

# E4S: The Extreme-scale Scientific Software Stack Release 22.11



Release 22.11 notes

November 13, 2022

# 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 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).
- 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\\_Oct22.pdf](https://e4s.io/talks/E4S_Support_Oct22.pdf)
- E4S for commercial cloud platforms: AWS image supports multiple MPI implementations and containers with remote desktop (DCV).
  - Intel MPI, NVHPC, MVAPICH2, MPICH, 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 22.11 released on November 13, 2022: [https://e4s.io/talks/E4S\\_22.11.pdf](https://e4s.io/talks/E4S_22.11.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 a single distribution
- 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

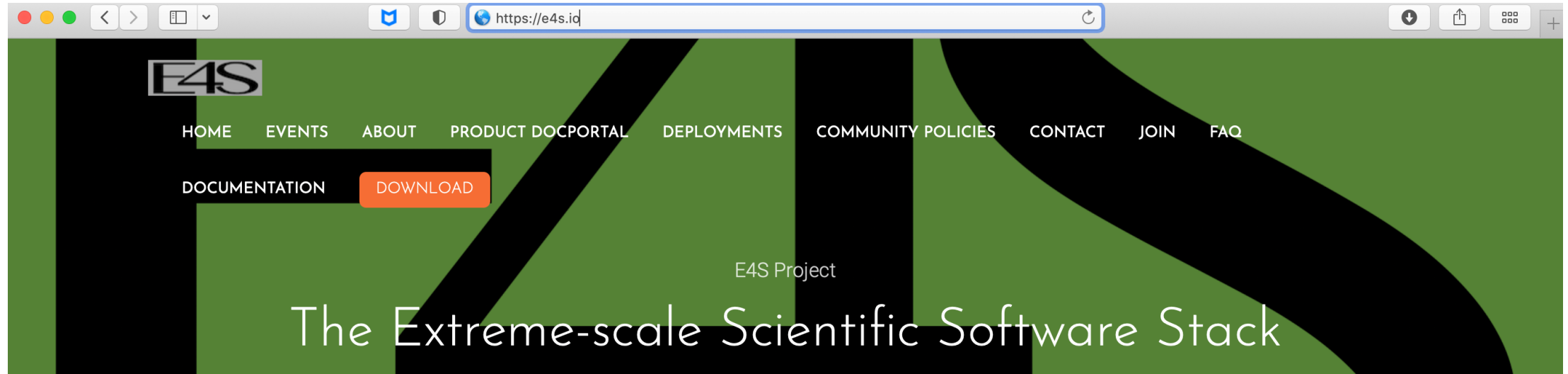


<https://e4s.io>

Lead: Sameer Shende  
(U Oregon)

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

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



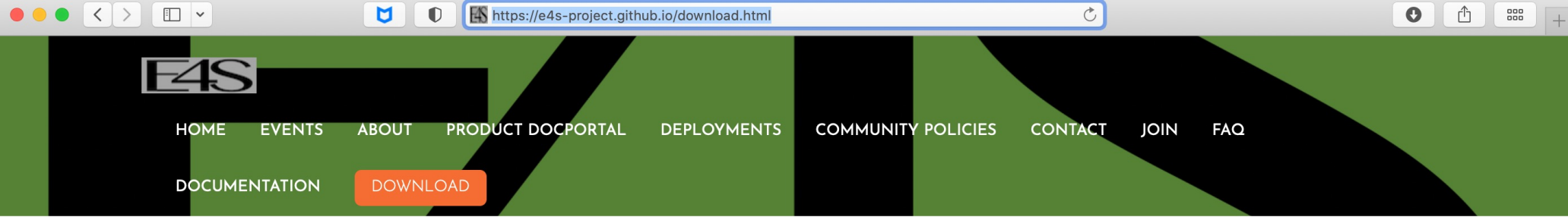
*E4S 22.11 container images now available!*

See [Downloads](#) for more information on E4S 22.11.

## 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](#).

# E4S Download from https://e4s.io



## Acquiring E4S Containers

The current E4S container offerings include Docker images based on Red Hat Enterprise Linux 7, Red Hat Enterprise Linux 8, Ubuntu 18.04 (Bionic), and Ubuntu 20.04 (Focal Fossa) for Continuous Integration. Our images can run on X86\_64, PPC64LE, and AARCH64 depending on the particular image. Our full E4S Release images (not for Continuous Integration) 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](#).



### Container Releases

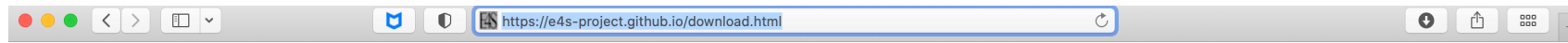
[📄 Docker Downloads - CUDA](#)



### From source with Spack

[🔗 Visit the Spack Project](#)

# Download E4S 22.11 GPU Container Images: NVIDIA, AMD, Intel



Docker images are available on the [E4S Docker Hub](#).



## Container Releases

📄 Docker Downloads - CUDA

📄 Docker Downloads - ROCm

📄 Docker Downloads - OneAPI

📄 Singularity x86\_64 Download - CUDA

📄 Singularity ppc64le Download - CUDA

📄 Singularity aarch64 Download - CUDA

📄 Singularity x86\_64 Download - ROCm

📄 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 22.11 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) NEW!
- Full featured images available on Dockerhub
- 100+ products on 3 architectures

# Download E4S 22.11 GPU Container Images: NVIDIA, AMD, Intel



## 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:22.11
```

```
# docker pull ecpe4s/e4s-rocm:22.11
```

```
# docker pull ecpe4s/e4s-oneapi:22.11
```

## 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:22.11
- e4s-rocm-22.11.sif

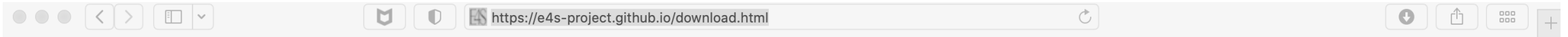
### NVIDIA CUDA (X86\_64, PPC64LE, AARCH64)

- ecpe4s/e4s-cuda:22.11
- e4s-cuda-x86\_64-22.11.sif
- e4s-cuda-ppc64le-22.11.sif
- e4s-cuda-aarch64-22.11.sif

### Intel OneAPI (x86\_64)

- ecpe4s/e4s-oneapi:22.11
- e4s-oneapi-22.11.sif

# E4S 22.11 Base images and Minimal Spack images with MPI



## 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:22.11  docker

e4s-base-rocm-22.11.sif  mirror 1

### NVIDIA Multi-Arch (X86\_64, PPC64LE, AARCH64)

ecpe4s/e4s-base-cuda:22.11  docker

e4s-base-cuda-x86\_64-22.11.sif  mirror 1

e4s-base-cuda-aarch64-22.11.sif  mirror 1

e4s-base-cuda-ppc64le-22.11.sif  mirror 1

### Intel OneAPI (X86\_64)

ecpe4s/e4s-base-oneapi:22.11  docker

e4s-base-oneapi-22.11.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

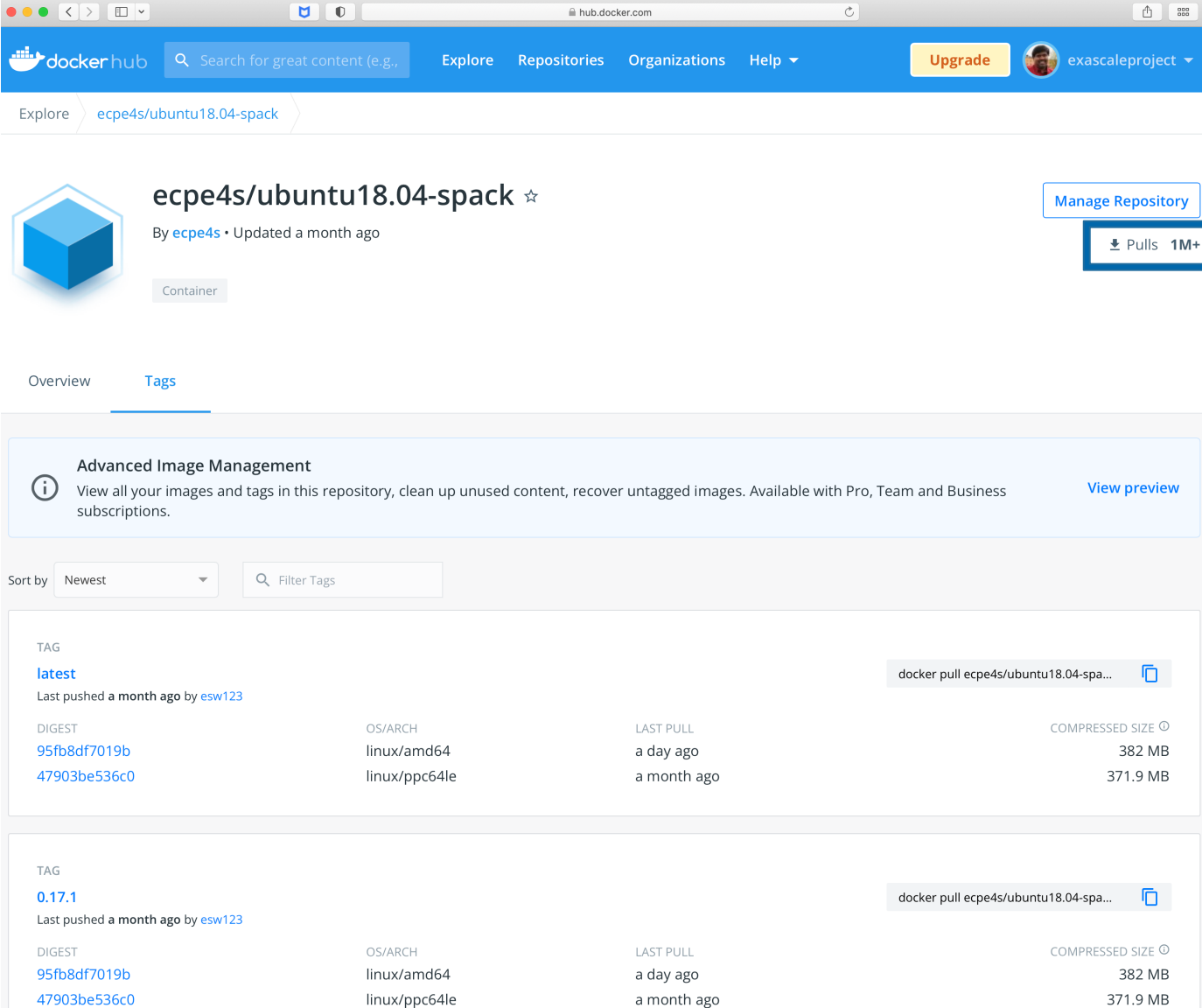
ecpe4s-ubuntu20.04-x86\_64-22.11.sif  mirror 1

ecpe4s-ubuntu20.04-ppc64le-22.11.sif  mirror 1

ecpe4s-ubuntu20.04-aarch64-22.11.sif  mirror 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 was updated a month ago. A blue box highlights the 'Pulls 1M+' badge. Below the repository information, there is an 'Advanced Image Management' section and a table of tags. The table lists two tags: 'latest' and '0.17.1', both pushed a month ago. Each tag entry includes a 'docker pull' command snippet, a digest, OS/ARCH information, last pull time, and compressed size.

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

- Create custom container images
- 1M+ downloads!

# 22.11 Release: 100+ Official Products + dependencies (gcc, x86\_64)

1:	adios2	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/adios2-2.8.3-3ajbsxge3eu6pxmyaeou3zdkvvhqdf6k
2:	alquimia	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/alquimia-1.0.10-qdyaifl16q7muq6fvjyfkxjnun5zagn4
3:	aml	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/aml-0.2.0-kj2y4vne6ffor425wpgqmtvfyubkvtk
4:	amrex	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/amrex-22.11-w34ivhpukaxvubuakvvgg5wf2rlfuio
5:	arborx	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/arborx-1.3-ugykp4hy14bx7hreg4yxqskoc21dntnh
6:	archer	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/archer-2.0.0-ikmxk25q3eq3euq4qgs5f76zybsfd4a2
7:	argobots	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/argobots-1.1-f6b6was4pd7d2u2fwvpxdoqffdbate2o
8:	ascent	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/ascent-0.8.0-drnzjcefdaozbbpjrjvxxum47gmcpgx2t
9:	axom	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/axom-0.7.0-c3gkccvhjxhpktsggi2ur2s3g54uo6iy
10:	bolt	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/bolt-2.0-4t2fedw3xwcm4ypowb3c34zzeglebe26
11:	bricks	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/bricks-r0.1-ufe1xtoylwegoqfca2vme7snpoqfi2bd
12:	butterflypack	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/butterflypack-2.2.2-dsj6epc3js6oseemdmhuzkty5f1s64y
13:	cabana	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/cabana-0.5.0-6ti6ogglfqu2igvq6ezowu4t3ehw77xf
14:	caliper	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/caliper-2.8.0-aweu5lqptfd5usw527hgxmpogun55u6j
15:	chai	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/chai-2022.03.0-7na7b7nf16ssypwkxzyu5mfrsy7fzpj
16:	charliecloud	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/charliecloud-0.29-hf25ge13q5ovgnhejztrupy4dh2svbo
17:	conduit	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/conduit-0.8.4-hfqsozz6eu46zccqfwgjm2hkwrlrtyk
18:	darshan-runtime	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/darshan-runtime-3.4.0-yrxz4npozgkhewkvnvggioni3espodiaf
19:	datatransferkit	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/datatransferkit-3.1-rc3-g6nalqnmmax5b7wpxxpru5nouxlm7i6bm
20:	dyninst	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/dyninst-12.2.0-6srff62fbqa3t4rgvim22s4qkfdvbl7
21:	ecp-data-vis-sdk	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/ecp-data-vis-sdk-1.0-vf57ba63borcvqkbg3au2fj3rmo3robh
22:	exaworks	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/exaworks-0.1.0-nhzb7c7pcggbdvvt3pi3qscvm423t4a1
23:	faodel	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/faodel-1.2108.1-h73xh332hnyi27j4g4fsgqbbhbvqmxj1
24:	flecsi	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/flecsi-2.1.0-lcwpm2aartvrvroisqmlflluujt6bt7kzhz
25:	flit	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/flit-2.1.0-ykzntwke3go3l3p2rzucvxxarrqamuno3
26:	flux-sched	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/flux-sched-0.25.0-hc52tymt1r4n427vzqmx6roazynwnata
27:	fortrilinos	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/fortrilinos-2.1.0-qbx567j5rchrjtjxh6uytpehcg3ilyyk
28:	gasnet	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/gasnet-2022.9.0-ut4wf6tncotjukmgfhndh5qdxj4tnqqe
29:	ginkgo	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/ginkgo-1.4.0-kk6x7pnc3sfvqovkrbn2yxk6s3y5uvb
30:	globalarrays	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/globalarrays-5.8-7iss2kycfby5lvmzmvbox7i5dt3t3kg
31:	gotcha	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/gotcha-1.0.4-36borpi6gemf3a7wuglm67wrqh5gdzly
32:	gptune	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/gptune-3.0.0-snfcqpefftp5z6yyfwdkrnc3gq5a2yyi
33:	h5bench	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/h5bench-1.3-fkoffwicyfuwtdfkrkhilxmigfu4p12
34:	hdf5	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/hdf5-1.12.2-mt44ijmcpqjg32g3lue3pfmv76adtvs
35:	heffte	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/heffte-2.3.0-5jfsnayaonnnpjy6p3d6i3jqdvdwhdpye
36:	hpctoolkit	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/hpctoolkit-2022.10.01-d16s6jzzzarpb7r75evrvjvtxtqqj4e5
37:	hpx	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/hpx-1.8.1-vpsaguio7f7iwcihwmzev7hnew2dsouj
38:	hypre	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/hypre-2.26.0-yorxzh7r7pdm5r5js363q2kwutapoyul
39:	kokkos	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/kokkos-3.7.0-2sitezkcfcvqajvj5dos5vjcls5zpqw4
40:	kokkos-kernels	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/kokkos-kernels-3.7.0-rlz3cuw7kg5qgspxzqetzwwzxi3hhg4
41:	lammps	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/lammps-20220623-upn4cjkfa3zx5a5zgt6k6uca7qktsyno
42:	legion	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/legion-21.03.0-hxm6epkjrboobnoq56ofcwtuzpzy47eo
43:	libnrm	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/libnrm-0.1.0-5vfy6mqkxsfemtrbrwutr6vidontqyhm
44:	libpressio	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/libpressio-0.88.0-v6eds2pj35vyvxyoor67hc2rlq6sh24
45:	libquo	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/libquo-1.3.1-7qbm6sey5z6z6p6dbvb5dijnqbix03dus
46:	magma	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/magma-2.6.2-i7tvhq6qqmrzybnkeqwdvthufprkvefy
47:	mercury	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/mercury-2.1.0-o2bzwoucsvq4yjatxzfa03j6ri4qhat
48:	metal	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/metal-0.21-d3di35ikbrylkkbh2azk4vgcc6djbxfx
49:	mfem	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/mfem-4.5.0-jtnyqpk7ij5emhjboqkvspi4e7bxmdl6
50:	mpark-variant	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/mpark-variant-1.4.0-cojotckrc4x4gymspggwupll56gposcp
51:	mpich	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/mpich-4.0.2-ts6t7znbvzfyth7jxzwiryfv7sc4v2z

## GPU runtimes

- AMD (ROCm)
  - 5.2.0
- Intel (oneAPI)
  - 2022.1.0
- NVIDIA (CUDA)
  - 11.4.2
- NVHPC
  - 22.9

# 22.11 Release: 100 Official Products + dependencies (gcc, x86\_64)

52:	mpifileutils	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/mpifileutils-0.11.1-ugd4fcf55nmpjwgmmropsy2sh4wh42ca
53:	nccmp	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/nccmp-1.9.0.1-glrrqptc5dmsgtkdi6matefyxa64ivoh
54:	nco	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/nco-5.0.1-fzunxjdmu7hdnhwhvdvd3r537qxcfxglg
55:	netlib-scalapack	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/netlib-scalapack-2.2.0-awvctx4s6tn37bu3irs3qxgi5b313e2c
56:	nrm	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/nrm-0.1.0-35ftcszjbgrr2s6wodzdyqig6qwxhdaj
57:	omega-h	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/omega-h-9.34.13-eyshakan2stlj7z12xlwln3bowg5f5pd
58:	openmpi	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/openmpi-4.1.4-6ycgzqotgsg3vfbzdnjngfplwqzbzfz
59:	openpmd-api	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/openpmd-api-0.14.5-zhvh6pd2ubpohrnkbeuiap7v1aqc7ne
60:	papi	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/papi-6.0.0-1-7mdhp4vhvvhv34zxjkd7fdxkmb6w4atz
61:	papyrus	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/papyrus-1.0.2-lmzmxz23fhht6supkjicdkbyyudb35q
62:	parallel-netcdf	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/parallel-netcdf-1.12.3-xbjo2gzly3df2k6ju2bqxypsgpj74av6
63:	paraview	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/paraview-5.10.1-4h5qdhzypcniaez2kuuvcdj6d4xhns4
64:	parsec	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/parsec-3.0.2209-7extkamumzt72g7v7j63yteyplgftyz5e
65:	pdtd	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/pdtd-3.25.1-1x67nrs24pkbnmnmj7am3t75sowntwfc5
66:	petsc	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/petsc-3.18.1-dedl2zpkohzwsnf25c76mw4m24ve3raa
67:	phist	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/phist-1.11.2-06oyojfq63ig32aprawafeemr5korrrpm
68:	plasma	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/plasma-22.9.29-1z12zqxszecrubvztpjppfytumjgg
69:	plumed	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/plumed-2.8.0-epvuukmxngij4wbuvpad6tbx7mpredyf
70:	precice	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/precice-2.5.0-y5ig3rxwfeupuk7odzsi5bbnqlbdeu25
71:	pumi	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/pumi-2.2.7-vrz5nche4gokubfuzmc46qz4mfqvcsg
72:	py-cinemasci	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-cinemasci-1.3-jtx4it414a6aooajjeodp5pwt4lghghw
73:	py-jupyterhub	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-jupyterhub-1.4.1-wi2zbgjgkigxwila5ok2pski2g7qzyw1
74:	py-libensemble	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-libensemble-0.9.3-exsvyi4ve2itudyzoldfkskyppuqegdj
75:	py-parsl	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-parsl-1.1.0-rsijhwc7q4qlo7kh4furvo7muyouwdz6
76:	py-radical-saga	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-radical-saga-1.16.0-bzyd6sofsz5cxlyuk2xrpugyuxflxtee
77:	qthreads	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/qthreads-1.16-xjrlin56oaf1tc3ehvxdy74pz5zvcpkn
78:	quantum-espresso	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/quantum-espresso-7.1-pf4cmxbnqmswamoxn12ihjgtz4p7kqp
79:	raja	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/raja-2022.03.0-kf7ckzhggoh3u3cshwonj5mafjkmgp1
80:	scr	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/scr-3.0.1-47wtxqrwipia77oeyavpp5qkhdokgkuvu
81:	slate	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/slate-2022.07.00-ofiigavw7kcyneulkfbazl3m45mufmvu
82:	slepc	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/slepc-3.18.1-pi6plqtsnssyp37d2wlz3wfpylrrrcvh
83:	stc	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/stc-0.9.0-wnlngxjsz04rg3yw2jtlzgnxvgr5nax
84:	strumpack	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/strumpack-7.0.1-bcxv6bhl6e5e77wvzv3ambzaciqi4bb6h
85:	sundials	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/sundials-6.4.1-nal5sibiqezc45fbz53cwr34rxfcb4f
86:	superlu-dist	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/superlu-dist-8.1.1-k7k4dihxf1zall4wqz66r8s7agshu3bj
87:	swig	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/swig-4.0.2-fortran-f6qkx5yz47aagoww12rtbz4kucc6gh3j
88:	sz	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/sz-2.1.12.2-2ilgy7ishmc2ubz2ghbtkaooasaltbiek
89:	tasmanian	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/tasmanian-7.9-izwrkvljnjevthorhquesa6rkkmc6t7x
90:	tau	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/tau-2.32-qoombzmdp3qhettxr4f4d44erxzd5
91:	trilinos	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/trilinos-13.4.0-xnlfgmz4zeb7jdfdlx7bm5nnc4qkr71
92:	turbine	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/turbine-1.3.0-mymxhgxtddpdowytshsotcm3zvs2arpak
93:	umap	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/umap-2.1.0-wpqbk1c3pxmcyacmk6f3g5gxovariibg5
94:	umfire	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/umfire-2022.03.1-2vs73ks3sglgqveks2awdrvuzbcx3quq
95:	unifyfs	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/unifyfs-1.0-omawjudjffjow2xikrcraqn3u3cvmjwzy
96:	upcxx	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/upcxx-2022.9.0-nbwjd4sgirqp1rgct4qamdivwskluxvy
97:	variorum	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/variorum-0.6.0-azdafc4zoaosrpn5sfmbfsl5m4d4b3d7
98:	veloc	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/veloc-1.5-rhta4y7xmuhj4sxsykgfyzfb3y4etenk
99:	visit	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/visit-3.2.2-h7vjzflnfk2zbvz2ono4wok3rutuy4
100:	vtk-m	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/vtk-m-1.9.0-j52zqfh35h5qofzyzcu3uhndap3b4vlbx
101:	wannier90	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/wannier90-3.1.0-npbjfygy4n64yzk2ni1tbjfm5z3li7dag
102:	warpx	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/warpx-22.10-xcdmruk6bkvf24npzxhk3ha5ydyymmnh
103:	zfp	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/zfp-0.5.5-dkanfr4t75fh3gwkgpsdzhpshs25h24npx

## Languages:

- Julia
- Python

## AI products with GPU support

- Tensorflow
- Pytorch

## 3D Visualization

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

# E4S Support for CUDA variants on x86\_64

```
Singularity> spack find +cuda cuda_arch=80
-- linux-ubuntu20.04-x86_64 / gcc@11.1.0 -----
adios2@2.8.3      camp@2022.03.2  ginkgo@1.4.0    kokkos@3.7.00   omega-h@9.34.13  strumpack@7.0.1  umpire@2022.03.1
amrex@22.11      camp@2022.03.2  heffte@2.3.0    kokkos-kernels@3.7.00  petsc@3.18.1    sundials@6.4.1   vtk-m@1.9.0
arborx@1.3       chai@2022.03.0  hpx@1.8.1       lapackpp@2022.07.00  raja@2022.03.0  superlu-dist@8.1.1  zfp@0.5.5
blaspp@2022.07.00 dealii@9.4.0    hypre@2.26.0    magma@2.6.2      slate@2022.07.00  tasmanian@7.9    trilinos@13.4.0
caliper@2.8.0    flecsi@2.1.0   kokkos@3.7.00   mfem@4.5.0      slepc@3.18.1
==> 33 installed packages
Singularity> spack find +cuda cuda_arch=70
-- linux-ubuntu20.04-x86_64 / gcc@11.1.0 -----
adios2@2.8.3      camp@2022.03.2  ginkgo@1.4.0    kokkos@3.7.00   omega-h@9.34.13  strumpack@7.0.1  umpire@2022.03.1
amrex@22.11      camp@2022.03.2  heffte@2.3.0    kokkos-kernels@3.7.00  petsc@3.18.1    sundials@6.4.1   vtk-m@1.9.0
arborx@1.3       chai@2022.03.0  hpx@1.8.1       lapackpp@2022.07.00  raja@2022.03.0  superlu-dist@8.1.1  zfp@0.5.5
blaspp@2022.07.00 dealii@9.4.0    hypre@2.26.0    magma@2.6.2      slate@2022.07.00  tasmanian@7.9    trilinos@13.4.0
caliper@2.8.0    flecsi@2.1.0   kokkos@3.7.00   mfem@4.5.0      slepc@3.18.1
==> 33 installed packages
Singularity> █
```

# E4S Support for ROCm variants for MI250X (gfx90a) on x86\_64

```
[Singularity> spack find +rocm amdgpu_target=gfx90a
-- linux-ubuntu20.04-x86_64 / gcc@11.1.0 -----
amrex@22.11          gasnet@2022.9.0  lapackpp@2022.07.00  strumpack@7.0.1      upcxx@2022.9.0
arborx@1.3          ginkgo@1.4.0    magma@2.6.2         sundials@6.4.1      vtk-m@1.9.0
blaspp@2022.07.00  heffte@2.3.0   petsc@3.18.1       superlu-dist@8.1.1
camp@2022.03.2     hpx@1.8.1      raja@2022.03.0     tasmanian@7.9
chai@2022.03.0     hypre@2.26.0   slate@2022.07.00   trilinos@13.4.0
ecp-data-vis-sdk@1.0 kokkos@3.7.00  slepc@3.18.1      umpire@2022.03.1
==> 26 installed packages
Singularity> █
```

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

1: adios2	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/adios2-2.8.3-xstw7pb2wnuauxru23yle4fwxftprwub
2: alquimia	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/alquimia-1.0.10-imm7jcs2ouai2rxauouvyckx7jgq66
3: aml	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/aml-0.2.0-zcs62l6fotx3x3qd5n6dw2yk6nq6p2lu
4: amrex	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/amrex-22.11-qkh4nkmrfvy3rsjuot4itogkgs3ykbmh
5: arborx	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/arborx-1.3-sfc3s5436qqbeba3ifeuiphfnmby3c7s
6: archer	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/archer-2.0.0-256hr6lkoioqfejxvvgp5qrm23zjondko
7: argobots	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/argobots-main-6nktgpmhhyk4moukp5acd574r6tx645m
8: ascent	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/ascent-0.8.0-ue6c6ykcj22v6cuhbbuwjxvheshdy7mq
9: axom	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/axom-0.7.0-tbaeg6h7snyrv2zaf5shhmmxx322ilq3
10: bolt	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/bolt-2.0-qgdopshdcpztcnnda56mowvww2digyz
11: butterflypack	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/butterflypack-2.2.2-lrytvkx54c64nw7sp4sgj7ju6zfpzmzg
12: cabana	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/cabana-0.5.0-dbnndtwhieiqh23dhdzdirar616rygz7w
13: caliper	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/caliper-2.8.0-ardfzvqrw5xx3eygslqy3wn3673fp4yv
14: chai	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/chai-2022.03.0-y67sx56h67l3svnpgmywms2nj3k57u07
15: charliecloud	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/charliecloud-0.29-22lhik3wztz2lwgsp5ztaaxivczfnvts
16: conduit	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/conduit-0.8.4-i2dirqo5kdnc1zmo4z2g4py7wat2toil
17: darshan-runtime	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/darshan-runtime-3.4.0-6gwxbfzshgdkluszryiuq7yvwil77f
18: datatransferkit	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/datatransferkit-3.1-rc3-yw7yb5352jm7ebuszgc7gxfmhjm2a6pz
19: dyninst	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/dyninst-12.2.0-srymkr1xqo2uel246lxun4by46vc1tx
20: ecp-data-vis-sdk	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/ecp-data-vis-sdk-1.0-zx5zr5bjurfk46l2rjmmznmotrnrjj
21: exaworks	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/exaworks-0.1.0-xwvmorfkgk2pfzjuja5gwuqsf1b63ugu
22: faodel	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/faodel-1.2108.1-fi5cqlv5vqkmjd6xdlm5cfffq6gs7qa3c
23: flecsi	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/flecsi-2.1.0-ry6mptoqpps6zw5qp77o1l2oepq5foai
24: flit	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/flit-2.1.0-3xcjxzekst34gvmawehi7tpew6wbqim
25: flux-sched	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/flux-sched-0.25.0-lsqmafqe4fkerkss5hcc5p3f6ifv44xu
26: fortrilinos	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/fortrilinos-2.1.0-ou6tjphmra6k4fjxeh3uasrtzcc6ftlm
27: gasnet	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/gasnet-2022.9.0-hcednfbzdkoag6sayingfup5dgdz5f2ah2
28: ginkgo	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/ginkgo-1.4.0-ihmtmzji6hamhvcaw45mzbsmyihmayvp
29: globalarrays	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/globalarrays-5.8-wcasxk7bjcsbjiaathzocnfxdnx6pz5v5
30: gotcha	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/gotcha-1.0.4-pp3wx752o7eyg2bohct5nsh3j67ck7bs
31: gptune	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/gptune-3.0.0-dxrelx4x3iptauno23qpscx76gvgsag
32: h5bench	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/h5bench-1.3-64tk47z26t3ier5oet3nck563ofpe6su
33: hdf5	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hdf5-1.13.2-jtg6fulrjfl6tsvkkcam2faconpjozz
34: hdf5-vol-async	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hdf5-vol-async-1.3-2idxkq4o4yf33sih3wh64ddj22sjhj34
35: heffte	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/heffte-2.3.0-ybenwfs5whb623uwencjgds1hqnbyedc
36: hpctoolkit	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hpctoolkit-2022.10.01-3s4wo2fusrnfvteiqpjs5c4ainkmogzk
37: hpx	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hpx-1.8.1-k4taf7ds4wjeihmyvzk6ia7ececqdkpvh4
38: hypre	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hypre-2.26.0-xcdmzvzb5uv34kxzipugli72s24koebvx
39: kokkos	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/kokkos-3.7.00-ridq237k7wk7hmkosbkzjucnqg3avqwh
40: kokkos-kernels	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/kokkos-kernels-3.7.00-75g3c4e4vf13p2bfk3gna4ttju72eiu
41: lammps	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/lammps-20220623-hqrhjr62kdzr35js3av7te6fz2bfibwc
42: legion	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/legion-21.03.0-6lbyivddvseddjfuujmvmki56ipnk7cp
43: libnrm	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/libnrm-0.1.0-d7pffkzjjrmrisboiqcl7yie4o6r4vxc
44: libpressio	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/libpressio-0.88.0-tu7zmnqrh7cnvq46m7r54sp7ofpw2ko
45: libquo	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/libquo-1.3.1-gmno3vlx7vu25rtpshwyxkrbbpnyc1qw
46: magma	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/magma-2.6.2-rzszsgyer4k2bvbcv7367aumyeu4as54
47: mercury	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mercury-2.1.0-6pfx2hulyppvn5gla06nnfyerojnq5sq
48: metall	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/metall-0.21-7yh36oky4dmp5eujuzasx7vnnncucrow
49: mfem	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mfem-4.5.0-i3ozodxminhapjxouuwunz2huwla5v2qk
50: mpark-variant	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mpark-variant-1.4.0-tkootg76dnc7lkamebdz4v63aadtcow
51: mpich	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mpich-4.0.2-vuh7xcc7tiruyjep1retykmeui6jv52e

## GPU runtimes for IBM Power

- CUDA 11.4
- NVHPC 22.9

## Languages

- Julia
- Python

## AI packages for NVIDIA GPU

- TensorFlow
- PyTorch

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

52:	mpifileutils	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mpifileutils-0.11.1-shjxfjppjvnosjprrm2qzaqzbdpydp6yp
53:	nccmp	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/nccmp-1.9.0.1-7mveozgiw4pwwv3jdmg5f5re3liereay
54:	nco	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/nco-5.0.1-cuqirm6yoh4soh3m4jyuyjd65lwrhm4
55:	netcdf-c	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/netcdf-c-4.9.0-k6yoh3wmojyjj6zkc56cof3ybadgkshvz
56:	netlib-scalapack	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/netlib-scalapack-2.2.0-ceqsztw3ftqckwgudwacd2dgtowj5y2r
57:	nrm	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/nrm-0.1.0-jehz42dp6tq2cexmgxwiqfozxfjkobw
58:	omega-h	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/omega-h-9.34.13-m5bwhbsbeq21cplwaxhdvrad7dnljpyi
59:	openmpi	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/openmpi-4.1.4-se2ftqv5xsejkmzvfpxsdybdmqqwb1gkzr
60:	openpmd-api	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/openpmd-api-0.14.5-vynu7b5z3fbdx46raffz64dtdvtdejh
61:	papi	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/papi-6.0.0.1-zsplngh5qplinh4eegi5wzfw2qg6ru3
62:	papyrus	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/papyrus-1.0.2-a6qveegb6k2ahymzggglulee6ojoovqm
63:	parallel-netcdf	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/parallel-netcdf-1.12.3-1w3glwqyttaa1qt45k67owvf5hqjnbp
64:	parsec	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/parsec-3.0.2209-3xmk1hbil6k2fpo4uveury3qdq3ae2um
65:	pdtd	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/pdtd-3.25.1-v4rjp5vwznt7s3d2c2j4wawyhs2aagqye
66:	petsc	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/petsc-3.18.1-td7n4vxi46oatcimj3zfhf7g2o572b
67:	phist	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/phist-1.11.2-rf712cixm47puybop3ayjxrra5plxdg3
68:	plasma	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/plasma-22.9.29-feh4vff11k4qck7vhtcw2fphq2dxq3rg
69:	plumed	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/plumed-2.8.0-tmxzczerz46vn3j27rtwqpxxb3kpw5xs
70:	precice	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/precice-2.5.0-iw2o7zww7umgssru3hoxqiigxrgdtul
71:	pumi	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/pumi-2.2.7-qboyr63c55zhrtedw5dtrpgmky5bjpw
72:	py-cinemasci	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-cinemasci-1.7.0-p4rv2a3lrzfxr2jddgwrxbi2zc4xxa6z
73:	py-jupyterhub	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-jupyterhub-1.4.1-cf3tays414k5drhetd6vuobfaoxke4rq
74:	py-libensemble	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-libensemble-0.9.3-3ohso23ip2jgcwxf67zkrzsp2gkixa55
75:	py-parsl	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-parsl-1.1.0-wuk64tyhzm3o3jw352yupu7uwjvqvvtwn
76:	py-radical-pilot	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-radical-pilot-1.16.0-dps7t7pvkves3wwrphxagoj6ghhzzvb
77:	py-radical-saga	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-radical-saga-1.16.0-br3ptdqhlo5yze4qt662hb735wlkdgv
78:	qthreads	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/qthreads-1.16-rtnk7r26b3x5yilieufiga2ipw55daiiq
79:	quantum-espresso	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/quantum-espresso-7.1-hpsqg56frlyptn6ebpfvqx7zh17boaw
80:	raja	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/raja-2022.03.0-j51murozoyj2ny37vcyucaaws5dkqapmk
81:	scr	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/scr-3.0.1-owo4tln4v1w4rxym525alqrc2gykdud
82:	slate	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/slate-2022.07.00-gfetndk473optp5xbf7wjyphkvvicwv4
83:	slepc	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/slepc-3.18.1-q7wi72f1ehxqgpdft57gugcthrwx34
84:	stc	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/stc-0.9.0-myxazo2kbnkirwxshrqfca4bo5tzd
85:	strumpack	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/strumpack-7.0.1-wsv5cgcffg2bh5rdpobab6odkv6ngtokn
86:	sundials	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/sundials-6.4.1-be5o3gu3lyz6chq477jnkbe2aoin24u
87:	superlu-dist	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/superlu-dist-8.1.1-xaslzn7y2pkysine4ukuly6fn5ib724g
88:	swig	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/swig-4.0.2-fortran-ct3v7tcpfcx7gzyhgq7c47f2j6gj7oex
89:	sz	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/sz-2.1.12.2-djc27r3exk3ykrxr3dmku5f5vwc56d5d
90:	tasmanian	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/tasmanian-7.9-rlbvfdrbrea5ifsd3juqceyayrgyozd
91:	tau	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/tau-2.32-bx7zr6szk652qsvgx24pqqo7br4xprgl
92:	trilinos	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/trilinos-13.4.0-3jyearqfsvxc7j7eicaytfuzxr6hsny
93:	turbine	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/turbine-1.3.0-ahvy6fjzi4pqgni4wv6zadaj4g26nsbj
94:	umap	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/umap-2.1.0-fbkjmj3aseq4yn3xecmwlx3i2f31ogn
95:	umpire	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/umpire-2022.03.1-ngbjwhktklyap24fy7x2ixrflgzwdh26
96:	unifyfs	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/unifyfs-1.0-k4m4q726d6fgo4z227hy7g5y3l5zxmvgk
97:	upcxx	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/upcxx-2022.9.0-xngkg2e35w3hxeqg73jfuu4nm3hakmnc
98:	veloc	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/veloc-1.5-2kisertu7gukltw3hgwt4a3fogi5p5cp
99:	vtk-m	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/vtk-m-1.9.0-xby4bbn4rsbs2o7tmsdhrag5s4twtupk
100:	wannier90	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/wannier90-3.1.0-71bbjhbvmrm4tzvdvhlh3gcwvx6nfzii
101:	warpx	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/warpx-22.10-ciw2valpnmv7jmoq3eqcj552zrppbsy7
102:	yaksa	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/yaksa-0.2-htchdndgcdknrsytcxm2rmeths3tdeca
103:	zfp	/spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/zfp-0.5.5-5ynynd5oyhse132b3psgf32hv3b3cy4ub

## GPU runtimes for IBM Power

- CUDA 11.4
- NVHPC 22.9

## Languages

- Julia
- Python

## AI packages for NVIDIA GPU

- TensorFlow
- PyTorch

# E4S Support for CUDA variants on ppc64le

```
Singularity> spack find +cuda
-- linux-ubuntu20.04-ppc64le / gcc@9.4.0 -----
adios2@2.8.3      caliper@2.8.0    ecp-data-vis-sdk@1.0  hpx@1.8.1        lapackpp@2022.07.00  petsc@3.18.1      sundials@6.4.1      umpire@2022.03.1
amrex@22.11      camp@0.2.3       flecsi@2.1.0          hwloc@2.8.0      magma@2.6.2          raja@0.14.0       superlu-dist@8.1.1  vtk-h@0.8.1
arborx@1.3       camp@2022.03.2   flux-core@0.44.0     hypre@2.26.0     mfem@4.5.0           raja@2022.03.0    tasmanian@7.9       vtk-m@1.7.1
ascent@0.8.0     camp@2022.03.2   ginkgo@1.4.0          kokkos@3.7.00    omega-h@9.34.13     slate@2022.07.00  tau@2.32            trilinos@13.4.0
blaspp@2022.07.00  chai@2022.03.0  heffte@2.3.0          kokkos@3.7.00    papi@6.0.0.1        slepc@3.18.1      trilinos@13.4.0    zfp@0.5.5
cabana@0.5.0     dray@0.1.8       hpctoolkit@2022.10.01  kokkos-kernels@3.7.00  petsc@3.18.1        strumpack@7.0.1   umpire@6.0.0
==> 46 installed packages
Singularity> uname -a
Linux eagle 4.18.0-348.7.1.el8_5.ppc64le #1 SMP Wed Dec 8 21:26:34 EST 2021 ppc64le ppc64le ppc64le GNU/Linux
Singularity>
```



# 22.11 Release: 97 Official Products + dependencies (gcc, aarch64)

1: adios2	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/adios2-2.8.3-tn6yp5hy7pzu4dsbx4btezwtu4tlre
2: alquimia	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/alquimia-1.0.10-tdvinjiqt46eacm6pnrdr3ue6k6i4j
3: aml	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/aml-0.2.0-syvk6hnrriqj77ncazqzqlmcbnkpclgu
4: amrex	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/amrex-22.11-6ydr3w7ayovuh2y2vsvxoid2kgwfpws
5: arborx	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/arborx-1.3-jt7ve5rlwivzf5dzwyng26jam5fzjqci
6: archer	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/archer-2.0.0-7f5pa6xnn5dv4jfvu7b4646ycq16fzkc
7: argobots	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/argobots-1.1-l74kgroqqhmojgtla6jcc636nxy2dalfc
8: axom	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/axom-0.7.0-t3kotm4x4z52ekeuf6jo4rr4vbwze63w
9: bolt	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/bolt-2.0-yvwovujhly33eswru7y5u7hrm5wrlvpb
10: butterflypack	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/butterflypack-2.2.2-kpf7z2obladjl5oyh5v1irhnuurv3i3l
11: cabana	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/cabana-0.5.0-vr5m5k2oaifqa5rf3avouo64goreqvqx
12: caliper	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/caliper-2.8.0-jn2n6qmx4nr5wah2v74hobktmltdgl5y
13: chai	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/chai-2022.03.0-5u6vclovphu7jujakax5hbcukh6qhym
14: charliecloud	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/charliecloud-0.29-ktfm7t2k7hpgtzrjmhcwcvgpi3grl5a
15: conduit	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/conduit-0.8.4-hvuikr4sv2kfcx4g35jfo6c2rj2zccmj
16: dealii	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/dealii-9.4.0-falixullnfl4vjamcep2ljuuscwrglzc
17: datatransferkit	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/datatransferkit-3.1-rc3-zisyujfv4nttxhdnbnbcdv6co75z5pv
18: dyninst	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/dyninst-12.2.0-ypzolgjgzobolvpbgsi4jzfhcyk47vjg
19: exaworks	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/exaworks-0.1.0-3m2ruyseumhukyekm2q4nt7rdvd7k4wg
20: flecsi	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/flecsi-2.1.0-s6rs2yftyaxvxl7q7p22gvekqa4y3
21: flit	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/flit-2.1.0-emd4kewqega7ex6b7fsoj7ks2jgfp2r
22: flux-sched	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/flux-sched-0.25.0-lmqd4l4srk3jhviy5is6s63bhi3wss3l
23: fortrilinos	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/fortrilinos-2.1.0-exjnwqhy36jgk3wzihytuxmhpux37x
24: gasnet	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/gasnet-2022.9.0-6bes46634npapndf4hjcntlbn5iwrvp
25: ginkgo	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/ginkgo-1.4.0-acxgljw53cythdethxlzrhny4qsb5x2
26: globalarrays	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/globalarrays-5.8-wz17agux5xdxyi4xngmd4xtgl5g3old
27: gotcha	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/gotcha-1.0.4-gagcbny5lx6tabraefjzoiobwbmdiiq
28: gptune	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/gptune-3.0.0-4kplix3fdcstrt5dyppqlrqaqrpogexi
29: h5bench	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/h5bench-1.3-7lmvmdpwsk755x5wckemhryj64t6adku
30: hdf5	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/hdf5-1.12.2-asibqu6li16f2khy4wz4jgugvdt6nasw
31: heffte	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/heffte-2.3.0-52sxlh32xxlx7xqsu2hn67ituonhpetd
32: hpctoolkit	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/hpctoolkit-2022.10.01-bt53j fagmgfgymp6dcg3mma2xkj6z6j
33: hypre	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/hypre-2.26.0-ohgawpjqqug75igt37gvh42akacask
34: kokkos	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/kokkos-3.7.00-f7yk3y47vlms4qzwikqgkxfyc2w5w24
35: kokkos-kernels	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/kokkos-kernels-3.7.00-atdbg7a5fyhnqwc2aiffor522mtaeswv
36: lammps	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/lammps-20220623-erjtpwzq4kgfmywp5ydvcdnltujb7fo
37: legion	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/legion-21.03.0-o3f5hnenbldjwvb42que4kajwxgm4xs
38: libnrm	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/libnrm-0.1.0-xbrc2ijsh3z5yz7m5dqkzeblqtb4dow
39: libpressio	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/libpressio-0.88.0-ofdlcpliljgeket6wujc7s7cylphx2x
40: libquo	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/libquo-1.3.1-yrjwwdkcw2syql7wqkladcc65bfj3z3n
41: magma	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/magma-2.6.2-vlhdyh4rcsuyv63s2g3kxooazucnzm
42: mercury	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/mercury-2.1.0-32tjycyhtonefmschzspb4t56hgqavs
43: metall	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/metall-0.21-p62a12ga42ubtmfbya4rvlrltoxmyc
44: metis	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/metis-5.1.0-zmoxqrtl3klpelmjjeofnquikf2z3hktj
45: mfem	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/mfem-4.5.0-tf5sgtvrvnsxhij53nw6u53skhgis35j
46: mpark-variant	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/mpark-variant-1.4.0-ffmm7i4mno7mpx6weaevaizygyccerb
47: mpich	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/mpich-4.0.2-4f7mm6hpijp7475nhxulp7nffjbmwu
48: mpifileutils	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/mpifileutils-0.11.1-ptsvxvdtg57g5ppuxfwzsaba6wwnicnth

## GPU runtimes for aarch64

- CUDA 11.7.1
- NVHPC 22.9

## Languages

- Julia
- Python

## AI packages for NVIDIA GPU

- TensorFlow
- PyTorch

# 22.11 Release: 97 Official Products + dependencies (gcc, aarch64)

49:	netcdf-c	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/netcdf-c-4.9.0-2pfmvfxccyym2mcbvr7wf5fz4lhyn5e
50:	netlib-scalapack	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/netlib-scalapack-2.2.0-jibpglaaLgu14vdkthm2Xffgsaqyk6x
51:	nccmp	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/nccmp-1.9.0.1-bj5q4zadekltopllmpwap55t6rhp7bn
52:	nco	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/nco-5.0.1-37anulj3jhpj7uppvvauLv3rhiyfokp
53:	nrm	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/nrm-0.1.0-gaw4judk5h7leoarmhglx7anwmot7ss
54:	omega-h	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/omega-h-9.34.13-7akf22v6k6gez6z3laipkgvodstcbs4x
55:	openmpi	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/openmpi-4.1.4-tzjiius6vahp7gqtpmj5dufkhupnh
56:	openmpi-api	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/openmpi-api-0.14.5-7n4dyx2hfvaqlx42yczmptrbh6pjrw
57:	papi	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/papi-6.0.0.1-whxzalkc552oguusqeoyslud72dms63l
58:	papyrus	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/papyrus-1.0.2-4izhlazxbhfgsu5wqr5mfph7nreryu7u
59:	parmetis	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/parmetis-4.0.3-uf2q6w2obb3ff55saykavw64v4qxx77g
60:	parsec	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/parsec-3.0.2209-kok6u7t4ktjs5hbskcui3ij5k273t4n
61:	pdst	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/pdst-3.25.1-tips7k5urkb4e06ggs7h47dbtrr4w6x2
62:	petsc	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/petsc-3.18.1-wa3y5fd6bpo6l2zcf5aldzggzn3lzzgq
63:	plasma	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/plasma-22.9.29-4flv33ga6ms6tk42s2wrxbg1btg5fmpu
64:	plumed	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/plumed-2.8.0-a2mtftxdvwp4xui3h3o3hwj2cke3gsvq
65:	precice	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/precice-2.5.0-3u3kp2fd3lxd4paqhc0zknw362en4p4a
66:	pumi	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/pumi-2.2.7-7pmitcrr6vf6b6e7tomboz6g6p2kke5l
67:	py-jupyterhub	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/py-jupyterhub-1.4.1-xfggddo75bxjnh7kdnix53lwuo7gjfm
68:	py-libensemble	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/py-libensemble-0.9.3-ekr7nmfbbvrrkar6mafz3fzr42qigbz
69:	py-opentuner	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/py-opentuner-0.8.7-ym2rlh2zrgsyamcxioL4dnxjws7qm
70:	py-parsl	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/py-parsl-1.1.0-m7wtbpe4nxq5mqdxirf22gwettjebvug
71:	py-radical-entk	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/py-radical-entk-1.16.0-uspj343t5wdcgrqykrjabeqs3taa23x
72:	py-radical-pilot	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/py-radical-pilot-1.16.0-gslkf66oznl4wgL3njL3gnjuobczyx
73:	py-radical-saga	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/py-radical-saga-1.16.0-wcz7tksshluahyoyjofpsyzqhlcc3
74:	qthreads	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/qthreads-1.16-c6uuprrtqcdkq75g5d3pur5iblvkutak
75:	quantum-espresso	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/quantum-espresso-7.1-hw7oy3jvdlkkgaraslhbwetuxx72uxf
76:	raja	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/raja-2022.03.0-6lmk40lb4ikhrg52wenkruy3o7oae4a
77:	scr	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/scr-3.0.1-byaglsu6i6bbencntnibty42hv2jux7s
78:	slate	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/slate-2022.07.00-je6innhafk7it6nh6pb472c6q4zc5jwx
79:	slepc	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/slepc-3.18.1-yo2g4k4gimlkivptfwyz7zxc6qafnrnt
80:	stc	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/stc-0.9.0-66ur7lde4sehbiuhq725h4njmh67yn6t
81:	strumpack	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/strumpack-7.0.1-6b43dyoqnfaf5yge4u2ljmckfs4wjggwa
82:	sundials	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/sundials-6.4.1-t2k7smta36vv4sfpvr72qvky37kzbo
83:	superlu-dist	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/superlu-dist-8.1.1-ul3qouwm24cvprbxaeevg7zrhyn55dv
84:	swig	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/swig-4.0.2-fortran-wgukl4d4bbrvln2dko27vmsbz4vdoz
85:	sz	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/sz-2.1.12.2-6inw3xqodwku35vffczal7x7e32g6vzv
86:	tasmanian	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/tasmanian-7.9-xehgodjpanihpukedfppvijv4kviffhl
87:	tau	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/tau-2.32-oi5yvfxxkdx46hdjcwisatfnwapp2qga
88:	trilinos	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/trilinos-13.4.0-7ig32xrxhx2wjygha77bh4h3yraxgfw
89:	turbine	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/turbine-1.3.0-ttxgmsxu5juonlagdgr74ugifohitu65
90:	umap	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/umap-2.1.0-kglnikj3dpcmeuwex3twovw7msjgkngb
91:	umpire	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/umpire-2022.03.1-2aagqdhp5wysbf5zwanwjdpnf7mh7za4
92:	upcxx	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/upcxx-2022.9.0-gaktmfdhbhnuhnpwsrrnq3amjtlfffeg
93:	vtk-m	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/vtk-m-1.9.0-mievxnqsq2ok6ysvL5lfrhraedcwwtvm
94:	wannier90	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/wannier90-3.1.0-osqph5gscpas7ofgu5uedhlzacebeb5n
95:	warpx	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/warpx-22.10-2uknrmbuohzvoluLhiqidwyc5uneekn
96:	yaksa	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/yaksa-0.2-vpraougviqj2c2wncmc7ebfgbwqon2d
97:	zfp	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/zfp-0.5.5-r4wxkyawwtixm3pwh2peL5o2ihwzkp

## GPU runtimes for aarch64

- CUDA 11.7.1
- NVHPC 22.9

## Languages

- Julia
- Python

## AI packages for NVIDIA GPU

- TensorFlow
- PyTorch

# E4S Support for CUDA variants on aarch64

```
[Singularity> spack find +cuda cuda_arch=80
-- linux-ubuntu20.04-aarch64 / gcc@11.1.0 -----
adios2@2.8.3      camp@2022.03.2  ginkgo@1.4.0    kokkos-kernels@3.7.00  petsc@3.18.1    sundials@6.4.1  vtk-m@1.9.0
amrex@22.11      camp@2022.03.2  heffte@2.3.0    lapackpp@2022.07.00   raja@2022.03.0  superlu-dist@8.1.1  zfp@0.5.5
arborx@1.3       chai@2022.03.0  hypre@2.26.0    magma@2.6.2           slate@2022.07.00  tasmanian@7.9
blaspp@2022.07.00 dealii@9.4.0    kokkos@3.7.00   mfem@4.5.0            slepc@3.18.1    trilinos@13.4.0
caliper@2.8.0    flecsi@2.1.0    kokkos@3.7.00   omega-h@9.34.13      strumpack@7.0.1  umpire@2022.03.1
==> 32 installed packages
Singularity> █
```

Support for A100 and T4 GPUs under aarch64

# E4S 22.11 Release: GPU support for Docker Containers

ecpe4s/e4s-cuda ☆

By [ecpe4s](#) • Updated 2 days ago

Manage Repository

Pulls 77

Overview **Tags**

Sort by Newest Filter Tags

TAG

**22.11** Last pushed 2 days ago by [esw123](#)

TAG	DIGEST	OS/ARCH	LAST PULL	COMPRESSED SIZE
22.11	<a href="#">968cfc478e8d</a>	linux/amd64	---	44.61 GB
	<a href="#">482dd048cf67</a>	linux/arm64/v8	---	28.66 GB
	<a href="#">5ddb0fb0b5c</a>	linux/ppc64le	---	32.03 GB

docker pull ecpe4s/e4s-cuda:...

- 100+ E4S Products
- Support for GPUs
  - x86\_64
  - ppc64le
  - aarch64

% docker pull ecpe4s/e4s-cuda

# E4S Build Cache for Spack 0.19.0



## E4S Build Cache for Spack 0.19.0

To add this mirror to your Spack:

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

95,721 total packages

Last updated 2022-11-11 14:47 PST

- All Arch  PPC64LE  X86\_64
- 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](#) [adlhx@0.9.2](#) [adlhx@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](#) [amr-wind@main](#) [amrex@20.07](#) [amrex@20.09](#) [amrex@20.10](#) [amrex@20.11](#) [amrex@20.12](#) [amrex@21.01](#)
- [amrex@21.02](#) [amrex@21.03](#) [amrex@21.04](#) [amrex@21.05](#) [amrex@21.06](#) [amrex@21.07](#) [amrex@21.08](#) [amrex@21.09](#) [amrex@21.10](#)
- [amrex@21.11](#) [amrex@21.12](#) [amrex@22.01](#) [amrex@22.02](#) [amrex@22.03](#) [amrex@22.04](#) [amrex@22.05](#) [amrex@22.08](#) [amrex@22.11](#)

- Over 95,000 binaries!
- No need to recompile from source code.

# E4S 22.11 AWS image: US-West2 (OR)

The screenshot displays a desktop environment with the following components:

- ParaView 5.9.0:** A 3D visualization of a pressure field on a mesh. The color scale ranges from  $0.0e+00$  (blue) to  $1.2e-38$  (red).
- Terminal Window:** Shows the output of the `singularity run` command, listing installed modules such as `adiak/0.2.1-4vc`, `amrex/21.11-rocml6cm`, and `parmetis/4.0.3-vhi`.
- TAU ParaProf Statistics:** A table showing performance metrics for various operations. The table is as follows:
 

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

## E4S 22.11 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-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:

```
. /opt/intel/oneapi/setvars.sh
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
```

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

# New release of e4s-cl on GitHub

Product Solutions Open Source Pricing Search Sign in Sign up

E4S-Project / e4s-cl Public Notifications Fork 0 Star 5

Code Issues 3 Pull requests 1 Actions Projects Security Insights

master 7 branches 8 tags Go to file Code

spoutn1k Prepare release v1.0.1 ✓ b2c9299 3 days ago 1,222 commits

.github/workflows	Updated python	4 months ago
assets/images	Proper image conversion	5 months ago
docs	Prepare release v1.0.1	3 days ago
e4s_cl	Prepare release v1.0.1	3 days ago
requirements	Unfreeze dependency version	3 months ago
scripts	Reflect name changes in scripts	3 months ago
tests	Fail to fix safe_tar test; disabling it	last month
.coveragerc	Introduced the coverage tool	9 months ago

About

Container manager for E4S

- Readme
- MIT license
- 5 stars
- 4 watching
- 0 forks

Releases 8

**E4S-CL release v1.0.1** Latest 3 days ago

+ 7 releases

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



# New release of custom E4S images: Waggle and SAGE projects

The screenshot shows the Docker Hub repository for '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 SAGE as 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 website URL is www.sagecontinuum.org.

**SAGE**  
A Software-Defined Sensor Network  
Cyberinfrastructure for AI at the Edge  
www.sagecontinuum.org

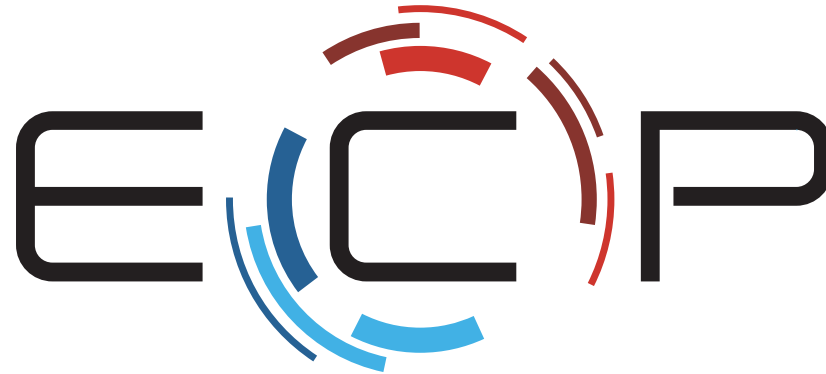
# Extreme-scale Scientific Software Stack (E4S)

- Three base images and three full featured images x86\_64
  - ROCm
  - CUDA
  - oneAPI
- Base image and full-featured image with CUDA for ppc64le and aarch64.
- 100+ HPC and AI/ML products (TensorFlow, PyTorch).
- New release of e4s-cl container launch tool v1.0 at SC22. e4s-cl is used to replace MPI in containerized application with host MPI. It includes MPICH ABI and OpenMPI support.
- Custom E4S images include support for Waggle (ecpe4s/waggle-ml) for x86\_64 and aarch64.

# 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.

