

E4S: The Extreme-scale Scientific Software Stack Release 23.05



Release 23.05 notes

May 31, 2023

E4S 23.05: What's New?

- E4S includes support for Intel oneAPI 2023.1 software (BaseKit and HPCToolkit) in containers on x86_64 with support for HPC packages built with Intel compilers
- E4S includes support for CUDA architectures
 - 70 (V100), 80 (A100), and 90 (H100) under x86_64
 - 70 under ppc64, and
 - 75 and 80 under aarch64
- E4S includes supports ROCm for gfx908 (MI100) and gfx90a (MI200) architectures under x86_64
- E4S includes support for DOE LLVM under x86_64, ppc64le, and aarch64
- E4S includes new applications: Xyce (with pyimi), LBANN, Quantum Espresso, LAMMPS, WARPX, Dealii, and OpenFOAM.
- E4S includes support for AI/ML frameworks such as TensorFlow and PyTorch support for A100 as well as H100 GPUs is integrated in E4S 23.02
- E4S supports updates to 100+ HPC packages on x86_64, aarch64, and ppc64le, 100K+ binaries in E4S Spack Build Cache
- New E4S tools: e4s-alc (à la carte) customizes container images, e4s-cl (container launch) replaces MPI at runtime!
- Detailed documentation for installing E4S on bare-metal and using containers

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 100+ HPC, EDA (e.g., Xyce), and AI/ML packages (e.g., TensorFlow, PyTorch).
- With E4S Spack binary build caches, E4S supports both bare-metal and containerized deployment for GPU based platforms.
 - X86_64, ppc64le (IBM Power 9), 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_Apr23.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.
- Quarterly releases: E4S 23.05 released on May 31, 2023: https://e4s.io/talks/E4S_23.05.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

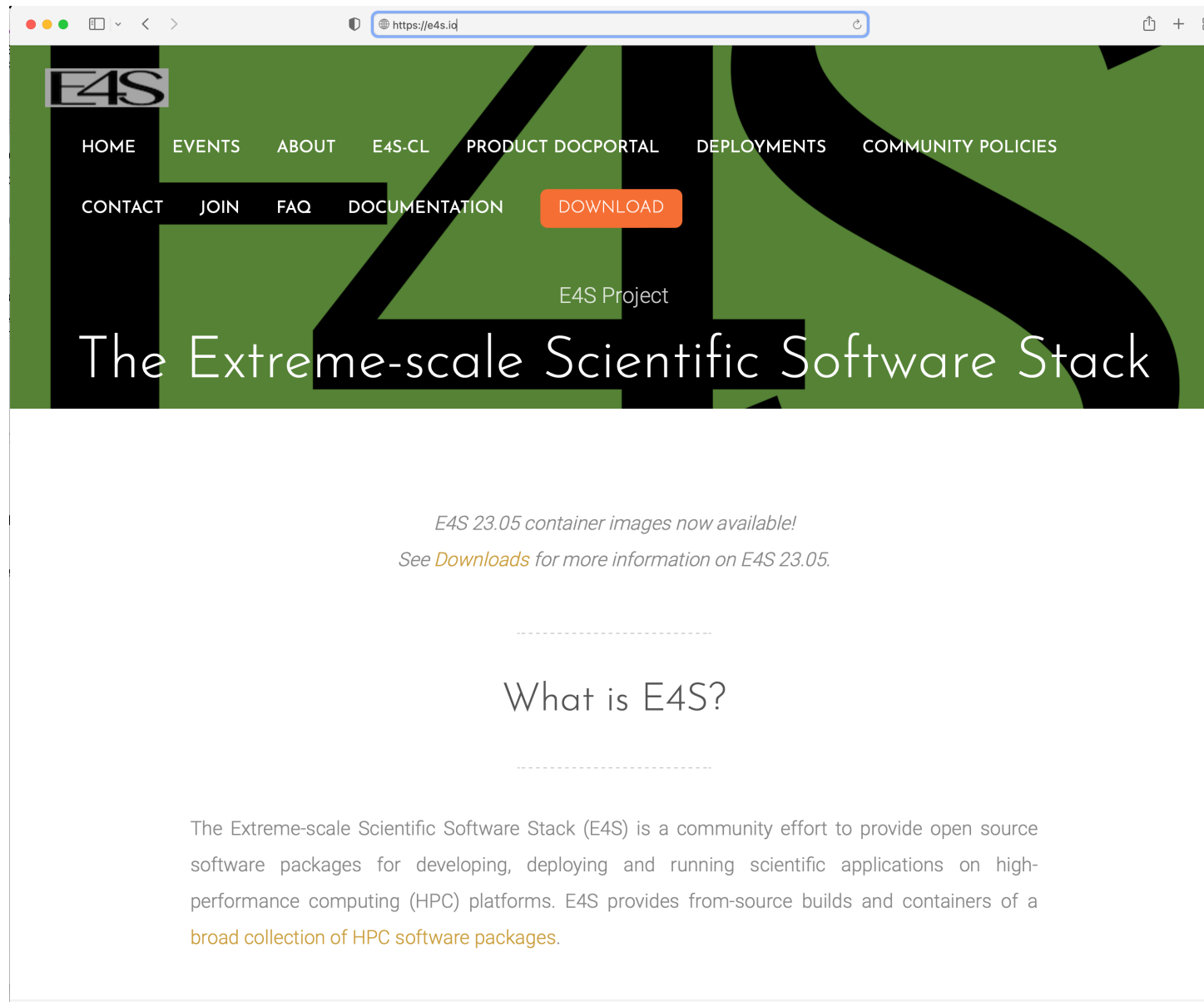


<https://e4s.io>

Lead: Sameer Shende
(U Oregon)

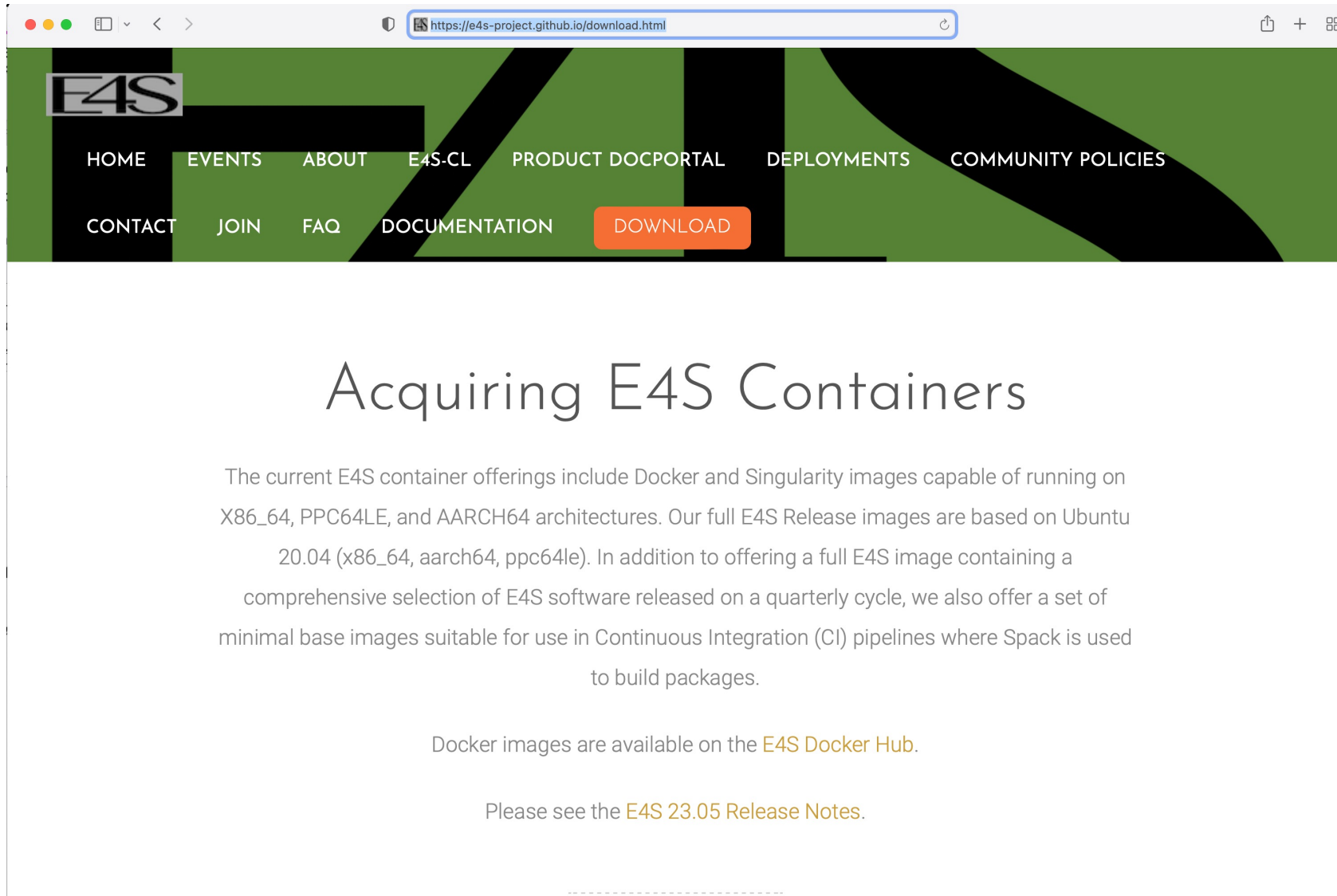
Also include other products .e.g.,
AI: PyTorch, TensorFlow (CUDA, ROCm)
Co-Design: AMReX, Cabana, MFEM
EDA: Xyce

E4S Download from https://e4s.io



The screenshot shows the E4S website homepage. The browser address bar displays "https://e4s.io". The navigation menu includes: HOME, EVENTS, ABOUT, E4S-CL, PRODUCT DOCPORTAL, DEPLOYMENTS, COMMUNITY POLICIES, CONTACT, JOIN, FAQ, DOCUMENTATION, and a prominent orange DOWNLOAD button. The main heading reads "E4S Project" followed by "The Extreme-scale Scientific Software Stack". A central announcement states: "E4S 23.05 container images now available! See [Downloads](#) for more information on E4S 23.05." Below this is a section titled "What is E4S?" with a dashed line above and below the title. The text describes E4S as a community effort to provide open source software packages for developing, deploying, and running scientific applications on high-performance computing (HPC) platforms. It mentions that E4S provides from-source builds and containers of a [broad collection of HPC software packages](#).

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



The screenshot shows a web browser window with the address bar displaying <https://e4s-project.github.io/download.html>. The website has a green and black header with the E4S logo and a navigation menu. The main content area features the title "Acquiring E4S Containers" and a paragraph of text describing the container offerings.

E4S

HOME EVENTS ABOUT E4S-CL PRODUCT DOCPORTAL DEPLOYMENTS COMMUNITY POLICIES

CONTACT JOIN FAQ DOCUMENTATION **DOWNLOAD**

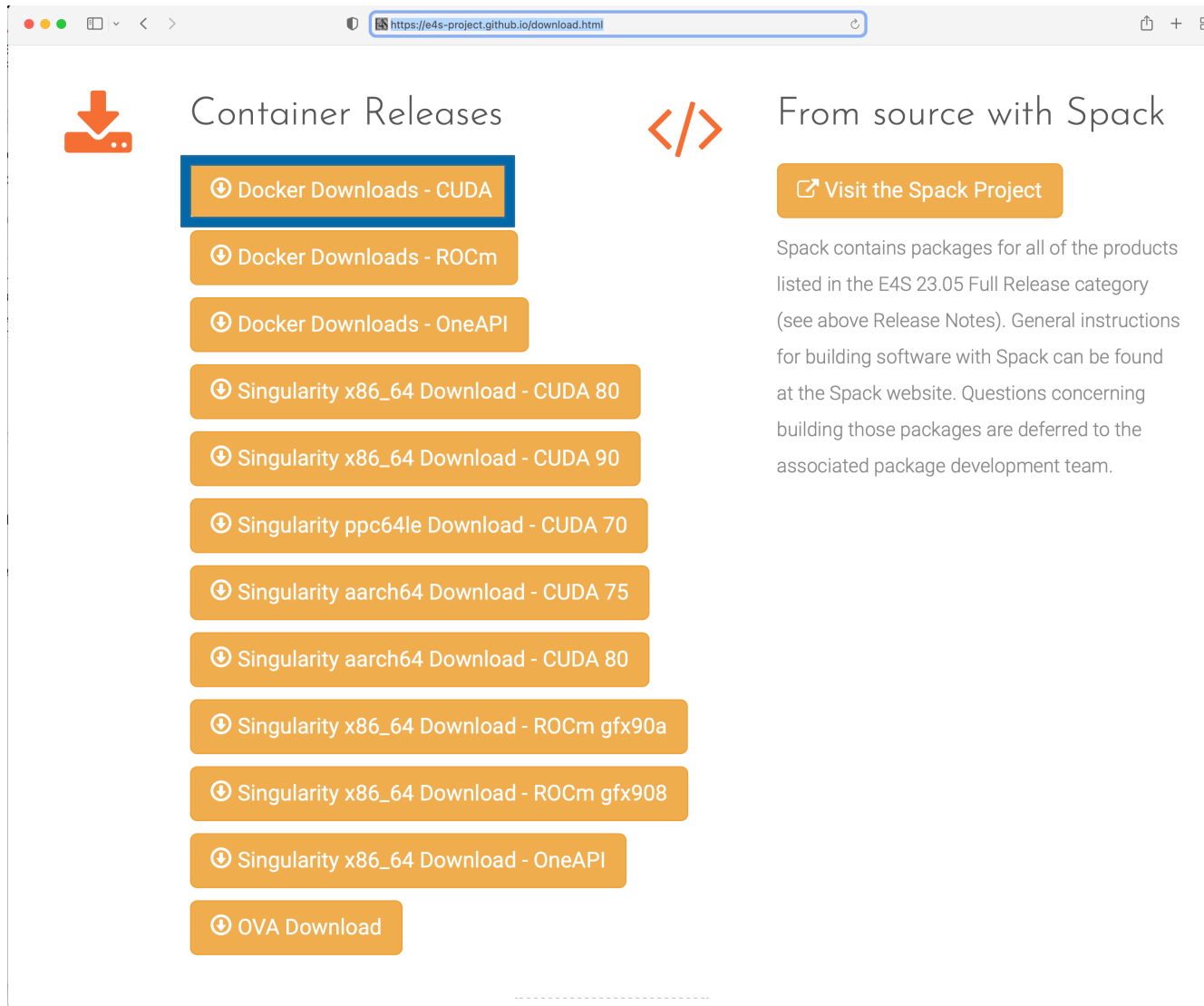
Acquiring E4S Containers

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 23.05 Release Notes](#).

Download E4S 23.05 GPU Container Images: NVIDIA, AMD, Intel



The screenshot shows a web browser window with the URL <https://e4s-project.github.io/download.html>. The page is divided into two main sections: 'Container Releases' and 'From source with Spack'. The 'Container Releases' section is highlighted with a blue border and contains a list of download links for various GPU architectures and container engines. The 'From source with Spack' section is also visible and contains a link to 'Visit the Spack Project' and a paragraph of text.

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 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 23.05 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
- 100+ products on 3 architectures

Download E4S 23.05 GPU Container Images: AMD, Intel, and NVIDIA

https://e4s-project.github.io/download.html

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:23.05  
# docker pull ecpe4s/e4s--rocm:23.05  
# docker pull ecpe4s/e4s--oneapi:23.05
```

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)	NVIDIA CUDA (X86_64, PPC64LE, AARCH64)	Intel OneAPI (x86_64)
ecpe4s/e4s-rocm:23.05	ecpe4s/e4s-cuda:23.05	ecpe4s/e4s-oneapi:23.05
e4s-rocm90a-x86_64-23.05.sif	e4s-cuda80-x86_64-23.05.sif	e4s-oneapi-x86_64-23.05.sif
e4s-rocm908-x86_64-23.05.sif	e4s-cuda90-x86_64-23.05.sif	
	e4s-cuda70-ppc64le-23.05.sif	
	e4s-cuda75-aarch64-23.05.sif	
	e4s-cuda80-aarch64-23.05.sif	

E4S base container images allow users to customize their containers

GPU Base Images

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:23.05 docker
e4s-base-rocm-x86_64-23.05.sif mirror 1

NVIDIA Multi-Arch (X86_64, PPC64LE, AARCH64)
ecpe4s/e4s-base-cuda:23.05 docker
e4s-base-cuda-x86_64-23.05.sif mirror 1
e4s-base-cuda-aarch64-23.05.sif mirror 1
e4s-base-cuda-ppc64le-23.05.sif mirror 1

Intel OneAPI (X86_64)
ecpe4s/e4s-base-oneapi:23.05 docker
e4s-base-oneapi-23.05.sif mirror 1

Minimal Spack

This image contains a minimal setup for using Spack 0.18.0 w/ GNU compilers

X86_64, PPC64LE, AARCH64
ecpe4s/ubuntu20.04 docker
ecpe4s-ubuntu20.04-x86_64-23.05.sif mirror 1
ecpe4s-ubuntu20.04-ppc64le-23.05.sif mirror 1
ecpe4s-ubuntu20.04-aarch64-23.05.sif mirror 1

- Intel oneAPI
- AMD ROCm
- NVIDIA NVHPC and CUDA

e4s-alc: a new tool to customize container images

The screenshot displays the GitHub repository for `E4S-Project/e4s-alc`. The repository is public and has 2 stars and 1 fork. The main content area shows a list of files and folders, including `e4s_alc`, `tests`, `.gitignore`, `LICENSE`, `Makefile`, `README.md`, `pyproject.toml`, and `tox.ini`. The `README.md` file is selected, showing the following content:

Operating Systems supported:

- Ubuntu ✓
- Red Hat ✓
- SUSE ✓

Backends supported:

- Docker ✓
- Podman ✓
- Singularity ✓

The right sidebar contains the following sections:

- About**: E4S à la carte is a tool that allows a user to customize a container image by adding packages to it. These can be system packages and Spack packages.
- Releases**: No releases published.
- Packages**: No packages published.
- Contributors**: 4 contributors: FrederickDeny, PlatinumCD Cameron Durbin, spoutn1k Jean-Baptiste Skutnik, sameershende Sameer Shende.

Add to a base image:

- Spack packages
- OS packages
- Tarballs

E4S 23.05 DOE LLVM and CI images

<https://e4s-project.github.io/download.html>

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](#) docker
- [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	PPC64LE	AARCH64
ecpe4s/ubuntu22.04-runner-x86_64 docker	ecpe4s/ubuntu22.04-runner-ppc64le	ecpe4s/ubuntu22.04-runner-aarch64
GitHub	docker GitHub	docker GitHub
ecpe4s/ubuntu20.04-runner-x86_64 docker	ecpe4s/ubuntu20.04-runner-ppc64le	ecpe4s/ubuntu20.04-runner-aarch64
GitHub	docker GitHub	docker GitHub
ecpe4s/ubuntu18.04-runner-x86_64 docker	ecpe4s/ubuntu18.04-runner-ppc64le	ecpe4s/rhel8-runner-aarch64 docker GitHub
GitHub	docker GitHub	
ecpe4s/rhel8-runner-x86_64 docker GitHub	ecpe4s/rhel8-runner-ppc64le docker GitHub	
ecpe4s/rhel7-runner-x86_64 docker GitHub	ecpe4s/rhel7-runner-ppc64le docker GitHub	

E4S 23.05 Detailed Documentation for Bare-metal Installation

https://e4s-project.github.io/documentation.html

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DOCUMENTATION [DOWNLOAD](#)

Extreme-scale Scientific Software Stack (E4S) version 23.05

Exascale Computing Project (ECP) Software Technologies (ST) software, Extreme-scale Scientific Software Stack (E4S) v23.05, 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 v23.05 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 v23.05 Release Notes PDF.](#)

[E4S v23.05 Spack Environment Notes.](#)

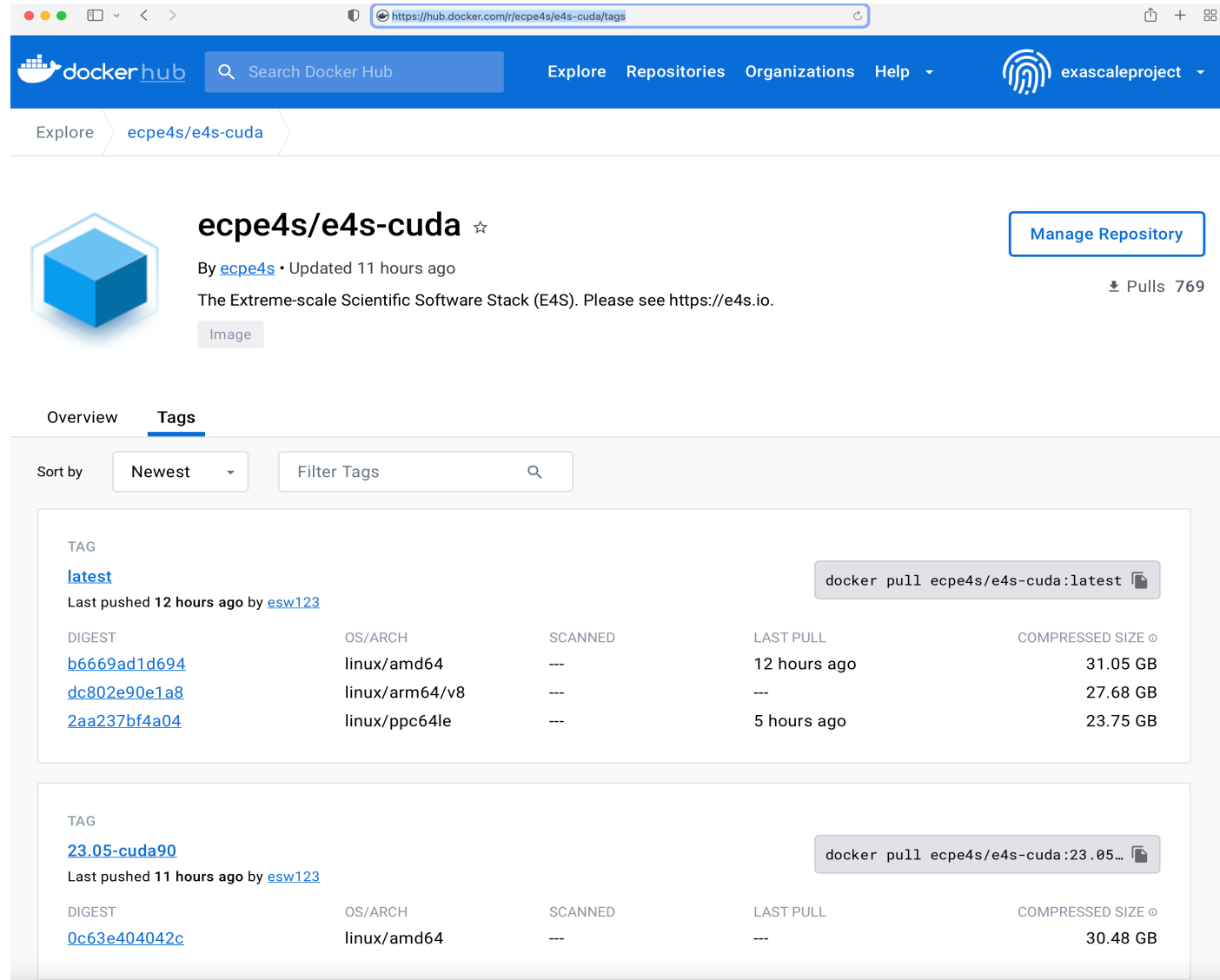
[E4S Manual Installation Instructions.](#)

[E4S Container Installation Instructions.](#)

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

Prebuilt binaries used in E4S images are stored in the E4S Build Cache.

E4S 23.05 full featured container release on Dockerhub



The screenshot shows the Docker Hub page for the repository `ecpe4s/e4s-cuda`. The page includes a search bar, navigation links, and a 'Manage Repository' button. The repository is described as 'The Extreme-scale Scientific Software Stack (E4S)'. The 'Tags' section is active, showing a list of tags with columns for TAG, DIGEST, OS/ARCH, SCANNED, LAST PULL, and COMPRESSED SIZE. The 'latest' tag is highlighted, and the '23.05-cuda90' tag is also visible.

TAG	DIGEST	OS/ARCH	SCANNED	LAST PULL	COMPRESSED SIZE
latest					
Last pushed 12 hours ago by esw123					
	b6669ad1d694	linux/amd64	---	12 hours ago	31.05 GB
	dc802e90e1a8	linux/arm64/v8	---	---	27.68 GB
	2aa237bf4a04	linux/ppc64le	---	5 hours ago	23.75 GB
TAG	DIGEST	OS/ARCH	SCANNED	LAST PULL	COMPRESSED SIZE
23.05-cuda90					
Last pushed 11 hours ago by esw123					
	0c63e404042c	linux/amd64	---	---	30.48 GB

Architectures:

- x86_64
- aarch64
- ppc64le

Software:

- CUDA 12.0
- NVHPC 23.3
- oneAPI 2023.1

E4S 23.05 base container release on DockerHub

docker hub Search Docker Hub Explore Repositories Organizations Help exascaleproject

Explore ecpe4s/e4s-base-cuda

ecpe4s/e4s-base-cuda ☆ Manage Repository

By [ecpe4s](#) • Updated 5 hours ago

Extreme-scale Scientific Software Stack (E4S) [https://e4s.io] Ubuntu 20.04 image with CUDA. ↓ Pulls 165

Image

Overview **Tags**

Sort by Newest Filter Tags

TAG [latest](#) `docker pull ecpe4s/e4s-base-cuda:...`

Last pushed 5 hours ago by [esw123](#)

DIGEST	OS/ARCH	SCANNED	LAST PULL	COMPRESSED SIZE
5ebe7f77a321	linux/amd64	---	---	18.7 GB
68b8a131065a	linux/arm64/v8	---	---	15.7 GB
9e19967783fa	linux/ppc64le	---	---	14.37 GB

TAG [23.05](#) `docker pull ecpe4s/e4s-base-cuda:...`

Last pushed 5 hours ago by [esw123](#)

DIGEST	OS/ARCH	SCANNED	LAST PULL	COMPRESSED SIZE
5ebe7f77a321	linux/amd64	---	---	18.7 GB
68b8a131065a	linux/arm64/v8	---	---	15.7 GB
9e19967783fa	linux/ppc64le	---	---	14.37 GB

Architectures:

- x86_64
- aarch64
- ppc64le

Software:

- CUDA 12.0
- NVHPC 23.3
- oneAPI 2023.1

Minimal Spack base image on Dockerhub

The screenshot shows the Docker Hub interface for the repository `ecpe4s/ubuntu18.04-spack`. The repository is categorized as a 'Container' and has been updated a month ago. It features a 'Manage Repository' button and a 'Pulls 1M+' badge. The 'Tags' section is active, showing two tags: `latest` and `0.17.1`. Both tags were pushed a month ago by user `esw123`. The table below details the digests and compressed sizes for different OS/ARCH combinations.

TAG	DIGEST	OS/ARCH	LAST PULL	COMPRESSED SIZE
<code>latest</code>	<code>95fb8df7019b</code>	linux/amd64	a day ago	382 MB
	<code>47903be536c0</code>	linux/ppc64le	a month ago	371.9 MB
<code>0.17.1</code>	<code>95fb8df7019b</code>	linux/amd64	a day ago	382 MB
	<code>47903be536c0</code>	linux/ppc64le	a month ago	371.9 MB

- Create custom container images
- 1M+ downloads!

23.05 Release: 100+ Official Products + dependencies (gcc, x86_64)

1: adios2	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/adios2-2.9.0-wr34ihoz2sk6iarctnuyxfhsctxwkvq4
2: alquimia	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/alquimia-1.0.10-gba5ayv4ps6ilmh5hc7krkoa4h3ksbvz
3: aml	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/aml-0.2.0-goqtywxw2lwciznqkc44paexlucn33v
4: amrex	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/amrex-23.05-2syxxbx3xwppc4ut7mbrmlev4ycty4ep
5: arborx	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/arborx-1.3-cvlmzk4kzetidsscc4nd4oprdivcsp31
6: archer	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/archer-2.0.0-vl5rv2ygrh4znug7rdk6jhh6t4nemk5l
7: argobots	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/argobots-1.1-f6b6was4pd7d2u2fwvpxdoqffdbate2o
8: axom	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/axom-0.7.0-epaxouqc4ul2kppggnhtvnl6fr3goik
9: bolt	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/bolt-2.0-zb4pgmqyozhf3ofvhdo26gpj2hibbc2t
10: bricks	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/bricks-r0.1-yuymne4nwfwtzckstwl6macyp6kkk2
11: butterflypack	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/butterflypack-2.2.2-kzdbd4fzvqfjn575hojafxlen2gzwx2n
12: cabana	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/cabana-0.5.0-hit7qxj2pwnvgmd5kkaeglbnvqsdgf7n
13: caliper	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/caliper-2.9.0-cthb1sk6ogn43qnufgbczjvcrawqzab
14: chai	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/chai-2022.03.0-6gi2vpoxdvy25sat6cdebunutp24i5sk
15: charliecloud	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/charliecloud-0.32-bmfm6chwp4g6mgnhjgcrh356gusbrzes
16: conduit	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/conduit-0.8.7-mfdfactk6xuqmyfqdwtiwszivxtrwho2
17: darshan-runtime	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/darshan-runtime-3.4.2-nfblomjg6ejmigmhu3dux6v7iojxnpf
18: datatransferkit	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/datatransferkit-3.1-rc3-enk32naiegjk42bex5mvuk3y3mefdef6
19: dyninst	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/dyninst-12.3.0-k3myl3szf7v3e2jccqowwglwyig4444o
20: ecp-data-vis-sdk	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/ecp-data-vis-sdk-1.0-s4ya3uqeb2ecyextvb42yprv5zy5l2qk
21: exaworks	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/exaworks-0.1.0-lxqvw3csw06pglbycqcacwatu6iln2
22: faodel	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/faodel-1.2108.1-gxc7m6ajdyb2jupcvx5qrvppe4jlcqt6
23: flecsi	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/flecsi-2.1.0-mfszzzew3vlkejgw43xuakoftuxrqnhm
24: flit	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/flit-2.1.0-3ptdgv522o5ng3euh56eci5nhaq4jctb
25: flux-sched	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/flux-sched-0.27.0-snqo4rzjtrmjkdv1kcixuw4vyt4ypie
26: fortrilinos	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/fortrilinos-2.2.0-dlxz63fh2tljmw2rje5srgfgdbx64adv
27: gasnet	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/gasnet-2023.3.0-aufps4j5ilwaosagcfyhwe4anrv6uknz
28: ginkgo	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/ginkgo-1.5.0-4gsh6pioh6qab3d67j7wtfk5qbfz7lnb
29: globalarrays	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/globalarrays-5.8.2-nzag4ztsjddm67gdurpwtirprgb3rkgz
30: gotcha	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/gotcha-1.0.4-3rwc6g46qxsit3vswvzi6icv67li57wi
31: gptune	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/gptune-4.0.0-dyxc7tkwnenjgl2edjqhvyg7eld643xx
32: h5bench	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/h5bench-1.3-34odudjnljbfxl7a44e32gwmuo6wn6
33: hdf5	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/hdf5-1.14.1-2-naucnfhfn57lxmlb3dcfls42m4hwdkeg
34: hdf5-vol-async	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/hdf5-vol-async-1.5-nwt25ouh2i5vtwvwsaijpnklgowag7ku
35: heffte	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/heffte-2.3.0-rib3o742d45ng7ukq4qq4vh3l5t5dccc
36: hpctoolkit	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/hpctoolkit-2023.03.01-sbct1delht4ntvzahpd6q5rj23fs25ar
37: hpv	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/hpv-1.9.0-374gqtjzm47p6ea3xsuahpagrq2ohgwy

GPU runtimes

- AMD (ROCm)
 - 5.4.3
- NVIDIA (CUDA)
 - 12.0
- NVHPC
 - 23.3
- Intel oneAPI
 - 2023.1

23.05 Release: 100+ Official Products + dependencies (gcc, x86_64)

38:	hypre	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/hypre-2.28.0-mozopbseodwvy7r7xklin7jnsuh5s7yi
39:	kokkos	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/kokkos-4.0.01-tgv5irdj4skczex6c2rvfty274vwuyk7
40:	kokkos-kernels	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/kokkos-kernels-3.7.00-2whrnzbzjyni42dytgehkuhke2zgaj5u
41:	lammgs	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/lammgs-20220623.3-cso7xzxuaz5jyld3n6seug2cexxbfnpc
42:	lbann	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/lbann-0.102-hf442maq5bbf5nndr4fqlyhxakndm23
43:	legion	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/legion-23.03.0-ksb4tvvggo6sfcfjiicnszyr5appehqxn
44:	libnrm	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/libnrm-0.1.0-h5ggd2cgai43porp2s2berqrsnki2j6c
45:	libpressio	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/libpressio-0.95.1-h54uerfc7gttwaokywa5cwntylrnklen
46:	libquo	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/libquo-1.3.1-e6ulmqbtpfcjjypvdqrbpkb4brzkgpf
47:	loki	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/loki-0.1.7-a4etdi45t2fbweddhjur5t5p56tiu2ca
48:	magma	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/magma-2.7.1-dapbrjq25hsqg2cztteusqkismcpnbu
49:	mercury	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/mercury-2.2.0-iap2sil3mo6g6aljvg34vtnxh2sglof
50:	metall	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/metall-0.25-2xic6pnhpbolhaknalu2qpjnw4bkvemi
51:	mfem	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/mfem-4.5.2-2f3kx62ogbv6bw6sdcybkawubvcyg2n
52:	mgard	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/mgard-2023-03-31-4maqkp6n3e2xshtu2y3tnve5ch7jdb43
53:	mpark-variant	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/mpark-variant-1.4.0-6f25xadnfdzmpweuit4yvp134katnt4s
54:	mpich	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/mpich-4.1.1-4cbi7qhusseuh6bcs6lokqwh6s3itl
55:	mpifileutils	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/mpifileutils-0.11.1-tuy2ycdl67kuv3ppp3diqy4o2bmvhok
56:	nccmp	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/nccmp-1.9.0.1-qmoiwfcpknknojwspffuvgrw3n3mphzb
57:	nco	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/nco-5.1.5-wwe7fm6df3zhc6d6qckvbcyxo5dqawpf
58:	netlib-scalapack	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/netlib-scalapack-2.2.0-3zhwrw6f2ohmbnpeec34ksb4h7svs65
59:	nrm	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/nrm-0.1.0-47ydygda2r3njdpkxyj4wrfpgfdt2zzl
60:	omega-h	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/omega-h-9.34.13-m2wmv5mmoxpoy622e6tbk7jzey2ufdvi
61:	openfoam	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/openfoam-2206-zftm6f5mhvnhxben2nzeqantgg41ll15d
62:	openmpi	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/openmpi-4.1.5-ed5u3cdcbs6dcve6ftb336v5uhwj4by
63:	openpmd-api	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/openpmd-api-0.15.1-uzamcamznyauzeem57j72gx2ascjpmju
64:	papi	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/papi-6.0.0.1-j7dmzprtcei2ifgjykb7rmkbf3gydfk7
65:	papyrus	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/papyrus-1.0.2-kuro7vtc7kh6fot5xmah6awfwgi5chm2
66:	parallel-netcdf	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/parallel-netcdf-1.12.3-mldyjplnyhw7qiljd327wda7exvpcvtf
67:	paraview	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/paraview-5.11.1-x4aqroj67nfq7gpk7w3pwlxhphfjyrno
68:	parsec	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/parsec-3.0.2209-wvchc4psqj3uotxff24xyc24xqwrzdg
69:	pdt	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/pdt-3.25.1-1x67nrs24pkbnmj7am3t75swtowtfc5
70:	petsc	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/petsc-3.19.1-bonrfxf3arijwltulzck4xqyd3ceik63
71:	phist	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/phist-1.11.2-qz36u6cuvuupj3gj5v7hmm4sdbzrdlrv
72:	plasma	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/plasma-22.9.29-2qwdll5vjs74mymdiugdhd32iibm2v3
73:	plumed	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/plumed-2.8.2-oq5243vtzgc16ex6zookbxqgaeofkzxh
74:	precice	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/precice-2.5.0-b7eniikqkee5veujb5xnuukfnz7wiwm2
75:	pumi	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/pumi-2.2.7-57q5bidz4mzlldkfpwaovebwqhvxgps3
76:	py-cinemasci	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-cinemasci-1.3-5tnt5kqnzrin5j5dmse6gdq77mteiiyz
77:	py-jupyterhub	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-jupyterhub-1.4.1-awj3cwfvd3irsm24dmr37gbhd5xniju

23.02 Release: 100 Official Products + dependencies (gcc, x86_64)

```
78: py-libensemble /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-libensemble-0.9.3-3d3tb25q2s3pa7uqscw7wlpz5rqmapa5
79: py-parsl /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-parsl-1.2.0-f7tbq4nmfecdu3nh5fw5zyddwj77zis5
80: py-radical-saga /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-radical-saga-1.20.0-wffrzdrccdd4cpst42gtqonbjni7m5pqq
81: qthreads /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/qthreads-1.16-r4ai62sxxg3os22n2xfntik7xabcvijgst
82: quantum-espresso /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/quantum-espresso-7.1-2hw2nzkjwtc4xi3hopd2oesn2ikmcb5e
83: raja /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/raja-2022.10.4-fffdno3g4c4wm6f2d5rbrehnjgv3ytw4
84: rempi /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/rempi-1.1.0-bsppojvqc4e4bf7re6u36f75dwo6wnuv
85: scr /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/scr-3.0.1-4twvdurdxeiv3ipees4y3nk64pmvtrbl
86: slate /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/slate-2022.07.00-5xkcozs6eabgn45t7uttghekbu4lanbwk
87: slepc /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/slepc-3.19.0-vqy6iy24c5wkpfdejjgql2bx32vjfbq
88: stc /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/stc-0.9.0-ocmzafclc6rsl2dop3poqjbnlyyk7vs2
89: strumpack /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/strumpack-7.1.1-7feghsapq3qe7stmbfodzcytm7tm441t
90: sundials /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/sundials-6.5.1-f23kbyw7bsam3cpka2mshks36d236yr3
91: superlu-dist /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/superlu-dist-8.1.2-ibmrgavx57kcy3fc7wdbcneuhk6axgv
92: swig /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/swig-4.1.1-cm45hunq4nk7x4ml756gur5wlaakaidha
93: sz /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/sz-2.1.12.2-bbc3ru73fa67nmr7j4jv53f6ji5e4xe
94: tasmanian /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/tasmanian-7.9-4skuz4cxghjjhlhad776xbixk3jvienk
95: tau /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/tau-2.32-qxwqmdsjoaxnrjed5mvlolax5ip273z
96: trilinos /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/trilinos-14.0.0-alm3rf45sel6ahz7ecfs5odq3eziqcah
97: turbine /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/turbine-1.3.0-sla74mxwn5michnji2aqmrf3gbphfcco
98: umap /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/umap-2.1.0-de4ftza63dmgjjgvv5uhceeunn2dvvkqig
99: umpire /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/umpire-2022.03.1-sprrgtmz5vvvsxxhwngyu7dxbghmdpij
100: unifyfs /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/unifyfs-1.0.1-q4bmwojbzaa2nnpnbc2q4flba5u5oshd
101: upcxx /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/upcxx-2023.3.0-ideeur7hshemz4ahe2col65tiryjfng
102: variorum /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/variorum-0.6.0-h3oif6j2nvgq4qzxjx773bjnef5owexx
103: veloc /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/veloc-1.6-5g5n244a6mo3i3dlcjxxlq7e3l5tv426
104: visit /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/visit-3.3.3-nt4yv7ecffq2onv5xznqja42uzt6tqlb
105: vtk-m /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/vtk-m-2.0.0-7rjk76kmbf4bmyvepvfj5qsc1kfz3uw
106: wannier90 /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/wannier90-3.1.0-dbfs2qlo2yvdxjtc65mn5d2xlnvplnzc
107: warpx /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/warpx-23.03-f2nbmfpld7xntj2lpy552upvwj6bq2
108: xyce /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/xyce-7.6.0-vt3rht5enpk1qck7m7d2z7ji64memqzw
109: zfp /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/zfp-1.0.0-ibmowr23apboprdgjrpr4eyblmibwd2w
```

Languages:

- Julia with support for MPI, and CUDA
- Python

AI products with GPU support

- Tensorflow
- Pytorch

EDA Tools:

- Xyce

3D Visualization

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

E4S 23.05 adds support for NVIDIA A100 (sm80), V100 (sm70), and H100 (sm90) GPUs

E4S Support for AI/ML frameworks with V100, A100, and H100 GPUs

```
Singularity> python
Python 3.8.10 (default, Nov 14 2022, 12:59:47)
[GCC 9.4.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import numpy
>>> import scipy
>>> import matplotlib
>>> import tensorflow
>>> tensorflow.__version__
'2.12.0'
>>> import torch
>>> torch.__version__
'2.0.0'
>>> torch.cuda.get_device_name(torch.cuda.current_device())
'NVIDIA H100 PCIe'
>>> █
```

E4S 23.05 supports NVIDIA H100 GPUs with TensorFlow 2.12.0 and PyTorch 2.0.0

E4S 23.05 Intel oneAPI 2023.1: Packages built with Intel compilers

```
Singularity> spack find -x
-- linux-ubuntu20.04-x86_64 / gcc@11.1.0 -----
papi@6.0.0.1

-- linux-ubuntu20.04-x86_64 / oneapi@2023.1.0 -----
adios@1.13.1      cabana@0.5.0      gmp@6.2.1         legion@23.03.0    netlib-scalapack@2.2.0  py-libensemble@0.9.3  sz3@3.1.7
aml@0.2.0         cabana@0.5.0      gotcha@1.0.4      libnrm@0.1.0     omega-h@9.34.13       py-petsc4py@3.19.1   tasmanian@7.9
aml@0.2.0         caliper@2.9.0     h5bench@1.3       libquo@1.3.1    openmpi@4.1.5         qthreads@1.16       tau@2.32
amrex@22.12       chai@2022.03.0    hdf5-vol-async@1.5  libunwind@1.6.2  openpmd-api@0.15.1   quantum-espresso@7.1  tau@2.32
amrex@23.05       charliecloud@0.32  hdf5-vol-log@1.4.0  loki@0.1.7      papyrus@1.0.2        raja@2022.10.4      trilinos@13.0.1
arborx@1.3        conduit@0.8.7     heffte@2.3.0      mercury@2.2.0   parsec@3.0.2209      rempi@1.1.0         turbine@1.3.0
arborx@1.3        datatransferkit@3.1-rc3  hpx@1.9.0        metall@0.25     pdt@3.25.1           slate@2022.07.00    umap@2.1.0
archer@2.0.0      exaworks@0.1.0    hypre@2.28.0      mfem@4.5.2     petsc@3.19.1         slepc@3.19.0       umpire@2022.03.1
argobots@1.1      flecsi@2.2.0      kokkos@4.0.01     mgard@2023-03-31  phist@1.11.2        stc@0.9.0          variorum@0.6.0
axom@0.7.0        flit@2.1.0        kokkos@4.0.01     mpark-variant@1.4.0  plasma@22.9.29      strumpack@7.1.1    wannier90@3.1.0
bolt@2.0          flux-core@0.49.0  kokkos-kernels@3.7.00  mpich@4.1.1    plumed@2.8.2        sundials@6.5.1
boost@1.82.0      fortrilinos@2.2.0  kokkos-kernels@3.7.00  mpifileutils@0.11.1  precice@2.5.0       superlu@5.3.0
bricks@r0.1       gasnet@2023.3.0   lammps@20220623.3  nccmp@1.9.0.1   pumi@2.2.7          superlu-dist@8.1.2
butterflypack@2.2.2  globalarrays@5.8.2  lbann@0.102       nco@5.1.5      py-h5py@3.7.0       swig@4.0.2-fortran
```

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

E4S 23.05 Intel oneAPI 2023.1: Packages built with Intel compilers

Singularity> module avail

----- /opt/intel/oneapi/modulefiles -----									
advisor/latest		compiler32/latest		dnnl-cpu-tbb/latest		inspector/latest		mpi/latest	
advisor/2023.1.0	(D)	compiler32/2023.1.0	(D)	dnnl-cpu-tbb/2023.1.0	(D)	inspector/2023.1.0	(D)	mpi/2021.9.0	(D)
ccl/latest		dal/latest		dnnl/latest		intel_ipp_intel64/latest		oclfpga/latest	
ccl/2021.9.0	(D)	dal/2023.1.0	(D)	dnnl/2023.1.0	(D)	intel_ipp_intel64/2021.8.0	(D)	oclfpga/2023.1.0	(D)
clck/latest		debugger/latest		dpl/latest		intel_ippcp_intel64/latest		tbb/latest	
clck/2021.7.3	(D)	debugger/2023.1.0	(D)	dpl/2022.1.0	(D)	intel_ippcp_intel64/2021.7.0	(D)	tbb/2021.9.0	(D)
compiler-rt/latest		dev-utilities/latest		icc/latest		itac/latest		vtune/latest	
compiler-rt/2023.1.0	(D)	dev-utilities/2021.9.0	(D)	icc/2023.1.0	(D)	itac/2021.9.0	(D)	vtune/2023.1.0	(D)
compiler-rt32/latest		dnnl-cpu-gomp/latest		icc32/latest		mkl/latest			
compiler-rt32/2023.1.0	(D)	dnnl-cpu-gomp/2023.1.0	(D)	icc32/2023.1.0	(D)	mkl/2023.1.0	(D)		
compiler/latest		dnnl-cpu-iomp/latest		init_openccl/latest		mkl32/latest			
compiler/2023.1.0	(D)	dnnl-cpu-iomp/2023.1.0	(D)	init_openccl/2023.1.0	(D)	mkl32/2023.1.0	(D)		
----- /spack/share/spack/lmod/linux-ubuntu20.04-x86_64/mpich/4.1.1/Core -----									
adios/1.13.1		datatransferkit/3.1-rc3		libnrm/0.1.0		petsc/3.19.1		strumpack/7.1.1-openmp	
amrex/22.12-sycl		exaworks/0.1.0		libquo/1.3.1		phist/1.11.2-openmp		sundials/6.5.1	
amrex/23.05	(D)	flecsi/2.2.0		mercury/2.2.0		plumed/2.8.2		superlu-dist/8.1.2	
arborx/1.3-sycl		fortrilinos/2.2.0		metall/0.25		precice/2.5.0		tasmanian/7.9	
arborx/1.3	(D)	globalarrays/5.8.2		mfem/4.5.2		pumi/2.2.7		tau/2.32-level-zero	(L)
axom/0.7.0-openmp		h5bench/1.3		mpifileutils/0.11.1		py-h5py/3.7.0		tau/2.32	(D)
boost/1.82.0		hdf5-vol-async/1.5		nccmp/1.9.0.1		py-libensemble/0.9.3		trilinos/13.0.1	
bricks/r0.1		hdf5-vol-log/1.4.0		nco/5.1.5		py-petsc4py/3.19.1		turbine/1.3.0	
butterflypack/2.2.2-openmp		heffte/2.3.0		netlib-scalapack/2.2.0		quantum-espresso/7.1-openmp		wannier90/3.1.0	
cabana/0.5.0-sycl		hpx/1.9.0		omega-h/9.34.13		rempi/1.1.0			
cabana/0.5.0	(D)	hypre/2.28.0		openpmd-api/0.15.1		slate/2022.07.00-openmp			
caliper/2.9.0		lammps/20220623.3-openmp		papyrus/1.0.2		slepc/3.19.0			
conduit/0.8.7		lbann/0.102		parsec/3.0.2209		stc/0.9.0			
----- /spack/share/spack/lmod/linux-ubuntu20.04-x86_64/Core -----									
aml/0.2.0-level-zero		flit/2.1.0		kokkos/4.0.01-openmp		mpich/4.1.1	(L)	superlu/5.3.0	
aml/0.2.0	(D)	flux-core/0.49.0		kokkos/4.0.01-sycl-openmp	(D)	openmpi/4.1.5		swig/4.0.2-fortran	
archer/2.0.0		gasnet/2023.3.0		legion/23.03.0		papi/6.0.0.1	(L)	sz3/3.1.7	
argobots/1.1		gmp/6.2.1		libunwind/1.6.2	(L)	pdtd/3.25.1		umap/2.1.0	
bolt/2.0		gotcha/1.0.4		loki/0.1.7		plasma/22.9.29		umpire/2022.03.1	
chai/2022.03.0		kokkos-kernels/3.7.00-openmp		mgard/2023-03-31-openmp		qthreads/1.16		variorum/0.6.0	
charliecloud/0.32		kokkos-kernels/3.7.00-sycl	(D)	mpark-variant/1.4.0		raja/2022.10.4-openmp			

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

E4S Support for ROCm variants for MI250X (gfx90a) on x86_64

```
Singularity> spack find -x
-- linux-ubuntu20.04-x86_64 / gcc@11.1.0 -----
adios@1.13.1      chai@2022.03.0      gptune@4.0.0      libcatalyst@2.0.0-rc3  openpmd-api@0.15.1  py-warp@23.03      tasmanian@7.9
adios2@2.9.0     charliecloud@0.32   h5bench@1.3       libnrn@0.1.0          papi@6.0.0.1       qthreads@1.16     tasmanian@7.9
alquimia@1.0.10  conduit@0.8.7       hdf5@1.12.2       libpressio@0.95.1    papyrus@1.0.2      quantum-espresso@7.1  tau@2.32
aml@0.2.0        darshan-runtime@3.4.2  hdf5@1.14.1-2    libquo@1.3.1         parallel-netcdf@1.12.3  raja@2022.10.4    tau@2.32
amrex@23.05     darshan-util@3.4.2   hdf5-vol-async@1.5  libunwind@1.6.2      paraview@5.11.1     raja@2022.10.4    trilinos@13.0.1
amrex@23.05     datatransferkit@3.1-rc3  hdf5-vol-cache@v1.1  loki@0.1.7          paraview@5.11.1     rempi@1.1.0       trilinos@14.0.0
arborx@1.3      dyninst@12.3.0      hdf5-vol-log@1.4.0  magma@2.7.1         parsec@3.0.2209     scr@3.0.1         turbine@1.3.0
arborx@1.3      ecp-data-vis-sdk@1.0  hdf5-vol-log@1.4.0  mercury@2.2.0       pdt@3.25.1         slate@2022.07.00  umap@2.1.0
archer@2.0.0    ecp-data-vis-sdk@1.0  heffte@2.3.0      metall@0.25         petsc@3.19.1       slate@2022.07.00  umpire@2022.03.1
argobots@1.1    exaworks@0.1.0      heffte@2.3.0      mfem@4.5.2         petsc@3.19.1       slepc@3.19.0     umpire@2022.03.1
ascent@0.9.1    faodel@1.2108.1     hpctoolkit@2023.03.01  mfem@4.5.2         phist@1.11.2      slepc@3.19.0     unifyfs@1.0.1
axom@0.7.0      flecsi@2.1.0        hpctoolkit@2023.03.01  mgard@2023-03-31   plasma@22.9.29     stc@0.9.0        upcxx@2023.3.0
bolt@2.0        flit@2.1.0          hpctoolkit@2023.03.01  mpark-variant@1.4.0  plumed@2.8.2      strumpack@7.1.1  upcxx@2023.3.0
boost@1.79.0    flux-core@0.49.0    hpx@1.9.0         mpi@4.1.1          precice@2.5.0     strumpack@7.1.1  variorum@0.6.0
bricks@r0.1     forttrilinos@2.2.0  hpx@1.9.0         mpifileutils@0.11.1  pumi@2.2.7        sundials@6.5.1   veloc@1.6
butterflypack@2.2.2  gasnet@2023.3.0    hypre@2.28.0      nccmp@1.9.0.1     py-cinemas@1.3     sundials@6.5.1   visit@3.3.3
cabana@0.5.0    gasnet@2023.3.0    kokkos@4.0.01     nco@5.1.5          py-h5py@3.7.0     superlu@5.3.0    vtk-m@1.9.0
cabana@0.5.0    ginkgo@1.5.0       kokkos@4.0.01     netlib-scalapack@2.2.0  py-jupyterhub@1.4.1  superlu-dist@8.1.2  vtk-m@2.0.0
cabana@0.5.0    ginkgo@1.5.0       kokkos-kernels@3.7.00  nrm@0.1.0         py-libensemble@0.9.3  superlu-dist@8.1.2  wannier90@3.1.0
caliper@2.9.0   globalarrays@5.8.2  lammps@20220623.3  omega-h@9.34.13    py-petsc4py@3.19.1  swig@4.0.2-fortran  xyce@7.6.0
caliper@2.9.0   gmp@6.2.1          lbann@0.102       openfoam@2206      py-warp@23.03      sz@2.1.12.2      zfp@0.5.5
chai@2022.03.0  gotcha@1.0.4       legion@23.03.0    openmpi@4.1.5     py-warp@23.03      sz3@3.1.7
==> 153 installed packages
```

E4S 23.05 supports AMD MI100 (gfx908) as well as MI250X (gfx90a) GPUs

E4S Support for ROCm variants for MI250X (gfx90a) on x86_64

Singularity> module avail

```
----- /spack/share/spack/lmod/linux-ubuntu20.04-x86_64/mpich/4.1.1/Core -----
adios/1.13.1                ginkgo/1.5.0-openmp      (D)  nccmp/1.9.0.1            slate/2022.07.00-openmp      (D)
adios2/2.9.0                globalarrays/5.8.2       nco/5.1.5                  slepc/3.19.0-gfx908
alquimia/1.0.10             gptune/4.0.0             netlib-scalapack/2.2.0     slepc/3.19.0              (D)
amrex/23.05-gfx908          h5bench/1.3              omega-h/9.34.13           stc/0.9.0
amrex/23.05                  (D)  hdf5-vol-async/1.5       openfoam/2206             strumpack/7.1.1-gfx908-openmp
arborx/1.3-gfx908          hdf5-vol-cache/v1.1     openpmd-api/0.15.1       strumpack/7.1.1-openmp    (D)
arborx/1.3                    (D)  hdf5-vol-log/1.4.0       papyrus/1.0.2            sundials/6.5.1-gfx908
ascent/0.9.1-openmp        hdf5/1.12.2              parallel-netcdf/1.12.3    sundials/6.5.1           (D)
axom/0.7.0-openmp          hdf5/1.14.1-2            paraview/5.11.1-gfx908    superlu-dist/8.1.2-gfx908
boost/1.79.0                heffte/2.3.0-gfx908     paraview/5.11.1           (D)  superlu-dist/8.1.2        (D)
bricks/r0.1                 heffte/2.3.0             parsec/3.0.2209           sz/2.1.12.2
butterflypack/2.2.2-openmp hpctoolkit/2023.03.01-rocm
cabana/0.5.0-rocm-gfx90a    hpctoolkit/2023.03.01   petsc/3.19.1-gfx908       tasmanian/7.9-gfx908
cabana/0.5.0-rocm-gfx908   (D)  hpx/1.9.0-gfx908         petsc/3.19.1              (D)  tasmanian/7.9             (D)
cabana/0.5.0                 (D)  hpx/1.9.0                phist/1.11.2-openmp      tau/2.32-rocm              (L)
caliper/2.9.0-gfx908       hypre/2.28.0-gfx908     plumed/2.8.2              tau/2.32                   (D)
caliper/2.9.0                (D)  hypre/2.28.0             precice/2.5.0            trilinos/13.0.1
conduit/0.8.7               lammps/20220623.3-openmp
darshan-runtime/3.4.2      lbann/0.102              py-cinemasci/1.3         turbine/1.3.0
datatransferkit/3.1-rc3    libcatalyst/2.0.0-rc3    py-h5py/3.7.0            unifyfs/1.0.1
dyninst/12.3.0-openmp      libnm/0.1.0              py-libensemble/0.9.3     upcxx/2023.3.0-gfx908
ecp-data-vis-sdk/1.0-gfx908
ecp-data-vis-sdk/1.0        (D)  libpressio/0.95.1-openmp
exaworks/0.1.0             mercury/2.2.0            py-warpX/23.03-dims2     upcxx/2023.3.0            (D)
faodel/1.2108.1            metall/0.25              py-warpX/23.03-dims3     veloc/1.6
flecsi/2.1.0               mfem/4.5.2-gfx908       py-warpX/23.03-dimsRZ    visit/3.3.3
fortrilinos/2.2.0          mfem/4.5.2               quantum-espresso/7.1-openmp
ginkgo/1.5.0-gfx908-openmp mpifileutils/0.11.1     rempi/1.1.0              vtk-m/1.9.0-openmp
                                (D)  scr/3.0.1                quantum-espresso/7.1-openmp
                                (D)  slate/2022.07.00-gfx908-openmp
                                (D)  vtk-m/2.0.0-gfx908      (D)
                                (D)  wannier90/3.1.0
                                (D)  xyce/7.6.0
----- /spack/share/spack/lmod/linux-ubuntu20.04-x86_64/Core -----
aml/0.2.0                    flux-core/0.49.0         libunwind/1.6.2           (L)  pdt/3.25.1                (L)  umap/2.1.0
archer/2.0.0                gasnet/2023.3.0-gfx908  loki/0.1.7                plasma/22.9.29            umpire/2022.03.1-gfx908
argobots/1.1                gasnet/2023.3.0         magma/2.7.1-gfx908        py-jupyterhub/1.4.1      umpire/2022.03.1        (D)
bolt/2.0                     gmp/6.2.1               mgard/2023-03-31-openmp  qthreads/1.16            variorum/0.6.0
chai/2022.03.0-gfx908      gotcha/1.0.4             mpark-variant/1.4.0      raja/2022.10.4-gfx908    zfp/0.5.5
chai/2022.03.0              (D)  kokkos-kernels/3.7.00-openmp
charliecloud/0.32          kokkos/4.0.01-gfx908    mpich/4.1.1               (L)  raja/2022.10.4-openmp    (D)
darshan-util/3.4.2         kokkos/4.0.01-openmp    nrm/0.1.0                 superlu/5.3.0
flit/2.1.0                  legion/23.03.0           openmpi/4.1.5             swig/4.0.2-fortran
                                (D)  papi/6.0.0.1             (L)  sz3/3.1.7
                                (D)  pdt/3.25.1                (L)  umap/2.1.0
                                (D)  plasma/22.9.29            umpire/2022.03.1-gfx908
                                (D)  py-jupyterhub/1.4.1      umpire/2022.03.1        (D)
                                (D)  qthreads/1.16            variorum/0.6.0
                                (D)  raja/2022.10.4-gfx908    zfp/0.5.5
                                (D)  raja/2022.10.4-openmp    (D)
                                (D)  superlu/5.3.0
                                (D)  swig/4.0.2-fortran
                                (D)  sz3/3.1.7
```

23.05 Release: 100+ Official Products + dependencies (gcc, ppc64le)

1: adios2	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/adios2-2.9.0-uhkh77nirxp3sudguz5rxipnrbv6q7pa
2: alquimia	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/alquimia-1.0.10-1rwnpnoqza5npucubt7qvohwyelcchjzm
3: aml	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/aml-0.2.0-tkoq4ljhmln6iiz2l1te73lihyajthqpt
4: amrex	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/amrex-23.05-wiqogp3iaawbi3sqamzqekkusfpohti4h
5: arborx	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/arborx-1.3-c5eh3umfgjppj2rs75m4pv7utjambftcx
6: argobots	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/argobots-1.1-6eibps3ungciczpzy2373gvh2x2bb3nw
7: axom	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/axom-0.7.0-vwaxdd5hftg7sdbvirqhz2iiznmtmgxf
8: bolt	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/bolt-2.0-3kxpzvmwolryeu6o62fu6rlldwlrptbtq
9: butterflypack	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/butterflypack-2.2.2-24f167yyab6ovh3ja5azxvk6lmcba7ip
10: cabana	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/cabana-0.5.0-ttgpqnm43orchppr4ki57ndo5zfk5bq
11: caliper	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/caliper-2.9.0-h12oh3r6fo5vfyhfc4r2ss5vza43bi3
12: chai	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/chai-2022.03.0-b6zqkir2oi2tn26fgtu3327inzsnwzcv
13: charliecloud	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/charliecloud-0.32-neljiquevqokng4xrimihj3tuj2pzfvk
14: conduit	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/conduit-0.8.7-npfozovam6jfff4244vxosppixn3wcxdc
15: darshan-runtime	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/darshan-runtime-3.4.2-shox5cmmmgv4ekjmrnibwsxbd3qwc4ch
16: datatransferkit	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/datatransferkit-3.1-rc3-vwlabziw5ps2g7o5mnv6qxdchgbhd24a
17: dyninst	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/dyninst-12.3.0-hbnm44zruygo5x6cotutoz2i47wvex2s
18: ecp-data-vis-sdk	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/ecp-data-vis-sdk-1.0-azvesz25koxjjc64c3vtu34yvsklmajw
19: exaworks	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/exaworks-0.1.0-myshgpanpgzydkb4depsdnz5aqs2i7s
20: faodel	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/faodel-1.2108.1-n7avkep4x61vmeq5gs2ib66r3w2jy4ne
21: flecsi	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/flecsi-2.2.0-cqk3rmkun6iibicwkcqwvjgeiarqsqfb
22: flit	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/flit-2.1.0-5jt3q4j0l4k5tvbtprojmybzvvyvr4byr
23: flux-sched	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/flux-sched-0.27.0-tvesdixlluglnnfthyhe2twbfukhvttm
24: fortrilinos	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/fortrilinos-2.2.0-q72sbvcasxw7qeigvviu6gssmt5sr4rm
25: gasnet	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/gasnet-2023.3.0-cwenku7fjq1qwp67g5zzdsihapucn7zn
26: ginkgo	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/ginkgo-1.5.0-5yhe6d2kbbfmm3m4d7x4vide4xhsngw
27: globalarrays	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/globalarrays-5.8.2-j44lneowmvsdu5eangnz6jvzef7qya5
28: gotcha	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/gotcha-1.0.4-wplg3bflnzou3ow46eyf45appgxs3hsu
29: gptune	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/gptune-4.0.0-snvgrpumuroxsimv2gtbnwmlfqvxr2cj
30: h5bench	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/h5bench-1.3-vght3dmobbjarqv3xaqe4nig7yjpjiv
31: hdf5	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hdf5-1.14.1-2-vwvt7vybeujyp6ukixkv5kjjyx5fuwfvsv
32: hdf5-vol-async	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hdf5-vol-async-1.5-cm4mfwwvs2qvhmdqcpoajxox3lqfa2x
33: heffte	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/heffte-2.3.0-veomxetlgrtctv33hhuzcfnnul6zygd
34: hpctoolkit	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hpctoolkit-2023.03.01-ictptpwympznphprjvsmabgxjz7sop
35: hpx	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hpx-1.9.0-ih6jtue5cqemjvzhg25gakdsyic6byna
36: hypre	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hypre-2.28.0-oulmotv3bpz16p45xz2skytz7fp65red

GPU runtimes for IBM Power

- CUDA 12
- NVHPC 23.3

Languages

- Julia with MPI and CUDA
- Python

EDA Tools

- Xyce

CFD Tools

- OpenFOAM

AI packages for NVIDIA GPU

- TensorFlow
- PyTorch
- LBANN

23.05 Release: 100+ Official Products + dependencies (gcc, ppc64le)

```
37: kokkos /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/kokkos-4.0.01-4aly3e4gp2msbsu2atqv6fjowokdia6g
38: kokkos-kernels /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/kokkos-kernels-3.7.00-bdbwp5djacbltdgb7ha6ts5quqblzpvf
39: lammmps /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/lammmps-20220623.3-sjfysx6gaw33hgjfeivfsesfrc4s5qew
40: lbann /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/lbann-0.102-r16d2nnswnlvk533l5oy2zmmwr2ka4lna
41: legion /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/legion-23.03.0-qib4igggl4ait3abpgomwkpqw7oqpvvu
42: libnrm /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/libnrm-0.1.0-nua4t4o7kqcumxoc27lxzyv17gmaqpd
43: libpressio /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/libpressio-0.95.1-pi5dwlrkfrpcf4hkjmn2pjtkdh6faxln
44: libquo /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/libquo-1.3.1-juwec3o3rtm3v54jas3n66wg6o22pewq
45: loki /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/loki-0.1.7-uceagjppgg5ehjmlnk4az5lv24hzafpzt
46: magma /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/magma-2.7.1-2ceqezqqs54vc5mpis6smcwrqwz4udcl
47: mgard /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mgard-2023-03-31-lup7aqnbw7f2tz3yzywzi3ws2kparbvjc
48: mercury /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mercury-2.2.0-t4cvhz2rv5depq2kr74n2tujqpuqe5sm
49: metall /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/metall-0.25-6j6ubufedstb3b3lg7hatgvi7nvqthmx
50: mfem /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mfem-4.5.2-56qrjn7fbnnavq7o4k7tylfsuypaqu5
51: mpark-variant /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mpark-variant-1.4.0-mzq76r65ntcog7mgmnic7sp4uvo3zxsh
52: mpich /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mpich-4.1.1-cvlcp63frcd4h7z7hd7gya2532d2c6qq
53: mpifileutils /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mpifileutils-0.11.1-gfzixrrmpypaazfprtag6ivuf53qgdy4
54: nccmp /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/nccmp-1.9.0.1-ce6gwybg32hjpjqe6ly2ddu4di6oplsa
55: nco /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/nco-5.1.5-5lvdidingb6w7zrjdsjb7bwn2lfazwjat
56: netcdf-c /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/netcdf-c-4.9.2-6iv3ckbdamojcaqcq3lo3lvkkyah2spr
57: netlib-scalapack /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/netlib-scalapack-2.2.0-dr2kie6hamsg6272m4jfb7ea4su7guoe
58: nrm /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/nrm-0.1.0-kw2s2wmu4xm3ljzt4ooxx56owasitblf
59: omega-h /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/omega-h-9.34.13-lfriczx7q2iyzbc24l6wq7s7vdm3tety
60: openfoam /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/openfoam-2206-ulcwiaylrstot7i23biajfuy4hk7mfqt
61: openmpi /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/openmpi-4.1.5-o2fpct2vymr4ca3lt35pdbu7mgrp3eydd
62: openpmd-api /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/openpmd-api-0.15.1-hr4yme2cyna7rifkx3tbgfhpbnjm4ux2
63: papi /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/papi-6.0.0.1-jwrwurntwmh3lwdkdx3pram72lmd5pt
64: papyrus /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/papyrus-1.0.2-nskpqf2denfhggrcvaukd1vlbn6avcv2
65: parallel-netcdf /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/parallel-netcdf-1.12.3-hsrpluhct5z3jhajcbuhmssx2fil4kkr
66: parsec /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/parsec-3.0.2209-h5us5t7szrt2yg57kn3ot6l4ehbx4fr3
67: pdt /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/pdt-3.25.1-rsjchybcj2rqz3g7qmb2kwvf6pxfwjql
68: petsc /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/petsc-3.19.1-zjwzezvirlsgk6i2t4l1trxm5zqbkk2or
69: plasma /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/plasma-22.9.29-so3zq77bpysp53hvr17zqsg2z2r6tkp
70: plumed /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/plumed-2.8.2-guxns5nkh3kesdsffzwap44ipc4vd55g
71: precice /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/precice-2.5.0-lmrwvzfrgmkxyxf2wlo62ctw3mvnhlwj
72: pumi /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/pumi-2.2.7-6hcz03aexr5fjz2aq37thxn6zsjsjp52bo
```

23.05 Release: 100+ Official Products + dependencies (gcc, ppc64le)

```
73: py-cinemasci /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-cinemasci-1.3-6f47e36iz5mdugjbumsr566whomnjwi5
74: py-jupyterhub /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-jupyterhub-1.4.1-a2fbq7jol4ysxrxe6r7vgj4bidgd4nat
75: py-libensemble /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-libensemble-0.9.3-g7sepw56p3p6i6lqyrcphiivhnrlykph
76: py-parsl /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-parsl-1.2.0-231f2ge7xdwaqoknvdq2d3gqn4han4ns
77: py-radical-pilot /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-radical-pilot-1.20.0-wx6pbcxqi4b5qjbfe344shp5cse7v6n
78: py-radical-saga /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-radical-saga-1.20.0-vszum2biikhiri42vmctwpdpxkjieq6y
79: qthreads /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/qthreads-1.16-ocziw7dq6fffr2mzdkomc5fzour5iuay
80: quantum-espresso /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/quantum-espresso-7.1-x54vzpf5t5l3r5h3xp5ejzuwsmqosi32
81: raja /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/raja-2022.10.4-7avifye7dznjssmdqknyv2jknkfvfkqm
82: scr /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/scr-3.0.1-xjbu4kvcthiovajxejmxxvjt6sdvtzbh
83: slate /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/slate-2022.07.00-rcmdjvvy6d6wr73ykrziwwscme4uxa6d
84: slepc /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/slepc-3.19.0-4kri4s2cainqvrlm66gz3eofzntfwssi
85: stc /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/stc-0.9.0-kkrsziha5tbctj7k5m6o7f7oeigaaajt
86: strumpack /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/strumpack-7.1.1-2pppj2vlykpqyogktxfrzztscp5v6g6n
87: sundials /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/sundials-6.5.1-wnfjm3sohjl4epqyy4azj3lhuepuzd3d
88: superlu /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/superlu-5.3.0-xdj3w4lzt5g2avn66zmhtsyulle5aene
89: superlu-dist /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/superlu-dist-8.1.2-ff2kn5ctx3wyrdaabholnwisu3cbiuax
90: swig /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/swig-4.1.1-hq4biusavaw42mpcis4pz755gillodze
91: sz /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/sz-2.1.12.2-oix6jt5d7lx7fb234wvuw4goptf23nv
92: tasmanian /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/tasmanian-7.9-coc3xp2za627mjknfyie5jmcvzr2rov
93: tau /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/tau-2.32-ielj7troxit4y5afdmtenjmiyucq645m
94: trilinos /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/trilinos-14.0.0-fpw4j1z44syyucukfcl2ldzab2t6ghee2
95: turbine /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/turbine-1.3.0-4qbitm42fmum3nfwxzzjyr2rd6ducpwuz
96: umap /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/umap-2.1.0-hhad4w3gcc4le5fttyzq7gkpofxreom3
97: umpire /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/umpire-2022.03.1-nandcjd1wbj1ksewhmbe7s4uj7cqst6
98: unifyfs /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/unifyfs-1.0.1-mrkrrypvvv6bsh334pvobcku7ilk5sgk
99: upcxx /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/upcxx-2023.3.0-3aepixv33clzkkdarjk73lpg7idfvp3p7
100: veloc /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/veloc-1.6-ahnr527j2jqazwc5szl5ufkyju7ufyl7
101: visit /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/visit-3.3.3-zfbx72nt6ibooshbnkuo5ebbehov5ayl
102: vtk-m /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/vtk-m-2.0.0-zzpe6kxkdc2jsz4fabxh5zdcnfcwzknf
103: wannier90 /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/wannier90-3.1.0-zpua7kk527xbealig23rzch27ppx5sr
104: warpx /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/warpx-23.03-wf3nq5wmc762reyf7nqp5don7qfsa4hr
105: xyce /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/xyce-7.6.0-fy27mi5xxhqihgyrguy3waepfdve465m
106: yaksa /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/yaksa-0.2-xhkfpsrkb3r3so7n4loastxwhsbe6xa7
107: zfp /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/zfp-1.0.0-5amyabiloytn5zy6m4hinokr4h3m2hha
```

23.05 Release: 100+ Official Products + dependencies (gcc, aarch64)

1:	adios2	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/adios2-2.9.0-5hx3ckkfc7lroseaizex64spckzzl42
2:	alquimia	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/alquimia-1.0.10-6vjvfknlq76tmhv3j4vryc77weqdrtya
3:	aml	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/aml-0.2.0-d2scnleqyhgsuhldi7vqee4azq7e7s54
4:	amrex	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/amrex-23.05-sxksck5lay6gmktguwlo7zprxyfti5y
5:	arborx	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/arborx-1.3-bblxreunovlfcabhcjpxwi76gmdni5mt
6:	archer	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/archer-2.0.0-cidpvhuyxxi3b5vrkfh65d7aobfpq15
7:	argobots	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/argobots-1.1-z6sgneii72i7b7g2qbbhrspzxx54j6fh
8:	axom	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/axom-0.7.0-vrwrzczihk6svtxx1ddqvleltljxofd3pf
9:	bolt	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/bolt-2.0-d7iczcaglrgtqwc2ukrmxqsqr76pylu
10:	butterflypack	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/butterflypack-2.2.2-66tcbf4wby2ixbdexadvgeokqv42wyer
11:	cabana	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/cabana-0.5.0-jc2w5p6ck7vejicvwcc6jclj3mduszuf
12:	caliper	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/caliper-2.9.0-r3ajaall6cyckgbjomyrujgg16f3mk6
13:	chai	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/chai-2022.03.0-r4esqowkacyw32giaedixg53ma4vsheq
14:	charliecloud	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/charliecloud-0.32-zp7v4vjguafh3ms25dd2b6q7v74cnb2k
15:	conduit	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/conduit-0.8.7-eomcxsrdqgz7osmtyon2jaapcx2yklqd
16:	datatransferkit	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/datatransferkit-3.1-rc3-6yqlphk2z2fjjugannywhlfnmvmcxsecl
17:	dealii	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/dealii-9.4.2-xjzryiysbioa7avpxb3nwsnwkdwfs2xh
18:	dyninst	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/dyninst-12.3.0-fux3ukyxtvfoo3un4ryjxvtu5kzzp63
19:	exaworks	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/exaworks-0.1.0-raljmy37oc52h65hkby4m7oxrbwzuqvt
20:	flecsi	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/flecsi-2.1.0-kwbqogveamct634zex4ioqvrbcyynvyi
21:	flit	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/flit-2.1.0-wsmxciiir4ouoevervbnvkrwwtonrtmtxp
22:	flux-core	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/flux-core-0.49.0-wlpcyowpzyhwzu54pkphvdmtd4ptxtn
23:	flux-sched	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/flux-sched-0.27.0-6cgiriueephagbfnzimijuv3og37snvt
24:	fortrilinos	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/fortrilinos-2.2.0-neydn4ekuuu5sfiwrmamn4vbe7igcten
25:	gasnet	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/gasnet-2023.3.0-mwtvy5h3r4p2hr4crbhp3esatgorxhin
26:	ginkgo	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/ginkgo-1.5.0-47b2pjjb7wohojpbob2xpuknouelm4o
27:	globalarrays	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/globalarrays-5.8.2-14xrdmmbvupr2w2u76uzsy444auvzhhs
28:	gotcha	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/gotcha-1.0.4-uszfpeta7asy5eeqys6dekipcefc63dn
29:	gptune	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/gptune-4.0.0-osk2uxrg2iesvaa3gi3rsbtukiacxuhm
30:	h5bench	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/h5bench-1.3-zmazqeyhfx73disvhhw5uzdtxh5johpv
31:	hdf5	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/hdf5-1.14.1-2-nt67ozrz53fo7ti4xc3r5niabpvqjfyf
32:	hdf5-vol-async	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/hdf5-vol-async-1.5-4xhckgg2oitnme2yckkgm4vkjv2wr62
33:	hdf5-vol-cache	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/hdf5-vol-cache-v1.1-7n64cdsi7mofmbixdtqal2bee32xwi5j

GPU runtimes for aarch64

- CUDA 12
- NVHPC 23.3

Languages

- Julia with MPI and CUDA
- Python

EDA

- Xyce

AI packages for NVIDIA GPU

- TensorFlow
- PyTorch

23.05 Release: 100+ Official Products + dependencies (gcc, aarch64)

```
34: hdf5-vol-log /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/hdf5-vol-log-1.4.0-ifklnjvhynjcsywqh32zztztzxffpi4ur
35: heffte /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/heffte-2.3.0-xsdldluhu6h4nisd5hilzuttsvyjc4nr
36: hpctoolkit /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/hpctoolkit-2023.03.01-2r53p52qrveuswgxmksu7i6x5bnyaia2
37: hypre /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/hypre-2.28.0-7xb2rd3aewwtu7xfkbb4wad7xmcn5ibv
38: kokkos /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/kokkos-4.0.01-nft3ud2oa2kdvkaundnejaz3de4r7hnw
39: kokkos-kernels /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/kokkos-kernels-3.7.00-ewcpxwfg3wlfprudptycluaj4q2x6rlp
40: lammps /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/lammps-20220623.3-ily3zw6pljr2n3y3ak4jomlgc5ohz4hq
41: lbann /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/lbann-0.102-ul5zbs7we3nez5jvli4xdvetv7vxqstl
42: legion /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/legion-23.03.0-kzdwjqdfqs77xzt3tx3sxsawuxputfv
43: libnrm /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/libnrm-0.1.0-2v6glsimsjnpjogz3wokna22phcvvfk
44: libpressio /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/libpressio-0.95.1-t2ly6fjw6ovrlxedii6gizzda37wc2xk
45: libquo /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/libquo-1.3.1-btmf455g2k7dd6gflsfusy4cijcz6jff
46: loki /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/loki-0.1.7-wefn27yr2azwytwllkfsj2on43225zw2
47: magma /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/magma-2.7.1-2gevflav2vjnd3tfbubpuxwhrulh4xix
48: mercury /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/mercury-2.2.0-3dmnkge46avczuwqd44iyjjnfsphckks
49: metall /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/metall-0.25-plujxrswrq3nyjylntdzmeheyppwgunc
50: mfem /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/mfem-4.5.2-yo5tcebpismq356ppcsymbv4uxmffela
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56: nco /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/nco-5.1.5-2ows33r6inafc26xqvufngwmhplfxbbm
57: netlib-scalapack /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/netlib-scalapack-2.2.0-secbwodbjj3quvl37eipcqawgoo36urd
58: nrm /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/nrm-0.1.0-uhquv6ifzjy5qwyztiozptf6fsdweckx
59: omega-h /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/omega-h-9.34.13-iim4vlzshckvwb3qdddr53tu46xnirq
60: openfoam /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/openfoam-2206-2mzdpojfxz547fngc3iedzkg33tjc3i2
61: openmpi /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/openmpi-4.1.5-iyad3f4boygpyqpvgt4y65cuviapc7s
62: openpmc-api /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/openpmc-api-0.15.1-vlypbqwnn5gvgkwk7qtervxoukqkbiz5
63: papi /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/papi-6.0.0.1-hkmm6nk3a6sjpc7vblrgq42aoc4xxdpb
64: papyrus /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/papyrus-1.0.2-moob7u474vchokhdsrllleykmygrpa7
65: parsec /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/parsec-3.0.2209-gkw22q2asdvsym7g656ypbjzbtogigt
66: pdt /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/pdt-3.25.1-dtetja2hxykx45ysshw7ng6w6nzb4j1w
```

23.05 Release: 100+ Official Products + dependencies (gcc, aarch64)

```
67: petsc /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/petsc-3.19.1-7hw5clqu4tbdbfjky6ajrgt3kxrs2mxk
68: plasma /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/plasma-22.9.29-pe5jv42353bw7cc73lba3fohq7uubl5n
69: plumed /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/plumed-2.8.2-bqf7jzhe2ymyip6nfamnnkmzjgh3razc
70: precice /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/precice-2.5.0-tu6kz7pwoo6qdfj7t4fwh7wbc2h75qay
71: pumi /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/pumi-2.2.7-v5ymezbyqcqldkcoj5aj3xif4sjgokxu
72: py-jupyterhub /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/py-jupyterhub-1.4.1-flaefn7k3v7usdijegqgxfcqdy4nqqm
73: py-libensemble /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/py-libensemble-0.9.3-exwo7uhq6on73rc2xedkji2urfn5atih
74: py-parsl /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/py-parsl-1.2.0-fg5mqkivy4hkexhx5552gaqaus5fbk5u
75: py-radical-saga /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/py-radical-saga-1.20.0-b3kg22bqahgym4okeuachcrlbw2wuf4y
76: qthreads /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/qthreads-1.16-viflrgzrzwejxcn4ngi5fvobp6e3vcwo
77: quantum-espresso /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/quantum-espresso-7.1-wra3slwi235jbr5r3ufh3wij3pszyk
78: raja /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/raja-2022.10.4-hvloxngdztictemnfi7qbhquwy7fypq7
79: rempi /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/rempi-1.1.0-yzxyzcnwogzevfjpdv2qmsz254y3lesx
80: scr /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/scr-3.0.1-vqgox3tntyakf3yttlxlwq6ns6olcmoj
81: slate /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/slate-2022.07.00-fztpoi2gpg5k7asalzg3udqvwwyuiqu3
82: slepc /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/slepc-3.19.0-mfwatst6iwfq6exk5cbaavhkdbphv5tb
83: stc /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/stc-0.9.0-tl7mhyoqd7smntrom3vi4rqy7yhk4n6l
84: strumpack /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/strumpack-7.1.1-vke6bsab5g66tozcx35wbcvxstew2ppi
85: sundials /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/sundials-6.5.1-xjrfkg6p5mmi6gh66wylnre5b5oblzaq
86: superlu /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/superlu-5.3.0-hyh23sh5627ene3zbel2h6tig5e7oinc
87: superlu-dist /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/superlu-dist-8.1.2-7i6t75nrjmzxfq4t77a4f6izwco4wmw6
88: swig /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/swig-4.1.1-i4ykb5ylcn43finrby5yf76gnbbpqwtr
89: sz /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/sz-2.1.12.2-pds4axmlwpjnpauhuci5uvf37c6cjoec
90: tasmanian /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/tasmanian-7.9-2ul5mesuqegth3hsv6c4z3tyadp5437i
91: tau /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/tau-2.32-spv5m5sefxfirdusuc67mzqr2lisrc2ij
92: trilinos /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/trilinos-14.0.0-j7qpf5b6l6ps3ursieqvc3iyumfzccn4
93: turbine /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/turbine-1.3.0-axykpyqi7p66tyecgayyhiwimjwh2a4
94: umap /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/umap-2.1.0-rz2jrkmcw7wydzkykg3veoxd3zgbwi
95: umpire /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/umpire-2022.03.1-xddybxhaitvw7cpjvgnvqd36wpt6bfux
96: upcxx /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/upcxx-2023.3.0-b3r3vumztano2tfrlby2h6sleyrkjudl
97: wannier90 /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/wannier90-3.1.0-aox2awcoj3tzmzhs2mruf3mfcldlwaah4
98: warpx /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/warpx-23.03-eosqswtnqjfobzz3zuwubvp4jmqkmid
99: xyce /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/xyce-7.6.0-qorkfm3d4pswfk22a2kmhkl32rbs7la
100: zfp /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/zfp-1.0.0-2mukw7csgccahz5cfa3pskf7jjnb7box
```

E4S 23.05 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 0.19.1 hosted at U. Oregon

E4S Build Cache for Spack 0.20.0

To add this mirror to your Spack:

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

102,289 total packages

Last updated 2023-05-31 16:38 PST

All Arch PPC64LE X86_64 AARCH64

All OS Centos 7 Centos 8 RHEL 7 RHEL 8 Ubuntu 18.04 Ubuntu 20.04

Search

[adiak@0.1.1](#) [adiak@0.2.1](#) [adiak@0.2.2](#) [adios2@2.5.0](#) [adios2@2.6.0](#) [adios2@2.7.0](#)

- Over 100K binaries!
- No need to recompile from source code.

E4S 23.05 AWS image: US-West2 (OR)

The screenshot displays a desktop environment with the following components:

- ParaView 5.9.0:** A 3D visualization of a mesh with a color scale for pressure, ranging from $0.0e+00$ to $1.2e-38$.
- Terminal Window:** Shows the execution of the Singularity command:


```
(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        openpm�-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
```
- TAU Performance 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
- TAU 3D Visualizer:** A 3D surface plot showing performance data over time, with a color scale for seconds ranging from 0 to 365.836.

E4S 23.05 AWS

- Intel oneAPI
- CUDA
- NVHPC
- ROCm
- AWS DCV
- Spack Build Cache
- ECP: Nalu-Wind
- Trilinos 13.4.0
- 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 several windows open:

- Xschem - top.sch**: A schematic editor window showing a circuit diagram with components like PERP, VPP, CAP, RERAM, VARACTORS, MIM, PFET, NFET, RES, DIODE, PNP, and NPN. It includes a 'Layers' menu and various simulation options.
- KLayout 0.28.5**: A layout editor window showing a 3D visualization of a component with a large 'K' on its surface.
- 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          qcvs-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      padring-021423     xschem-021323
iverilog-021423    pcb-3.0.98          xscheme-gaw-021423
klayout-0.28.5     qflow-1.4           yosys-021123
magic-8.3           qrouter-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_dev.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 tasks for project preparation, synthesis, placement, static timing analysis, routing, post-route STA, migration, DRC, LVS, and GDS.

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

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	Xscheme	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

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

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

On the right side, the 'About' section describes the repository as a 'Container manager for E4S' and lists related technologies: 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 in a blue box. This release was published on Mar 31.

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

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 image tags:

TAG	OS/ARCH	LAST PULL	COMPRESSED SIZE
latest			
Last pushed 13 days ago by <code>esaw123</code>			
DIGEST			
<code>ecdde88d2622</code>	linux/amd64	3 days ago	9.15 GB
<code>6985b191a048</code>	linux/arm64	3 days ago	1.58 GB

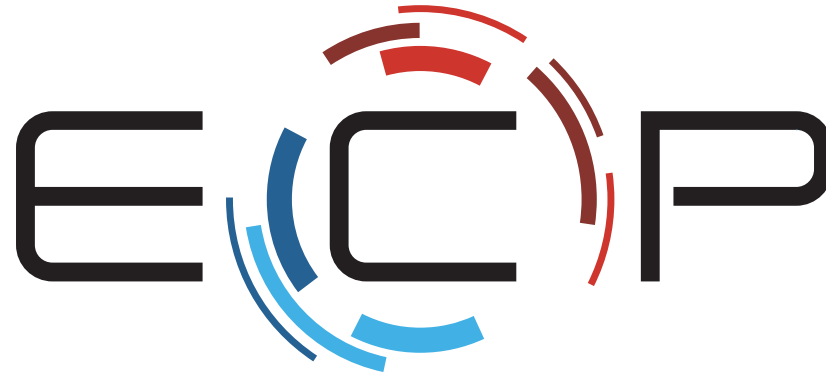
`% docker pull ecpe4s/waggle-ml`

The screenshot shows the Argonne National Laboratory website for the SAGE project. 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 includes a navigation menu with "RESEARCH", "WORK WITH US", "COMMUNITY", and "ABOUT US". A sidebar on the right lists "MCS Division" with links to "About MCS", "Research", "News", "Events", and "Publications". The SAGE logo features a stylized plant and the text "SAGE A Software-Defined Sensor Network Cyberinfrastructure for AI at the Edge". The website URL is www.sagecontinuum.org.

Thank you

<https://www.exascaleproject.org>

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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.

