface with a color scale ranging from 0 to 1. The x and y axes range from -5 to 5, and the z axis ranges from -2 to 1. A color bar on the right indicates the mapping from z values to colors, with 0 being dark purple and 1 being bright yellow.



E4S: VisIt

Heidi Cloud On-Demand Data C X VNC Connection - motra x + Private browsing

uobddc.nic.uoregon.edu/clusters/67916edad084b35febbafb81

Activities gui

```
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 127.0.0.1
```

Nov 7 06:35

Window 1 (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

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)

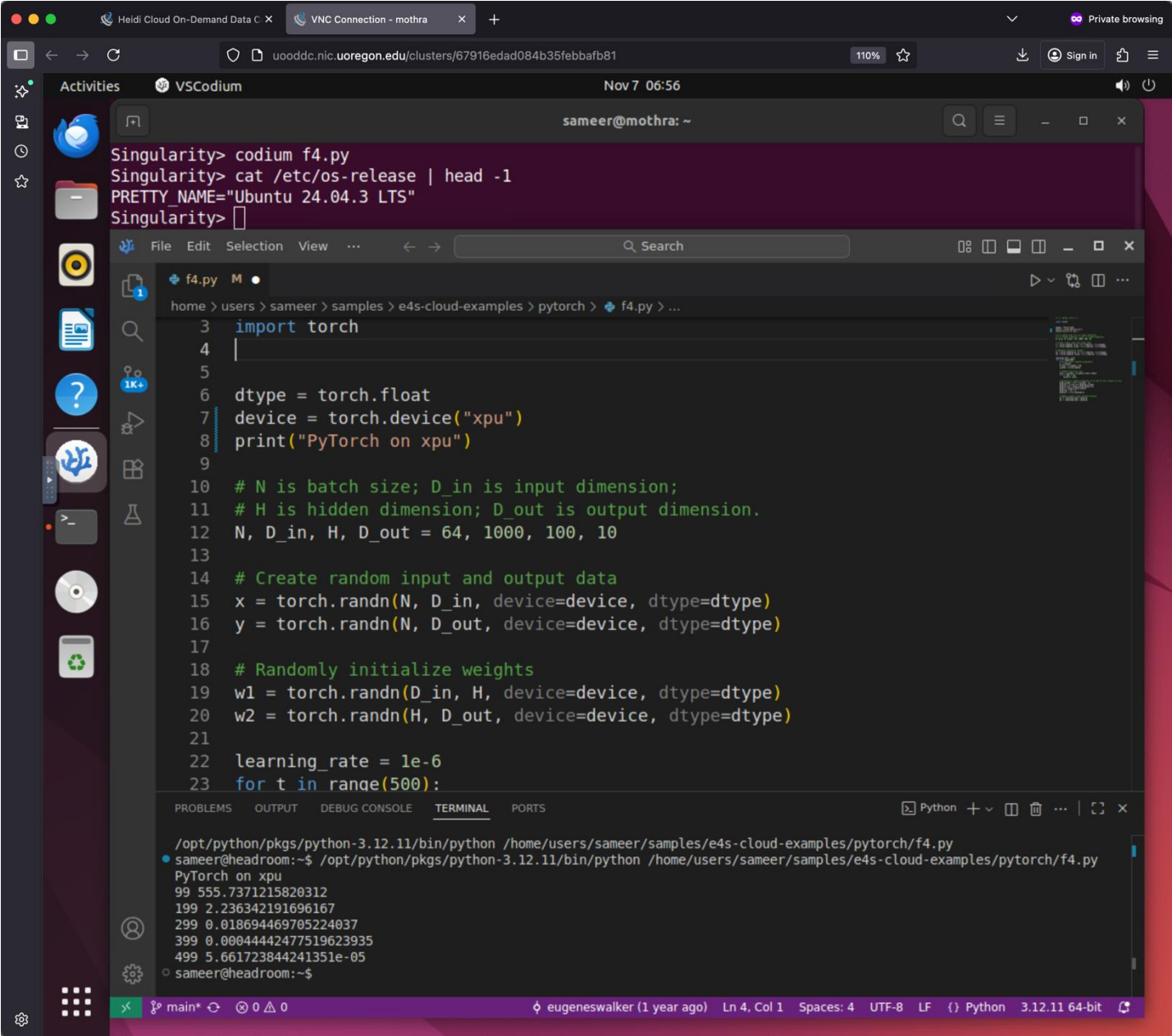
Width (parsec)

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

The screenshot displays the VS Code interface with a Jupyter Notebook open. The notebook title is "Zero-shot prediction of BRCA1 variant effects with Evo 2". The content includes a "Deploy this tutorial on brev.dev:" button, a note about the notebook being a reproduction of The Arc Institute's work, and a description of Evo2 as a foundation AI model trained on 9.3 trillion DNA base pairs. It also discusses the human BRCA1 gene and its association with cancer risk. The notebook contains two code cells:

```
%%capture
import os

# Runs a subset of the model layers to test that the notebook runs in CI, but the output will be incorrect.
FAST_CI_MODE = bool = os.environ.get("FAST_CI_MODE", False)
[1] ✓ 0.0s Python
```

```
import glob
import gzip
import json
import math
import os
from pathlib import Path

import matplotlib.pyplot as plt
import pandas as pd
import seaborn as sns
import torch
from Bio import SeqIO
from sklearn.metrics import auc, roc_auc_score, roc_curve
[2] ✓ 2.3s Python
```

The notebook also includes a function definition for downloading data:

```
def download_data(data_dir="brca1", commit_hash="3819474bee6c24938016614411f1fa025e542bbe"):
    """Download required data files if they don't exist locally.

    Parameters:
    -----
    data_dir : str
        Directory to store downloaded files
    commit_hash : str
        GitHub commit hash for data version
    """
```

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

The screenshot shows a Linux desktop environment with a terminal window and a ParaView 5.13.3 application window.

Terminal Output:

```
paratoolsadmin@e4s-ibm:~$ glxinfo | grep NVIDIA
client glx vendor string: NVIDIA Corporation
OpenGL vendor string: NVIDIA Corporation
OpenGL renderer string: NVIDIA L4/PCIe/SSE2
OpenGL core profile version string: 4.6.0 NVIDIA 570.195.03
OpenGL core profile shading language version string: 4.60 NVIDIA
OpenGL version string: 4.6.0 NVIDIA 570.195.03
OpenGL shading language version string: 4.60 NVIDIA
OpenGL ES profile version string: OpenGL ES 3.2 NVIDIA
paratoolsadmin@e4s-ibm:~$ which paraview
/usr/local/paraview-5.13.3/bin/paraview
paratoolsadmin@e4s-ibm:~$ paraview &
paratoolsadmin@e4s-ibm:~$ glxgears &
[2] 57076
paratoolsadmin@e4s-ibm:~$ Running synchronized to
approximately the same as the monitor refresh rate
28913 frames in 5.0 seconds = 5782.519 FPS
25233 frames in 5.0 seconds = 5046.367 FPS
25470 frames in 5.0 seconds = 5093.550 FPS
24694 frames in 5.0 seconds = 4938.712 FPS
26629 frames in 5.0 seconds = 5325.770 FPS
31803 frames in 5.0 seconds = 6360.508 FPS
22320 frames in 5.0 seconds = 4464.000 FPS
22320 frames in 5.0 seconds = 4464.000 FPS
```

ParaView 5.13.3 Interface:

- Pipeline Browser:** Shows a pipeline with objects: Clip1, StreamTracer1, Tube1, and Glyph1.
- RenderView1:** Displays a 3D visualization of a complex structure, possibly a turbine or engine component, with a color scale ranging from 2.029e to 9.132e.
- Properties Panel:** Shows properties for the selected object (disk_out), including variables like Object Ids, Global Element Ids, Global Node Ids, AqH3, Ch4, GaMe3, H2, Pres, Temp, and V. It also includes options for Apply Displacements, Element Blocks, and Face Blocks.



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Science

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

