E4S: The Extreme-scale Scientific Software Stack Release 22.08



Release 22.08 notes

August 31, 2022





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







https://e4s.io

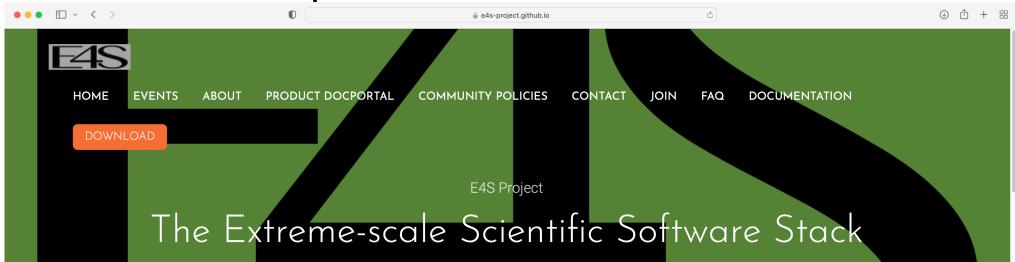
Lead: Sameer Shende (U Oregon)

Also include other products .e.g.,

AI: PyTorch, TensorFlow (CUDA, ROCm)

Co-Design: AMReX, Cabana, MFEM

E4S Download from https://e4s.io



Deadline to submit changes for E4S 22.11 is November 15, 2022

See Downloads for more information on E4S 22.08.

What is E4S?

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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.



Download E4S 22.08 GPU Container Images: NVIDIA, AMD, Intel



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 18.04 (ppc64le) and Ubuntu 20.04 (x86_64). 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.



From source with Spack

☑ Visit the Spack Project

Spack contains packages for all of the products listed in the E4S 22.08 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 22.05 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:22.08
# docker pull ecpe4s/e4s-rocm:22.08
# docker pull ecpe4s/e4s-oneapi:22.08
```

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:22.08 docker

e4s-rocm-22.08.sif (s) mirror 1

NVIDIA CUDA (x86_64, ppc64le, aarch64)

ecpe4s/e4s-cuda:22.08 docker

e4s-cuda-x86_64-22.08.sif (s) mirror 1

e4s-cuda-ppc64le-22.08.sif s mirror 1

e4s-cuda-aarch64-22.08.sif s mirror 1

https://e4s.io

Intel OneAPI (x86_64)

ecpe4s/e4s-oneapi:22.08 docker

e4s-oneapi-22.08.sif S mirror 1



E4S 22.08 Full Featured and Base Images

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:22.08 docker

e4s-rocm-22.08.sif (S) mirror 1

NVIDIA CUDA (x86_64, ppc64le, aarch64)

ecpe4s/e4s-cuda:22.08 docker

e4s-cuda-x86_64-22.08.sif (S) mirror 1

e4s-cuda-ppc64le-22.08.sif (S) mirror 1

e4s-cuda-aarch64-22.08.sif (S) mirror 1

Intel OneAPI (x86_64)

ecpe4s/e4s-oneapi:22.08 docker

e4s-oneapi-22.08.sif (S) mirror 1



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:22.08 docker

e4s-base-cuda-x86_64-22.08.sif (S) mirror 1

e4s-base-cuda-aarch64-22.08.sif (S) mirror 1

e4s-base-cuda-ppc64le-22.08.sif s mirror 1

ROCM X86_64

ecpe4s/e4s-base-rocm:22.08 docker

e4s-base-rocm-22.08.sif s mirror 1

Intel OneAPI X86_64

ecpe4s/e4s-base-oneapi:22.08 docker

e4s-base-oneapi-22.08.sif (S) mirror 1





22.08 Release: 102 Official Products + dependencies (gcc, cuda, x86_64)

```
1: adios2
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/adios2-2.8.3-ifkuulgk4fcrwgcizlflfquna2x5ofay
2: alguimia
                       /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/alguimia-1.0.9-2lrac7o4ffv4rgt4h2vgzjud3tkjwkrd
                       /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/aml-0.2.0-pwiapieu4qrmlv64dvz6ztnlryomtxov
3: aml
                       /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/amrex-22.08-2k6mn7x6c6bn37e4gghcijpof5l663ec
4: amrex
5: arborx
                       /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/arborx-1.2-hpgevuvvjogfpgt3334czuut4secym7u
6: archer
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/archer-2.0.0-ubhbdonoquovu6i6yh6byf5vkjqdst2s
7: argobots
                       /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/argobots-main-62s4jy7ijfzur2pw2rzadwo5ixgnizjl
8: ascent
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/ascent-0.8.0-k6pkjgeaxjbtjngv4galvfi76a3tecyn
9: axom
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/axom-0.6.1-adc6pqaau33eh47lt62cd7gx6qv3qebj
10: bolt
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/bolt-2.0-t3nxvx37r4r4b4v6o4tmjplwxosamm65
11: bricks
                       /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/bricks-r0.1-75cmpltikrkwriklzkss7khaiif72lco
12: butterflypack
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/butterflypack-2.1.1-q5eimvsxo5jzoyxlaq7mrkoe715o3y2n
13: cabana
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/cabana-0.5.0-uzm7qvptohoxhz3fpxqbob2sq4a5bbli
14: caliper
                       /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/caliper-2.8.0-v4tngpfc5dcnxslg4ltugkhxcr6aydfa
15: chai
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/chai-2022.03.0-v4q3jdzv5zvmq4x2gswjxscqonewm43j
16: conduit
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/conduit-0.8.3-zphidjxhjkiwukbg4sdftgsrjbfov5y3
17: darshan-runtime
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/darshan-runtime-3.4.0-caydqukivwqaecivrajoj5nusrqzql7t
18: datatransferkit
                       /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/datatransferkit-3.1-rc3-blednv72j7co7xf7j3wspaswy6jtxbwy
19: dyninst
                       /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/dyninst-12.2.0-3dwen3nn22mkgjsivikdd43rrl4vehvz
20: faodel
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/faodel-1.2108.1-kqkwty5hn4cvjrgbvutzgk3p45tb5sdc
21: flecsi
                       /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/flecsi-2.1.0-jdt5s7vgugxngcco3higygdtc6p3jlp3
22: flit
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/flit-2.1.0-hh43s4mmqrw3p7zj2hlkylklgr3tggf5
23: flux-sched
                       /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/flux-sched-0.23.0-qod4dtvrvmat3npnpwysrpebxjexsxhr
24: fortrilinos
                       /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/fortrilinos-2.0.0-61ceg2wvliv7xgkif2es47bpgm3ztvxi
25: gasnet
                       /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/gasnet-2022.3.0-mjam365gep6iigr36s454x4psmgrkwp6
26: geopm
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/geopm-1.1.0-vzi6bgaktmcahuvu66oozto2wtoe27la
27: ginkgo
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/ginkgo-1.4.0-7iqzf3oxknmk2iv3i74eu4d44otnqh37
28: globalarrays
                       /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/globalarrays-5.8-2qdtkpndvwvqylybsfxps2px3ansltxn
29: gotcha
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/gotcha-1.0.3-a2gy4enms44svpeek5vzlvnalx3pr6ia
30: gptune
                       /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/gptune-3.0.0-db3njgcxugdun5d452wiw7goxw4hhykx
31: h5bench
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/h5bench-1.2-hul73s3xtl2srumekg7cuo2bb533fmot
32: hdf5
                       /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/hdf5-1.13.2-doki3exhfk6ofx2qum2nv6fdjs3lab4s
33: hdf5-vol-async
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/hdf5-vol-async-1.2-34dt32yinsj52cwxykv6jzcpbnejdptf
34: heffte
                       /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/heffte-2.2.0-goupv4n2hgxdtezc3g6r7isf4h5jvsm3
35: hpctoolkit
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/hpctoolkit-2022.05.15-xjug5nhvocxzdrbooncuk3te6t3rw7wa
36: hpx
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/hpx-1.8.1-lrb5wsjktqgsswclupnaayb2ohq3ptkw
37: hypre
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/hypre-2.25.0-4nmvphj2dtfh7uisr44f7oftptmenl31
38: kokkos
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/kokkos-3.6.01-7vuflt6v5ahimf6e3noa6o67kx5ut3ns
39: kokkos-kernels
                       /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/kokkos-kernels-3.6.00-uihsgkd6swlogua3hdkxe6kr5oaolkxz
40: lammps
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/lammps-20220623-5cqu3suoycin5fgoz4cvc3qzq7elqqif
41: legion
                       /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/legion-21.03.0-v36c4daichtlrig3zlarfzdcenlndktb
42: libnrm
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/libnrm-0.1.0-tj463dbbvyerlzhtesccp525byjmug5n
43: libquo
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/libquo-1.3.1-zihxwoeobknjaj3bmaybfaoqn3jwfvso
44: loki
                       /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/loki-0.1.7-rgel6sujgugxzgvtddd2jibhuw7dmhai
45: magma
                       /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/magma-2.6.2-zw7i6ultwiuxsvztuvijix72fle7vtil
                       /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/mercury-2.1.0-ubcppuuys2e6mbwe26kg5rerwuzfrgno
46: mercury
47: metall
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/metall-0.21-vi6z32g7zotumjtcgonykfhje35z4lmr
48: mfem
                       /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/mfem-4.4.0-bcbkjqqyj26nvx7ojhxyats3mbm57ycl
49: mpark-variant
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mpark-variant-1.4.0-fokhy42s3yd7uh75qo43ifjnzchsbr3g
50: mpich
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mpich-4.0.2-yurg3uwktdw4kw76r5djfsnjdzdmp6cm
51: mpifileutils
                       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mpifileutils-0.11.1-6dj2vqlpw5qydyg7v52ubu55op3ajpq7
```

- NVHPC 22.7 with CUDA 11.7
- Support for A100 and V100 GPUs
- TensorFlow v2.9.1 and
- PyTorch v1.12.1 optimized for GPUs



22.08 Release: 102 Official Products + dependencies (gcc, cuda, x86_64) (contd.)

52: netlib-scalapack /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/netlib-scalapack-2.2.0-25vd6rfg4ufuesofo57jysj5x53nxu74 53: nccmp /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/nccmp-1.9.0.1-ftszrngzc2cygogrtioee6h3fjx6w6yv 54: nco /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/nco-5.0.1-rlffrgp2xzm4uvdwgqodtn3exrr2dlnd 55: nrm /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/nrm-0.1.0-uwg666h4ka32lj2bxmc4nj36liyil3zq /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/omega-h-9.34.1-27heb5almci24q7zq7mfn2mdgq6562va 56: omega-h /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/openmpi-4.1.4-7co3hc3hfqfsziffum3fu7c3q23ozqv4 57: openmpi /spack/opt/spack/linux-ubuntu20.04-x86_64/qcc-9.4.0/openpmd-api-0.14.5-pj2hi5r2m5wubpacflddd3tivqjwunbi 58: openpmd-api 59: papi /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/papi-6.0.0.1-yjnzh45s2nzeeb553xpx5qxinm73jdgz 60: papyrus /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/papyrus-1.0.2-ae7pgcjs72utsbtgg6x3g4e5tgzpgocb 61: parallel-netcdf /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/parallel-netcdf-1.12.2-v7h7r3hqjw6vakzqj6uarb465ss4oj6v 62: paraview /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/paraview-5.10.1-lf7udp3dnwkptjh5mxr4xotc4wuf2jfm 63: parsec /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/parsec-3.0.2012-7hbcudupjmlfcgihhtfp7pe2moszdvcl 64: pdt /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/pdt-3.25.1-22x4lgxduh2ejs477htndgxuiha5uo2s 65: petsc /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/petsc-3.17.4-vwoni5xmzv4nsiahsq5oww6f246t7r62 66: phist /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/phist-1.9.5-ey2e2xjqrkoqucncqlcaiay5pi5yqnpo 67: plasma /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/plasma-21.8.29-q4m6euppnulfmxi5aufltyd3kgdhvtts 68: plumed /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/plumed-2.8.0-z265gsvzvb43xn42lajf6d3fa6k6jpn2 69: precice /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/precice-2.5.0-mojal5gfigzzseifja5xdulveukdziml 70: pruners-ninja /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/pruners-ninja-1.0.1-okgyfnztj2rfcyitth4n4oexghk445hr 71: pumi /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/pumi-2.2.7-whec6o6kj7qpo53s2yyqch5xda5akdgp 72: py-cinemasci /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/py-cinemasci-1.7.0-n3pshnjlwj5mdpp4m3w5xc42h3cufci3 73: py-jupyterhub /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/py-jupyterhub-1.4.1-odbpt2k2xolyk4qnfeti6pyjlrxm7n2a 74: py-libensemble /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/py-libensemble-0.9.2-2zefvm7ymmap5i66nie5ocfq7a7ewz7v 75: py-parsl /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/py-parsl-1.1.0-w6buwwgyvx7qk3d66an6nzhlh2d7fe3f 76: pv-radical-saga /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/pv-radical-saga-1.16.0-qkvigeig5dwb7x2245wgah6h7vobzvto 77: qthreads /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/qthreads-1.16-vujctsewvsjga2drshoekdnv1416cp6d 78: raja /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/raja-2022.03.0-shzxmdu6mmyuwlxfwsa6k54njfu34r23 79: rempi /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/rempi-1.1.0-3fg5re7uwjzb33j7dq2mathtmosmmisq 80: scr /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/scr-3.0-7wiky6bzgzdc3tit5ifb2migohp2vfs7 81: slate /spack/opt/spack/linux-ubuntu20.04-x86_64/qcc-9.4.0/slate-2022.06.00-7cfrzgha7dslzh7b5z5ut5al5msxt3gr 82: slepc /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/slepc-3.17.2-5r2ldqn5hlnnwqv32vp7esc7whvkx32r 83: stc /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/stc-0.9.0-qhahav5nnvq512nrp4duimrhao6baxem 84: strumpack /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/strumpack-6.3.1-7vhcwyrwmc5tnexxg35ldxg5uqa4r5vx 85: sundials /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/sundials-6.2.0-aput4a22o2yszv7gs56wiphtwhlpnh3r 86: superlu-dist 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- NVHPC 22.7 with CUDA 11.7
- Support for A100 and V100 GPUs
- TensorFlow v2.9.1 and
- PyTorch v1.12.1 optimized for GPUs



22.08 Release: 102 Official Products + dependencies (gcc, rocm, x86_64)

```
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 3: aml
 4: amrex
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 6: archer
7: argobots
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 8: ascent
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9: axom
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10: bolt
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11: bricks
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12: butterflypack
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13: cabana
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14: caliper
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15: chai
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16: conduit
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17: darshan-runtime
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18: datatransferkit
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19: dyninst
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21: flecsi
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22: flit
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23: flux-sched
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24: fortrilinos
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26: geopm
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27: ginkgo
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                       /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/qlobalarrays-5.8-2qdtkpndvwvqylybsfxps2px3ansltxn
28: globalarrays
29: gotcha
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30: gptune
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31: h5bench
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32: hdf5
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33: hdf5-vol-async
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34: heffte
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36: hpx
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37: hypre
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38: kokkos
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39: kokkos-kernels
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40: lammps
41: legion
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42: libnrm
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43: libauo
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44: loki
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45: magma
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46: mercury
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47: metall
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48: mfem
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49: mpark-variant
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50: mpich
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51: mpifileutils
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```

- ROCm 5.2.0
- Support for MI100 as well as MI250X
- TensorFlow v2.9.1 and
- PyTorch v1.12.1 optimized for GPUs



22.08 Release: 102 Official Products + dependencies (gcc, rocm, x86_64) (contd.)

52: netlib-scalapack /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/netlib-scalapack-2.2.0-25vd6rfg4ufuesofo57jysj5x53nxu74 /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/nccmp-1.9.0.1-ftszrngzc2cygogrtioee6h3fix6w6vv 53: nccmp 54: nco /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/nco-5.0.1-rlffrqp2xzm4uvdwqqodtn3exrr2dlnd 55: nrm /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/nrm-0.1.0-uwg666h4ka32lj2bxmc4nj36liyil3zq 56: omega-h /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/omega-h-9.34.1-27heb5almci24g7zg7mfn2mdgg6562va /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/openmpi-4.1.4-7co3hc3hfgfszjffum3fu7c3q23ozqy4 57: openmpi 58: openpmd-api /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/openpmd-api-0.14.5-pj2hi5r2m5wubpacflddd3tivqjwunbi /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/papi-6.0.0.1-c3oavnkaeczxhe52todjoxwugiwfiygx 59: papi /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/papyrus-1.0.2-ae7pqcjs72utsbtgq6x3q4e5tqzpgocb 60: papyrus 61: parallel-netcdf /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/parallel-netcdf-1.12.2-v7h7r3hgjw6vakzgj6uarb465ss4oj6v 62: paraview /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/paraview-5.10.1-lf7udp3dnwkptjh5mxr4xotc4wuf2jfm 63: parsec /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/parsec-3.0.2012-jcncq7zogrwo7jpyms4gwtdtdr2zvbdd 64: pdt /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/pdt-3.25.1-22x4lgxduh2ejs477htndgxuiha5uo2s 65: petsc /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/petsc-3.17.4-7njjpmskey2xjmfqiiksdncjfsfmw3w4 66: phist /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/phist-1.9.5-ey2e2xjgrkogucncglcaiay5pi5ygnpo 67: plasma /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/plasma-21.8.29-g4m6euppnulfmxi5aufltvd3kgdhvtts /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/plumed-2.8.0-z265gsvzvb43xn42lajf6d3fa6k6jpn2 68: plumed 69: precice 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- ROCm 5.2.0
- Support for MI100 as well as MI250X
- TensorFlow v2.9.1 and
- PyTorch v1.12.1 optimized for GPUs



22.08 Release: 102 Official Products + dependencies (gcc, oneAPI, x86_64)

1: adios2 /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/adios2-2.8.3-a4apzfywnvv2emsljo2xk4damq24xzv2 2: alguimia /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/alguimia-1.0.9-2lrac7o4ffv4rgt4h2vgzjud3tkjwkrd 3: aml /spack/opt/spack/linux-ubuntu20.04-x86 64/oneapi-2022.1.0/aml-0.2.0-av6pzg2cygtm2oeonnnylxaof5iaf5bb 4: amrex /spack/opt/spack/linux-ubuntu20.04-x86_64/oneapi-2022.1.0/amrex-22.08-k7etpgmun4z6gqi3twjuyyucjpo4jwsg 5: arborx /spack/opt/spack/linux-ubuntu20.04-x86 64/oneapi-2022.1.0/arborx-1.2-x3hj7gi56h3s2xwb5gb5mbmaf7s157eb /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/archer-2.0.0-ubhbdonoquovu6i6yh6byf5vkjqdst2s 6: archer 7: argobots /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/argobots-main-62s4jy7ijfzur2pw2rzadwo5ixgnizjl 8: ascent /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/ascent-0.8.0-oia5j2hoeitlarm4vck76f5djoza3zf4 9: axom /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/axom-0.6.1-adc6pgaau33eh47lt62cd7gx6gv3gebj 10: bolt 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- oneAPI 5.2.0
- Support for Intel GPUs (DG1,...)
- TensorFlow v2.9.1 and
- PyTorch v1.12.1



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

1: adios2 /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/adios2-2.8.3-a4apzfywnvv2emsljo2xk4damq24xzv2 2: alguimia /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/alguimia-1.0.9-2lrac7o4ffv4rgt4h2vgzjud3tkjwkrd 3: aml /spack/opt/spack/linux-ubuntu20.04-x86 64/oneapi-2022.1.0/aml-0.2.0-av6pzg2cygtm2oeonnnylxaof5iaf5bb 4: amrex /spack/opt/spack/linux-ubuntu20.04-x86_64/oneapi-2022.1.0/amrex-22.08-k7etpgmun4z6gqi3twjuyyucjpo4jwsg 5: arborx /spack/opt/spack/linux-ubuntu20.04-x86 64/oneapi-2022.1.0/arborx-1.2-x3hj7gi56h3s2xwb5gb5mbmaf7s157eb 6: archer /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/archer-2.0.0-ubhbdonoquovu6i6yh6byf5vkjqdst2s 7: argobots /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/argobots-main-62s4jy7ijfzur2pw2rzadwo5ixgnizjl 8: ascent /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/ascent-0.8.0-oia5j2hoeitlarm4vck76f5djoza3zf4 9: axom /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/axom-0.6.1-adc6pgaau33eh47lt62cd7gx6gv3gebj 10: bolt 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/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/hpctoolkit-2022.05.15-kb2yvndwj7j247idlusc2uroqpx5fc5v /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/hpx-1.8.1-gbrz4os5rrogiudxr26by2vwoeog53kd 36: hpx 37: hypre /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/hypre-2.25.0-taa2gtk4x2xsuf2tpjsy34gtofg3ikhr 38: kokkos /spack/opt/spack/linux-ubuntu20.04-x86_64/oneapi-2022.1.0/kokkos-3.6.00-e3aolvmpjxbtwihjvn24v47sats3bw3m 39: kokkos-kernels /spack/opt/spack/linux-ubuntu20.04-x86 64/oneapi-2022.1.0/kokkos-kernels-3.6.00-hhupbyutxfmvzoetc3idq4ph7m2hx364 40: lammps /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/lammps-20220623-5cqu3suoycin5fgoz4cvc3qzq7elqqif 41: legion /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/legion-21.03.0-y36c4daichtlrjq3zlarfzdcenlndktb 42: libnrm /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/libnrm-0.1.0-ti463dbbvverlzhtesccp525bvimug5n 43: libquo /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/libquo-1.3.1-zihxwoeobknjaj3bmaybfaogn3jwfvso 44: loki /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/loki-0.1.7-rgel6sujgugxzqvtddd2jibhuw7dmhai 45: mercury /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/mercury-2.1.0-ubcppuuys2e6mbwe26kg5rerwuzfrgno 46: metall /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/metall-0.21-vi6z32g7zotumjtcgonykfhje35z4lmr 47: mfem /spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/mfem-4.4.0-nf5ukqqvpyzdfkxjuqqkoiktootmsbbx 48: mpark-variant /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/mpark-variant-1.4.0-fokhv42s3vd7uh75go43ifinzchsbr3g 49: mpich /spack/opt/spack/linux-ubuntu20.04-x86 64/oneapi-2022.1.0/mpich-4.0.2-sxre2qqfpvyak2hchnp3qeqdncxzvvco 50: mpifileutils /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mpifileutils-0.11.1-6dj2vqlpw5qydyq7v52ubu55op3ajpq7 51: netlib-scalapack /spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/netlib-scalapack-2.2.0-25vd6rfq4ufuesofo57jysj5x53nxu74

- oneAPI 2022.1.0
- Support for Intel GPUs (DG1,...)
- TensorFlow v2.9.1 and
- PyTorch v1.12.1



22.08 Release: 101 Official Products + dependencies (gcc, oneAPI, x86_64) (contd.)

```
52: nccmp
53: nco
54: nrm
55: omega-h
56: openmpi
57: openpmd-api
58: papi
59: papyrus
60: parallel-netcdf
61: paraview
62: parsec
63: pdt
64: petsc
65: phist
66: plasma
67: plumed
68: precice
69: pruners-ninja
70: pumi
71: pv-cinemasci
72: py-jupyterhub
73: py-libensemble
74: py-parsl
75: pv-radical-saga
76: gthreads
77: raja
78: rempi
79: scr
80: slate
81: slepc
82: stc
83: strumpack
84: sundials
85: superlu-dist
86: swig
87: sz
88: tasmanian
89: tau
90: trilinos
91: turbine
92: umap
93: umpire
94: unifyfs
95: upcxx
96: variorum
97: veloc
98: vtk-m
99: wannier90
100: warpx
```

```
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/spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/umap-2.1.0-4pteduzi242vxrweax7fx3mpqcrd42bl
/spack/opt/spack/linux-ubuntu20.04-x86 64/qcc-9.4.0/umpire-2022.03.1-mnn3tttwlzyasrh7zbwqskffj6qnkpcz
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/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/upcxx-2022.3.0-rafoonfubm2nlnwdwftgg4zmr2vcbg36
/spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/variorum-0.4.1-yso3svxygafgtn3yzjbnmb3eiycyhzsd
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/spack/opt/spack/linux-ubuntu20.04-x86 64/gcc-9.4.0/warpx-22.08-llgiiakur6amductbpxoagd2gslv6c2g
/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/zfp-0.5.5-6csn5bcuypuo3lteydiwsykoyjgylbz2
```

- oneAPI 2022.1.0
- Support for Intel GPUs (DG1,...)
- TensorFlow v2.9.1 and
- PyTorch v1.12.1



101: zfp

22.08 Release: 102 Official Products + dependencies (gcc, cuda, ppc64le)

1: adios2 spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/adios2-2.8.3-7nsyrc6kahbnbl2tggbv322ufie35pzt/ 2: alguimia spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/alguimia-1.0.9-g6nhgxj5eaitwniowal6nfip72wmkzx4/ spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/aml-0.2.0-s5it2fyntsesracr6txvi5kncwwvttla/ 3: aml 4: amrex spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/amrex-22.08-34gawx6htudsd6wgagrt5ru3eo7z4np5/ 5: arborx spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/arborx-1.2-65osfgiogccjutjvu2hmngh6z6e2jrjr/ 6: archer spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/archer-2.0.0-rcjtr3w4r2tteedz24jhfpsfojod6nuh/ 7: argobots spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/argobots-main-ilx5nitwe7gaacifewubp2dvxc2uskug/ 8: ascent spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/ascent-0.8.0-totua2ppnyfhxdysz5saikevjlala5gj/ spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/axom-0.6.1-dej5vhwggy2vnydantd3haclvnh5y55m/ 9: axom 10: bolt 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- NVHPC 22.7 with CUDA 11.7
- Support for NVIDIA GPUs
- TensorFlow v2.5.1 and
- PyTorch v1.9.0a0



22.08 Release: 102 Official Products + dependencies (gcc, cuda, ppc64le) (contd.)

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- NVHPC 22.7 with CUDA 11.7
- Support for NVIDIA GPUs
- TensorFlow v2.5.1 and
- PyTorch v1.9.0a0



22.08 Release: 101 Official Products + dependencies (gcc, cuda, aarch64) NEW!

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/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/loki-0.1.7-q5dtcfozzf4p7pycx4gtlgkvvglrworn 43: magma /spack/opt/spack/linux-ubuntu20.04-aarch64/qcc-9.4.0/magma-2.6.2-4u3qt62dtczmlvv2c7nt5qpru6vzmmze 44: mercury /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/mercury-2.1.0-fv5bxgdvgb3lv57s77xw3pmmjlk45gcg 45: metall /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/metall-0.21-op6ltaipplev2llrmget3e5frtyp73y7 /spack/opt/spack/linux-ubuntu20.04-aarch64/qcc-9.4.0/mfem-4.4.0-uvizvyebucxiqhbq4y7twveiqfydtzsi 46: mfem 47: mpark-variant /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/mpark-variant-1.4.0-hhfriafnm45uljscabscmahuhfclvmql 48: mpich /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/mpich-4.0.2-g3ba3kgzkdsuc2cl2eii665iltbk4pd4 49: mpifileutils /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-9.4.0/mpifileutils-0.11.1-guvx7all5mei2i4ouihkxu7taauznrrv 50: netlib-scalapack 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- NVHPC 22.7 with CUDA 11.7
- Support for NVIDIA GPUs
- PyTorch v1.12.1



22.08 Release: 101 Official Products + dependencies (gcc, cuda, aarch64) NEW!

```
52: nco
 53: nrm
 54: omega-h
 55: openmpi
 56: openpmd-api
 57: papi
 58: papyrus
 59: parallel-netcdf
 60: paraview
 61: parsec
 62: pdt
 63: petsc
 64: plasma
 65: plumed
 66: precice
 67: pruners-ninja
 68: pumi
 69: py-cinemasci
 70: py-jupyterhub
 71: py-libensemble
 72: py-opentuner
 73: py-parsl
 74: py-radical-pilot
 75: pv-radical-saga
 76: gthreads
 77: raja
 78: rempi
 79: scr
 80: slate
 81: slepc
 82: stc
 83: strumpack
 84: sundials
 85: superlu-dist
 86: swig
 87: sz
 88: tasmanian
 89: tau
 90: trilinos
 91: turbine
 92: umap
 93: umpire
 94: unifyfs
 95: upcxx
 96: veloc
 97: vtk-m
 98: wannier90
 99: warpx
100: yaksa
101: zfp
```

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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).



Thank you

https://www.exascaleproject.org

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