E4S: The Extreme-scale Scientific Software Stack Release 22.02

Release 22.05 notes

May 31, 2022

U.S. DEPARTMENT OF **ENERGY** | Office of Science

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

https://e4s.io

Lead: Sameer Shende
(U Oregon)

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

EXASCALE COMPUTING PROJECT

E4S Download from https://e4s.io
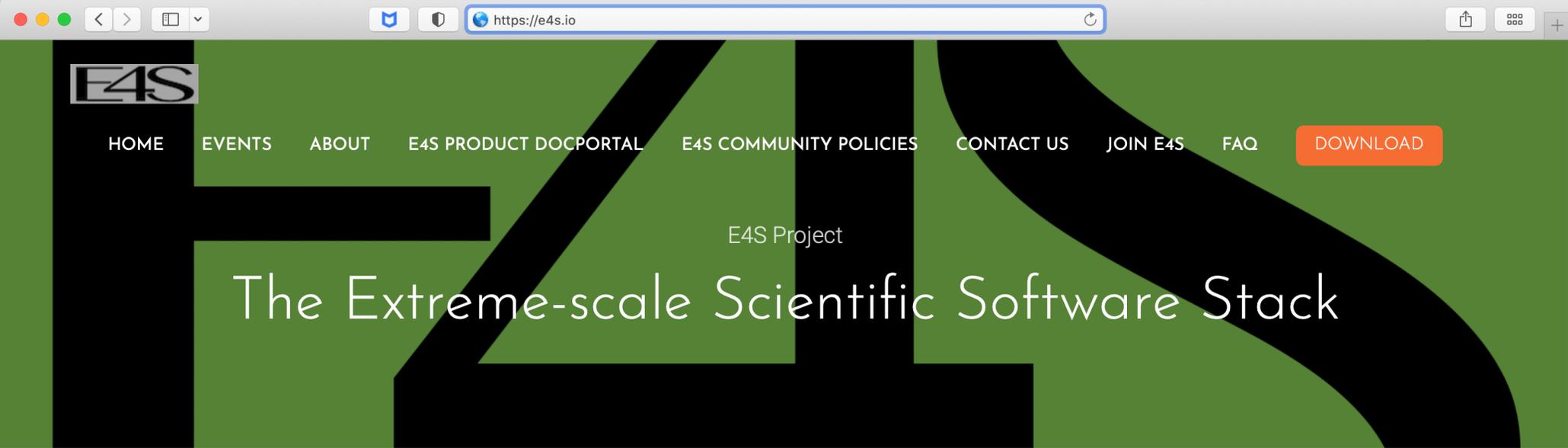
Download E4S 22.05 GPU Container Images: NVIDIA, AMD, Intel

Container Releases

⊕ Docker Downloads - CUDA

⊕ Docker Downloads - ROCm

⊕ Docker Downloads - OneAPI

⊕ Singularity x86_64 Download - CUDA

⊕ Singularity ppc64le 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 22.05 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 base images for
  - x86_64 (Intel, AMD, NVIDIA)
  - ppc64le
  - aarch64

https://e4s.io

Download E4S 22.05 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:22.05
```

```
# docker pull ecpe4s/e4s-rocm:22.05
```

```
# docker pull ecpe4s/e4s-oneapi:22.05
```

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)	Intel OneAPI (x86_64)
ecpe4s/e4s-rocm:22.05 🐳 docker	ecpe4s/e4s-cuda:22.05 🐳 docker	ecpe4s/e4s-oneapi:22.05 🐳 docker
e4s-rocm-22.05.sif ⓢ mirror 1	e4s-cuda-x86_64-22.05.sif ⓢ mirror 1	e4s-oneapi-22.05.sif ⓢ mirror 1
	e4s-cuda-ppc64le-22.05.sif ⓢ mirror 1	

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Download E4S 22.05 Base GPU Container Images

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.

NVIDIA Multi-Arch (X86_64, PPC64LE, AARCH64)

ecpe4s/e4s-base-cuda:22.05 🐳 docker

e4s-base-cuda-x86_64-22.05.sif Ⓢ mirror 1

e4s-base-cuda-aarch64-22.05.sif Ⓢ mirror 1

e4s-base-cuda-ppc64le-22.05.sif Ⓢ mirror 1

ROCM X86_64

ecpe4s/e4s-base-rocm:22.05 🐳 docker

e4s-base-rocm-22.05.sif Ⓢ mirror 1

Intel OneAPI X86_64

ecpe4s/e4s-base-oneapi:22.05 🐳 docker

e4s-base-oneapi-22.05.sif Ⓢ mirror 1

https://e4s.io

22.05 Release: 101 Official Products + dependencies (gcc, x86_64)

```
 1: adios2             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/adios2-2.8.0-5fxpauervqbotprybms3mwkgh7t6jc6v
 2: alquimia           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/alquimia-1.0.9-mkugz7joihpf4umcyidflg3dwik2nvlr
 3: aml                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/aml-0.1.0-ogtiuh4diyg4tq47tfjdpw7nue7sa5ka
 4: amrex              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/amrex-22.05-7tgphdtmt3fmoijkfrfsnwbqzpikxqfs
 5: arborx             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/arborx-1.2-a5j5wjdwqatoqsvs6xjckootv76g5h32
 6: archer             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/archer-2.0.0-zurunmhys3lwxhqn3ffapnelmezog2gl
 7: argobots           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/argobots-1.1-prj5il35vpp7sgcclenbh2thzqvrylwf
 8: ascent             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/ascent-0.8.0-qgivng4ownyfzct535vkvzle6irkjaq2
 9: axom               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/axom-0.6.1-ammuobdcyxxfsoyl7pyvbgyvw3kysoaj
10: bolt               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/bolt-2.0-mb62bsxs7cvgisgkww4m46qffxvfknfz
11: bricks             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/bricks-r0.1-5qkeva7iiqimec7zwsgvd33tz4mddslz
12: butterflypack      /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/butterflypack-2.1.1-fhncpxhwa4agoogz7magi6flubctqdp6
13: cabana             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/cabana-0.4.0-obd2epyboqn4pifoqwfiojyszqi6npoc
14: caliper            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/caliper-2.7.0-5scpuxjsztlwgbpclgpw3kafmfvbp3ub
15: chai               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/chai-2.4.0-l6nclfuapgjlbctkriikyeo3mhdatl5l
16: charliecloud       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/charliecloud-0.26-wgnmvl3rceimjvrcstuogmhlzhelz466
17: conduit            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/conduit-0.8.3-hm2j65mka5alpsg4uc4dswqvp7fusqvz
18: darshan-runtime    /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/darshan-runtime-3.3.1-ausjp6wozamwgyhgxiv22qcsarxvoixy
19: datatransferkit    /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/datatransferkit-3.1-rc3-xd57qoqxv4ikmz7ypfowrmnboqtohwq4
20: dyninst            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/dyninst-12.1.0-du56qu4uijap4synulxijiwury3dni5h
21: faodel             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/faodel-1.2108.1-kvw27w57ny2achbuhpiu3cweudqnin7h
22: flecsi             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/flecsi-1.4.2-fzhunvoffnf7l4sssl6l5ufukbrftc5u
23: flit               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/flit-2.1.0-j4naqyymm6h4mofj5id6sfit5ngr4xh6
24: flux-sched         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/flux-sched-0.22.0-nfljuuoxqlk4r7zx3yoepyzjjjfxsqkz
25: fortrilinos        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/fortrilinos-2.0.0-uobhjnniqweeclzx7awlhcmvxitktwo5
26: gasnet             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/gasnet-2022.3.0-ep4xyqocdziblie475bojotd6qgpfpse
27: geopm              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/geopm-1.1.0-3bxmokjvkuh4gmymmu6b4iqhss5zq352
28: ginkgo             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/ginkgo-1.4.0-l6ahxdmshvwqrl6rmke7w4p3i5d5ehyd
29: globalarrays       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/globalarrays-5.8-y42lqtmfsq6nddv7vu5z3bjxbqjz6yww
30: gotcha             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/gotcha-1.0.3-cidwbtn2h7xjqzvajljks3idskhr3dcv
31: gptune             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/gptune-3.0.0-bjtlsqmghh24awymzp5g3fxt6wiequ3n
32: h5bench            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/h5bench-1.2-x5gqhbii26t7f4e3bpscw5wbhfg5qlhb
33: hdf5               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/hdf5-1.12.2-75qn37lp7leuvlsrbizprz5o5yr3ekjo
```

22.05 Release: 101 Official Products + dependencies (gcc, x86_64)

```
34: heffte            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/heffte-2.2.0-hqigomw3nlexreke2rgquwvdazenvhb2
35: hpctoolkit        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/hpctoolkit-2022.04.15-cqz4vlmjclq6qmxp4sonlrqiz4twl2sh
36: hpx               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/hpx-1.7.1-o7y77tofbg4jg2vcvfhjgdsqtckzhw3v
37: hypre             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/hypre-2.24.0-c7vk7oprzxpfs6njr42xn632tksu64ax
38: kokkos            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/kokkos-3.6.00-fy3onzyijziq2x2laoxu7rttrwhaqufj
39: kokkos-kernels    /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/kokkos-kernels-3.6.00-gn7fvng67ekhwt324xo45lizuxea327n
40: lammps            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/lammps-20220107-pmr5l5hzxruzhpzkucukg7qqr6os5iir
41: legion            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/legion-21.03.0-g3tu5cdevxuzsrvcqinaxrgduik3ea54
42: libnrm            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/libnrm-0.1.0-gjllhvje7in4rp3kvvaywywr7uyjprxj
43: libquo            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/libquo-1.3.1-2o7zqn3e2f7je3o3z4hcwsqgkn6bjmme
44: loki              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/loki-0.1.7-66nzpehhmoidzifzm6khyxhnbfgmppoa
45: magma             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/magma-2.6.2-mmx2xmmz7cbcjbc2j3vn6eoxrwgivu24
46: mercury           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mercury-2.1.0-yzp4mkdsnmcf5dgsein4ek2co7eag763
47: metall            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/metall-0.20-6o2ewhyu2ilxbco74j5qqdeunqjkmgta
48: mfem              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mfem-4.4.0-cra7q4353kgqdow7futlc5vik5hf4bu6
49: mpich             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mpich-4.0.2-ssbmd2ccbxzkbxk7fzrlekupe23rokw2
50: mpifileutils      /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mpifileutils-0.11.1-zvlai7bnjegicp5dzelxnvwmvu6sye5j
51: netlib-scalapack  /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/netlib-scalapack-2.2.0-l2chii6rgvnp6rswldzqxza7trgpdkib
52: nccmp             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/nccmp-1.9.0.1-ef6vn4ls3rj7wieuygnpf5c2i4trzpvo
53: nco               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/nco-5.0.1-xlix5wvr6bprihee7rryknegskv4sjho
54: nrm               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/nrm-0.1.0-cyiqhjsurt3q4bkn37u2ylvzhgdtmuuu
55: omega-h           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/omega-h-9.34.1-3d4zvshz6tj7twd3nqcnebls4zwryrvm
56: openpmd-api       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/openpmd-api-0.14.4-6ktbupm7eqmq73vflxkjiapn3kanomm4
57: openmpi           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/openmpi-4.1.3-p5q2yggpo7lhcn2n26deo25ymx3thdwt
58: papi              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/papi-6.0.0.1-fxfxybh2varhxhnu6jcrqsg5ixrrcxp2
59: papyrus           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/papyrus-1.0.2-r2wef2ldj24dluqgd43hjn23fxowxet2
60: parallel-netcdf   /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/parallel-netcdf-1.12.2-7ruhgcy35hofq4goi6c3d42tteuhqlwl
61: paraview          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/paraview-5.10.1-ohruf5tnfp2yeywlslszty5jfbq6pjw7
62: parsec            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/parsec-3.0.2012-dcaz2iwq6nrz7l6kcwpwsbeftpb3urv6
63: pdt               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/pdt-3.25.1-d5jyjfrocerrcl5cxqwsfrbv5l776d7r
64: petsc             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/petsc-3.17.1-vffv6b2ykiy3a4lxuoe7dzi4zggbrdqb
65: phist             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/phist-1.9.5-vxmwjbns3kywtogpldhhmouoehgi7d2m
66: plasma            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/plasma-21.8.29-hwpchnbrscxsmzgyioeepsjwddgnunxm
```

22.05 Release: 101 Official Products + dependencies (gcc, x86_64)

```
 67: plumed          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/plumed-2.6.3-g6dn67baochvycvcicgeltwjnvotgjk2
 68: precice         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/precice-2.4.0-orye5yx46n4mm2zey7xeg5k5i222twiw
 69: pruners-ninja   /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/pruners-ninja-1.0.1-hn6y2kevr5hgmlykfverjadgbgxkppcn
 70: pumi            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/pumi-2.2.7-zkipah7wz3a4eksedht2syqpx3tcg6ki
 71: py-cinemasci    /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/py-cinemasci-1.7.0-77yj2xigharoeq6lciw4mzngexnegxmc
 72: py-jupyterhub   /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/py-jupyterhub-1.4.1-3cebk5prfze6najqsdabftwxgqkccmwm
 73: py-libensemble  /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/py-libensemble-0.9.1-noalxjfvyidhsvps4zn7mhu4j5hf2wo6
 74: py-parsl        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/py-parsl-1.1.0-ul2cthsh524npmv6zrseklzodp6ej4en
 75: py-radical-saga /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/py-radical-saga-1.11.1-naxx4rp2e6wr7oo24jw3catzys26loya
 76: qthreads        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/qthreads-1.16-v7vcyz7vakzdyzpa3mjdbnov4s55a6vw
 77: raja            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/raja-0.14.0-edjvff74mwcz7fngfj4qlatpplxs5vzl
 78: rempi           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/rempi-1.1.0-yoa3gfri6iafv2l2avkhg25pzpgiftwg
 79: scr             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/scr-3.0rc2-mibyx3jm6nkm4gq7ovpbwe4kpwxnwou6
 80: slate           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/slate-2021.05.02-6krdeny5oeki4o2slafxstn7wa6vgmlq
 81: slepc           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/slepc-3.17.1-fzx6e3h2jqmsvhgbeclbwuirqrax7hkl
 82: stc             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/stc-0.9.0-vd4xaiuv4ryo4tzqzqvnsr4qwtndyyxq
 83: strumpack       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/strumpack-6.3.1-du3qimqp3yrjcso22pw2zsbbswgrtsay
 84: sundials        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/sundials-6.2.0-5iz6lim5mabrkkukic63lipmz5r6lmvb
 85: superlu-dist    /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/superlu-dist-7.2.0-2jp6torp4rjf44hhffm56glemlegfoyb
 86: swig            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/swig-4.0.2-fortran-fjva3hpwop4b3dmrmguisinqdrt2ixyk
 87: sz              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/sz-2.1.12-kzqvvvdo5fvv2s6sgheei7ikwgsbsd7m
 88: tasmanian       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/tasmanian-7.7-5q6657fcerfpwshuhdmrowzvxpoo25tt
 89: tau             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/tau-2.31.1-ikx2r2pk34hej3rmjqoam5ma6rvzbuqm
 90: trilinos        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/trilinos-13.2.0-hmpjtr4o7fnpffcg6m6b4pl73ipr422e
 91: turbine         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/turbine-1.3.0-aztpwwbbjeogl5bwiznmpx2lcyos64cz
 92: umap            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/umap-2.1.0-blwc2edy5e3lkrylgbrwfd55slyuuy4s
 93: umpire          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/umpire-6.0.0-gwbap637zehqkvjwmetuqcgjtkwhzzlo
 94: unifyfs         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/unifyfs-0.9.2-hcid7bugnj4vzetl4oh4zfnah2gzsctb
 95: upcxx           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/upcxx-2022.3.0-fpv2zorgjpac5iuqibffz57h6x3xhrjr
 96: variorum        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/variorum-0.4.1-fcfi26hd2dfvnwe5gehtv4iqx36hafj7
 97: veloc           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/veloc-1.5-avca7jodby7efy3be63siav4mqao2big
 98: vtk-m           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/vtk-m-1.7.1-hbilfvhsgkelno7jrvr6fffyn6guusxf
 99: wannier90       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/wannier90-3.1.0-vzfixrlicq5jrtzj2wpd6bg7nbkqdit6
100: warpx           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/warpx-22.05-gtg2e5dwy3lzr53t7fsyzscbj25gzu2m
101: zfp             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/zfp-0.5.5-3cc5y5ffuvxtdsiurtrt4blcbodbxj2p
```

GPU runtimes
- Intel (oneAPI)
  - 2022.1.0
- AMD (ROCm)
  - 5.1.1
- NVIDIA (CUDA)
  - 11.4
- NVHPC
  - 22.3

EXASCALE COMPUTING PROJECT

22.05 Release: 101 Official Products + dependencies (gcc, ppc64le)

```
 1: adios2            /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/adios2-2.8.0-l3uoqxbcqtdw6acjkm2mkilrsz4cplhn
 2: alquimia          /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/alquimia-1.0.9-uur6z7y5odoyby6umwxdorfo2nbbnohw
 3: aml               /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/aml-0.1.0-zfgeqmb6632fta22ytmomo4mu2fw3lvb
 4: amrex             /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/amrex-22.05-km2isnpb7l3muxey6hnbnoju2llw5hjo
 5: arborx            /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/arborx-1.2-rm7wnlzo3wcam6briglal22oyrictnb5
 6: archer            /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/archer-2.0.0-vsljqh3qhilsqgpqnqkgmeld267kgkrd
 7: argobots          /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/argobots-1.1-53v35i6gn2swvvrtl7bxalwzuc2tq3ty
 8: ascent            /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/ascent-0.8.0-y3gnx7ztjofbiwwgc537bmnix32dhoe4
 9: axom              /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/axom-0.6.1-g552mnzr43bnkz6pnozqplpqgc77qktk
10: bolt              /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/bolt-2.0-nbievusty3ohurw66gybj3ylsx57wrex
11: butterflypack     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/butterflypack-2.1.1-6cfpnjkfjtyrcrkr5uds3utwgdiun4rh
12: cabana            /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/cabana-0.4.0-qtngrrdxuwr2dvcfw6cq7ooi5itfw5sp
13: caliper           /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/caliper-2.7.0-6yob3cnulacurei4r74wqywbiddi2zqx
14: chai              /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/chai-2.4.0-gdjlgtnw37djx77ub6loueiozpwyrwz4
15: charliecloud      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/charliecloud-0.26-gfvv4zs2da4lmjry5pcv7bgiulq53dkh
16: conduit           /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/conduit-0.8.3-nt23fkfvsdc7vvgphhzugk5k3fr5hry7
17: darshan-runtime   /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/darshan-runtime-3.3.1-3tri6deqykmvo5l2yb5dpeyya7qy52p3
18: datatransferkit   /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/datatransferkit-3.1-rc3-34axhs5y4fphnqrxqeoatq23xmfhy64y
19: dyninst           /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/dyninst-12.1.0-qjucp4hbzk73utkjer2u6iauookgc5xk
20: exaworks          /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/exaworks-0.1.0-j4oyws2l6b3oa3ehiph7hr3qsu3xwcny
21: faodel            /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/faodel-1.2108.1-5uvp7odssmdoy3u3kwcyb4imvhsifkpc
22: flecsi            /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/flecsi-1.4.2-w6mhu5bfumqzg27v4nw4nu35l7xkbbeq
23: flit              /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/flit-2.1.0-4mnclif2iiayhwkhndemxo24ligjzq7v
24: flux-sched        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/flux-sched-0.22.0-rfqrabahnjutfgmss7377d7rtmhhknf2
25: fortrilinos       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/fortrilinos-2.0.0-xqopkkdcnj32t6ujpkpia5s5i5fj3dkz
26: gasnet            /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/gasnet-2022.3.0-rtr5lpjjrbzca6fdbvfxsmhqsywbixhc
27: ginkgo            /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/ginkgo-1.4.0-zhjkhwtzcfthnzr57o7fex57m4ausb7l
28: globalarrays      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/globalarrays-5.8-n4sze7tqf4ty3x65a6vnyoos6ninzuzf
29: gotcha            /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/gotcha-1.0.3-ygplgppjszeiftecygig3zpnk34m7nva
30: gptune            /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/gptune-3.0.0-rf7kag2a4ntxlqp5geggeyqrodosmad7
31: h5bench           /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/h5bench-1.2-f4dxdpglnt5i6ll3pxwqobm24vpr5fhy
32: hdf5              /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/hdf5-1.12.2-np7u5ivkhh2dljmeboekev5mgalipou7
33: heffte            /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/heffte-2.2.0-jshdo5of5p6nzqyurrtovgv4ymntx7iw
```

22.05 Release: 101 Official Products + dependencies (gcc, ppc64le)

```
34: hpctoolkit          /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/hpctoolkit-2022.04.15-yfhefus2qk7nb2dpvcnfmljud5wimyl5
35: hpx                 /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/hpx-1.7.1-ubdtwy7do6h3awjh2wyiaddui2yxz5sx
36: hypre               /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/hypre-2.24.0-v7hkiurnu6bo2dz5zfhmbb77xztik6c4
37: kokkos              /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/kokkos-3.6.00-4asspnluai7wx5mmeralzei6xtba6eud
38: kokkos-kernels      /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/kokkos-kernels-3.6.00-rna5swth72aqfwag2a62icyg5gxqdahc
39: lammps              /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/lammps-20220107-i4wdut62blpbwr6kitptivbyapb525f2
40: legion              /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/legion-21.03.0-kp4fz7au7ttb2cfoqsvt3t2wdfgjy4i2
41: libnrm              /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/libnrm-0.1.0-nn7mpcrk7fdevym4zpeeha6m7nqg3cis
42: libquo              /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/libquo-1.3.1-cv3vcijmffuutay6rkidwmbh7eajc4x6
43: loki                /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/loki-0.1.7-k52kcqywvu6ftfymw3lvqqldrwcwmxy2
44: magma               /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/magma-2.6.2-c3oionxxjnja35pbkriliexlncqocmpk
45: mercury             /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mercury-2.1.0-hzpwx73vc6p5cuyn5echuh63emzio5nv
46: metall              /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/metall-0.20-wcjaceek46d6jgk3kaz3rlkppugvfmhr
47: mfem                /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mfem-4.4.0-noytuh65o4hmxcgtojvufel35yrdpp4m
48: mpark-variant       /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mpark-variant-1.4.0-m5m6aixgdol2wyqw3jicr55zipd3dkut
49: mpich               /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mpich-4.0.2-66lytwzbos3xsv5ulxlrauggcggunxli
50: mpifileutils        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mpifileutils-0.11.1-vfp3xeqlizyp2fxbgzdwum5yuxczqcpa
51: netlib-scalapack    /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/netlib-scalapack-2.2.0-qf2uni4wwakywf2to6bcs2v6o5ezeryp
52: nccmp               /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/nccmp-1.9.0.1-avgfcvvac7k2hq7cpv7zjgkwh5eontgk
53: nco                 /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/nco-5.0.1-zizmp6sgjstd5rrtuu6oayuuzcrxmeoi
54: nrm                 /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/nrm-0.1.0-ea2gwqxrymwiszsb36uz2iprgc5oi4zt
55: omega-h             /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/omega-h-9.34.1-c5gj526wkjvrmjzywtc4lmgrqh6ewvly
56: openpmd-api         /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/openpmd-api-0.14.4-wdkkdo2v2xnzshojxl4p5ytqiyelxbmf
57: openmpi             /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/openmpi-4.1.3-s3g3qrtiqwjrjxj5bnosfngquuc3vs5x
58: papi                /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/papi-6.0.0.1-vghyjh55fu6mmal6czcaqciaboserw5e
59: papyrus             /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/papyrus-1.0.2-vsxqqctyjiyfgpazqdsyejkubkecmswj
60: parallel-netcdf     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/parallel-netcdf-1.12.2-zagedvigrmexckbaqhfhhijk5c5py526
61: parsec              /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/parsec-3.0.2012-77zuvm5ioe5schjyba55dsd2fhgxfmzk
62: pdt                 /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/pdt-3.25.1-hdxejnfp32dsvceukljn4orbehsw7ble
63: petsc               /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/petsc-3.17.1-pbri2lcnrritfkk6xx3qvg4tqalo77fu
64: plasma              /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/plasma-21.8.29-ow5ip3dmcfwjj2bg34hllruotrdrdlnr
65: plumed              /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/plumed-2.6.3-yw57pgxlhdwgnabprd235yv2q43gb4j4
66: precice             /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/precice-2.4.0-brfbvpkoo6vdtewk542jw2amzqilycxa
```

22.05 Release: 101 Official Products + dependencies (gcc, ppc64le)

```
 67: pruners-ninja    /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/pruners-ninja-1.0.1-xri4wt2pkvv54tsto3zl2njriblfnqei
 68: pumi             /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/pumi-2.2.7-5uqwyt4a5b7p372ptvekosyeaol5bqno
 69: py-cinemasci     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-cinemasci-1.7.0-ovv4qw4vp6ao3ukyt7yffqo2dr76hcix
 70: py-jupyterhub    /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-jupyterhub-1.4.1-jloxcbs7x6hsbzktls25mqv3p4nfni26
 71: py-libensemble   /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-libensemble-0.9.1-5bs6ugzqcdrhw2cuwjkbuydd2jrutwpg
 72: py-opentuner     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-opentuner-0.8.7-xqcv6l6vmpmp7p5nw4nl47vlshoogl4w
 73: py-parsl         /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-parsl-1.1.0-hqnojotjauv4o5na5yhnyqs7eodedd4r
 74: py-radical-pilo  /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-radical-pilot-1.11.2-tieorl4fju5za2n2vdtbkquqjxphw6ui
 75: py-radical-saga  /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-radical-saga-1.11.1-sjv4nhrhvlvhgtku2lat27fmvf7kveyd
 76: qthreads         /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/qthreads-1.16-md7z53zbdffm3zmgpqji4tcno7aqo6bb
 77: raja             /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/raja-0.14.0-fmvdypdhro2n7k6xovmfgmkc26aekdof
 78: rempi            /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/rempi-1.1.0-bultj4j7ef7qsdffo3gapameeyftjx4n
 79: scr              /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/scr-3.0rc2-xip4gfjzkzjar73urcab7mqwp6p3lqn2
 80: slate            /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/slate-2021.05.02-rvxg3qm3bc4orccwvnnfxt6j35i5tuws
 81: slepc            /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/slepc-3.17.1-bur33hbhnucmsk6uktqhg4tjco6sdmri
 82: stc              /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/stc-0.9.0-vcqy4zscq5mktfdxsk36j5www6wbl55l
 83: strumpack        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/strumpack-6.3.1-4i5oyjylpm27o4zecxegpn7imrhok5lb
 84: sundials         /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/sundials-6.2.0-h4xo2zqezj6ef5y7v3727srlratiqs5l
 85: superlu-dist     /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/superlu-dist-7.2.0-6rwclsr7fo5rfybu3mylfjozwblydznu
 86: swig             /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/swig-4.0.2-fortran-zpsyg6fhwuekaff4fqyvnd7cypnevcjs
 87: sz               /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/sz-2.1.12-xobq2pzb6l25htimlhuokwqvtggwxgfs
 88: tasmanian        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/tasmanian-7.7-a2rk5ujjed542bqp3vpmo235532qzdqk
 89: tau              /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/tau-2.31-fym3ff54vwfgbw53rj2ntvakfbwirgcj
 90: trilinos         /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/trilinos-13.2.0-mmz5acf7trnptodope3jv3lucnugylcd
 91: turbine          /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/turbine-1.3.0-df2lqm4bnlo6vvjbutnzpayfsphaee4m
 92: umap             /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/umap-2.1.0-6nh3hjzgbisu2wcigrwqusvdugkzvxkg
 93: umpire           /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/umpire-6.0.0-2phff7zj3b4sht6qkdtb3im46nzoe774
 94: unifyfs          /spack/opz/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/unifyfs-0.9.2-h33e2ceufqjlvqopz456vluituxlrfor
 95: upcxx            /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/upcxx-2022.3.0-hfzxekrtpjvvgg5p3ndjphkuh5y4cl65
 96: veloc            /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/veloc-1.5-sy2ht5e34kry5gqmamq2i5eiba4baz54
 97: vtk-m            /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/vtk-m-1.7.1-vjkewsjwisjtnrhjqgee72krlu2takbl
 98: wannier90        /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/wannier90-3.1.0-4xbesxrnwafmset7hv3ydunlpwjfeyqx
 99: warpx            /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/warpx-22.05-33bd7p6hkocl3iayodejy3fua77wfpb5
100: yaksa            /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/yaksa-0.2-32f626altydcxrvpeukiigbpy7ibtgkd
101: zfp              /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/zfp-0.5.5-mcame7nbb22fh27n44nkimbokt6azel6
```

GPU runtimes
- NVIDIA (CUDA)
  - 11.0
- NVHPC
  - 22.3

E4S 22.05 Release: Support for AMD GPUs

```
Singularity> python
Python 3.9.7 (default, Sep 16 2021, 13:09:58)
[GCC 7.5.0] :: Anaconda, Inc. on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import tensorflow
>>> tensorflow.__version__
'2.8.0'
>>> import torch
>>> torch.__version__
'1.11.0+rocm4.5.2'
>>>
Singularity> which hipcc
/opt/rocm/hip/bin/hipcc
Singularity> spack find -l amdgpu_target=gfx90a +rocm
==> 17 installed packages
-- linux-ubuntu20.04-x86_64 / gcc@9.4.0 -------------------------
357tvji amrex@22.05        egwwklq ginkgo@1.4.0   pmri64c petsc@3.17.1        t2bsxuz umpire@6.0.0
uawks2x arborx@1.2         m75ci6i heffte@2.2.0   aoo762y raja@0.14.0         tboqlrc upcxx@2022.3.0
2h2jnil camp@0.2.2         ddpp5a7 hpx@1.7.1      w3wwqzx slepc@3.17.1
uh7nqyy chai@2.4.0         aegedco kokkos@3.6.00  dvyddsb strumpack@6.3.1
c2pvxtt gasnet@2022.3.0    zwsqooc magma@2.6.2    ypavztb superlu-dist@7.2.0
Singularity> spack find -l amdgpu_target=gfx908 +rocm
==> 17 installed packages
-- linux-ubuntu20.04-x86_64 / gcc@9.4.0 -------------------------
5rbk2or amrex@22.05        wsnjvv4 ginkgo@1.4.0   w67sm7w petsc@3.17.1        oijpipf umpire@6.0.0
3n5fwfv arborx@1.2         6bksj3x heffte@2.2.0   qbdnr3o raja@0.14.0         yuzwxoy upcxx@2022.3.0
yuk323w camp@0.2.2         kxqzrjt hpx@1.7.1      te425aa slepc@3.17.1
sntvjjs chai@2.4.0         vmsecny kokkos@3.6.00  x3yv3xj strumpack@6.3.1
afhffop gasnet@2022.3.0    bsj3ldg magma@2.6.2    q25hplz superlu-dist@7.2.0
Singularity>
```

E4S 22.05 Release: Support for NVIDIA GPUs

```
〔Singularity〕> python
Python 3.9.7 (default, Sep 16 2021, 13:09:58)
[GCC 7.5.0] :: Anaconda, Inc. on linux
Type "help", "copyright", "credits" or "license" for more information.
▷>>> import tensorflow as tf
▷>>> tf.__version__
 '2.9.1'
▷>>> tf.config.list_physical_devices('GPU')
 [PhysicalDevice(name='/physical_device:GPU:0', device_type='GPU'), PhysicalDevice(name='/physical_device:GPU:1', device_type='GPU')]
▷>>> import torch
▷>>> torch.__version__
 '1.11.0+cu113'
>>> torch.cuda.get_device_name(torch.cuda.current_device())
 'NVIDIA A100-PCIE-40GB'
▷>>>
〔Singularity〕> spack find -l +cuda cuda_arch=80
==> 27 installed packages
-- linux-ubuntu20.04-x86_64 / gcc@9.4.0 --------------------------
5fxpaue adios2@2.8.0    hqigomw heffte@2.2.0         mmx2xmm magma@2.6.2       fzx6e3h slepc@3.17.1       gwbap63 umpire@6.0.0
a5j5wjd arborx@1.2      o7y77to hpx@1.7.1            cra7q43 mfem@4.4.0        du3qimq strumpack@6.3.1    hbilfvh vtk-m@1.7.1
5scpuxj caliper@2.7.0   c7vk7op hypre@2.24.0         dcaz2iw parsec@3.0.2012   5iz6lim sundials@6.2.0     3cc5y5f zfp@0.5.5
5nftkwe camp@0.2.2      kn4ult3 kokkos@3.6.00        mvt3juo petsc@3.17.1      2jp6tor superlu-dist@7.2.0
l6nclfu chai@2.4.0      fy3onzy kokkos@3.6.00        edjvff7 raja@0.14.0       5q6657f tasmanian@7.7
l6ahxdm ginkgo@1.4.0    gn7fvng kokkos-kernels@3.6.00 6krdeny slate@2021.05.02 hmpjtr4 trilinos@13.2.0
〔Singularity〕> spack find -l +cuda cuda_arch=70
==> 27 installed packages
-- linux-ubuntu20.04-x86_64 / gcc@9.4.0 --------------------------
mvzqvxg adios2@2.8.0    zz33g5c heffte@2.2.0         7ddf6kl magma@2.6.2       td7e334 slepc@3.17.1       hjgbyxh umpire@6.0.0
2wllnpi arborx@1.2      zrpfbiq hpx@1.7.1            hyuvayy mfem@4.4.0        66zzxrb strumpack@6.3.1    stzpxgb vtk-m@1.7.1
xb3ix2x caliper@2.7.0   m735zlc hypre@2.24.0         37dtmme parsec@3.0.2012   ykvyvrc sundials@6.2.0     ldaf46p zfp@0.5.5
etalgqv camp@0.2.2      dmru53c kokkos@3.6.00        2lsmpfg petsc@3.17.1      7bbqseb superlu-dist@7.2.0
rjky53t chai@2.4.0      xwt7ck4 kokkos@3.6.00        ttunttv raja@0.14.0       r7artq7 tasmanian@7.7
36fsm5m ginkgo@1.4.0    k47b42d kokkos-kernels@3.6.00 yeairhs slate@2021.05.02 qpycht6 trilinos@13.2.0
Singularity> ▊
```

E4S 22.05 Release: GUI Tools

```
[Singularity> module load paraview
[Singularity> which paraview
/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/paraview-5.10.1-ohruf5tnfp2yeywlslszty5jfbq6pjw7/bin/paraview
[Singularity> module load visit
[Singularity> which visit
/usr/local/visit/bin/visit
[Singularity> which paraprof
/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/tau-2.31.1-ikx2r2pk34hej3rmjqoam5ma6rvzbuqm/bin/paraprof
[Singularity> module load julia
[Singularity> julia
                   _
       _       _ _(_)_     |  Documentation: https://docs.julialang.org
      (_)     | (_) (_)    |
       _ _   _| |_  __ _   |  Type "?" for help, "]?" for Pkg help.
      | | | | | | |/ _` |  |
      | | |_| | | | (_| |  |  Version 1.7.3 (2022-05-06)
     _/ |\__'_|_|_|\__'_|  |  Official https://julialang.org/ release
    |__/                   |

[julia>
[Singularity> nvidia-smi
Tue May 31 23:33:39 2022
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 470.57.02    Driver Version: 470.57.02    CUDA Version: 11.4      |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|                               |                      |               MIG M. |
|===============================+======================+======================|
|   0  NVIDIA A100-PCI...  Off  | 00000000:25:00.0 Off |                    0 |
| N/A   42C    P0    37W / 250W |      0MiB / 40536MiB |      0%      Default |
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+
|   1  NVIDIA A100-PCI...  Off  | 00000000:E1:00.0 Off |                    0 |
| N/A   38C    P0    37W / 250W |      0MiB / 40536MiB |     32%      Default |
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+
```
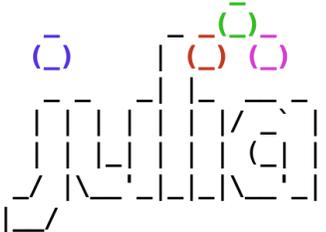
E4S 22.05 Release: Intel oneAPI with support for Intel GPUs

```
〖Singularity> which clinfo
/usr/bin/clinfo
〖Singularity> clinfo -l
Platform #0: Intel(R) FPGA Emulation Platform for OpenCL(TM)
 `-- Device #0: Intel(R) FPGA Emulation Device
Platform #1: Intel(R) OpenCL
 `-- Device #0: Intel(R) Xeon(R) Gold 6348H CPU @ 2.30GHz
Platform #2: Intel(R) OpenCL HD Graphics
 `-- Device #0: Intel(R) Iris(R) Xe MAX Graphics [0x4905]
〖Singularity> spack find -dl -v kokkos+sycl
==> 1 installed package
-- linux-ubuntu20.04-x86_64 / oneapi@2022.1.0 --------------------
rdujf3d kokkos@3.6.00~aggressive_vectorization~compiler_warnings~cuda~cuda_constexpr~cuda_lambda~cuda_ldg_intrinsic~cuda_relocatable_d
evice_code~cuda_uvm~debug~debug_bounds_check~debug_dualview_modify_check~deprecated_code+examples~explicit_instantiation~hpx~hpx_async
_dispatch~hwloc~ipo~memkind~numactl+openmp~pic+profiling~profiling_load_print~pthread~qthread~rocm+serial+shared+sycl~tests~tuning~wra
pper build_type=RelWithDebInfo std=17
xoj37yl     cmake@3.23.1~doc+ncurses+ownlibs~qt build_type=Release
az4hpr4       ncurses@6.2~symlinks+termlib abi=none
uycnlmy         pkgconf@1.8.0
w4cv7zw       openssl@1.1.1o~docs~shared certs=system
uqtpe2z         perl@5.34.1+cpanm+shared+threads
sngm6aa           berkeley-db@18.1.40+cxx~docs+stl patches=b231fcc
ndilfww           bzip2@1.0.8~debug~pic+shared
yzcfxcb             diffutils@3.8
zf2ftv4               libiconv@1.16 libs=shared,static
4hns3dz           gdbm@1.19
s63k2n3             readline@8.1
nxdjy7n           zlib@1.2.12+optimize+pic+shared patches=0d38234

〖Singularity> ls /spack.yaml
/spack.yaml
〖Singularity> which dpcpp
/opt/intel/oneapi/compiler/2022.1.0/linux/bin/dpcpp
〖Singularity> which mpiicpc
/opt/intel/oneapi/mpi/2021.6.0/bin/mpiicpc
```

EXASCALE COMPUTING PROJECT

E4S 22.05 AWS image: US-West2 (OR) ami-0d7295416d1c63e3a

E4S 22.05 AWS
- Intel oneAPI
- CUDA
- NVHPC
- ROCm
- AWS DCV
- Spack Build Cache
- ECP: Nalu-Wind
- OpenFOAM
- ParaView
- VisIt
- TAU
- Docker
- Shifter
- Charliecloud
- E4S Singularity…

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 for ppc64le.

- 101 HPC and AI/ML products (TensorFlow, PyTorch).

- Updated E4S AWS image with E4S 22.05 Singularity container.

Thank you

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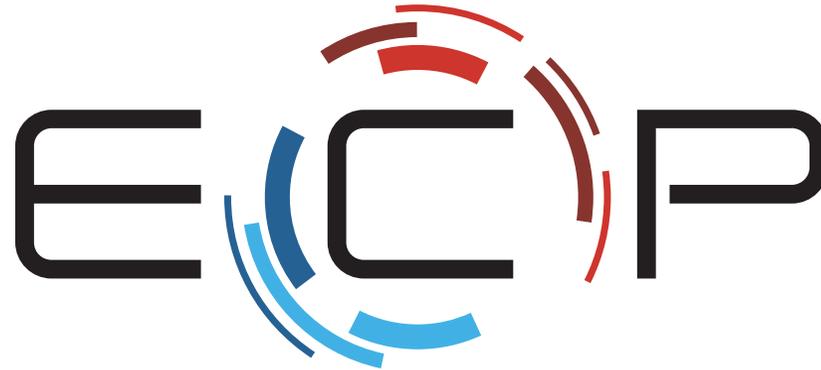
Thank you to all collaborators in the ECP and broader computational science communities. The work discussed in this presentation represents creative contributions of many people who are passionately working toward next-generation computational science.