

E4S: The Extreme-scale Scientific Software Stack Release 24.02

Release 24.02 notes
February 14, 2024



U.S. DEPARTMENT OF
ENERGY

Office of
Science

E4S 24.11: What's New?

- E4S includes 122+ HPC packages on ARM, x86_64, and ppc64le platforms, 123K+ binaries in E4S Spack Build Cache
- E4S includes a comprehensive suite of AI/ML packages including TorchBraid, OpenAI, Pandas, Scikit-Learn, along with previously supported JAX, PyTorch, TensorFlow, Horovod, OpenCV, and LBANN. Updated Python tools including Seaborn, Plotly, and Jupyter notebook.
- VSCodium (MIT License) Integrated Development Environment GUI.
- E4S includes new applications: GROMACS and CP2K and previously supported Xyce, Quantum Espresso, ExaGo, LAMMPS, WARPX, Dealii, and OpenFOAM.
- E4S includes support for Intel oneAPI 2024.0.2 software (BaseKit and HPCToolkit) in containers on x86_64 with support for HPC packages built with Intel compilers and Intel MPI with support for Intel Data Center GPU Max 1000 series (aka PVC).
- New tool e4s-chain-spack.sh to chain two Spack instances allowing a user to install new packages in home directory while using prebuilt E4S packages.
 - `. /etc/e4s/e4s-chain-spack.sh $HOME/tmp/spack ; spack install valgrind`
- Support for new platforms: NVIDIA Grace-Grace and Grace-Hopper (GH200)
- E4S includes support for CUDA architectures
 - 80 (A100), and 90 (H100) under x86_64
 - 70 under ppc64le (IBM Power 10)
 - 75, 80, and 90 (GH200) under aarch64
- Adaptive Computing's ODDC platform for multi-node E4S images on AWS, GCP, OCI, and Azure with support for VNC based remote desktop:
 - <https://adaptivecomputing.com/cherry-services/adaptive-ai-as-a-service/>

E4S: Extreme-scale Scientific Software Stack

- E4S is a community effort to provide open-source software packages for developing, deploying and running scientific applications on HPC platforms.
- E4S has built a comprehensive, coherent software stack that enables application developers to productively develop highly parallel applications that effectively target diverse exascale architectures.
- E4S provides a curated, Spack based software distribution of 120+ HPC, EDA (e.g., Xyce), and AI/ML packages (e.g., TorchBraid, Scikit-Learn, Pandas, TensorFlow, PyTorch, JAX, Horovod, and LBANN).
- 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 GPUs from NVIDIA, AMD, and Intel
 - HPC and AI/ML packages are optimized for GPUs and CPUs.
- Container images on DockerHub and E4S website of pre-built binaries of ECP ST products.
- Base images and full featured containers (with GPU support) and DOE LLVM containers.
- Commercial support for E4S through ParaTools, Inc. for installation, maintaining an issue tracker, and ECP AD engagement.
 - <https://dashboard.e4s.io> https://e4s.io/talks/E4S_Support_Dec23.pdf
- E4S for commercial cloud platforms: AWS image supports MPI implementations and containers with remote desktop (DCV).
 - Intel MPI, NVHPC, MVAPICH2, MPICH, MPC, OpenMPI
- e4s-cl container launch tool allows binary distribution of applications by substituting MPI in the containerized app with the system MPI. A-la-carte tool to customize container images: e4s-alc.
- Quarterly releases: E4S 24.02 released on Feb. 14, 2024: https://e4s.io/talks/E4S_24.02.pdf

Extreme-scale Scientific Software Stack (E4S)



- E4S: HPC Software Ecosystem – a curated software portfolio
- A **Spack-based** distribution of software tested for interoperability and portability to multiple architectures with support for GPUs from NVIDIA, AMD, and Intel in each release
- Available from **source, containers, cloud, binary caches**
- Leverages and enhances SDK interoperability thrust
- Not a commercial product – an open resource for all
- Oct 2018: E4S 0.1 - 24 full, 24 partial release products
- Jan 2019: E4S 0.2 - 37 full, 10 partial release products
- Nov 2019: E4S 1.0 - 50 full, 5 partial release products
- Feb 2020: E4S 1.1 - 61 full release products
- Nov 2020: E4S 1.2 (aka, 20.10) - 67 full release products
- Feb 2021: E4S 21.02 - 67 full release, 4 partial release
- May 2021: E4S 21.05 - 76 full release products
- Aug 2021: E4S 21.08 - 88 full release products
- Nov 2021: E4S 21.11 - 91 full release products
- Feb 2022: E4S 22.02 – 100 full release products
- May 2022: E4S 22.05 – 101 full release products
- August 2022: E4S 22.08 – 102 full release products
- November 2022: E4S 22.11 – 103 full release products
- February 2023: E4S 23.02 – 106 full release products
- May 2023: E4S 23.05 – 109 full release products
- Aug 2023: E4S 23.08 – 115 full release products
- Nov 2023: E4S 23.11 – 120 full release products
- Feb 2024: E4S 24.02 – 122 full release products



<https://e4s.io>

Lead: Sameer Shende
(U Oregon)

Also include other products .e.g.,
AI: TorchBraid, Scikit-Learn, JAX, PyTorch,
TensorFlow, Horovod, LBANN
Co-Design: AMReX, Cabana, MFEM
EDA: Xyce



E4S Download from https://e4s.io



E4S 24.02 has been released!

See [Downloads](#) for more information on the latest E4S 24.02 release.

What is E4S?

The Extreme-scale Scientific Software Stack (E4S) is a community effort to provide open source software packages for developing, deploying and running scientific applications on high-performance computing (HPC) platforms. E4S provides from-source builds and containers of a [broad collection of HPC software packages](#).



Purpose

E4S exists to accelerate the development, deployment and use of HPC software, lowering the barriers for HPC users. E4S provides containers and turn-key, from-source builds of more than 80 popular HPC products in programming models, such as MPI; development tools such as HPCToolkit, TAU and PAPI; math libraries such as PETSc and Trilinos; and Data and Viz tools such as HDF5 and Paraview.



Approach

By using Spack as the meta-build tool and providing containers of pre-built binaries for Docker, Singularity, Shifter and CharlieCloud, E4S enables the flexible use and testing of a [large collection of reusable HPC software packages](#).

E4S Container Download from <https://e4s.io>



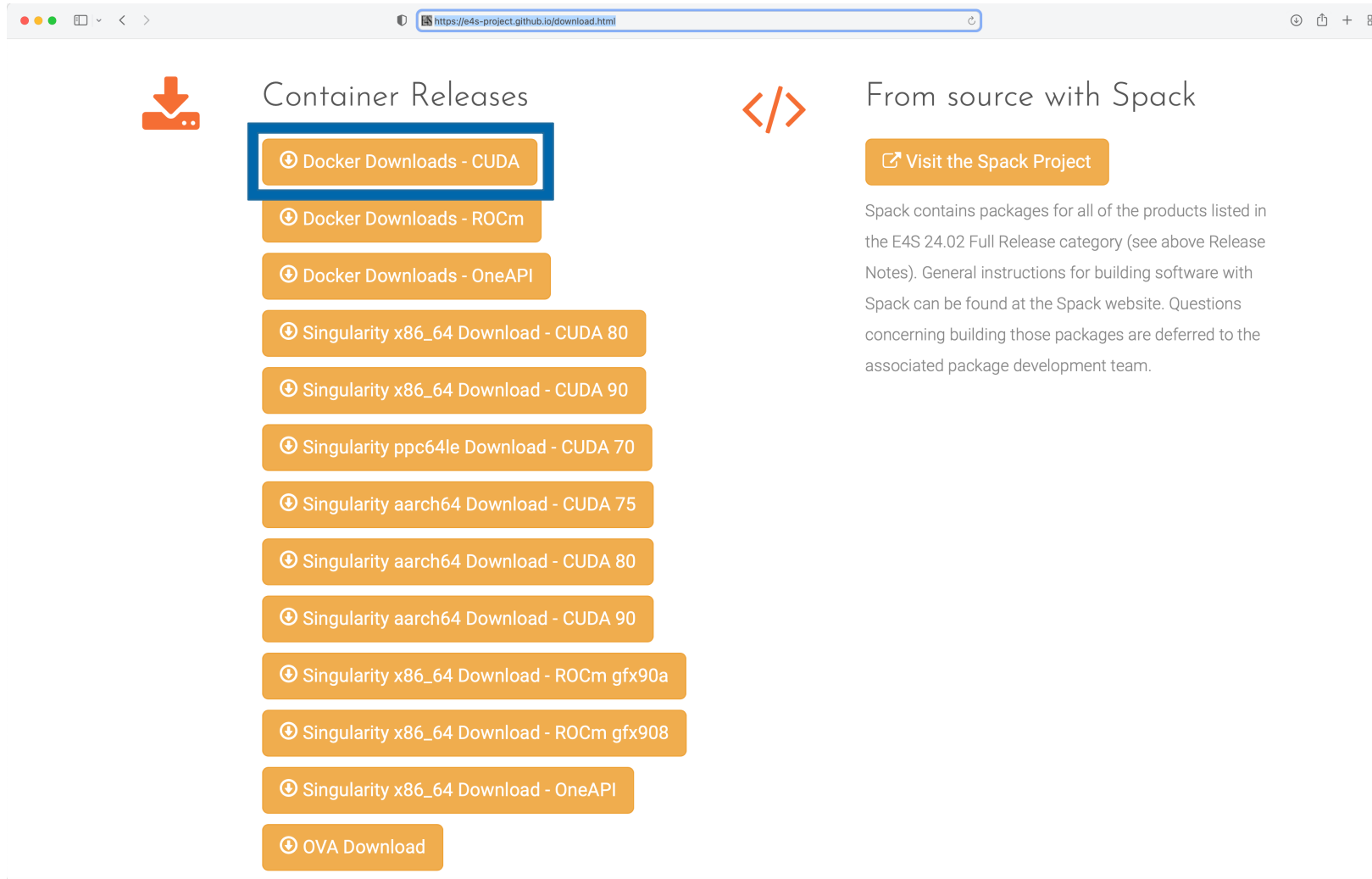
Acquiring E4S Containers

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 20.04 (x86_64, aarch64, ppc64le). In addition to offering a full E4S image containing a comprehensive selection of E4S software released on a quarterly 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 24.02 Release Notes](#).

E4S Container Download from https://e4s.io



Container Releases

- ⌚ Docker Downloads - CUDA
- ⌚ Docker Downloads - ROCm
- ⌚ Docker Downloads - OneAPI
- ⌚ Singularity x86_64 Download - CUDA 80
- ⌚ Singularity x86_64 Download - CUDA 90
- ⌚ Singularity ppc64le Download - CUDA 70
- ⌚ Singularity aarch64 Download - CUDA 75
- ⌚ Singularity aarch64 Download - CUDA 80
- ⌚ Singularity aarch64 Download - CUDA 90
- ⌚ Singularity x86_64 Download - ROCm gfx90a
- ⌚ Singularity x86_64 Download - ROCm gfx908
- ⌚ Singularity x86_64 Download - OneAPI
- ⌚ OVA Download

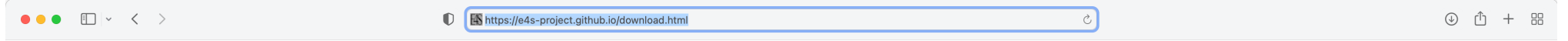
From source with Spack

[Visit the Spack Project](#)

Spack contains packages for all of the products listed in the E4S 24.02 Full Release category (see above Release Notes). General instructions for building software with Spack can be found at the Spack website. Questions concerning building those packages are deferred to the associated package development team.

- Separate full featured Singularity images for 3 GPU architectures
- GPU full featured images for
 - x86_64 (Intel, AMD, NVIDIA)
 - ppc64le (NVIDIA)
 - aarch64 (NVIDIA)
- Full featured images available on Dockerhub
- 122+ products on 3 architectures

Download E4S 24.02 GPU Container Images: AMD, Intel, and NVIDIA



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:24.02
```

```
# docker pull ecpe4s/e4s-rocm:24.02
```

```
# docker pull ecpe4s/e4s-oneapi:24.02
```

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 TensorFlow, PyTorch, and TAU.


AMD ROCm (x86_64)

ecpe4s/e4s-rocm:24.02 

e4s-rocm90a-x86_64-24.02.sif  mirror 1

e4s-rocm908-x86_64-24.02.sif  mirror 1

NVIDIA CUDA (X86_64, PPC64LE, AARCH64)


ecpe4s/e4s-cuda:24.02 

e4s-cuda80-x86_64-24.02.sif  mirror 1

e4s-cuda90-x86_64-24.02.sif  mirror 1

e4s-cuda70-ppc64le-24.02.sif  mirror 1

e4s-cuda75-aarch64-24.02.sif  mirror 1

e4s-cuda80-aarch64-24.02.sif  mirror 1

e4s-cuda90-aarch64-24.02.sif  mirror 1

Intel OneAPI (x86_64)

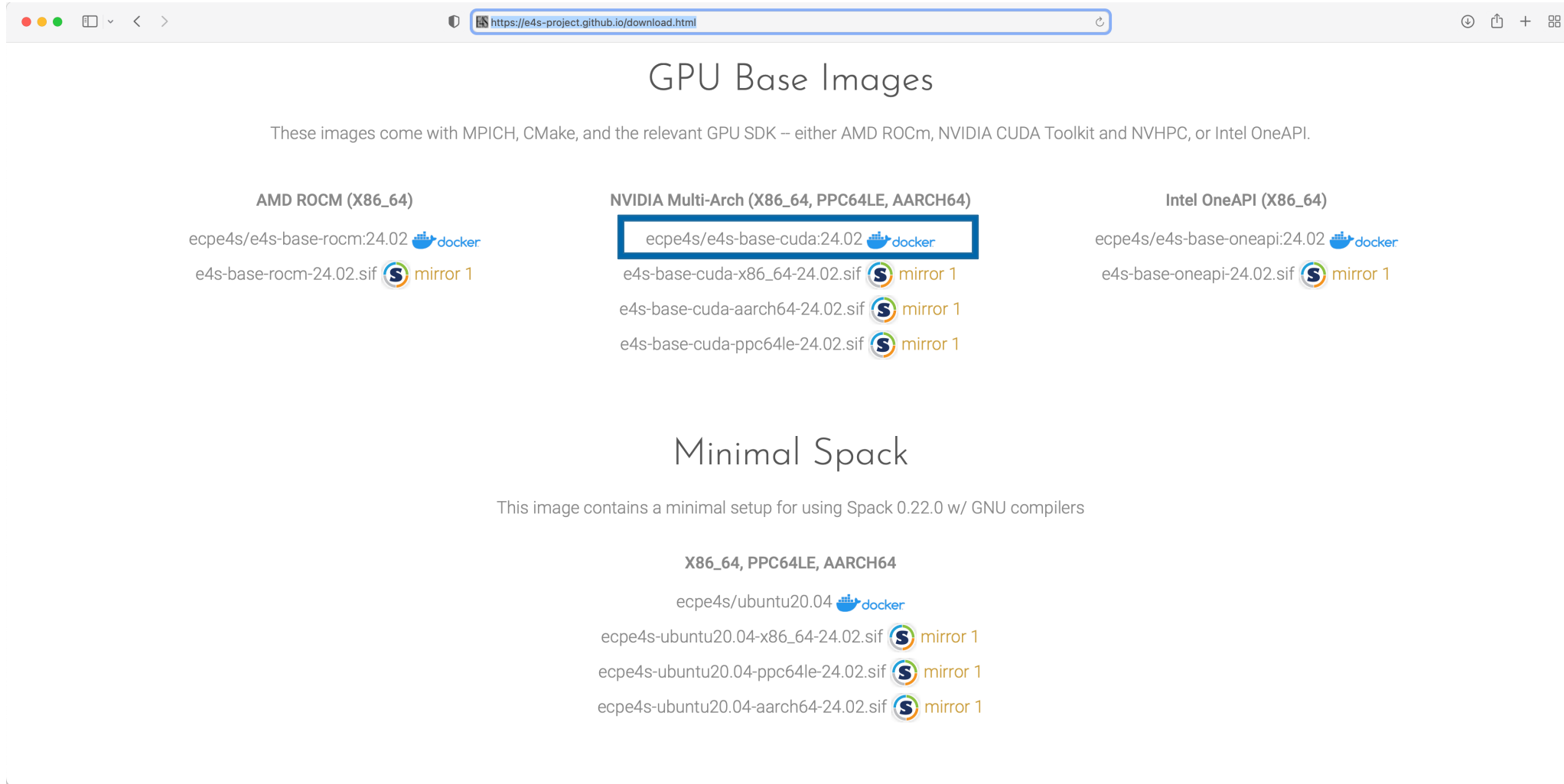
ecpe4s/e4s-oneapi:24.02 

e4s-oneapi-x86_64-24.02.sif  mirror 1



<https://e4s.io>



E4S base container images allow users to customize their containers







The screenshot shows a web browser window with the URL <https://e4s-project.github.io/download.html>. The page is titled "GPU Base Images" and contains the following content:

These images come with MPICH, CMake, and the relevant GPU SDK -- either AMD ROCm, NVIDIA CUDA Toolkit and NVHPC, or Intel OneAPI.



AMD ROCM (X86_64)

- ecpe4s/e4s-base-rocm:24.02 
- e4s-base-rocm-24.02.sif  mirror 1

NVIDIA Multi-Arch (X86_64, PPC64LE, AARCH64)

- ecpe4s/e4s-base-cuda:24.02 
- e4s-base-cuda-x86_64-24.02.sif  mirror 1
- e4s-base-cuda-aarch64-24.02.sif  mirror 1
- e4s-base-cuda-ppc64le-24.02.sif  mirror 1





Intel OneAPI (X86_64)

- ecpe4s/e4s-base-oneapi:24.02 
- e4s-base-oneapi-24.02.sif  mirror 1

Minimal Spack

This image contains a minimal setup for using Spack 0.22.0 w/ GNU compilers

X86_64, PPC64LE, AARCH64

- ecpe4s/ubuntu20.04 
- ecpe4s-ubuntu20.04-x86_64-24.02.sif  mirror 1
- ecpe4s-ubuntu20.04-ppc64le-24.02.sif  mirror 1
- ecpe4s-ubuntu20.04-aarch64-24.02.sif  mirror 1

- Intel oneAPI
- AMD ROCm
- NVIDIA NVHPC and CUDA

e4s-alc: a new tool to customize container images. Version 1.0

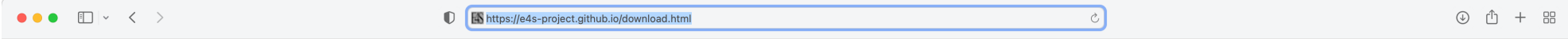
The screenshot displays the GitHub repository page for `E4S-Project/e4s-alc`. The repository is public and has 16 branches and 1 tag. The main branch is not protected. The repository contains several files and folders, including `docs`, `e4s_alc`, `examples`, `.gitignore`, `.readthedocs.yaml`, `LICENSE`, `Makefile`, `README.md`, and `pyproject.toml`. The `README.md` file is expanded, showing the project description and documentation link. The `Releases` section is highlighted with a blue box, showing version `v1.0.0` as the latest release on Jul 20. The `Contributors` section lists four contributors: FrederickDeny, PlatinumCD Cameron Durbin, spoutn1k Jean-Baptiste Skutnik, and sameershende Sameer Shende. The `Languages` section shows Python at 96.4% and Makefile at 3.6%. The `Suggested Workflows` section is also visible.

Add to a base image:

- Spack packages
- OS packages
- Tarballs
- Can create a Dockerfile



E4S DOE LLVM and CI images



DOE LLVM E4S Image

This multi-architecture image contains E4S products compiled with DOE LLVM 16 and Flang using Spack

Multi-Arch (X86_64, PPC64LE, AARCH64)

- ecpe4s/e4s-doe-llvm:23.05
- e4s-doe-llvm-x86_64-23.05.sif mirror 1
- e4s-doe-llvm-aarch64-23.05.sif mirror 1
- e4s-doe-llvm-ppc64le-23.05.sif mirror 1

Continuous Integration Images

These are barebones operating system images which contain only essential build tools and python packages needed by Spack.

These images are intended to be used in continuous integration workflows where Spack is first cloned and then used to build and test software.

X86_64

- ecpe4s/ubuntu22.04-runner-x86_64
- ecpe4s/ubuntu20.04-runner-x86_64
- ecpe4s/ubuntu18.04-runner-x86_64
- ecpe4s/rhel8-runner-x86_64
- ecpe4s/rhel7-runner-x86_64

PPC64LE

- ecpe4s/ubuntu22.04-runner-ppc64le
- ecpe4s/ubuntu20.04-runner-ppc64le
- ecpe4s/ubuntu18.04-runner-ppc64le
- ecpe4s/rhel8-runner-ppc64le
- ecpe4s/rhel7-runner-ppc64le

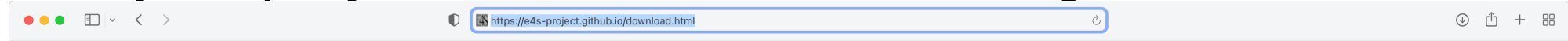
AARCH64

- ecpe4s/ubuntu22.04-runner-aarch64
- ecpe4s/ubuntu20.04-runner-aarch64
- ecpe4s/rhel8-runner-aarch64



<https://e4s.io>

E4S Facility Deployment and AWS EC2 Image



Custom Images

ecpe4s/waggle-ml  docker

ecpe4s/exawind-snapshot  docker

ecpe4s/superlu_sc  docker

E4S Facility Deployment

NERSC

OLCF

AWS EC2 Image

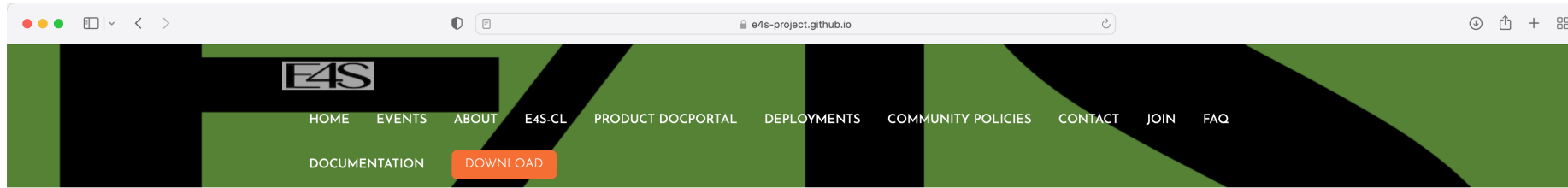
The E4S 24.02 release is also available on [AWS](#) as an EC2 AMI with ID ami-08c2daa0fb4864b90 in the US-West-2 (Oregon) region.

Created for The Extreme-scale Scientific Software Stack (E4S) Project by Michael A. Heroux



DOE Facility Deployment Dashboard: <https://dashboard.e4s.io>

E4S 24.02 Detailed Documentation for Bare-metal Installation



Extreme-scale Scientific Software Stack (E4S) version 24.02

Exascale Computing Project (ECP) Software Technologies (ST) software, Extreme-scale Scientific Software Stack (E4S) v24.02, includes a subset of ECP ST software products, and demonstrates the target approach for future delivery of the full ECP ST software stack. Also available are a number of ECP ST software products that support a Spack package, but are not yet fully interoperable. As the primary purpose of the v24.02 is demonstrating the ST software stack release approach, not all ECP ST software products were targeted for this release. Software products were targeted primarily based on existing Spack package maturity, location within the scientific software stack, and ECP SDK developer experience with the software. Each release will include additional software products, with the ultimate goal of including all ECP ST software products.

[E4S ReadTheDocs: Full Documentation.](#)

[E4S ReadTheDocs: Support Guide.](#)

[E4S Deployment Dashboard.](#)

[E4S v24.02 Release Notes PDF.](#)

[E4S v24.02 Spack Environment Notes.](#)

[E4S Manual Installation Instructions.](#)

[E4S Container Installation Instructions.](#)

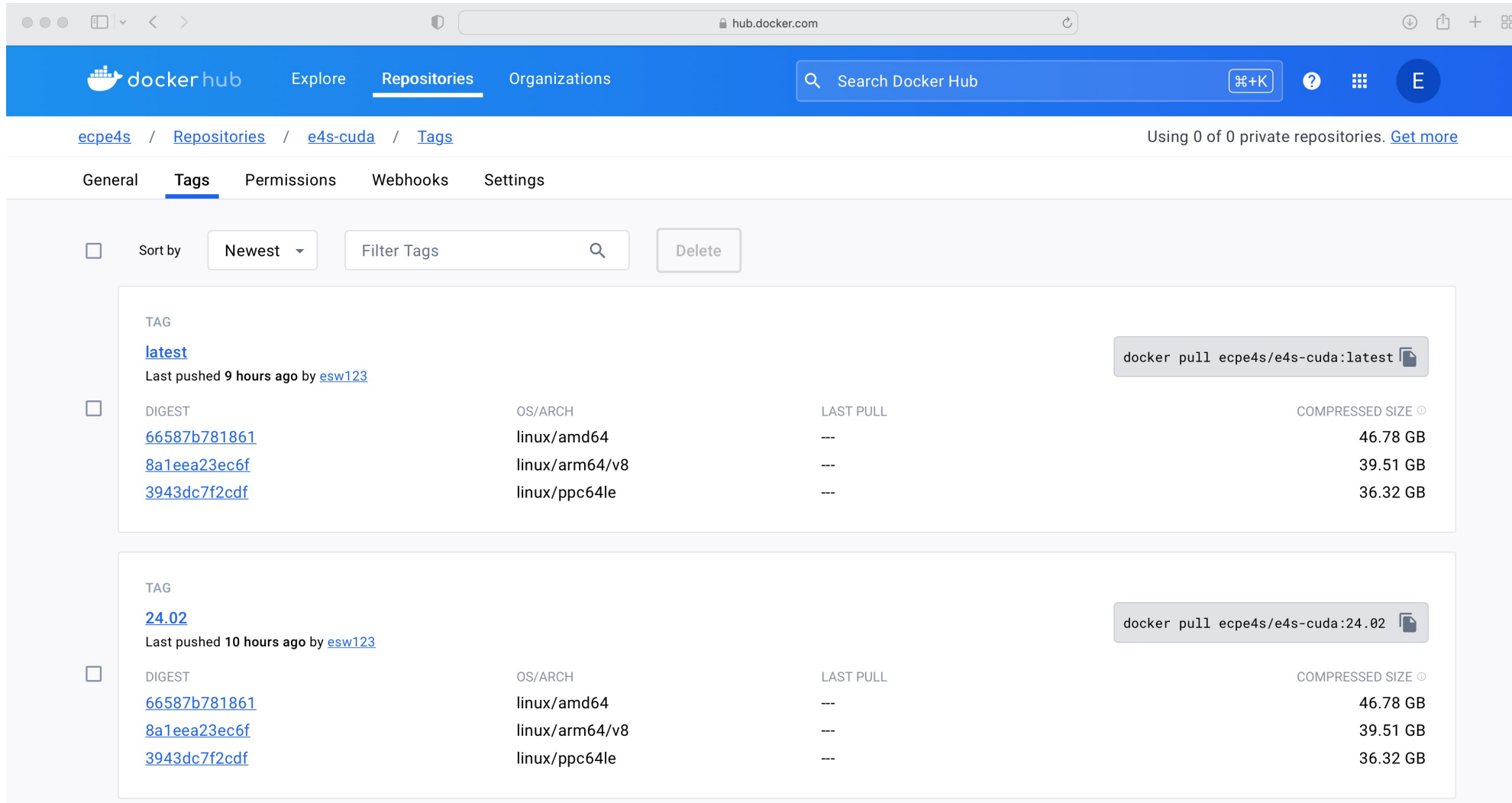
[Recipes for building E4S images from scratch.](#)

[Prebuilt binaries used in E4S images are stored in the E4S Build Cache.](#)



<https://e4s.io>

E4S 24.02 full featured container release on Dockerhub



The screenshot shows the Docker Hub interface for the repository `ecpe4s/e4s-cuda`. The page is viewed from the 'Tags' tab. The 'latest' tag is selected, showing it was pushed 9 hours ago by `esw123`. Below the tag information is a table of digests for different architectures. The '24.02' tag is also visible, pushed 10 hours ago by `esw123`, with its own table of digests. A 'Delete' button is present at the top of the tag list.

DIGEST	OS/ARCH	LAST PULL	COMPRESSED SIZE
66587b781861	linux/amd64	---	46.78 GB
8a1eea23ec6f	linux/arm64/v8	---	39.51 GB
3943dc7f2cdf	linux/ppc64le	---	36.32 GB

DIGEST	OS/ARCH	LAST PULL	COMPRESSED SIZE
66587b781861	linux/amd64	---	46.78 GB
8a1eea23ec6f	linux/arm64/v8	---	39.51 GB
3943dc7f2cdf	linux/ppc64le	---	36.32 GB

Architectures:

- x86_64
- aarch64
- ppc64le

Software:

- CUDA 12.3
- NVHPC 23.11
- ROCm 5.4.3
- oneAPI 2024.0.2



```
docker pull ecpe4s/e4s-cuda:24.02
```

E4S 24.02 base container release on Dockerhub

The screenshot shows the Docker Hub interface for the repository `ecpe4s/ubuntu20.04`. The page is viewed on a desktop browser. The navigation bar includes 'docker hub', 'Explore', 'Repositories', and 'Organizations'. A search bar is present with the text 'Search Docker Hub'. The breadcrumb trail is `ecpe4s / Repositories / ubuntu20.04 / Tags`. The main content area has tabs for 'General', 'Tags', 'Permissions', 'Webhooks', and 'Settings'. The 'Tags' tab is active, showing a list of tags. At the top of the tag list, there is a 'Sort by' dropdown set to 'Newest', a 'Filter Tags' search box, and a 'Delete' button. Each tag entry includes a 'TAG' section with the tag name and a 'Last pushed' timestamp, a 'DIGEST' section with three links for different architectures, an 'OS/ARCH' section with the architecture name, a 'LAST PULL' section with the time since last pull, and a 'COMPRESSED SIZE' section with the size in MB. A 'docker pull' command snippet is provided for each tag.

TAG	DIGEST	OS/ARCH	LAST PULL	COMPRESSED SIZE
latest Last pushed 10 hours ago by esw123	4bff25e25500	linux/amd64	41 minutes ago	931.92 MB
	d62cf76b7826	linux/arm64/v8	---	862.12 MB
	bc38b965be0a	linux/ppc64le	---	812.6 MB
	<code>docker pull ecpe4s/ubuntu20.04:latest</code>			
24.02 Last pushed 10 hours ago by esw123	4bff25e25500	linux/amd64	41 minutes ago	931.92 MB
	d62cf76b7826	linux/arm64/v8	---	862.12 MB
	bc38b965be0a	linux/ppc64le	---	812.6 MB
	<code>docker pull ecpe4s/ubuntu20.04:24.02</code>			
23.11 Last pushed 3 months ago by esw123	0bad20ec8b73	linux/amd64	an hour ago	934.68 MB
	cc0456ea5d27	linux/arm64/v8	4 days ago	863.94 MB
	ce4c85ec19c5	linux/ppc64le	---	814.89 MB
	<code>docker pull ecpe4s/ubuntu20.04:23.11</code>			

Architectures:

- x86_64
- aarch64
- ppc64le



`docker pull ecpe4s/ubuntu20.04`

E4S 24.02 ROCm release on Dockerhub

The screenshot shows the Docker Hub interface for the repository `ecpe4s/e4s-rocm`. The page is viewed on a browser with the URL `https://hub.docker.com/repository/docker/ecpe4s/e4s-rocm/tags?page=1&ordering=last_updated`. The navigation bar includes 'docker hub', 'Explore', 'Repositories', and 'Organizations'. The breadcrumb trail is `ecpe4s / Repositories / e4s-rocm / Tags`. The 'Tags' tab is active, showing a list of tags sorted by 'Newest'. Each tag entry includes a checkbox, the tag name, the user 'esw123', the digest 'd354902ea7c5', the OS/ARCH 'linux/amd64', the last pull status '---', and the compressed size '31.02 GB'. A 'docker pull' button is provided for each tag.

Sort by	Filter Tags	Delete
Newest		
<input type="checkbox"/>	latest	<code>docker pull ecpe4s/e4s-rocm:latest</code>
<input type="checkbox"/>	24.02	<code>docker pull ecpe4s/e4s-rocm:24.02</code>
<input type="checkbox"/>	24.02-gfx90a	<code>docker pull ecpe4s/e4s-rocm:24.02...</code>



`docker pull ecpe4s/e4s-rocm:24.02`

E4S 24.02 oneAPI release on Dockerhub

The screenshot shows the Docker Hub interface for the repository `ecpe4s/e4s-oneapi`. The page is viewed on a browser with the URL `https://hub.docker.com/repository/docker/ecpe4s/e4s-oneapi/tags?page=1&ordering=last_updated`. The navigation bar includes 'docker hub', 'Explore', 'Repositories', and 'Organizations'. A search bar is present with the text 'Search Docker Hub'. The breadcrumb trail is `ecpe4s / Repositories / e4s-oneapi / Tags`. The 'Tags' tab is selected, showing a list of tags. The 'latest' tag is the most recent, pushed 5 hours ago by `esw123`. The '24.02' tag is also pushed 5 hours ago by `esw123`. Both tags have a digest of `ef165253d7e1` and are for the `linux/amd64` architecture. The compressed size for both is 20.59 GB. A 'Delete' button is visible at the top of the tag list. A 'docker pull' command snippet is shown for each tag.

TAG	DIGEST	OS/ARCH	LAST PULL	COMPRESSED SIZE
latest Last pushed 5 hours ago by <code>esw123</code>	ef165253d7e1	linux/amd64	---	20.59 GB
24.02 Last pushed 5 hours ago by <code>esw123</code>	ef165253d7e1	linux/amd64	---	20.59 GB



```
docker pull ecpe4s/e4s-oneapi:24.02
```

24.02 Release: 122+ Official Products + dependencies (gcc, x86_64)

1: adios2	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/adios2-2.9.2-su4tc6nl2te2mues3iqgeqltc2mrsfcu
2: alquimia	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/alquimia-1.1.0-ngm6n4fpaxruwdkbrotkrswpyjsb24g
3: aml	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/aml-0.2.1-4zzl1trirh4xalxkdi77uvosx7moy5w1
4: amrex	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/amrex-24.01-lcm7tyxjk7xrmu31chjcm4jqyu3z6hnx
5: arborx	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/arborx-1.5-7yerbzkysthcwqsfsktolj5k767eobt
6: argobots	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/argobots-1.1-2xylrhey2pjpvfddafegoomse4d37psk
7: ascent	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/ascent-0.9.2-4hjb5u5bwtppqzfwk2xjmxv3t1bybq65
8: axom	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/axom-0.8.1-wh23ue5cudzdggeburrvvwc5tmlogot
9: bolt	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/bolt-2.0-teiskaivfavvwj47u3kuwxghin5abmis
10: blaspp	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/blaspp-2023.11.05-d3vyunwy7gy5mm4yjo3jsznt5czhqhp
11: bricks	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/bricks-2023.08.25-cujzqmsvdhfvxh2dyu7ttrme6gat4t4
12: butterflypack	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/butterflypack-2.4.0-t7popaaelqkrdjrrwtuwp6frujflqlw
13: cabana	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/cabana-0.6.0-dbjkjp624ab3ojxgqlzzncuh4v3cauw
14: caliper	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/caliper-2.10.0-orwuspl2gsgqgvjlkzvy1jc4fyqxdxaj
15: camp	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/camp-2022.10.1-rxn44cbqw43syp47iqnw3skfaa2mk6os
16: chai	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/chai-2022.03.0-bhwnrvx5xwqnbfnftbdbmsxeredhhe5k
17: charliecloud	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/charliecloud-0.35-5sn2iuuuef3dek57ag61q5nvkc6iz3sj
18: conduit	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/conduit-0.8.8-f5tg6yo6i2glhggntx6x465kp33b5bln
19: cp2k	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/cp2k-2024.1-ksmkbf6xv7pcqh2pqsh2hc55zqx7bfgc
20: cusz	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/cusz-0.3.1-uqzup3z7xv6yimma6grqt4jtdhpcng57d
21: darshan-runtime	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/darshan-runtime-3.4.4-fx2xt4efwcx7apdhmijwuv4sxgh45qko
22: datatransferkit	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/datatransferkit-3.1.1-qbghfa62oceht3zgolx3sy5a47hnhmo
23: dealii	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/dealii-9.5.1-myseb7q5uj3jq5qvkqebjchp6hsdveje
24: dyninst	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/dyninst-12.3.0-zkqtqt5zpnue6mhbmomfdf2h5d4nnv7q4j
25: ecp-data-vis-sdk	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/ecp-data-vis-sdk-1.0-wjz52roa6dgpfvvg5x53zgtf6jkdns5
26: exago	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/exago-1.6.0-znuyivt7map35ckt4ghaeqee2zodgbz
27: exaworks	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/exaworks-0.1.0-izru16w3eyq2uhsol17pbv3w3xxbdp667
28: faodel	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/faodel-1.2108.1-g2jj4bkm552x7rfu76fqsdsdh26dp5fr
29: flecsi	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/flecsi-2.2.1-pvampcxzo2ab5wqs22qowci4g4p12qpn
30: flit	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/flit-2.1.0-2x7pdvrfwfdqw44udcpxba7zoevslvz3
31: flux-core	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/flux-core-0.58.0-wc3uhn7dzdmewi7lxysm3t6ksy3e7nn
32: flux-sched	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/flux-sched-0.32.0-wsu7iphaprrwpdhsrthgugyssh47qe2
33: fortrilinos	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/fortrilinos-2.3.0-n5cxts5apobuq5djbdaqnrdq67fbcgo
34: gasnet	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/gasnet-2023.9.0-jq3gdqkdm3nurvcduzbsko5pw3jlozbl
35: ginkgo	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/ginkgo-1.7.0-nmthpjjvjomel35zf6erfzvcp5sxnzb6j
36: globalarrays	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/globalarrays-5.8.2-3lrzv36gr3zv3674gvdc5cx3eodc7lj
37: gotcha	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/gotcha-1.0.5-nuzj2eyugqdnswxs212ceinc34u6lyzf
38: gptune	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/gptune-4.0.0-sg2nhpbbwywh17axka7ik6di5fu5eocxc
39: gromacs	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/gromacs-2023.3-jnx6atxejgau7zab64hsoin66s5ggz1r
40: h5bench	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/h5bench-1.4-2wpa6knuhk5ln7ijlzbv4kncpfcvccskb
41: hdf5	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/hdf5-1.14.3-eygnixicmaiitcgdbovz1b4dzwowo24f

GPU runtimes

- AMD (ROCm)
 - 5.4.3
- NVIDIA (CUDA)
 - 12.3
- NVHPC
 - 23.11
- Intel oneAPI
2024.0.2



24.02 Release: 122+ Official Products + dependencies (gcc, x86_64)

```
42: hdf5-vol-cache /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/hdf5-vol-cache-v1.1-u4ns554sa6p6i3eejktla4ylona33ztb
43: hdf5-vol-async /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/hdf5-vol-async-1.7-h54dmdpdvejwkke7bhrcmuhqudoac37e
44: hdf5-vol-log /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/hdf5-vol-log-1.4.0-j3p4alkrmlfidrszm7kmbdewtntd42
45: heffte /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/heffte-2.4.0-lmn6xnuhfwxsjhmt33ouab6scayxthx
46: hpctoolkit /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/hpctoolkit-2023.08.1-cuzxhycgmrokgy4a53vq5a73ggfyb4n
47: hpx /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/hpx-1.9.1-js3yv4vz73lmk3wd3hr67tii44dbyhst
48: hypre /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/hypre-2.30.0-tlpuke7ccklavodwkaj3yclqzqfgqjsy
49: kokkos /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/kokkos-4.2.00-oim2tyxa4ijqjkemg7j7axu24fovvyfj
50: kokkos-kernels /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/kokkos-kernels-4.2.00-uehtixq4rmwrkoa3lupmtk53vk46upak
51: lammmps /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/lammmps-20230802.2-r2l656f3d4imvjwo5f2uua5r6tf4mfyy
52: lapackpp /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/lapackpp-2023.11.05-vsjrqqghfb4bsbdxs5vleboww5iroe4m
53: lbann /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/lbann-0.104-dhmqx fjkhjfgb47fdwd7wph5n7bohjsf
54: legion /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/legion-23.06.0-5f7lytnp7o4a2e2fp6332dcpds4a7vy
55: libcatalyst /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/libcatalyst-2.0.0-rc4-7foztrrn2w4ihu7osgu6vivy42tbljun
56: libnrm /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/libnrm-0.1.0-nrkqdt63sexo4d4rumpjamle6djggpxb
57: libpressio /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/libpressio-0.95.1-5tf23tmbhe7cad6ywuyngpb6he6gdiyd
58: libquo /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/libquo-1.3.1-ndp7emlx5lqwscpvhpfykaowxychnft7
59: loki /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/loki-0.1.7-mxejb3m44hhtb6wnpc5uppgqtah53dux
60: magma /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/magma-2.7.2-edrr5tibzpd5jc4xqe4t4lvwhauueh7
61: mercury /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/mercury-2.3.1-izoh2mdb4qyxhi5avj3ljzxrxtlmbz2z
62: metall /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/metall-0.25-jee6ww6ys2zfm dyqfyuro3dv5f2r7t7v
63: mfem /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/mfem-4.6.0-x7rnzhmikmbulmhwoeoa7fjxswmq2hyt
64: mgard /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/mgard-2023-03-31-n7ahfp6qcab6ykj4o7ptch35g6zc3r7a
65: mpark-variant /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/mpark-variant-1.4.0-3q7w6rg2n7z545w2vbqjve52ghy4bf6x
66: mpich /usr/local/mpich/install/mpich
67: mpifileutils /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/mpifileutils-0.11.1-rm4pm3kdybdgl7nc4bbtphaszzfotp4j
68: nccmp /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/nccmp-1.9.1.0-35vdd7ep5s12p34ddd7eybyzygvic22f
69: nco /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/nco-5.1.6-zy5qp3ojyqz7mg17kqp2a2lluedlrjoj
70: netlib-scalapack /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/netlib-scalapack-2.2.0-imu7mfp2anmcbcbwhbbg50ehgthks63zp
71: nrm /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/nrm-0.1.0-haqjftkngind32vhel4t4xs23oqsvtpk
72: omega-h /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/omega-h-9.34.13-ynfydwyldgjxfvvqsh4cwflrg3tndefz
73: openfoam /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/openfoam-2312-irhy7qllmi3fmdr7vec5hg34apalcy7q
74: openmpi /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/openmpi-5.0.1-vuexbeezm47ykepcwj6dxhpzrshmett
75: openpmd-api /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/openpmd-api-0.15.2-cp2xfyj2b2uclt3qceomu56pjgidlmk
76: papi /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/papi-7.1.0-gzqkp7tyhbbxptkp7tbz7z2a53bzcfmq
77: papyrus /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/papyrus-1.0.2-dal2ge6cl62mnaoxlqaalb jxpbjnz3mq
78: parallel-netcdf /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/parallel-netcdf-1.12.3-kchqz5bxj5rfahqgadbllynconijrvunk
79: paraview /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/paraview-5.11.2-h7qeicup7xh5flfvcw6m6mvbvfgjhdq
80: parsec /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/parsec-3.0.2209-r6q7fpyhfuoxrugoizspohwj2wjwykgh
81: pdt /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/pdt-3.25.2-ktev65bmn3juabdf42vvjxkq4tzmbzspg
82: petsc /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/petsc-3.20.3-ynxsrrj6tstvlpnrjh2g46iykghsjldhc
```

24.02 Release: 122+ Official Products + dependencies (gcc, x86_64)

```
83: phist /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/phist-1.12.0-nd4p1qezkinza6roz5ke3o56niitvyud
84: plasma /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/plasma-23.8.2-2no2xnu7uwyjcwqg6h5jgfnigbft5tct
85: plumed /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/plumed-2.9.0-ppsp6ufipkmcDCzm4xgcwang3oyzc25ai
86: precice /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/precice-2.5.0-wxwlqxa5ob6mezuxhto32luz43ze5wyb
87: pruners-ninja /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/pruners-ninja-1.0.1-sna5i226xpggia5pgs75lkipjiefmukxq
88: pumi /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/pumi-2.2.8-cf5t7ivcx3q7ly2bgantpjjfb63pkh52b
89: py-cinemascope /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/py-cinemascope-1.3-evtrst67j7hhojumi2konvisczhbja
90: py-jupyterhub /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/py-jupyterhub-1.4.1-647zpath2qhl1linprlz2ipeha4yqpmDM
91: py-libensemble /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/py-libensemble-1.1.0-4paduo2pz2ouohfvnmpegsvebcby32w
92: py-parsl /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/py-parsl-2023.08.21-l6qftilw2rsy2bynypwabmen2tevqo4n
93: py-radical-saga /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/py-radical-saga-1.20.0-2jcadlsefjs3lhef4fswfml7c65wi6d
94: qthreads /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/qthreads-1.18-7l5aok4kxvqsh3xcyhmcf1vp2nkr2nqv
95: quantum-espresso /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/quantum-espresso-7.3-ve2alec2o23sdlvljz3fgglN7vjpt6y6
96: raja /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/raja-2022.10.4-xrrmkgcP4iepub2mmetkend77ppnret6
97: rempi /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/rempi-1.1.0-dtv6mjpc6ozhs62w4f2oh2cwsrqy5ex
98: scr /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/scr-3.0.1-kl7ubaujbxqg7rty6ggjyussf6gc3lvn
99: slate /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/slate-2023.08.25-fxd6cphgxymdtxwendoicf3ra3erh2ya
100: slepc /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/slepc-3.20.1-7yaga344vvuj7kp7bfrmvghffaur5rc3
101: stc /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/stc-0.9.0-fni2k4fuvC7ertn7qowhgaiuedb536b
102: strumpack /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/strumpack-7.2.0-gnqbe6uvvrk3oyxzxrb6mcdffghuxlu
103: sundials /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/sundials-6.7.0-r36lglynuHz35injuyh7aftmno4amg5
104: superlu-dist /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/superlu-dist-8.2.1-nxoqlgbrvt3q76azfoipxarpyuu3hqa
105: swig /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/swig-4.1.1-jzchgz2v5smcinkr4dbjqdbn4dxqbt
106: sz3 /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/sz3-3.1.7-lhvfD143gxuhx3mblo3b6m7f3mul5hlv
107: tasmanian /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/tasmanian-8.0-l2u44psagjgpv32oftluhyah7dvkpygt
108: tau /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/tau-2.33.1-tjdyusn3gxzx3nmbiwr7d3np24evwpo
109: trillinos /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/trillinos-15.0.0-ozanynohqjbqa653ftuddhvuevkb3pm
110: turbine /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/turbine-1.3.0-4mehzhgmiehwjxqiaV47hedro5np6bg
111: umap /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/umap-2.1.0-7bhxbhmotchkgnzf3ypdtr6s3ousjo3m
112: umpire /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/umpire-2022.10.0-34iyblbowuwhlm3dg6o4swtbarbdfxexf
113: unifyfs /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/unifyfs-2.0-rlbigm2a4qp7wedcz7dmswt53z4auo7c
114: upcxx /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/upcxx-2023.9.0-kftns1ls5djcuV7onpbaax5h63jzrf5o
115: variorum /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/variorum-0.7.0-fk3kofdfqckelbsu2cywukqzsj7m3c3p
116: veloc /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/veloc-1.7-bb3dqeyamm6pqr7rio4a7ltbrnxi77
117: visit /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/visit-3.3.3-4xtlxhcjdemxlf2o3rzqppxf3rvuvr
118: vtk-m /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/vtk-m-2.1.0-hocvo42bxzdmkjmg5kagj2bi2rcn3vvp
119: wannier90 /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/wannier90-3.1.0-y2cc142fxetuw3x4baywju5i4foxvlgb
120: warpx /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/warpx-23.08-ccutnxiBazcgs6wq4mezyniq4k4f6jch
121: xyce /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/xyce-7.8.0-hilbds1uwxfqe7gepc23dbouoot3nkv
122: zfp /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.4.0/zfp-1.0.0-vnvxgiuplecwyiwqgzxycbav5adhszla
```

Languages:

- Rust
- Julia with support for MPI, and CUDA
- Python

AI products

- TensorBraid
- OpenAI
- Tensorflow
- Pytorch
- JAX
- Horovod

EDA Tools:

- Xyce

3D Visualization

- Paraview
- VisIt
- TAU's paraprof
- Jupyter notebook ...



New Tool in E4S 24.02: e4s-chain-spack.sh

```
Singularity> rm -rf ~/tmp/spack
Singularity> . /etc/e4s/e4s-chain-spack.sh ~/tmp/spack
Cloning into '/home/users/sameer/tmp/spack'...
remote: Enumerating objects: 531987, done.
remote: Counting objects: 100% (180/180), done.
remote: Compressing objects: 100% (92/92), done.
remote: Total 531987 (delta 83), reused 139 (delta 60), pack-reused 531807
Receiving objects: 100% (531987/531987), 176.96 MiB | 32.95 MiB/s, done.
Resolving deltas: 100% (249575/249575), done.
Updating files: 100% (11224/11224), done.
Singularity> spack find valgrind
==> Error: No package matches the query: valgrind
Singularity> spack install valgrind
[+] /opt/intel/oneapi (external intel-oneapi-mpi-2021.11.0-2qi2xp2qs4kxwddgnibhixhgjmwvngvo)
[+] /spack/opt/spack/linux-ubuntu22.04-x86_64/oneapi-2024.0.2/gmake-4.4.1-zpg4uz3bbxf4ljfzxsm5uhhepceiwdwd
[+] /spack/opt/spack/linux-ubuntu22.04-x86_64/oneapi-2024.0.2/boost-1.84.0-zualrbbikg6f5cvkjif227s3mebjfnov
==> Installing valgrind-3.20.0-7t4aj3mw3fokiyun6ofcjpgxaj6teseas [4/4]
==> No binary for valgrind-3.20.0-7t4aj3mw3fokiyun6ofcjpgxaj6teseas found: installing from source
==> Fetching https://mirror.spack.io/_source-cache/archive/85/8536c031dbe078d342f121fa881a9ecd205cb5a78e639005ad570011bdb9f3c6.tar.bz2
==> Ran patch() for valgrind
==> valgrind: Executing phase: 'autoreconf'
==> valgrind: Executing phase: 'configure'
==> valgrind: Executing phase: 'build'
==> valgrind: Executing phase: 'install'
==> valgrind: Successfully installed valgrind-3.20.0-7t4aj3mw3fokiyun6ofcjpgxaj6teseas
  Stage: 3.53s. Autoreconf: 0.00s. Configure: 45.60s. Build: 28.97s. Install: 3.15s. Post-install: 1.32s. Total: 1m 22.86s
[+] /home/users/sameer/tmp/spack/opt/spack/linux-ubuntu22.04-x86_64/oneapi-2024.0.2/valgrind-3.20.0-7t4aj3mw3fokiyun6ofcjpgxaj6teseas
Singularity> spack load valgrind
Singularity> which valgrind
/home/users/sameer/tmp/spack/opt/spack/linux-ubuntu22.04-x86_64/oneapi-2024.0.2/valgrind-3.20.0-7t4aj3mw3fokiyun6ofcjpgxaj6teseas/bin/valgrind
Singularity> valgrind --help | head
usage: valgrind [options] prog-and-args

  tool-selection option, with default in [ ]:
  --tool=<name>          use the Valgrind tool named <name> [memcheck]

  basic user options for all Valgrind tools, with defaults in [ ]:
  -h --help              show this message
  --help-debug           show this message, plus debugging options
  --help-dyn-options     show the dynamically changeable options
  --version              show version
Singularity> █
```

e4s-chain-spack.sh allows a user to extend and add new tools to an existing Spack installation in a read-only filesystem in a container and chain both Spack installations!



E4S Support for AI/ML frameworks with NVIDIA GPUs

```
$ singularity run --nv e4s-cuda90-aarch64-24.02.sif
```

```
Singularity> nvidia-smi
```

```
Wed Feb 14 21:35:06 2024
```

```
+-----+
| NVIDIA-SMI 535.146.02                Driver Version: 535.146.02   CUDA Version: 12.2   |
+-----+-----+-----+-----+-----+-----+
| GPU  Name           Persistence-M | Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp   Perf          Pwr:Usage/Cap |      Memory-Usage | GPU-Util  Compute M. |
|====+=====+====+=====+=====+=====+
|   0   NVIDIA GH200 480GB           On   | 00000009:01:00:0 Off |             0         |
| N/A   23C    P0              77W / 900W | 229MiB / 97871MiB |    0%      Default  |
|                                           |                       | Disabled         |
+-----+-----+-----+-----+-----+-----+

```

```
+-----+
| Processes:
| GPU  GI  CI           PID  Type  Process name                        GPU Memory
|   ID  ID  ID                                 Usage
|=====+=====+=====+=====+=====+=====+
| No running processes found
+-----+

```

```
Singularity> python
Python 3.8.10 (default, May 26 2023, 14:05:08)
[GCC 9.4.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import tensorflow
>>> import torch
>>> torch.cuda.get_device_name(0)
'NVIDIA GH200 480GB'
>>> print(torch.cuda.get_arch_list())
['sm_35', 'sm_70', 'sm_75', 'sm_80', 'sm_90']
>>> █
```



E4S 24.02 supports NVIDIA Grace-Hopper GH200 GPUs with TensorFlow and PyTorch

E4S Support for AI/ML and Python tools

```
$ singularity run --nv e4s-cuda90-x86_64-24.02.sif
Singularity> python
Python 3.8.10 (default, May 26 2023, 14:05:08)
[GCC 9.4.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import tensorflow
>>> import torchbraid
>>> import torch
>>> import jax
>>> import keras
>>> import pandas
>>> import cv2
>>> import sklearn
>>> import numpy
>>> import scipy
>>> import matplotlib
>>> import plotly
>>> import seaborn
>>> import open3d
>>> import openai
>>> █
```

E4S 24.02 Support for GPUs: NVIDIA

```
$ singularity run --nv e4s-cuda90-x86_64-24.02.sif
Singularity> spack find -x +cuda
-- linux-ubuntu20.04-x86_64 / gcc@11.4.0 -----
adios2@2.9.2      chai@2022.03.0    gromacs@2023.3    libpressio@0.95.1  raja@2022.10.4    tau@2.33.1
amrex@24.01      cusz@0.3.1        heffte@2.4.0     magma@2.7.2        slate@2023.08.25  trilinos@14.4.0
arborx@1.5       ecp-data-vis-sdk@1.0  hpctoolkit@2023.08.1  mfem@4.6.0        slepc@3.20.1      umpire@2022.10.0
axom@0.8.1       exago@1.6.0       hpx@1.9.1        mgard@2023-03-31  strumpack@7.2.0   vtk-m@2.1.0
bricks@2023.08.25  flecsi@2.2.1      kokkos@4.2.00    papi@7.1.0         sundials@6.7.0    zfp@0.5.5
cabana@0.6.0     flux-core@0.58.0   kokkos-kernels@4.2.00  parsec@3.0.2209   superlu-dist@8.2.1
caliper@2.10.0    ginkgo@1.7.0      legion@23.06.0    petsc@3.20.3       tasmanian@8.0
==> 40 installed packages
Singularity> spack find -x
-- linux-ubuntu20.04-x86_64 / gcc@11.4.0 -----
adios@1.13.1     cuda@12.3.0       h5bench@1.4       mercury@2.3.1      phist@1.12.0      superlu-dist@8.2.1
adios2@2.7.1     cusz@0.3.1        hdf5@1.12.3      metall@0.25        plasma@23.8.2     superlu-dist@8.2.1
adios2@2.9.2     darshan-runtime@3.4.4  hdf5-vol-async@1.7  mfem@4.6.0        plumed@2.9.0      swig@4.0.2-fortran
alquimia@1.1.0   darshan-util@3.4.4   hdf5-vol-cache@v1.1  mfem@4.6.0        precice@2.5.0     sz@2.1.12.5
aml@0.2.1        datatransferkit@3.1.1  hdf5-vol-log@1.4.0  mgard@2023-03-31  pruners-ninja@1.0.1  sz3@3.1.7
amrex@24.01      dealii@9.5.1       heffte@2.4.0     mgard@2023-03-31  pumi@2.2.8        tasmanian@8.0
amrex@24.01      dyninst@12.3.0     heffte@2.4.0     mpark-variant@1.4.0  py-cinemasci@1.3  tasmanian@8.0
arborx@1.5       ecp-data-vis-sdk@1.0  hpctoolkit@2023.08.1  mpich@4.1.2        py-h5py@3.8.0     tau@2.33.1
arborx@1.5       ecp-data-vis-sdk@1.0  hpctoolkit@2023.08.1  mpiutils@0.11.1    py-jupyterhub@1.4.1  tau@2.33.1
argobots@1.1     exago@1.6.0        hpx@1.9.1        nccmp@1.9.1.0     py-libensemble@1.1.0  trilinos@13.0.1
ascent@0.9.2     exago@1.6.0        hpx@1.9.1        nco@5.1.6          py-petsc4py@3.20.2  trilinos@14.4.0
axom@0.8.1       exaworks@0.1.0     hypre@2.30.0      netlib-scalapack@2.2.0  py-warp@23.08     trilinos@15.0.0
axom@0.8.1       faodel@1.2108.1    kokkos@4.2.00    nrm@0.1.0          qthreads@1.18      turbine@1.3.0
bolt@2.0         flecsi@2.2.1       kokkos@4.2.00    nvhpc@23.11        quantum-espresso@7.3  umap@2.1.0
boost@1.79.0     flecsi@2.2.1       kokkos-kernels@4.2.00  omega-h@9.34.13    raja@2022.10.4     umpire@2022.10.0
bricks@2023.08.25  flit@2.1.0        kokkos-kernels@4.2.00  openfoam@2312     raja@2022.10.4     umpire@2022.10.0
bricks@2023.08.25  flux-core@0.58.0   lammps@20230802.2  openmpi@5.0.1      rempi@1.1.0        unifyfs@2.0
butterflypack@2.4.0  flux-core@0.58.0  lbann@0.104       openpmd-api@0.15.2  scr@3.0.1          upcxx@2023.9.0
cabana@0.6.0     fortlinos@2.3.0    legion@23.06.0    papi@7.1.0         slate@2023.08.25  variorum@0.7.0
cabana@0.6.0     gasnet@2023.9.0    legion@23.06.0    papi@7.1.0         slate@2023.08.25  veloc@1.7
caliper@2.10.0    ginkgo@1.7.0      libcat@2.0.0-rc4  papyrus@1.0.2     slepc@3.20.1       visit@3.3.3
caliper@2.10.0    ginkgo@1.7.0      libcat@2.0.0-rc4  papyrus@1.0.2     slepc@3.20.1       vtk-m@2.0.0
chai@2022.03.0   globalarrays@5.8.2  libpressio@0.95.1  parallel-netcdf@1.12.3  stc@0.9.0         vtk-m@2.1.0
chai@2022.03.0   gmp@6.2.1          libpressio@0.95.1  paraview@5.11.2    strumpack@7.2.0    wannier90@3.1.0
charliecloud@0.35  gotcha@1.0.5       libquo@1.3.1      parsec@3.0.2209   strumpack@7.2.0    xyce@7.8.0
conduit@0.8.8    gptune@4.0.0       libunwind@1.6.2    parsec@3.0.2209   sundials@6.7.0     zfp@0.5.5
cp2k@2024.1      gromacs@2023.3     loki@0.1.7        pdt@3.25.2         sundials@6.7.0     zfp@0.5.5
cuda@11.8.0      gromacs@2023.3     magma@2.7.2        petsc@3.20.3       superlu@5.3.0
==> 167 installed packages
Singularity> █
```


E4S 24.02 Support for GPUs: AMD

```
$ singularity run --rocm e4s-rocm90a-x86_64-24.02.sif
Singularity> spack find -x +rocm
-- linux-ubuntu20.04-x86_64 / gcc@11.4.0 -----
amrex@24.01      ecp-data-vis-sdk@1.0  hpctoolkit@2023.08.1  magma@2.7.2      slate@2023.08.25     tasmanian@8.0      vtk-m@2.1.0
arborx@1.5      exago@1.6.0          hpx@1.9.1            mfem@4.6.0      slepc@3.20.1        tau@2.33.1
cabana@0.6.0    gasnet@2023.9.0     hypre@2.30.0        paraview@5.11.2  strumpack@7.2.0     trilinos@15.0.0
caliper@2.10.0  ginkgo@1.7.0        kokkos@4.2.00       petsc@3.20.3    sundials@6.7.0     umpire@2022.10.0
chai@2022.03.0  heffte@2.4.0        legion@23.06.0      raja@2022.10.4  superlu-dist@8.2.1  upcxx@2023.9.0
==> 31 installed packages
Singularity> spack find -x
-- linux-ubuntu20.04-x86_64 / gcc@11.4.0 -----
adios@1.13.1      dealii@9.5.1          hdf5-vol-log@1.4.0  mgard@2023-03-31  pumi@2.2.8          sz3@3.1.7
adios2@2.7.1     dyninst@12.3.0       heffte@2.4.0       mpark-variant@1.4.0  py-cinemasci@1.3   tasmanian@8.0
alquimia@1.1.0   ecp-data-vis-sdk@1.0  heffte@2.4.0       mpich@4.1.2        py-h5py@3.8.0      tasmanian@8.0
aml@0.2.1        ecp-data-vis-sdk@1.0  hpctoolkit@2023.08.1  mpiutils@0.11.1    py-jupyterhub@1.4.1  tau@2.33.1
amrex@24.01      exago@1.6.0          hpctoolkit@2023.08.1  nccmp@1.9.1.0     py-libensemble@1.1.0  tau@2.33.1
amrex@24.01      exago@1.6.0          hpx@1.9.1          nco@5.1.6          py-petsc4py@3.20.2  trilinos@13.0.1
arborx@1.5      exaworks@0.1.0       hypre@2.30.0       netlib-scalapack@2.2.0  py-warpx@23.08     trilinos@15.0.0
arborx@1.5      faodel@1.2108.1      hypre@2.30.0       nrm@0.1.0          qthreads@1.18       trilinos@15.0.0
argobots@1.1     flecsi@2.2.1         hypre@2.30.0       nvhpc@23.11        quantum-espresso@7.3  turbine@1.3.0
ascent@0.9.2     flit@2.1.0           kokkos@4.2.00      omega-h@9.34.13    raja@2022.10.4     umap@2.1.0
axom@0.8.1       flux-core@0.58.0     kokkos@4.2.00      openfoam@2312     raja@2022.10.4     umpire@2022.10.0
bolt@2.0         fortrilinos@2.3.0    kokkos-kernels@4.2.00  openmpi@5.0.1     rempi@1.1.0         umpire@2022.10.0
boost@1.79.0     gasnet@2023.9.0     lammps@20230802.2   openpmd-api@0.15.2  scr@3.0.1           unifyfs@2.0
bricks@2023.08.25  gasnet@2023.9.0     lbann@0.104        papi@7.1.0         slate@2023.08.25    upcxx@2023.9.0
butterflypack@2.4.0  ginkgo@1.7.0        legion@23.06.0     papyrus@1.0.2     slate@2023.08.25    upcxx@2023.9.0
cabana@0.6.0     ginkgo@1.7.0        legion@23.06.0     parallel-netcdf@1.12.3  slepc@3.20.1       variorum@0.7.0
cabana@0.6.0     globalarrays@5.8.2  libcatalyst@2.0.0-rc4  paraview@5.11.2    slepc@3.20.1       veloc@1.7
caliper@2.10.0   gmp@6.2.1           libnm@0.1.0        paraview@5.11.2    stc@0.9.0           visit@3.3.3
caliper@2.10.0   gotcha@1.0.5        libpressio@0.95.1  parsec@3.0.2209   strumpack@7.2.0     vtk-m@2.0.0
chai@2022.03.0   gptune@4.0.0        libquo@1.3.1       pdt@3.25.2        strumpack@7.2.0     vtk-m@2.1.0
chai@2022.03.0   gromacs@2023.3      libunwind@1.6.2    petsc@3.20.3      sundials@6.7.0     wannier90@3.1.0
charliecloud@0.35  h5bench@1.4         loki@0.1.7         petsc@3.20.3      sundials@6.7.0     xyce@7.8.0
conduit@0.8.8    hdf5@1.12.3         magma@2.7.2        phist@1.12.0      superlu@5.3.0       zfp@0.5.5
cp2k@2024.1      hdf5@1.14.3         mercury@2.3.1     plasma@23.8.2     superlu-dist@8.2.1  superlu-dist@8.2.1
darshan-runtime@3.4.4  hdf5-vol-async@1.7  metall@0.25        plumed@2.9.0      swig@4.0.2-fortran  sz@2.1.12.5
darshan-util@3.4.4  hdf5-vol-cache@v1.1  mfem@4.6.0        precice@2.5.0     pruners-ninja@1.0.1
datatransferkit@3.1.1  hdf5-vol-log@1.4.0  mfem@4.6.0
==> 158 installed packages
Singularity> █
```

E4S 24.02 Support for GPUs: Intel

```
$ singularity run e4s-oneapi-x86_64-24.02.sif
Singularity> H1=$(spack find --format /{hash} +level_zero)
Singularity> H2=$(spack find --format /{hash} +sycl)
Singularity> spack find $H1 $H2
-- linux-ubuntu22.04-x86_64 / oneapi@2024.0.2 -----
amrex@24.01 blaspp@2023.11.05 ginkgo@1.7.0 kokkos@4.2.00 lapackpp@2023.11.05 slate@2023.08.25 tau@2.33.1
arborx@1.5 cabana@0.6.0 heffte@2.4.0 kokkos@4.2.00 petsc@3.20.3 sundials@6.7.0 upcxx@2023.9.0
==> 14 installed packages
Singularity> spack find -x
-- linux-ubuntu22.04-x86_64 / gcc@11.4.0 -----
hdf5@1.12.3 papi@7.1.0

-- linux-ubuntu22.04-x86_64 / oneapi@2024.0.2 -----
adios@1.13.1 darshan-runtime@3.4.4 hdf5-vol-async@1.7 mgard@2023-03-31 pumi@2.2.8 sz@2.1.12.5
adios2@2.8.3 darshan-util@3.4.4 hdf5-vol-cache@v1.1 mpark-variant@1.4.0 py-cinemas@1.3 sz3@3.1.7
aml@0.2.1 datatransferkit@3.1.1 hdf5-vol-log@1.4.0 mpiutils@0.11.1 py-h5py@3.8.0 tasmanian@8.0
aml@0.2.1 dealii@9.5.1 heffte@2.4.0 nccmp@1.9.1.0 py-jupyterhub@1.4.1 tau@2.33.1
amrex@24.01 ecp-data-vis-sdk@1.0 heffte@2.4.0 nco@5.1.6 py-libensemble@1.1.0 tau@2.33.1
amrex@24.01 exago@1.6.0 hpx@1.9.1 netlib-scalapack@2.2.0 py-petsc4py@3.20.2 trilinos@13.0.1
arborx@1.5 exaworks@0.1.0 hypre@2.30.0 nrm@0.1.0 py-warp@23.08 trilinos@15.0.0
arborx@1.5 faodel@1.2108.1 intel-oneapi-mpi@2021.11.0 omega-h@9.34.13 qthreads@1.18 turbine@1.3.0
argobots@1.1 flecsi@2.2.1 kokkos@4.2.00 openmpi@5.0.1 raja@2022.10.4 umap@2.1.0
ascent@0.9.2 flit@2.1.0 kokkos@4.2.00 openpmd-api@0.15.2 rempi@1.1.0 umpire@2022.10.0
axom@0.8.1 flux-core@0.58.0 kokkos-kernels@4.2.00 papyrus@1.0.2 scr@3.0.1 unifyfs@2.0
bolt@2.0 fortrilinos@2.3.0 kokkos-kernels@4.2.00 parallel-netcdf@1.12.3 slate@2023.08.25 upcxx@2023.9.0
boost@1.84.0 gasnet@2023.9.0 lammps@20230802.2 parsec@3.0.2209 slate@2023.08.25 upcxx@2023.9.0
bricks@2023.08.25 ginkgo@1.7.0 legion@23.06.0 pdt@3.25.2 slepc@3.20.1 variorum@0.7.0
butterflypack@2.4.0 ginkgo@1.7.0 libnrm@0.1.0 petsc@3.20.3 stc@0.9.0 veloc@1.7
cabana@0.6.0 globalarrays@5.8.2 libquoo@1.3.1 petsc@3.20.3 strumpack@7.2.0 vtk-m@2.0.0
cabana@0.6.0 gmp@6.2.1 libunwind@1.6.2 phist@1.12.0 sundials@6.7.0 wannier90@3.1.0
caliper@2.10.0 gotcha@1.0.5 loki@0.1.7 plasma@23.8.2 sundials@6.7.0 xyce@7.8.0
chai@2022.03.0 gptune@4.0.0 mercury@2.3.1 plumed@2.9.0 superlu@5.3.0 zfp@0.5.5
charliecloud@0.35 gromacs@2023.3 metall@0.25 precice@2.5.0 superlu-dist@8.2.1
conduit@0.8.8 h5bench@1.4 mfem@4.6.0 pruners-ninja@1.0.1 swig@4.0.2-fortran
==> 126 installed packages
Singularity> █
```

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



E4S 24.02 Support for GPUs: Intel Data Center GPU Max (aka PVC)

```
[$ singularity run e4s-oneapi-x86_64-24.02.sif
[Singularity> clinfo -l
Platform #0: Intel(R) FPGA Emulation Platform for OpenCL(TM)
  |-- Device #0: Intel(R) FPGA Emulation Device
Platform #1: Intel(R) OpenCL
  |-- Device #0: Intel(R) Xeon(R) Silver 4410T
Platform #2: Intel(R) OpenCL Graphics
  |-- Device #0: Intel(R) Data Center GPU Max 1100
[Singularity> spack find -dl hypre
-- linux-ubuntu22.04-x86_64 / oneapi@2024.0.2 -----
zru7exj hypre@2.30.0
zpg4uz3      gmake@4.4.1
2qi2xp2      intel-oneapi-mpi@2021.11.0
bfvkvxz      openblas@0.3.26
kpcnpil      perl@5.38.0
3hes7b4      berkeley-db@18.1.40
tpb5mkt      bzip2@1.0.8
7zwrc6j      diffutils@3.9
dlt7okv      libiconv@1.17
z6er6dm      gdbm@1.23
mc7mfjt      readline@8.2
py23jjv      ncurses@6.4
ja3taxz      pkgconf@1.9.5
qzqmxiw      zlib-ng@2.1.5

==> 1 installed package
[Singularity> which dpcpp
/opt/intel/oneapi/compiler/2024.0/bin/dpcpp
[Singularity> which icpx
/opt/intel/oneapi/compiler/2024.0/bin/icpx
[Singularity> which mpiifx
/opt/intel/oneapi/mpi/2021.11/bin/mpiifx
Singularity> █
```

E4S 24.02 packages in oneAPI containers are now built with Intel compilers with Intel MPI

24.02 Release: 122+ Official Products + dependencies (gcc, ppc64le)

1: adios2	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/adios2-2.9.2-5q5v15lpzmxobujst2v2ts6qqultqjnl
2: alquimia	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/alquimia-1.1.0-xke5dbutys22d77dfqlpi3wqpp4sr4we
3: aml	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/aml-0.2.1-xxrddsxxdrno2rvbfw2lqsnwauuc5t1j
4: amrex	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/amrex-24.01-hugvv5o35nm36pudyvuxx5y7g5bp3zzr
5: arborx	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/arborx-1.5-dpfdgdcggo5c256pmvpesaxj653ete2iw
6: argobots	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/argobots-1.1-mkrjub4uyen7hoali3kr63kj2m4cfduv
7: ascent	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/ascent-0.9.2-an7y4an2q3z553usqq4xm6zr25cmeyeh
8: axom	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/axom-0.8.1-wv3xmeenyloprjo55w4mcroryshbemhyp
9: blaspp	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/blaspp-2023.11.05-item4osempfzcyjg2bcdc7spygepttj
10: bolt	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/bolt-2.0-wuf4ig4oqsopggcjoxwy3r6d3rw5xou4
11: bricks	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/bricks-2023.08.25-2ivsswy2lmez4yboxz2g45qgdzh5zbp4
12: butterflypack	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/butterflypack-2.4.0-vblaiupihjvwbjdnby5mo3yaops2khfa
13: cabana	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/cabana-0.6.0-ll dih6scvktwauvlx246c3i4sfkcdni
14: caliper	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/caliper-2.10.0-cyqwbftchbznrbm3nc5razd7qqg4utw
15: camp	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/camp-2022.10.1-57yc2wvrd4uq2xmzqgftsjsksh6ceinx
16: chai	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/chai-2022.03.0-mnj2xurzajvvrn27rdzmy7wdfnokcc3
17: charliecloud	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/charliecloud-0.35-o4uwfvhtvss2t7oxiur4fb6aakkheo3i
18: cp2k	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/cp2k-2024.1-xey7kmuo7q2jvzpjfifdexnmpvj36rxt
19: conduit	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/conduit-0.8.8-srp3zkdkxsn7ikqas6fwltameppjg5on
20: darshan-runtime	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/darshan-runtime-3.4.4-6mbdtvt53dff32qqet22h7zbjy7vr35c
21: datatransferkit	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/datatransferkit-3.1.1-7pkvazhicpyf6yrb4qcqzmkreilm2xmz
22: dyninst	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/dyninst-12.3.0-vn3kabflea4xm24obvrq5j4wt2tu2wh
23: ecp-data-vis-sdk	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/ecp-data-vis-sdk-1.0-wvdbjlwlycbcg4fhgqzmajrco4pd4wp
24: exago	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/exago-1.6.0-ykzmjwbhwsdmagv5gy3nygyxyqywp2h
25: exaworks	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/exaworks-0.1.0-f5qqslmipih3ghxdlucokurcn6wsmc
26: faodel	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/faodel-1.2108.1-r6wixzybad26e6x7zsu753nsaggb7kt4
27: flecsi	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/flecsi-2.2.1-x5vwlk7oxtonkjpaaqnhmlcvkyzspeh
28: flit	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/flit-2.1.0-6uvpzojtp4lwl2yuyucpavqcfukoqcd
29: flux-core	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/flux-core-0.58.0-julahjgbbhoiml6qsolptzcidtzf5jkuc
30: flux-sched	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/flux-sched-0.32.0-okcabo755ab2k33e43y7ewy5wfkvr2
31: fortrilinos	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/fortrilinos-2.3.0-6php2j7p3dhs3j27tkh4udlu3wi5smxq
32: gasnet	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/gasnet-2023.9.0-ys2azjjk6u4xvt2s6ca6v2v26lukifg
33: ginkgo	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/ginkgo-1.7.0-7sjpvydbjg33l6zoorxxbcrcp3xupdrj
34: globalarrays	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/globalarrays-5.8.2-6nfjxqc6h4okj17pne2dpqppcy4hmzom
35: gotcha	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/gotcha-1.0.5-5ilfdy2gfwswjy64wmvogy323kf6ho3in
36: gptune	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/gptune-4.0.0-ws7pwxr5vyndzewaantjrf1jqticjv7o
37: gromacs	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/gromacs-2023.3-dcqe575bzst3gqizhxytgd3iukw3a
38: h5bench	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/h5bench-1.4-nh6ctn6jgklu3tnohldzrdjwoajyxns
39: hdf5	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hdf5-1.14.3-uwyt7vvgj76xfelfifm6w3if2xz5xz
40: hdf5-vol-async	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hdf5-vol-async-1.7-rjymicz5wglrg3vnxlv2yfituh4in5by
41: hdf5-vol-cache	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hdf5-vol-cache-v1.1-ak6dzztxzvqebwg6rujue4eusunkee6

GPU runtimes for IBM Power

- CUDA 12.3
- NVHPC 23.11

Languages

- Julia with MPI and CUDA
- Python

EDA Tools

- Xyce

CFD Tools

- OpenFOAM

AI packages for NVIDIA GPU

- TensorFlow
- PyTorch
- LBANN



24.02 Release: 122+ Official Products + dependencies (gcc, ppc64le)

42:	hdf5-vol-log	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hdf5-vol-log-1.4.0-rnxshnopjahslo2aprakh5r437een3ep
43:	heffte	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/heffte-2.4.0-jbajlownymgk2jdss2ihx6jbaiekni4
44:	hiop	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hiop-1.0.0-udfo2pbsp6t7pj5eltile2ohghgalhvv
45:	hpctoolkit	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hpctoolkit-2023.08.1-q4gwj53adcbssbiiqsd6icjuobqpaезу
46:	hpx	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hpx-1.9.1-hzzez7mprcseh3t653avyrwhvcir24b6
47:	hypre	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hypre-2.30.0-werssrxnmvjzghjid67z4lqmdtcj56jd
48:	kokkos	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/kokkos-4.2.00-o3jqfghg6ipv4tppkpnpn53gidhfnqde
49:	kokkos-kernels	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/kokkos-kernels-4.2.00-q3dufrmkjyrrk4txxrmzx63dgsfftt7g
50:	lammps	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/lammps-20230802.2-lnvoktfrtidpitdcccnoabaqfv5oua4c6
51:	lapackpp	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/lapackpp-2023.11.05-7q3mjxzt4z4hzby3pig2lpn7pj54wxw5
52:	lbann	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/lbann-0.104-imdc66dotonmerc5camppe6rpw4ljdqn
53:	legion	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/legion-23.06.0-pimbo3z4xauc2p6pljgappyioblosmft
54:	libnrm	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/libnrm-0.1.0-laxddnxsiqu6gncdifektjrrj6wkddiy6
55:	libpressio	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/libpressio-0.95.1-thqddw3jjh3phdtl3ief03vreh3u33uk
56:	libquo	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/libquo-1.3.1-hpxkhdcy2wo7yy4a7p3plbdysjfybnp
57:	loki	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/loki-0.1.7-zzjmrbyhvyvnh2tm43pwjxrxz6xkzyt
58:	magma	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/magma-2.7.2-cahm2antfbfsf3rug52dc7ntj6jbdg2j
59:	mercury	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mercury-2.3.1-uy72eqdfvqgodcnzlx4wtdwvkrbdurzd
60:	mgard	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mgard-2023-03-31-qdbs3q12p2bhs6f2vaerrbibod3efqc3
61:	metall	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/metall-0.25-47w5sph2pk2qgczc5cmkmlt235oxmvfd
62:	mfem	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mfem-4.6.0-xlcp32lyuf6l5lywrmkzne4rwftorzj4
63:	mpark-variant	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mpark-variant-1.4.0-sh43qm5a2wghz5iwkum7mynee7t5zdr2
64:	mpich	/usr/local/mpich/install/mpich
65:	mpifileutils	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mpifileutils-0.11.1-bzmwd5n66ye34v3tu34mv3jrhtdied3f
66:	nccmp	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/nccmp-1.9.1.0-bpmjwz3rdfueuly4f4crulkwakt dhjt g
67:	nco	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/nco-5.1.6-3csraps4ul2kbrxgbdpamozsisd26gne
68:	netcdf-c	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/netcdf-c-4.9.2-w5r17olreipvypjbhfdwjmmdlhtmh2wp
69:	netlib-scalapack	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/netlib-scalapack-2.2.0-qcazeqm74tya6lvmddgcjbniswkrwk6dd
70:	nrm	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/nrm-0.1.0-ih2k72yhpc65yfsr14yrirb4okvfx7
71:	omega-h	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/omega-h-9.34.13-wu6hvonq25egioejq3qxldslmfknkxr
72:	openfoam	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/openfoam-2312-uhzwt46n14z2iwoeciuybkg16ccml1x
73:	openmpi	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/openmpi-5.0.1-zitxe4u4wewwo4lvzgrbdemy55furrx6
74:	openpmd-api	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/openpmd-api-0.15.2-2nq5pwnp4trxmjn7ai7j26fkbfdysbb
75:	papi	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/papi-7.1.0-eyp6czwm2uuqnaj4lvck752k34kfawfa
76:	papyrus	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/papyrus-1.0.2-gmf6werpe36rfn4wixpi3xaxsigcgsst
77:	parallel-netcdf	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/parallel-netcdf-1.12.3-cjfc773cnory3f3yrerz434z7ygi56f
78:	paraview	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/paraview-5.11.2-o7alhry656hkb22uhkwmroalntyo2crv
79:	parsec	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/parsec-3.0.2209-5p25ds0ea4d75yzfgtutpvwdjiahfcny
80:	pdt	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/pdt-3.25.2-6hncbcwj66y2kuhvxehihmi7rtwkgc2
81:	petsc	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/petsc-3.20.3-qid2evxvlotunbv4gapbtmstl7i3alu5
82:	plasma	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/plasma-23.8.2-jbn7mcyexzteeaugk5jkolecqc4emr

24.02 Release: 122+ Official Products + dependencies (gcc, ppc64le)

```
83: plumed /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/plumed-2.9.0-swuscal3rdncfcpsh3dx6yvtvbhsmkx5
84: precice /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/precice-2.5.0-ijqnoc3purfo7ruquw4w7dd4676szcin
85: pruners-ninja /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/pruners-ninja-1.0.1-2snxci4tchnkjbvxjknbmqivv4cslik7
86: pumi /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/pumi-2.2.8-2zi5iehwapnzrrn3ens5frvvhqay7in3
87: py-cinemasci /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-cinemasci-1.3-27c5hriwor4arwer3bhvim6cgecokzzz
88: py-jupyterhub /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-jupyterhub-1.4.1-f52md365puankvcdtqd4w7unz7j3kysw
89: py-libensemble /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-libensemble-1.1.0-txrv7geddljxgkn64vzmgfiwz7s6ijty
90: py-parsl /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-parsl-2023.08.21-prai3jybytzgciicd6yofaumniudbcb
91: py-radical-pilot /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-radical-pilot-1.20.0-kpjih2zqwfvugpakf5y5fqixxsj2oly5
92: py-radical-saga /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-radical-saga-1.20.0-tjohn4jmmmm4gyx4pundtlqzbzzkhcsp
93: qthreads /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/qthreads-1.18-ccjrdytsccqpgm3ywr4xm7aqis7v4m5p
94: quantum-espresso /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/quantum-espresso-7.3-66qrplfwrw65foppips47mqzk7pt52xh
95: raja /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/raja-2022.10.4-hqzbr7jeronbqciie6qlabcai3w5grl
96: rempi /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/rempi-1.1.0-mtrxdw5ycr4lzs5qeuf4npsvtc5mygj
97: scr /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/scr-3.0.1-wcax6z2zdqro3mncw5zlrkfbjjqsyw
98: slate /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/slate-2023.08.25-xezth23gtyb36ztx52savc2nwhoqzuda
99: slepc /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/slepc-3.20.1-vy62tnc25xhgeapzbrxtoiwbhmqszilm
100: stc /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/stc-0.9.0-b7cmomhumzdf3kvpcyk3potr7x5ctox
101: strumpack /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/strumpack-7.2.0-y6dzyt2qqp3pw622e33nvhqamfhw71a
102: sundials /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/sundials-6.7.0-rwqqownyhpmdzo6pua44tclqsb4a6q
103: superlu /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/superlu-5.3.0-cwpgjefdt54c6mtuaixzh6pexbvipn7
104: superlu-dist /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/superlu-dist-8.2.1-7dkdt5lvocjay27nfag7yas16jpkarlj
105: swig /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/swig-4.1.1-7zdl5y7gugwv7bze5x553hxghirgpm
106: sz /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/sz-2.1.12.5-klmqlixoyiuzxnmkgnbgey5esiueb5di
107: sz3 /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/sz3-3.1.7-cwxvy7sit4yp4413tw266po542s5u57a
108: tasmanian /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/tasmanian-8.0-ioosv7a6xiyjbv2n6iq762mmyhtr7ijo
109: tau /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/tau-2.33.1-qibd4g5h35s7kyreky51wgthxo5nswmu
110: trilinos /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/trilinos-15.0.0-j4nq5pboovqkvcapswtsdllh3mkzdc7
111: turbine /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/turbine-1.3.0-p4ebye3wtev26zgbibimcqdttxfutiha
112: umap /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/umap-2.1.0-ktzs6eefjmva2dj2s72ubtqnx2oi4yae
113: umpire /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/umpire-2022.10.0-fdqmw5moex2tew7i4aq3dvlpsgm1qnty
114: unifyfs /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/unifyfs-2.0-kiotvsqahcr254ng46anfamn13kpljfy
115: upcxx /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/upcxx-2023.9.0-zhmoyegt2ogbdbl157lndqvo5t5m5l1tr
116: veloc /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/veloc-1.7-yn4gvj2l2ucybj7kqqnhe6tjkyggjec
117: visit /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/visit-3.3.3-lwfls3dyzg4aslir2japfkx5dz7q3jzmz
118: vtk-m /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/vtk-m-2.1.0-z2y3jp5pk7fedztcdbfhuaks7c14p6t
119: wannier90 /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/wannier90-3.1.0-fzvxevlqxa4refd6c7jrl7k77ilxfpx
120: warpx /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/warpx-23.08-yt3vytjmxp62ho5vbjdmb2oi7cjdrr
121: xyce /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/xyce-7.8.0-fyvke3w6kf324fh5536tsnxhgjhcxdp
122: zfp /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/zfp-1.0.0-tdfdz4m5keequkl12gfbh3pc1b6bgnm2
```

Supports
IBM Power10 and
Power 9 processors



E4S 24.02 Support for GPUs: NVIDIA CUDA on IBM ppc64le

```
$ singularity run e4s-cuda70-ppc64le-24.02.sif
[Singularity> lscpu | grep "Model name"
Model name: POWER10 (architected), altivec supported
[Singularity> spack find +cuda
-- linux-ubuntu20.04-ppc64le / gcc@9.4.0 -----
adios2@2.9.2      camp@2022.10.1   gromacs@2023.3   kokkos@4.2.00    ncc1@2.19.3-1    slate@2023.08.25  umpire@2022.10.0
aluminum@1.4.1   camp@2022.10.1   hefffte@2.4.0    kokkos@4.2.00    nvcomp@2.2.0     slepc@3.20.1      upcxx@2023.9.0
amrex@24.01      chai@2022.03.0   hiop@1.0.0       kokkos-kernels@4.2.00  omega-h@9.34.13  strumpack@7.2.0   vtk-m@2.1.0
arborx@1.5       cusz@0.3.1       hpctoolkit@2023.08.1  lammps@20230802.2  papi@7.1.0       sundials@6.7.0    zfp@0.5.5
axom@0.8.1       dihydrogen@0.3.0  hp@1.9.1         lapackpp@2023.11.05  paraview@5.11.2  superlu-dist@8.2.1
blaspp@2023.11.05  ecp-data-vis-sdk@1.0  hwloc@2.9.1     lbann@0.104       parsec@3.0.2209  tasmanian@8.0
bricks@2023.08.25  exago@1.6.0      hwloc@2.9.1     legion@23.06.0    petsc@3.20.3     tau@2.33.1
cabana@0.6.0     flecsi@2.2.1     hydrogen@1.5.3   magma@2.7.2       petsc@3.20.3     trilinos@14.4.0
caliper@2.10.0   flux-core@0.58.0  hypre@2.30.0    mgard@2.7.2       raja@0.14.0      umpire@6.0.0
camp@0.2.3       ginkgo@1.7.0     kokkos@4.1.00   mgard@2023-03-31  raja@2022.10.4   umpire@2022.10.0
==> 64 installed packages
[Singularity> spack find -x
-- linux-ubuntu20.04-ppc64le / gcc@9.4.0 -----
adios@1.13.1     darshan-runtime@3.4.4  hdf5-vol-cache@v1.1  metall@0.25      plasma@23.8.2     swig@4.0.2-fortran
adios2@2.7.1    darshan-util@3.4.4    hdf5-vol-log@1.4.0   mfem@4.6.0       plumed@2.9.0      sz@2.1.12.5
adios2@2.9.2    datatransferkit@3.1.1  hdf5-vol-log@1.4.0   mfem@4.6.0       precice@2.5.0     sz3@3.1.7
alquimia@1.1.0  dyninst@12.3.0        hefffte@2.4.0        mgard@2023-03-31  pruners-ninja@1.0.1  tasmanian@8.0
aml@0.2.1       ecp-data-vis-sdk@1.0  hefffte@2.4.0        mgard@2023-03-31  pumi@2.2.8        tasmanian@8.0
amrex@24.01     ecp-data-vis-sdk@1.0  hpctoolkit@2023.08.1  mpark-variant@1.4.0  py-cinemasci@1.3  tau@2.33.1
amrex@24.01     exago@1.6.0          hpctoolkit@2023.08.1  mpich@4.1.2       py-h5py@3.8.0     tau@2.33.1
arborx@1.5      exago@1.6.0          hp@1.9.1             mpifileutils@0.11.1  py-jupyterhub@1.4.1  trilinos@13.0.1
arborx@1.5      exaworks@0.1.0       hpx@1.9.1            nccmp@1.9.1.0     py-libensemble@1.1.0  trilinos@14.4.0
argobots@1.1    faodel@1.2108.1      hypre@2.30.0         nco@5.1.6         py-petsc4py@3.20.2  trilinos@15.0.0
ascent@0.9.2    flecsi@2.2.1         hypre@2.30.0         netlib-scalapack@2.2.0  py-warpx@23.08     turbine@1.3.0
axom@0.8.1      flecsi@2.2.1         kokkos@4.2.00        nrm@0.1.0         qthreads@1.18      umap@2.1.0
axom@0.8.1      flit@2.1.0          kokkos@4.2.00        nvhpc@23.11       quantum-espresso@7.3  umpire@2022.10.0
bolt@2.0        flux-core@0.58.0     kokkos-kernels@4.2.00  omega-h@9.34.13   raja@2022.10.4     umpire@2022.10.0
boost@1.84.0    flux-core@0.58.0     kokkos-kernels@4.2.00  omega-h@9.34.13   raja@2022.10.4     unifyfs@2.0
bricks@2023.08.25  fortrilinos@2.3.0    lammps@20230802.2    openfoam@2312     rempi@1.1.0        upcxx@2023.9.0
bricks@2023.08.25  gasnet@2023.9.0     lammps@20230802.2    openmpi@5.0.1     scr@3.0.1          upcxx@2023.9.0
butterflypack@2.4.0  ginkgo@1.7.0        lbann@0.104         openpmd-api@0.15.2  slate@2023.08.25   veloc@1.7
cabana@0.6.0     ginkgo@1.7.0        lbann@0.104         papi@7.1.0        slate@2023.08.25   visit@3.3.3
cabana@0.6.0     globalarrays@5.8.2   legion@23.06.0     papi@7.1.0        slepc@3.20.1       vtk-m@2.0.0
caliper@2.10.0   gmp@6.2.1           legion@23.06.0     papyrus@1.0.2     slepc@3.20.1       vtk-m@2.1.0
caliper@2.10.0   gotcha@1.0.5        libcatlyst@2.0.0-rc4  parallel-netcdf@1.12.3  stc@0.9.0          wannier90@3.1.0
chai@2022.03.0  gptune@4.0.0        libnm@0.1.0         paraview@5.11.2    strumpack@7.2.0    xyce@7.8.0
chai@2022.03.0  gromacs@2023.3     libpressio@0.95.1   paraview@5.11.2   strumpack@7.2.0    zfp@0.5.5
charliecloud@0.35  gromacs@2023.3     libquo@1.3.1        parsec@3.0.2209   sundials@6.7.0     zfp@0.5.5
conduit@0.8.8    h5bench@1.4         libunwind@1.6.2     parsec@3.0.2209   sundials@6.7.0
cp2k@2024.1     hdf5@1.12.3         loki@0.1.7          parsec@3.0.2209   superlu@5.3.0
cuda@11.4.4     hdf5@1.14.3         magma@2.7.2         pdt@3.25.2        superlu-dist@8.2.1
cusz@0.3.1      hdf5-vol-async@1.7  mercury@2.3.1       petsc@3.20.3     superlu-dist@8.2.1
==> 170 installed packages
Singularity> █
```



24.02 Release: 122+ Official Products + dependencies (gcc, aarch64)

1: adios2	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/adios2-2.9.2-kttrkhmb3t53w6e6bd6zjwrnpkagpu
2: alquimia	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/alquimia-1.1.0-oo37weogbknwcqits34cymzjg7k57ytg
3: aml	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/aml-0.2.1-emjezjsnrhvb3osv7fimjtyrfd4va3fg
4: amrex	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/amrex-24.01-a6eukfnxd4i3zpmah3asgje5owmaufxz
5: arborx	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/arborx-1.5-wuufubz7c2xaijj4io35tbmnlmltbtwr
6: argobots	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/argobots-1.1-6xtoicjumtncj4mfjvw6bamxqth6hy
7: ascent	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/ascent-0.9.2-p23zg3o3rn27okh6eeao5cdztzpfcoch
8: axom	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/axom-0.8.1-qv7krybgptvdhgzp427sdf677khfgb4b
9: blaspp	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/blaspp-2023.11.05-1jjudzxc6c6b4qmkiwme6gvrdrwvztb5p
10: bolt	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/bolt-2.0-mtvbvpvng2vo2dserystizqva51lt64p
11: butterflypack	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/butterflypack-2.4.0-3cgnbhiqma43le6qdlndupnxrcldbunf
12: cabana	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/cabana-0.6.0-tsw33wg452v55y5oxouwsp3u7gcjwv3m
13: caliper	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/caliper-2.10.0-zp6m12jdbt3gffulid5ustuqsi7bgnqx
14: camp	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/camp-2022.10.1-eessck5jqyxc4ra7imggzj4pbohasdp
15: chai	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/chai-2022.03.0-aflnyzsbitb6t4nipojgds1m76ggj
16: charliecloud	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/charliecloud-0.35-wg7p6gfhnbu6z2odd2ag4fhgjm4rdo6t
17: conduit	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/conduit-0.8.8-jqougwpnw6goknh2pcxjhgfkkxspq7sv
18: cp2k	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/cp2k-2024.1-pf176kwc2lweumbjppfizj7j3wzsq7u
19: cusz	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/cusz-0.3.1-vpgfbjaqtctsss232cgp2mtduzwohy6g
20: darshan-runtime	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/darshan-runtime-3.4.4-p433exfriwrrwgbuopxndnuq7as7ox
21: datatransferkit	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/datatransferkit-3.1.1-k6vo4hvqijy4n57ugtne1tgqwod347wo
22: dealii	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/dealii-9.5.1-oslws4c4aj7zzm5hmgwsv3v37x37rmve
23: dyninst	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/dyninst-12.3.0-4czjfp3xlngisn3qvez3o56m7upvzwig
24: ecp-data-vis-sdk	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/ecp-data-vis-sdk-1.0-kwzcykrkvid15xb7rztas7r6e6ynzc4m
25: exago	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/exago-1.6.0-to7iejuw4d5esrxhyl3zrim4ybkikhag
26: exaworks	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/exaworks-0.1.0-65isqloxfijbasgzmn3me67dje27r4zy
27: exago	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/exago-1.6.0-to7iejuw4d5esrxhyl3zrim4ybkikhag
28: faodel	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/faodel-1.2108.1-kuky2hpmesdgbhfykzgzunwoc2f23c
29: flecsi	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/flecsi-2.2.1-2cilao4m4i6263sjfuvt6prg3qd7czh
30: flit	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/flit-2.1.0-xpwmclbwhi6slwq4feukhrr2uovhlgm
31: flux-core	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/flux-core-0.58.0-nmbkrfi32fkhkvidg2fuyj2fttus2x6g
32: flux-sched	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/flux-sched-0.32.0-qorvsiz57y2oreiwk2y3fhkg4jayd354
33: forttilinos	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/forttilinos-2.3.0-bjhsopv3froe2lszxaomrawhqzpk4i
34: gasnet	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/gasnet-2023.9.0-5pqtqpjoqgmzjbz374bhrihqarc2fsn2
35: ginkgo	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/ginkgo-1.7.0-oorqdf6at7joazfu7b3w7yrq6jphhkof
36: globalarrays	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/globalarrays-5.8.2-avjllwizcic3tzxydpa5dkqw7edcc5jgx
37: gotcha	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/gotcha-1.0.5-dqqwcqkia73u472n375ogjmswsv4hbo
38: gptune	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/gptune-4.0.0-52zv7j6opfqx3dwz2jdyz2lqdbvghi752
39: gromacs	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/gromacs-2023.3-7sauoid7w4hrnwvt615qlvfb5gwmeac5
40: h5bench	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/h5bench-1.4-whmhqgy7jccyhi4o2h2reyyhfwykr
41: hdf5	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/hdf5-1.14.3-vsbqwqsrrv2fomnxpobi2tj77ahwxz4

GPU runtimes for aarch64

- CUDA 12.3
- NVHPC 23.11

Languages

- Julia with MPI and CUDA
- Rust
- Python

EDA

- Xyce

AI packages for NVIDIA GPU

- TensorFlow
- PyTorch
- JAX
- Horovod
- LBANN



24.02 Release: 122+ Official Products + dependencies (gcc, aarch64)

```
42: hdf5-vol-async /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/hdf5-vol-async-1.7-hplf4ehpy4od42hn54f6dm2lninac2gg
43: hdf5-vol-cache /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/hdf5-vol-cache-v1.1-ursgc6bix4jdsnix43ncp22sweaapabd
44: hdf5-vol-log /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/hdf5-vol-log-1.4.0-wi33ys5absjy2itb6sgip3dim6dnfubg
45: heffte /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/heffte-2.4.0-ondtnrv6c2tm264olzbvmpmu2fnxryg5
46: hiop /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/hiop-1.0.0-u6bo5itjyeeonmynbcnllqhv33xt5hda
47: hpctoolkit /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/hpctoolkit-2023.08.1-hcvzvnvipgrlvvygpheigz3ikqboepdad
48: hpx /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/hpx-1.9.1-gtzswputhxdl5rdfwr6uxm64qrda3355
49: hypre /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/hypre-2.30.0-wx5bd6pnchocdtxope4dvbjando7s52r
50: kokkos /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/kokkos-4.2.00-j2i2ww6lr7h6beljspveimfmgsgolq2t5
51: kokkos-kernels /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/kokkos-kernels-4.2.00-4wvtjqjp5yqoo5cniwzcey4jqhyobkn6
52: lammmps /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/lammmps-20230802.2-p6awcyjum55npgaliwzjnoeff6hsenb
53: lapackpp /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/lapackpp-2023.11.05-mos1264wawa5xemuo3hmxfvuti25p6hx
54: lbann /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/lbann-0.104-zuy7dtkca4if3jg3wqrcsrbylar7cvzk
55: legion /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/legion-23.06.0-ytxhii33m7djm2rva6toanx2gtfy6p7y
56: libnm /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/libnm-0.1.0-l6p3f4kl5wmayhe2ucgj6zw6pcoz3p3r
57: libpressio /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/libpressio-0.95.1-imn2jqomrqgyjsjia4rmlq6zje4t5mae
58: libquo /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/libquo-1.3.1-hdz4nk334p5l6yfmua5o77f3knepkncv
59: loki /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/loki-0.1.7-fsnaymhtxgwjcof535t6gsbiud6nfnngk
60: magma /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/magma-2.7.2-zuhv6fsxqpubt7kvpxnjbd5fkmkzpx7ck
61: mercury /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/mercury-2.3.1-imbfgwq7e56anrwiighpsyppt5yxfzn
62: metall /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/metall-0.25-we2qcvtur32lepbuona3t7wycql3rrpmz
63: mfem /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/mfem-4.6.0-3gqjclu75t2skwt6hid3wvox5axh5fub
64: mgard /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/mgard-2023-03-31-ldyiz5yrpxdsduccj4xkgclcktz6m7k6s
65: mpark-variant /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/mpark-variant-1.4.0-snnlmg6fxrta3lm3jbmzh4mdsww36uq6
66: mpich /usr/local/mpich/install/mpich
67: mpifileutils /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/mpifileutils-0.11.1-ydvweshg35oark26q2gxyclrjtkg2fyfa
68: nccmp /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/nccmp-1.9.1.0-imwubvqkqn7woobnx737uh7zffejsmte
69: nco /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/nco-5.1.6-56d3wsdenoymgvbxah62rrylo5poa6zc
70: netcdf-c /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/netcdf-c-4.9.2-hi5nh7qhetrxfl5zoursctu77ujjkhf
71: netlib-scalapack /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/netlib-scalapack-2.2.0-e7wblchppr7uiuurjgk754cwgxgoanka
72: nrm /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/nrm-0.1.0-v2xg7jkb5r7azf5zc3qi7rfj4uaodatg
73: omega-h /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/omega-h-9.34.13-vir2a5xgolu5swcehhoin4jz13rdwz6m
74: openfoam /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/openfoam-2312-lntbxzjw5avn2ufpsfoawxtfquvwcgtn
75: openmpi /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/openmpi-5.0.1-pyx1mtwchnud3tcsjdx3jneuzjyogn4
76: openpmd-api /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/openpmd-api-0.15.2-qt6n6yobl7hhkeuj67qk2k4nciu2vfqex
77: papi /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/papi-7.1.0-n6haxpbq6qfy3ht6ldiuykrqksfhhw4m
78: papyrus /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/papyrus-1.0.2-vf65ruavmkv3kjsotcehxohfolw7fuce
79: parallel-netcdf /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/parallel-netcdf-1.12.3-2le7h7gwpd6maacpwhqwy6bh32o6vwa5
80: paraview /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/paraview-5.11.2-3nfbg2zvczifh5xbaeowuncscbkhqrft
81: parsec /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/parsec-3.0.2209-n5yoym5akc54xomtcoi2mjaiej5ivmqv
82: pdt /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/pdt-3.25.2-6x6wii1314r7xyuxbhkdlix7izbyjb3
```



24.02 Release: 122+ Official Products + dependencies (gcc, aarch64)

```
83: petsc /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/petsc-3.20.3-omqpk5efvmzyetd4huvop73anggpdmqi
84: phist /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/phist-1.12.0-v7v7pduhppy5taynj2p45uiesfehlp4
85: plasma /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/plasma-23.8.2-m22imniq5hhokzn43p52vyba2hycrswx
86: plumed /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/plumed-2.9.0-fnuqluohdkeyvk4vkvzju3kr5i3wign
87: precice /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/precice-2.5.0-niv4xglfod5nyaz76sr6pdzgp6ramxu4
88: pruners-ninja /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/pruners-ninja-1.0.1-z3tyciuu4srnzworfkrpr3omk2upm44
89: pumi /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/pumi-2.2.8-n4zpvkyveu6q2kqsg5dccioc7hzhvkjs
90: py-cinemasci /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/py-cinemasci-1.3-2iy5evmiwx2hpsi4pwbvd2ng2cqnvf7
91: py-jupyterhub /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/py-jupyterhub-1.4.1-xrgyxvpdwc7vkz3twjkcj3pkkb6zpe4
92: py-libensemble /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/py-libensemble-1.1.0-6eb5eqwxgsiihpsb4mmhjb2vo5opsofy
93: py-parisl /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/py-parisl-2023.08.21-gs373547qgilqjztipvar2dr4yd6hrw2
94: py-radical-saga /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/py-radical-saga-1.20.0-7tnqeth4po7d7fa2h2l1jgyoyga32ew4b
95: qthreads /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/qthreads-1.18-t5lv5dms6poie4bw3lidymy6y532kfv
96: quantum-espresso /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/quantum-espresso-7.3-5tbttdtpouky5ipzadlmznmh74izt
97: raja /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/raja-2022.10.4-w5actnsbdcqrfrfkgdqncvtl6bw736d
98: rempi /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/rempi-1.1.0-4lze5q42irsf7edwjdlt2z3mxwmjoiqj
99: scr /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/scr-3.0.1-bgmd6qvsnedhncppgx7re2p2z1zn7me
100: slate /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/slate-2023.08.25-3gtrgnbhmy6r7eumapbsnc3iidjw544
101: slepc /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/slepc-3.20.1-io4hsewq4vga2zsi7loy22kwjdrk5cqcx
102: stc /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/stc-0.9.0-22fdtc4m3hdekqqvriycdhgbxzlutord
103: strumpack /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/strumpack-7.2.0-gq2atgdcx7mfqnbfasnrvdqqccpurq3my
104: sundials /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/sundials-6.7.0-4n6qxnbnh2wu3kqqsrpw7hjziwklw4plh
105: superlu-dist /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/superlu-dist-8.2.1-5m7y53hi4co2uvc5f4hhfjjjthkhtti6
106: swig /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/swig-4.1.1-3yzbd7cq4pdeqnwxmqwbl7qvcx4ha3s
107: sz3 /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/sz3-3.1.7-hxyhqh2djdjvk4jn4eidb4pakelcfnml
108: tasmanian /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/tasmanian-8.0-xqj2bp74b54jiwyzwphle7bhlqtsfafv
109: tau /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/tau-2.33.1-5olezrmv5wqk34p5np26olnj7pakanqa
110: trilinos /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/trilinos-15.0.0-yfrrczlecy3o4jrrg7kmjyljyepemip
111: turbine /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/turbine-1.3.0-utwgcuprl5wepymfmuuqms44d2ve5yqc
112: umap /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/umap-2.1.0-ltyeodewetaq4mf4obrjycougfhjvxsx
113: umpire /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/umpire-2022.10.0-bfpnmpiad5zknfqrwgp65hbwdtdsviyh
114: unifyfs /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/unifyfs-2.0-iwpegkfejeaznznnot6zmdj6aqrscsq475
115: upcxx /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/upcxx-2023.9.0-js4qzj2sed4p27xoz4x3zwetvtymw25e
116: veloc /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/veloc-1.7-g32acxiez7e73hyngs725wcv2ubg57h
117: visit /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/visit-3.3.3-hzxnqhtqgyjxudy7lqonooyxnjwiy7ir
118: vtk-m /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/vtk-m-2.1.0-435mjexttfgenzrzk4mumhb3ljg2q7w
119: wannier90 /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/wannier90-3.1.0-zg5hgk3aqt1zvypyezfk6ywuua4drfv1
120: warpx /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/warpx-23.08-t2oobl2ebymaioxgcrd4k1sv6h7ect4
121: xyce /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/xyce-7.8.0-i3mxbzw63ld7xxazpmpcbwej55g2af7v
122: zfp /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.4.0/zfp-1.0.0-4pwayxi462jhmlsyyy3cxqzjkygucu
```

E4S Support for GPUs: CUDA on aarch64

```

$ singularity run --nv e4s-cuda90-aarch64-24.02.sif
Singularity> spack find -x +cuda
-- linux-ubuntu20.04-aarch64 / gcc@11.4.0 -----
adios2@2.9.2      chai@2022.03.0    gromacs@2023.3    kokkos-kernels@4.2.00  papi@7.1.0        strumpack@7.2.0    umpire@2022.10.0
amrex@24.01      cusz@0.3.1        heffte@2.4.0      legion@23.06.0         parsec@3.0.2209    sundials@6.7.0     vtk-m@2.1.0
arborx@1.5       ecp-data-vis-sdk@1.0  hpctoolkit@2023.08.1  libpressio@0.95.1      petsc@3.20.3       superlu-dist@8.2.1  zfp@0.5.5
axom@0.8.1       flecsi@2.2.1      hp@1.9.1          magma@2.7.2            raja@2022.10.4     tasmanian@8.0
cabana@0.6.0     flux-core@0.58.0   hypre@2.30.0      mfem@4.6.0            slate@2023.08.25   tau@2.33.1
caliper@2.10.0   ginkgo@1.7.0      kokkos@4.2.00     mgard@2023-03-31      slepc@3.20.1       trilinos@14.4.0
==> 39 installed packages
Singularity> spack find -x
-- linux-ubuntu20.04-aarch64 / gcc@11.4.0 -----
adios@1.13.1      darshan-runtime@3.4.4  hdf5-vol-cache@v1.1  mfem@4.6.0            plumed@2.9.0       swig@4.0.2-fortran
adios2@2.7.1      darshan-util@3.4.4    hdf5-vol-log@1.4.0   mfem@4.6.0            precice@2.5.0       sz@2.1.12.5
adios2@2.9.2      datatransferkit@3.1.1  heffte@2.4.0         mgard@2023-03-31      pruners-ninja@1.0.1  sz3@3.1.7
alquimia@1.1.0    dealii@9.5.1          heffte@2.4.0         mgard@2023-03-31      pumi@2.2.8          tasmanian@8.0
aml@0.2.1         dyninst@12.3.0        hpctoolkit@2023.08.1  mpark-variant@1.4.0  py-cinemasci@1.3    tasmanian@8.0
amrex@24.01       ecp-data-vis-sdk@1.0  hpctoolkit@2023.08.1  mpich@4.1.2          py-h5py@3.8.0       tau@2.33.1
amrex@24.01       ecp-data-vis-sdk@1.0  hp@1.9.1            mpifileutils@0.11.1  py-jupyterhub@1.4.1  tau@2.33.1
arborx@1.5        exago@1.6.0           hp@1.9.1            nccmp@1.9.1.0        py-libensemble@1.1.0  trilinos@13.0.1
arborx@1.5        exaworks@0.1.0        hypre@2.30.0         nco@5.1.6            py-petsc4py@3.20.2  trilinos@14.4.0
argobots@1.1      faodel@1.2108.1       hypre@2.30.0         netlib-scalapack@2.2.0  py-warp@23.08       trilinos@15.0.0
ascent@0.9.2      flecsi@2.2.1          kokkos@4.2.00        nrm@0.1.0            qthreads@1.18       turbine@1.3.0
axom@0.8.1        flecsi@2.2.1          kokkos@4.2.00        nvhpc@23.11          quantum-espresso@7.3  umap@2.1.0
axom@0.8.1        flit@2.1.0           kokkos-kernels@4.2.00  omega-h@9.34.13      raja@2022.10.4       umpire@2022.10.0
bolt@2.0          flux-core@0.58.0      kokkos-kernels@4.2.00  openfoam@2312        raja@2022.10.4       umpire@2022.10.0
boost@1.79.0      flux-core@0.58.0      lammps@20230802.2    openmpi@5.0.1        rempi@1.1.0          unifyfs@2.0
butterflypack@2.4.0  fortrilinos@2.3.0    lbann@0.104          openpmd-api@0.15.2   scr@3.0.1            upcxx@2023.9.0
cabana@0.6.0      gasnet@2023.9.0       legion@23.06.0       papi@7.1.0           slate@2023.08.25     veloc@1.7
cabana@0.6.0      ginkgo@1.7.0          legion@23.06.0       papi@7.1.0           slate@2023.08.25     visit@3.3.3
caliper@2.10.0    ginkgo@1.7.0          libcatalyst@2.0.0-rc4  papyrus@1.0.2        slepc@3.20.1         vtk-m@2.0.0
caliper@2.10.0    globalarrays@5.8.2    libnm@0.1.0          parallel-netcdf@1.12.3  slepc@3.20.1         vtk-m@2.1.0
chai@2022.03.0    gmp@6.2.1             libpressio@0.95.1    paraview@5.11.2      stc@0.9.0            wannier90@3.1.0
chai@2022.03.0    gotcha@1.0.5          libpressio@0.95.1    parsec@3.0.2209      strumpack@7.2.0      xyce@7.8.0
charliecloud@0.35  gptune@4.0.0          libquo@1.3.1         parsec@3.0.2209      strumpack@7.2.0      zfp@0.5.5
conduit@0.8.8     gromacs@2023.3        libunwind@1.6.2      pdt@3.25.2           sundials@6.7.0       zfp@0.5.5
cp2k@2024.1       gromacs@2023.3        loki@0.1.7           petsc@3.20.3          sundials@6.7.0
cuda@11.8.0       h5bench@1.4           magma@2.7.2          petsc@3.20.3          superlu@5.3.0
cuda@12.3.0       hdf5@1.12.3           mercury@2.3.1        phist@1.12.0          superlu-dist@8.2.1
cusz@0.3.1        hdf5-vol-async@1.7    metall@0.25          plasma@23.8.2         superlu-dist@8.2.1
==> 164 installed packages
Singularity>

```

E4S 24.02 supports CUDA architectures 75 (T4), 80 (A100), as well as 90 (H100/GH200)



E4S DOE LLVM Release: x86_64, ppc64le, and aarch64

```
Singularity> spack find -x
```

```
-- linux-ubuntu20.04-x86_64 / clang@16.0.2 -----
```

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

```
-- linux-ubuntu20.04-x86_64 / gcc@11.1.0 -----
```

```
cmake@3.26.3 llvm-doe@16.0.2
```

```
Singularity> spack find -x
```

```
-- linux-ubuntu20.04-ppc64le / clang@16.0.2 -----
```

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

```
-- linux-ubuntu20.04-ppc64le / gcc@11.1.0 -----
```

```
cmake@3.26.3 llvm-doe@16.0.2
```

```
Singularity> spack find -x
```

```
-- linux-ubuntu20.04-aarch64 / clang@16.0.2 -----
```

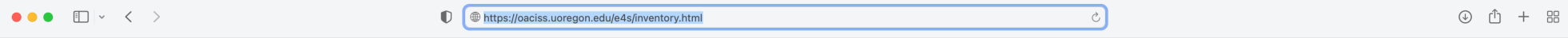
```
adios@1.13.1 cabana@0.5.0 globalarrays@5.8.2 heffte@2.3.0 mfem@4.5.2 parsec@3.0.2209 sundials@6.5.1 umpire@2022.03.1  
aml@0.2.0 chai@2022.03.0 gmp@6.2.1 hypre@2.28.0 mpark-variant@1.4.0 pdt@3.25.1 superlu@5.3.0 upcxx@2023.3.0  
amrex@23.05 charliecloud@0.32 gotcha@1.0.4 legion@23.03.0 mpich@4.1.1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

```
-- linux-ubuntu20.04-aarch64 / gcc@11.1.0 -----
```

```
cmake@3.26.3 llvm-doe@16.0.2
```



E4S Build Cache for Spack 0.22.0 hosted at U. Oregon



E4S Build Cache for Spack 0.22.0

To add the latest release mirror to your Spack (recommended):

```
$> spack mirror add E4S https://cache.e4s.io/24.02
$> spack buildcache keys -it
```

Or, add the combined cache to your Spack:

```
$> spack mirror add E4S https://cache.e4s.io
$> spack buildcache keys -it
```

123,589 total packages

Last updated 2024-02-14 13:35 PST

- All Arch
- PPC64LE
- X86_64
- AARCH64
- All OS
- Centos 7
- Centos 8
- RHEL 7
- RHEL 8
- Ubuntu 18.04
- Ubuntu 20.04

- [adiak@0.1.1](#)
- [adiak@0.2.1](#)
- [adiak@0.2.2](#)
- [adios2@2.5.0](#)
- [adios2@2.6.0](#)
- [adios2@2.7.0](#)
- [adios2@2.7.1](#)
- [adios2@2.8.0](#)
- [adios2@2.8.3](#)
- [adios@1.13.1](#)
- [adlbx@0.9.2](#)
- [adlbx@1.0.0](#)
- [adol-c@2.7.2](#)
- [alquimia@1.0.10](#)
- [alquimia@1.0.9](#)
- [alsa-lib@1.2.3.2](#)
- [amg@1.2](#)
- [aml@0.1.0](#)
- [aml@0.2.0](#)
- [amr-wind@ascent](#)

- Over 120K binaries!
- No need to recompile from source code



E4S 24.02 AWS image: ami-08c2daa0fb4864b90 in US-West-2 (OR)

The screenshot displays a Linux desktop environment with the following components:

- Desktop Environment:** Includes icons for Home, Trash, Firefox, and Gnome-terminal.
- ParaView 5.9.0:** A 3D visualization of a mesh with a color scale for pressure, ranging from 0.0e+00 to 1.2e-38.
- TAU ParaProf Statistics:** A table showing performance metrics for various components.

Name	Exclusive TIME	Inclusive TIME
.TAU application	8.784	218.852
Belos: Operation Op*x	0.629	0.706
Belos: PseudoBlockGmresSolMgr total solve time	0.615	65.591
Belos: ICGS[2]: Orthogonalization	0.22	18.854
Belos: Operation Op*x	1.672	2.32
Belos: Operation Prec*x	7.617	43.327
Ifpack2::Chebyshev::apply	4.76	25.865
Kokkos::parallel_for Kokkos::View::initialization [DualV	0.003	0.003
Kokkos::parallel_for Kokkos::View::initialization [MV::D	0.004	0.004
Kokkos::parallel_for Kokkos::View::initialization [export	0.002	0.002
Kokkos::parallel_for Kokkos::View::initialization [import	0.002	0.002
- Terminal Window:** Shows the output of the Singularity module command, listing various software modules and their versions.


```
(base) [tutorial@ip-172-31-6-250 Zoltan]$ singularity run --/ecp.sing
Singularity> module avail
Rebuilding cache, please wait ... (written to file) done.

----- /spack/modules/linux-ubuntu20.04-x86_64/mpich/3.4.2-jpicv6o/Core -----
adiak/0.2.1-4vc          omega-h/9.34.1-wt2
adios/1.13.1-zh4        openpmd-api/0.14.3-el6
adios2/2.7.1-4qz       papyrus/1.0.1-3g6
adlbx/1.0.0-h27         parallel-netcdf/1.12.2-phc
alquimia/1.0.9-m25     paraview/5.9.1-s6m
amrex/21.11-cuda-7bb    parmetis/4.0.3-vhi
amrex/21.11-cuda-zxc    parsec/3.0.2012-cuda-qxe
amrex/21.11-ny5         parsec/3.0.2012-cuda-45r
amrex/21.11-rocm-6cm   parsec/3.0.2012-ljc
arborx/1.1-qda         petsc/3.16.1-cuda-prk
arpack-ng/3.8.0-xhd     petsc/3.16.1-cuda-sjk
ascent/0.7.1-aij       petsc/3.16.1-cuda-372
axl/0.3.0-6n4          petsc/3.16.1-dor
axl/0.5.0-xdi          pflotran/3.0.2-wqt
axom/0.5.0-xaa         pfunit/3.3.3-7ln
butterflypack/2.0.0-oto phist/1.9.5-dsi
cabana/0.4.0-hcz       precice/2.3.0-hov
```

E4S AWS

- Intel oneAPI
- CUDA
- NVHPC
- ROCm
- AWS DCV
- Spack Build Cache
- ECP: Nalu-Wind
- Trinos
- OpenFOAM
- ParaView
- TAU
- Docker
- Shifter
- Charliecloud
- E4S Singularity...

E4S for Commercial Cloud Platforms for EDA on AWS

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

The screenshot displays a Linux desktop environment with the following components:

- Xschem - top.sch:** A schematic editor window showing a circuit diagram with components like PERP, VPP, CAP, RERAM, ES, VARACTORS, MIM, PFET, NFET, RES, DIODE, PNP, and NPN. It includes a 'Layers' menu and various simulation options.
- Terminal:** A terminal window showing the installation and configuration of EDA tools. The commands and output are as follows:


```
[tutorial@ip-172-31-43-167 eda]$ module load eda
[tutorial@ip-172-31-43-167 eda]$ pwd
/usr/local/packages/eda
[tutorial@ip-172-31-43-167 eda]$ ls
act-022223          netgen-1.5          qucs-s-0.0.23
adms-022223        ngspice-39          rggen-021423
boost-1.80.0       nvc-021423          riscv-gnu-toolchain-rv32ia-021423
fault-021423       open_pdks-1.0.393  SRC
gds3d-021423       openroad-021123    swift-5.7.3
ghdl-021423        opensta-021123     tar
graywolf-0.1.6     opentimer-021123   verilator-021423
gtkwave-gtk3-021423 or-tools-021123    xcircuit-3.10.30
irsim-9.7.116      padding-021423     xschem-021323
iverilog-021423    pcb-3.0.98          xscheme-gaw-021423
klayout-0.28.5     qflow-1.4           yosys-021123
magic-8.3           grouter-1.4
[tutorial@ip-172-31-43-167 eda]$ python3
Python 3.7.16 (default, Dec 15 2022, 23:24:54)
[GCC 7.3.1 20180712 (Red Hat 7.3.1-15)] on linux
Type "help", "copyright", "credits" or "license()" for more information.
>>> import openram
>>> import cocotb
>>> import amaranth
>>> import edalize
>>> import gdsfactory
2023-02-23 02:21:35.822 | INFO | gdsfactory.config:<module>:51 - Load '/home/tutorial/.local/lib/python3.7/site-packages/gdsfactory' 6.38.0
2023-02-23 02:21:35.876 | INFO | gdsfactory.technology.layer_views: _init_
:780 - Importing LayerViews from KLayout layer properties file: /home/tutorial/.local/lib/python3.7/site-packages/gdsfactory/generic_tech/klayout/tech/layers.lyp.
mp>>> import gdspys
>>> import pyverilog
>>> import spyci
>>> import volare
>>> import siliconcompiler
>>>
[tutorial@ip-172-31-43-167 eda]$ ls /usr/local/packages/eda/SRC/OpenLane/
AUTHORS.md      designs         install         pdks             requirements.txt
configuration   docker          Jenkinsfile    README.md        run_designs.py
CONTRIBUTING.md docs            klayoutrc      regression_results scripts
default.cvcrc   env.py          LICENSE        requirements_dev.txt tests
dependencies    flow.tcl        Makefile       requirements_lint.txt venv
[tutorial@ip-172-31-43-167 eda]$ magic --version
8.3.365
[tutorial@ip-172-31-43-167 eda]$ conda activate openfasoc
(openfasoc) [tutorial@ip-172-31-43-167 eda]$ magic --version
8.3.303
(openfasoc) [tutorial@ip-172-31-43-167 eda]$
```
- Qflow Manager:** A window showing a checklist of EDA tasks such as Preparation, Synthesis, Placement, Static Timing Analysis, Routing, Post-Route STA, Migration, DRC, LVS, and GDS.
- KLayout 0.28.5:** A window showing a 3D visualization of a circuit component, likely a capacitor or inductor, with a large 'K' overlaid on it.

E4S EDA on AWS

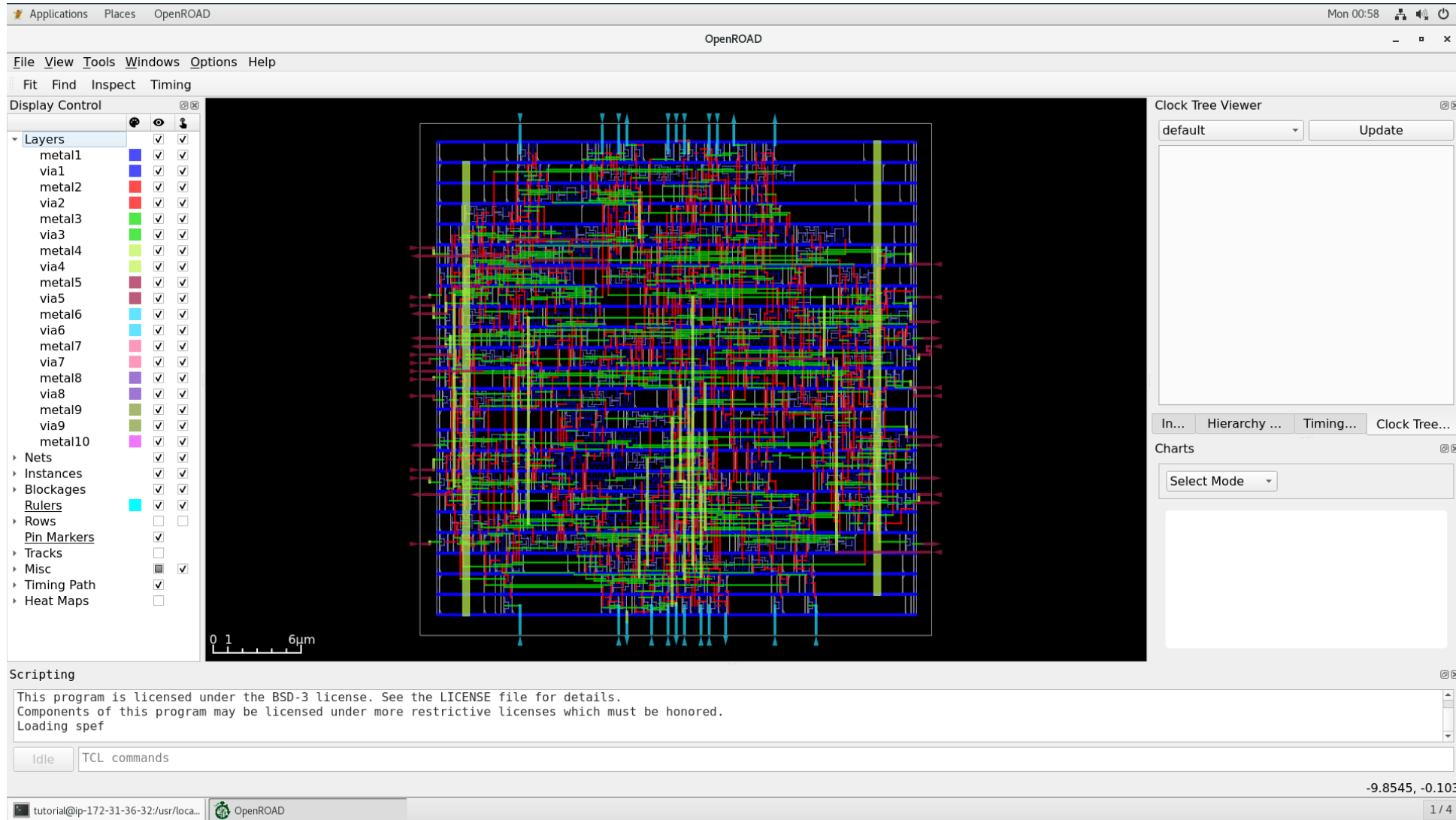
- Magic
- ACT
- Klayout
- Qflow
- Xschem
- Xcircuit
- Yosys
- Volator
- OpenROAD
- OpenLane
- iVerilog
- Gtkwave
- Irsim
- Qrouter
- Fault
- GDS3D
- Rggen
- Python tools
 - Cocotb
 - Amaranth
 - Edalize
 - Gdsfactory
 - Gdspys
 - OpenRAM
 - Gdstk
 - Silicon compiler
 - Volare ...
- PDKs
 - GF
 - Skywater



<https://e4s.io/eda>

E4S for Commercial Cloud Platforms for EDA on AWS

- E4S: HPC Software Ecosystem – a curated software portfolio for Electronic Design Automation. Microwatt CPU (IBM) in OpenROAD.



E4S EDA on AWS

- Magic
- ACT
- Klayout
- Qflow
- Xschem
- Xcircuit
- Yosys
- Volator
- OpenROAD
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- Gtkwave
- Irsim
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 - Edalize
 - Gdsfactory
 - Gdspy
 - OpenRAM
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OpenROAD GUI

E4S for Commercial Cloud Platforms for EDA on AWS

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

#	Packages currently in E4S	URL	#	Packages currently in E4S	URL
1	Magic	http://opencircuitdesign.com/magic/	13	Yosys	https://github.com/YosysHQ/yosys
2	Xyce	https://xyce.sandia.gov	14	Xcircuit	http://opencircuitdesign.com/xcircuit/
3	NGSPICE	https://ngspice.sourceforge.io	15	Graywolf	https://github.com/rubund/graywolf
4	KLayout	https://www.klayout.de	16	OpenSTA	https://github.com/The-OpenROAD-Project/OpenSTA
5	Qflow	http://opencircuitdesign.com/qflow	17	OpenTimer	https://github.com/OpenTimer/OpenTimer
6	OR-Tools	https://developers.google.com/optimization	18	Qrouter	http://opencircuitdesign.com/qrouter/
7	IRSIM	http://opencircuitdesign.com/irsim/	19	Xschem	https://github.com/silicon-vlsi-org/eda-xschem
8	OpenROAD	https://github.com/The-OpenROAD-Project/OpenROAD	20	RISC-V GNU Toolchain	https://github.com/riscv-collab/riscv-gnu-toolchain
9	OpenLane	https://openlane.readthedocs.io/	21	Fault: Design for Test	https://github.com/AUCOHL/Fault
10	OpenFASOC	https://openfasoc.readthedocs.io/	22	NVC	https://github.com/nickg/nvc
11	Open_PDKs	http://opencircuitdesign.com/open_pdks/	23	Amaranth	https://github.com/amaranth-lang/amaranth
12	Netgen	http://opencircuitdesign.com/netgen/	24	Cocotb	https://github.com/cocotb/cocotb



<https://e4s.io/eda>

E4S for Commercial Cloud Platforms for EDA on AWS

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

#	Packages currently in E4S	URL	#	Packages currently in E4S	URL
25	Covered	https://github.com/hpretl/verilog-covered	37	Padring	https://github.com/donn/padring
26	Edalize	https://github.com/olofk/edalize	38	Pyverilog	https://github.com/PyHDI/Pyverilog
27	Gaw3-xschem	https://github.com/StefanSchippers/xschem-gaw.git	39	OpenRAM	https://github.com/VLSIDA/OpenRAM
28	GDSFactory	https://github.com/gdsfactory/gdsfactory	40	Rggen	https://github.com/rggen/rggen
29	GDSPy	https://github.com/heitzmann/gdspy	41	Spyci	https://github.com/gmagno/spyci
30	GDS3D	https://github.com/trilomix/GDS3D	42	Volare	https://github.com/efabless/volare
31	Ghdl	https://github.com/ghdl/ghdl	43	Siliconcompiler	https://github.com/siliconcompiler/siliconcompiler
32	Gtkwave	https://github.com/gtkwave/gtkwave	44	Verilator	https://github.com/verilator/verilator
33	iic-osic	https://github.com/hpretl/iic-osic.git	45	Sky130	SkyWater Technologies 130nm CMOS PDK
34	Iverilog	https://github.com/steveicarus/iverilog.git	46	Actflow	https://github.com/asynclsi/actflow.git
35	Netlistsvg	https://github.com/nturley/netlistsvg	47	Qucs-s	https://github.com/Qucs
36	Ngspyce	https://github.com/ignamv/ngspyce	48	ADMS	https://github.com/Qucs/ADMS.git
			49	Gdstk	https://heitzmann.github.io/gdstk/
			50	xcell	https://github.com/asynclsi/xcell.git



<https://e4s.io/eda>

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

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

- Usage:

```
% e4s-cl init --backend singularity --image ~/images/e4s-gpu-x86.sif --source ~/source.sh
% cat ~/source.sh
  . /spack/share/spack/setup-env.sh
  spack load trilinos+cuda cuda_arch=80
% e4s-cl mpirun -np 4 ./a.out
```



New release of e4s-cl on GitHub

The screenshot shows the GitHub repository page for `E4S-Project/e4s-cl`. The repository is public and has 11 stars and 1 fork. The main content area displays a list of files and folders with their commit history:

File/Folder	Commit Message	Time
<code>.github/workflows</code>	Updated python	10 months ago
<code>assets/images</code>	Proper image conversion	last year
<code>docs</code>	Sameer report sync	last month
<code>e4s_cl</code>	Allow non-existing paths to source scripts	last month
<code>scripts</code>	Merge branch 'makefile-cleanup' into init-update	last month
<code>tests</code>	Merge branch 'makefile-cleanup' into init-update	last month
<code>.coveragerc</code>	Introduced the coverage tool	last year
<code>.gitignore</code>	Replace setup.py with pyproject.toml	2 months ago
<code>.gitlab-ci.yml</code>	added .gitlab-ci.yml file in order to use gitlab's continuous inte...	8 months ago
<code>.readthedocs.yaml</code>	Adapt documentation build to PEP518	2 months ago
<code>CHANGELOG</code>	Update CHANGELOG	last month
<code>LICENSE</code>	Updated LICENSE	2 years ago

The right sidebar contains the 'About' section, which includes the repository description 'Container manager for E4S', the documentation link `e4s-cl.readthedocs.io`, and various tags like 'containers', 'mpi', 'singularity-container', 'shifter', 'podman', 'apptainer', and 'e4s'. The 'Releases' section shows 9 releases, with the latest release 'E4S-CL release v1.0.2' highlighted by a blue box. This release was published on Mar 31.

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



E4S: Open Source Development on GitHub

The screenshot shows the GitHub repository page for `E4S-Project / e4s`. The left sidebar displays the file structure, with the `environments/24.02` directory selected. The main content area shows the file list for `e4s / environments / 24.02 /`, including subdirectories for various architectures and a `README.md` file. The `README.md` content is displayed below, detailing the E4S Release 24.02 (February 2024) and listing the files for different hardware configurations.

Name	Last commit message	Last commit date
..		
amd64-gcc-cpu-ubuntu20.04	e4s 24.02	9 hours ago
amd64-gcc-cuda-ubuntu20.04	e4s 24.02	9 hours ago
amd64-gcc-rocm-ubuntu20.04	e4s 24.02	9 hours ago
amd64-oneapi-ubuntu22.04	e4s 24.02	9 hours ago
arm64-gcc-cpu-ubuntu20.04	e4s 24.02	9 hours ago
arm64-gcc-cuda-ubuntu20.04	e4s 24.02	9 hours ago
ppc64-gcc-cpu-ubuntu20.04	e4s 24.02	9 hours ago
ppc64-gcc-cuda-ubuntu20.04	e4s 24.02	9 hours ago
README.md	e4s 24.02	9 hours ago

E4S Release 24.02

February 2024 release of E4S

Files

- `amd64-gcc-cpu-ubuntu20.04/spack.yaml` -- Model Spack Environment for systems without GPU (amd64)
- `amd64-gcc-cuda-ubuntu20.04/spack.yaml` -- Model Spack Environment for systems with NVIDIA GPUs (amd64)
- `amd64-gcc-rocm-ubuntu20.04/spack.yaml` -- Model Spack Environment for systems with AMD GPUs (amd64)
- `amd64-oneapi-ubuntu22.04/spack.yaml` -- Model Spack Environment for systems with Intel GPUs (amd64)



<https://github.com/E4S-Project>

Release of custom E4S images: Waggle and SAGE projects

The screenshot shows the Docker Hub page for the repository `ecpe4s/waggle-ml`. The repository is owned by `ecpe4s` and was updated 13 days ago. It has 137 pulls. The 'Tags' section is active, showing a table of tags with columns for TAG, OS/ARCH, LAST PULL, and COMPRESSED SIZE. The 'latest' tag is highlighted with a blue border.

TAG	OS/ARCH	LAST PULL	COMPRESSED SIZE
latest	linux/amd64	3 days ago	9.15 GB
	linux/arm64	3 days ago	1.58 GB

`% docker pull ecpe4s/waggle-ml`

The screenshot shows the website for the SAGE project at Argonne National Laboratory. The page title is "SAGE: A Software-Defined Sensor Network". The text describes the project as building a national research infrastructure of new sensors that support programmable edge computers and machine learning within an interconnected cyberinfrastructure, spanning multiple major science instruments. The website features the Argonne National Laboratory logo, navigation menus for CAREERS, NEWS, EVENTS, STAFF DIRECTORY, RESEARCH, WORK WITH US, COMMUNITY, and ABOUT US. A sidebar on the right lists navigation options for the MCS Division, including About MCS, Research, News, Events, and Publications. Social media sharing icons for Facebook, Twitter, LinkedIn, and Email are also present. The project status is listed as "Active".

SAGE
A Software-Defined Sensor Network
Cyberinfrastructure for AI at the Edge

www.sagecontinuum.org

Thank you

<https://www.exascaleproject.org>

This research was supported by the Exascale Computing Project (17-SC-20-SC), a joint project of the U.S. Department of Energy's Office of Science and National Nuclear Security Administration, responsible for delivering a capable exascale ecosystem, including software, applications, and hardware technology, to support the nation's exascale computing imperative.

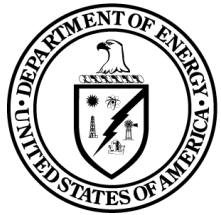


EXASCALE COMPUTING PROJECT

Thank you to all collaborators in the ECP and broader computational science communities. The work discussed in this presentation represents creative contributions of many people who are passionately working toward next-generation computational science.

Acknowledgment

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- <https://science.osti.gov/ascr>
- <https://www.pesoproject.org>

