E4S: The Extreme-scale Scientific Software Stack
Release 22.02

Release 22.02 notes

February 28, 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
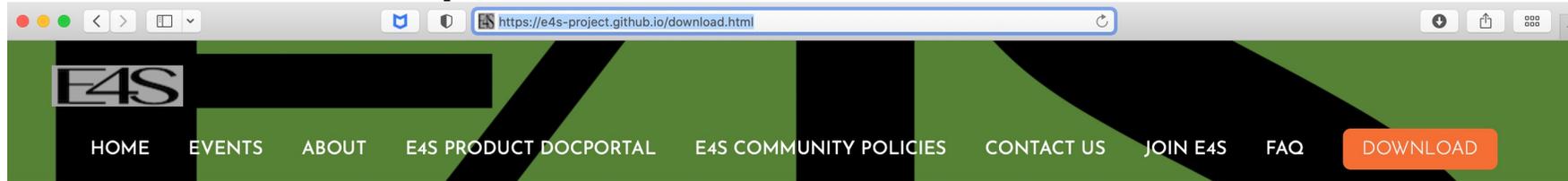
- Feb 2022: E4S 22.02 – 100 full release products

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

Download E4S 22.02 GPU Container Image: NVIDIA, AMD, Intel
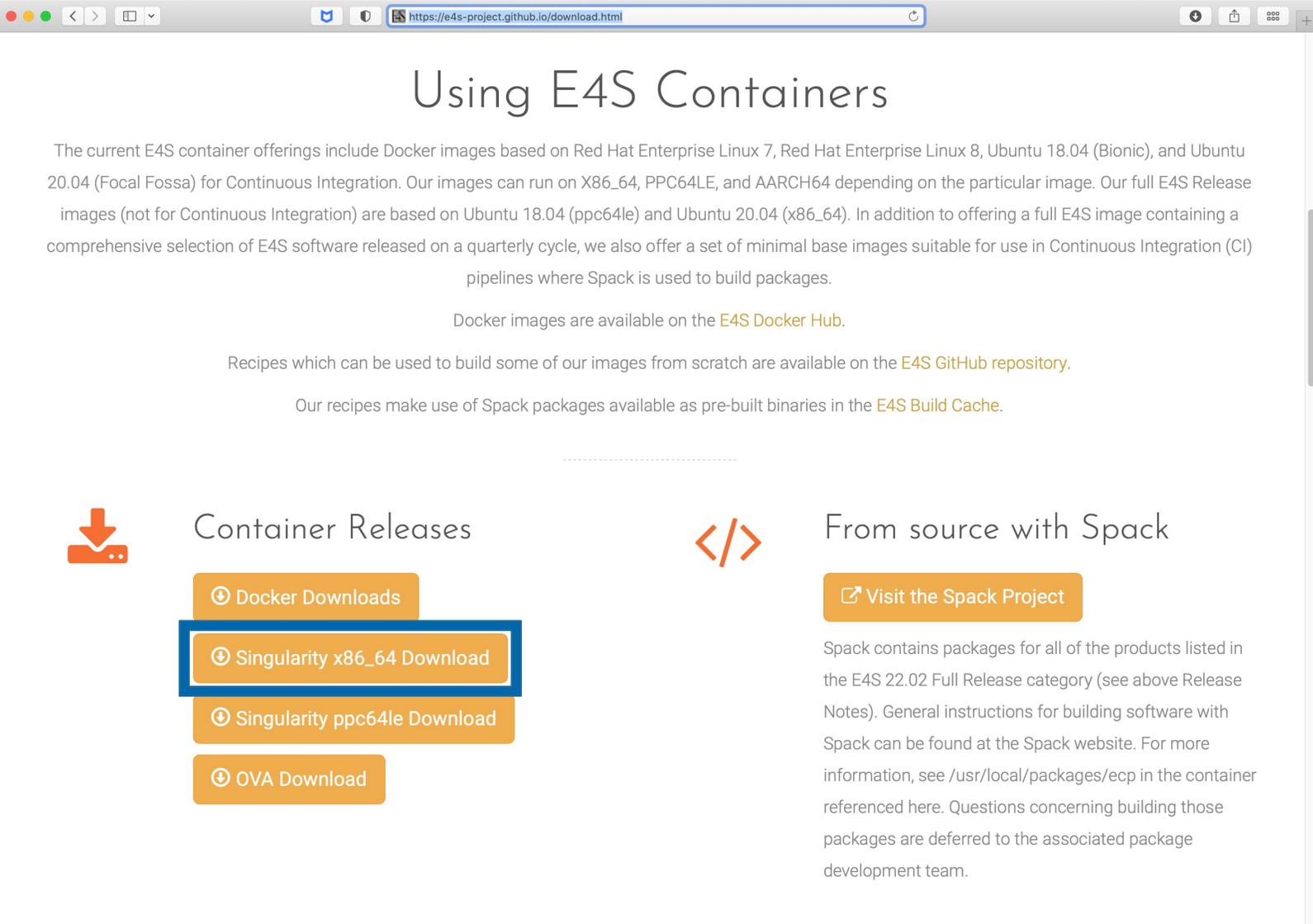
Using E4S Containers

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.

Recipes which can be used to build some of our images from scratch are available on the E4S GitHub repository.

Our recipes make use of Spack packages available as pre-built binaries in the E4S Build Cache.

Container Releases

- ⊕ Docker Downloads
- ⊕ Singularity x86_64 Download
- ⊕ Singularity ppc64le Download
- ⊕ OVA Download

From source with Spack

⊕ Visit the Spack Project

Spack contains packages for all of the products listed in the E4S 22.02 Full Release category (see above Release Notes). General instructions for building software with Spack can be found at the Spack website. For more information, see /usr/local/packages/ecp in the container referenced here. Questions concerning building those packages are deferred to the associated package development team.

- Full featured Singularity image
- GPU base images for
  - x86_64 (Intel, AMD, NVIDIA)
  - ppc64le
  - aarch64
- Packages with support for all three GPU runtimes:
  - Kokkos
  - TAU

https://e4s.io

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

```
 1: adios2              spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/adios2-2.7.1-vrqqwksvvumpvuvi2f3zvhrudbhrgvr7
 2: alquimia            spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/alquimia-1.0.9-5pxq2rf35knkrbdjz2hdqifjpsvsj2ay
 3: aml                 spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/aml-0.1.0-52bcp4rwi6xzklr2qpl3a3huqle6sszh
 4: amrex               spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/amrex-22.02-xjb77ajgucyfcyswmioly672gck3s2fy
 5: arborx              spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/arborx-1.1-x54ta6aq3vgvzhqaznybw63nbpwgp2c7
 6: archer              spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/archer-2.0.0-wkdybteqjoqfupcjcnr3syh4kgjza4mv
 7: argobots            spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/argobots-1.1-6vbx4fbx3ert23po2fzeuddnyal2wniy
 8: ascent              spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/ascent-0.7.1-y6ozlrcntdjrten3eel7di6fuuoe6f7x
 9: axom                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/axom-0.6.1-vbde3r3uveb6n37vzqq6xuobett2y7l2
10: bolt                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/bolt-2.0-fh7dq6fzfeie5fl3nzgindyzvggges6v
11: butterflypack       spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/butterflypack-2.1.0-vwr7qf256rg2n63auewcyuko3wy3gzzt
12: cabana              spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/cabana-0.4.0-ubam723mz433hemjuepsvmq553v3geln
13: caliper             spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/caliper-2.7.0-xvpd7krs6gxtyqekpaulssn4efm72zlj
14: catalyst            spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/catalyst-5.6.0-5ao2vfmbfis3na5p4a5j7uvykihdgxaf
15: chai                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/chai-2.4.0-nkjjn2do7p747ysc2ywxa4n7nqhnmh2v
16: charliecloud        spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/charliecloud-0.26-imxvh6utmc4icpeieodkonunb7zn4eez
17: conduit             spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/conduit-0.8.2-nhruflxgas6lzwjy5scaucveyncwox44
18: darshan-runtime     spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/darshan-runtime-3.3.1-ws6gpwomoa7nmgzcc4ztga6lwx55oeg2
19: datatransferkit     spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/datatransferkit-3.1-rc3-euqumxqzcu7f3c4hvsvhbc3mtpvi2jpu
20: dyninst             spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/dyninst-12.0.1-dslp7foewbfnxe2pn2z3mbiqwztmf57c
21: faodel              spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/faodel-1.2108.1-rdn5dmxtyf2rpiz5cimijutrqr7p2zwk
22: flecsi              spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/flecsi-2.1.0-gcqxn654rmz4vxndkmup62o3wmoebtiu
23: flit                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/flit-2.1.0-qfegiopjkolncxhhraopx6s3nr4g23xi
24: flux-sched          spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/flux-sched-0.20.0-eaf5kwa3r46vxwnyuljl7zhpitjthp3k
25: fortrilinos         spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/fortrilinos-2.0.0-nh7wozfevbp3rdy3iu3wei5f7u2kzzl2
26: gasnet              spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/gasnet-2021.9.0-37bcasne2t26z4f7rju7fy52eeqooolx
27: geopm               spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/geopm-1.1.0-o2b57hvdpzkd7as754onu5cdzhg6boc6
28: ginkgo              spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/ginkgo-1.4.0-tlueryyabtnd6yg7sen6iknpyyzkpfbt
29: globalarrays        spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/globalarrays-5.8-auttuj4uxg5s45agb2pr4oih7rhjchbv
30: gotcha              spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/gotcha-1.0.3-u6ttykuc7w75fpckuy4piy72uhdxvdxy
31: gptune              spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/gptune-2.1.0-yocmmqkzvmaqewybyn2o4i7qu6x73f7i
32: hdf5                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/hdf5-1.10.7-ydvek2t5h4kz2bc7qxrnborep7ljkye6
33: heffte              spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/heffte-2.2.0-gt4xlhl6oe2abi5tc6psrdqdnz2hs2gj
34: hpctoolkit          spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/hpctoolkit-2022.01.15-5bpxdxxdkagebetg4c2vqa3ca36elwvs
35: hpx                 spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/hpx-1.7.1-udoriqk2dx6vactf3gl6746r2ykw7s5j
36: hypre               spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/hypre-2.24.0-rubtvtyzb7i6fk52vryghtcr62bgnlvt
37: kokkos              spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/kokkos-3.5.00-jcqkaxownuoufxxbsiw5tm2s7p763rkc
38: kokkos-kernels      spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/kokkos-kernels-3.5.00-w6r3jgo7i5qzb5crtr3wqlo7l3a2gskn
39: lammps              spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/lammps-20220107-dxuaklopsx4q3t4gtwx274l7ear3d6v5
40: legion              spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/legion-21.03.0-ewj6mv6kyslktjgj5reeyoasegc5insn
41: libnrm              spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/libnrm-0.1.0-zt2trrdexkcjkcxsag4hvlry7q7x2aqv
42: libquo              spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/libquo-1.3.1-ot45gb6c3cbjddanrmoy4yxpqfdapoey
43: loki                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/loki-0.1.7-2zpo6dh6bdrko47n4gziacm6xteojflm
44: magma               spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/magma-2.6.1-hjnxgt33n2nwmg6jsolrilai6dnycxc3
45: mercury             spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/mercury-2.1.0-5by37sm7nto6t7tz6rfnq6355vu6fbnw
46: metall              spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/metall-0.17-a3qixbbz5hpkkvmocpiqbp4e5lehf2j2
47: mfem                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/mfem-4.3.0-7b7vcw33k4brllinosrhvii2oj63bwzs
48: mpich               spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/mpich-3.4.2-b2hsqqqnsiodzp3kw63u425osorilfty
49: mpifileutils        spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/mpifileutils-0.11.1-x6mkbu3osheeiba7rqb3xjsu4fequ7tu
50: netlib-scalapack    spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/netlib-scalapack-2.1.0-mu7sj7fu3nmrtzknsrkvquuoud2eupvf
```

```
Singularity> which dpcpp
/opt/intel/oneapi/compiler/2022.0.2/linux/bin/dpcpp
Singularity> which hipcc
/opt/rocm-4.5.2/bin/hipcc
Singularity> spack find cuda
==> 1 installed package
-- linux-ubuntu20.04-x86_64 / gcc@9.3.0 ------------------------
cuda@11.4.2
Singularity> spack find nvhpc
==> 1 installed package
-- linux-ubuntu20.04-x86_64 / gcc@9.3.0 ------------------------
nvhpc@22.1
Singularity> ▮
```

GPU runtimes
- Intel (oneAPI)
  - 2022.0.2
- AMD (ROCm)
  - 4.5.2
- NVIDIA (CUDA)
  - 11.4.2
- NVHPC
  - 22.1

EXASCALE COMPUTING PROJECT

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

```
51: nccmp            /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/nccmp-1.9.0.1-2hkqbcchaexl22f3lnkkozvznjr6h3g4
52: nco              /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/nco-5.0.1-nzqjzuwz3pvkslc32fnshotwr7nwlcgu
53: ninja            /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/ninja-1.10.2-2gpjomjrzlvinikx2qrm3rsasypnptvl
54: nrm              /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/nrm-0.1.0-omwezy5dwi7qshkr5v2eo64lj37scwhw
55: omega-h          /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/omega-h-9.34.1-syd6ahkexymz5ik24msxcki4fnatgvta
56: openpmd-api      /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/openpmd-api-0.14.4-k6wknbemtkoujp5fh3lxum5x5lklmf7u
57: openmpi          /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/openmpi-4.1.2-5yqclfs7ipo3u6ap4aeffacgvxqt5674
58: papi             /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/papi-6.0.0.1-mjwlkr6yrsrcnufl7nv47435mjmiifij
59: papyrus          /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/papyrus-1.0.1-oawas4327vvwwy7cpgkuftqnberp4dbj
60: parallel-netcdf  /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/parallel-netcdf-1.12.2-ojopqbmuz6rhdtxq3xl4icd7euvmhwoj
61: paraview         /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/paraview-5.10.0-ai6ih3nx3rhwtepdlojfx57oupjlht7j
62: parsec           /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/parsec-3.0.2012-mmut76y5frfk22qlraeihmyb6noruw3c
63: pdt              /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/pdt-3.25.1-c57l5pqsnjyt7f3tfa256lkotm3mwaow
64: petsc            /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/petsc-3.16.4-o3kxlwykh3lflqg3unx2vwykitgodpjh
65: phist            /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/phist-1.9.5-ejcz3wgujbcpi4wkoxcr63w4hkyb5yyp
66: plasma           /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/plasma-21.8.29-447maohfkz3idurx33gxypl5jc54cblq
67: plumed           /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/plumed-2.6.3-3d6ibkubuzle3a4pd3duhi56y6ajaclt
68: precice          /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/precice-2.3.0-rjrp7whhwk7x3ztvq6p4pfbxigpbkso5
69: pumi             /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/pumi-2.2.6-z26nhhtfcbhv62ceukc4hhy77wzkavut
70: py-cinemasci     /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/py-cinemasci-1.3-6ah5lcb5kno2owdxils677ngylt5asfv
71: py-jupyterhub    /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/py-jupyterhub-1.4.1-wdouha5jog55a6u2mnq34yw5hguohc2l
72: py-libensemble   /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/py-libensemble-0.8.0-6upb3t7cbizf2bzg2mkaufm52ki7n5zx
73: py-parsl         /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/py-parsl-1.1.0-qi4ema4wexehbxwiy4yfatdx4ltkqhdy
74: py-radical-saga  /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/py-radical-saga-1.11.1-yroolargjs4w3wid4copj6qqn7li4ji4
75: qthreads         /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/qthreads-1.16-oqsr5vtyypuqmjowxy7cf7l4c7o35hao
76: raja             /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/raja-0.14.0-wug2hk4iuvwdiqaylipykempp227o6ek
77: rempi            /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/rempi-1.1.0-7szviepug5lw2khdoxcwvs6d7pg2u2nt
78: scr              /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/scr-3.0rc2-wmnhwtvh7uzfwth7q6l3shphnunvqeoe
79: slate            /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/slate-2021.05.02-7ck5664dxjjhdn63dp7xrkxgr7b3zqzf
80: slepc            /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/slepc-3.16.2-tk2zp7s5kqqjbbw3unvqqebf2infp4us
81: strumpack        /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/strumpack-6.3.0-mdvvav6jov5rq2qk6gubl6xr7u7xeafz
82: sundials         /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/sundials-6.1.1-nin5qvr6nywydyqfoitwdmnueifvowhi
83: superlu-dist     /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/superlu-dist-develop-jbyhfjjr2s24yhiqhb2fop3o4qe72ugc
84: stc              /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/stc-0.9.0-4ldizggme2pk22wvbmxstlmdljz7daft
85: swig             /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/swig-4.0.2-fortran-hdwur55hnamozikupngwlygilofxgact
86: sz               /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/sz-2.1.12-ncwe7eipqstaikf6w5yuisut7ohu7cfo
87: tasmanian        /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/tasmanian-7.7-ntlsb3dbnklrlyqb44c7td7tln7y4ji4
88: tau              /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/tau-2.31-pbccumbiklduiftms63x2jqtviwvk764
89: trilinos         /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/trilinos-develop-d5semjk4u4axs7mlep2yj4aarwfgxttw
90: turbine          /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/turbine-1.3.0-lpu56cphuxnmonv5dpojvcbsecfxewo2
91: umap             /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/umap-2.1.0-qwldcv45isedxa2xiq2lui6eorvsknvd
92: umpire           /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/umpire-6.0.0-kfzrcgjnnisrevs422hgg622djvshvdp
93: unifyfs          /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/unifyfs-0.9.1-xfqgf74ejwrfo4y3ue45phglzh6hidmz
94: upcxx            /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/upcxx-2021.9.0-x7yedv4bmia4dsupr3x2elvngjw2e6ep
95: variorum         /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/variorum-0.4.1-iucjprimf7tpjo6jz7w2hyrouvfwflwe
96: veloc            /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/veloc-1.5-xnjowfax7ysawyyygo46mikk7ss36uw3
97: vtk-m            /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/vtk-m-1.7.1-iqkpaoty4ot66d5w6urgdpowyncgpoq2
98: wannier90        /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/wannier90-3.1.0-fz3t3zaslhan5fbgghjmzvo5xvaucub3
99: warpx            /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/warpx-22.02-yq75dzo7ycj6y5kpcuvc74mt6wvbeq7l
100: zfp             /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/zfp-0.5.5-glocwgycmhef4w4pnqemrcct6xpac3t5
```

Languages:
- Julia
- Python

AI products with GPU support
- Tensorflow
- Pytorch

3D Visualization
- Paraview
- VisIt
- TAU's paraprof …

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

```
 1: adios2            spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/adios2-2.7.1-4jqdeeg24ievjsmidstktyiwlv2kws55
 2: alquimia          spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/alquimia-1.0.9-kl2uuwk4ihcda7fhyxkedopuqhultaqf
 3: aml               spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/aml-0.1.0-dvzmjcuzox3ubd7lnxdgoggoksk5v43k
 4: amrex             spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/amrex-22.02-zc7mv3makq5c2qpw7jjlmwrb4k66rvvl
 5: arborx            spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/arborx-1.1-szs54gusdjuwibxshd27xq5pmds5por3
 6: archer            spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/archer-2.0.0-vcvzy6okrw4mjxtqgmuo3725ulboietr
 7: argobots          spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/argobots-1.1-trhfaqcmt2ib5tsw4axzqzls4tbxxt45
 8: ascent            spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/ascent-0.7.1-6nzrbj2mgi7fqfrseyuhjm5rencldn3c
 9: axom              spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/axom-0.6.1-ymb5ju6djdwurkxjbwo6yzpkgkybagan
10: bolt              spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/bolt-2.0-lfkm2qifo3qdvdgdgckeq2b7rgv3yesq
11: butterflypack     spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/butterflypack-2.1.0-eusmk3wvyju7wm4uekimknyl7ftz77j5
12: cabana            spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/cabana-0.4.0-bv6y5ek6w42tufhkgzztxnhz4nyzdmcy
13: caliper           spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/caliper-2.7.0-yt7las4hzzmk75a4mehej4c5klt62dnk
14: chai              spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/chai-2.4.0-k3mrmb3ywq6ixwrn6mn7jl4gcxmqxkmy
15: charliecloud      spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/charliecloud-0.26-2byo4we7isxo5m77ixm6hjb2wbevymrr
16: conduit           spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/conduit-0.8.2-lnpv6hggqcap5v4q4wkacna3id53wosr
17: darshan-runtime   spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/darshan-runtime-3.3.1-fig7a4dxy56f5xbibb6fbi5wbawyv6b4
18: datatransferkit   spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/datatransferkit-3.1-rc3-wa4d7h6s2ui3r375rirnsxs6mduiynu7
19: dyninst           spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/dyninst-12.0.1-h3kpxhzv7iqylpjvqbneegatif7qs67t
20: exaworks          spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/exaworks-0.1.0-vlseszxfohskd3t2wujfabjkqspdxhaa
21: faodel            spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/faodel-1.2108.1-7cbwmf5olgoff34nrf6aciayewwh5ol5
22: flecsi            spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/flecsi-1.4.2-2ny3vyzvo3kfe7oi37awx3im4pzuenem
23: flit              spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/flit-2.1.0-tiazm5zdjun5fpgbilqwuyv75sdng4yn
24: flux-sched        spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/flux-sched-0.20.0-ntaytdbybyy3d2vvr4yw3o6sqlmdautz
25: fortrilinos       spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/fortrilinos-2.0.0-5lwnkjhu2pfqa7i53r5dmjwrtdlfmchj
26: gasnet            spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/gasnet-2021.9.0-vov6viwltjtgd2xdcjebkcuysd22yk4f
27: ginkgo            spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/ginkgo-1.4.0-43puh65asdbyuppjvnkclvlhbcbypdxi
28: globalarrays      spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/globalarrays-5.8-u3ksyg4nk4q6hyzq2m7uhil5obsaej4s
29: gotcha            spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/gotcha-1.0.3-nyelkzzoqqa4ca4lug5wjl2jkhibrvpq
30: gptune            spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/gptune-2.1.0-ejaasogpqkkirlslnr4fa3xpjlkniuut
31: hdf5              spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/hdf5-1.10.7-55dzf6dfzrzfygclkniva73v3am77j7y
32: heffte            spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/heffte-2.2.0-zs4yjubwwqoplaxiyzeabe6ol4ytratl
33: hpctoolkit        spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/hpctoolkit-2022.01.15-qljk5ibsjxsvxbwbom5z7qj4hmhhzvwu
34: hpx               spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/hpx-1.7.1-usg36dncwef4p4ekynejmyaqv54rlqay
35: hypre             spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/hypre-2.24.0-35mmfx5qlvsjklkqblmbtxabp446f76h
36: kokkos            spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/kokkos-3.5.00-ooeb3ky7vlwbhwbatfdbqtgyxpwwa4ow
37: kokkos-kernels    spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/kokkos-kernels-3.5.00-elayrtzesapufvrxqqdeiwqjvplytpb4
38: lammps            spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/lammps-20220107-qfojnjyzxoyfzvtnxrswy4d22h5qm6vy
39: legion            spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/legion-21.03.0-mmgybyncfgefmdaj3v5nhztxtsjbjd2x
40: libnrm            spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/libnrm-0.1.0-icb2b2szd3gxcrmw5gewvdvoxxriyzar
41: libquo            spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/libquo-1.3.1-bqqr2ucgacsvbkdob2sjamurqjyqdcc4
42: loki              spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/loki-0.1.7-ggwkzpwhjztzezp5x2fnimeesnu5i6un
43: magma             spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/magma-2.6.1-cgwcbhobvdoxdbmz7laf6cvwusfq3pp4
44: mercury           spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mercury-2.1.0-rw3fop4oagnr7kn3pkv76u5fmahpv3ii
45: metall            spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/metall-0.17-m2umsb6xkpybnjb2ggd54bhk2d72yikf
46: mfem              spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mfem-4.3.0-cy43egzrzhl6qqsfo32iqyymkxqei6x6
47: mpark-variant     spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mpark-variant-1.4.0-xyf5xrvdszmtlswk35ayonajo2falqg5
48: mpich             spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mpich-3.4.2-ylw3nuwbq2kvtrmmtkohrqttkggksr4g
49: mpifileutils      spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mpifileutils-0.11.1-qdsthysxq4h5hievlaeiwhumdbc4pslt
50: netlib-scalapack  spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/netlib-scalapack-2.1.0-bdwubudmyuuvk4ddcqb46hmn4qnlk2bx
```

GPU runtimes for IBM Power
- CUDA 11
- NVHPC 22.1

Languages
- Julia
- Python

AI packages for NVIDIA GPU
- TensorFlow
- PyTorch

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

```
51: nccmp           /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/nccmp-1.9.0.1-pq554jkehwzda5aeebmj36h6maclzykk
52: nco             /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/nco-5.0.1-sdtngoaodihhafblfplykjwgegmelvvj
53: ninja           /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/ninja-1.10.2-txpvjbtkrg7ovnuluobagoqgn5gabg3d
54: nrm             /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/nrm-0.1.0-wr7vo4mitz3ig42i7vaezwebxiep4ky7
55: omega-h         /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/omega-h-9.34.1-6urugkbhaolrzpl4i5ligoelkyrmqqrq
56: openpmd-api     /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/openpmd-api-0.14.4-7gfvhisxtj5o37obnqgoh5r5oashdfyk
57: openmpi         /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/openmpi-4.1.2-wlurs7nh53mkbcff5xmm7cyzpfmhdahz
58: papi            /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/papi-6.0.0.1-j35bykhaeufp5heiaqly6q25qotqmttj
59: papyrus         /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/papyrus-1.0.1-str3rilmozozbsutftr5djq4cfkavoxv
60: parallel-netcdf /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/parallel-netcdf-1.12.2-33rzdxxg65zqr3cwezvjmb4jp547fs3t
61: paraview        /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/paraview-5.10.0-fo23tjskoerryh2j44d7dw6tfambrqv7
62: parsec          /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/parsec-3.0.2012-44e7355zpzsitd3umlxw33d5omdlowok
63: pdt             /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/pdt-3.25.1-dfzobkfuiqczpxae5hnfezqm6gpqi3wk
64: petsc           /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/petsc-3.16.4-4gppqwtlxqjcdlvxixgdifiu4qyfhfzk
65: plasma          /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/plasma-21.8.29-ym55wql2kluudjfmsnguxa5524urx6k5
66: plumed          /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/plumed-2.6.3-co5f5mocjw4tshji7qnskscjoeutnsay
67: precice         /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/precice-2.3.0-3lntwf73n3sxiiszhdmth3u7fgzdy6ab
68: pumi            /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/pumi-2.2.6-sognwzwhnjfhx4yjj43bvzy3k4fogzcj
69: py-cinemasci    /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-cinemasci-1.3-awg5ln4mavzhqtsj47zeq7yl3uf4f7ya
70: py-jupyterhub   /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-jupyterhub-1.4.1-tmqhrglytercluboxu7gsbnhrfkuwlep
71: py-libensemble  /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-libensemble-0.8.0-cnr27aysatnm6k54qpbcjhxvmjptw6ut
72: py-parsl        /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-parsl-1.1.0-qtfq7fr22pjynprxyhpaxjbemdqmvx5m
73: py-radical-pilot /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-radical-pilot-1.11.2-4yopypwcrqywxwg4tpzz4xi5uos3k4hy
74: py-radical-saga /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-radical-saga-1.11.1-e4vdj67jjokqimcrabtuqnrdb3kklmqd
75: qthreads        /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/qthreads-1.16-z2esuoqorzcr4tcuqyeh4zgx7kh2gy4j
76: raja            /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/raja-0.14.0-ow63lt5olwwomoxwfqbz7464df4ek2bl
77: rempi           /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/rempi-1.1.0-2tpsr2ppdahbbplqtur45vyvt6tdwlpb
78: scr             /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/scr-3.0rc2-wzvfcuxwbcwqx3rjg27wbwcpo53kjsc5
79: slate           /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/slate-2021.05.02-mnnpn3ezdopcraqjo5expxcyh7pa7zfo
80: slepc           /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/slepc-3.16.2-sklcgra3kvyrzfqanwuefezqrrinsllz
81: spot            /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/spot-2.9.4-y5pxssx23mkdiygis2jraucj3d6kdarp
82: strumpack       /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/strumpack-6.3.0-gjauyvljjlh6gew4egajp7x4i7q6xudu
83: sundials        /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/sundials-6.1.1-ycocpnjvrmncp7ttoxqno7p4kgr64aet
84: superlu-dist    /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/superlu-dist-7.2.0-o5sqg2lsaklwsqmbvct72epkivllsono
85: stc             /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/stc-0.9.0-id3urr2mljdhry2pu7bbkqhwt3o2a3as
86: swig            /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/swig-4.0.2-fortran-exxngdij3rqd7rgcnkn5go4vc7dugrxw
87: sz              /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/sz-2.1.12-n5wgbtryijanb6p6qh27p36daq4y2mce
88: tasmanian       /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/tasmanian-7.7-veo5oikqc5ajmubpa6f5jehy4xc7d2ev
89: tau             /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/tau-2.31-4bounoz2d6rchlf4h4lut5dn7r3tkkaq
90: trilinos        /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/trilinos-13.2.0-crlw734mrosiph5og5ashcz64df23qbi
91: turbine         /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/turbine-1.3.0-cldrv363ejpzhi3zpexxboapsbkyi6mr
92: umap            /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/umap-2.1.0-7sqkyikt6qkgfbgnxgwbjwy2ia47cc5d
93: umpire          /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/umpire-6.0.0-fje4b6sdckggwney53z2rnwdhrfswmja
94: unifyfs         /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/unifyfs-0.9.1-3sgocddzc3xyvog7vti54qr7owlnu5o5
95: upcxx           /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/upcxx-2021.9.0-ypki2vvo2isqf3xrtww55ww5arwbjudm
96: veloc           /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/veloc-1.5-new5o35pn6y7w4wn465xna6znfumwqzw
97: vtk-m           /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/vtk-m-1.7.1-nj4wujmfy5gos57ntvwc7m24raslrkoe
98: wannier90       /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/wannier90-3.1.0-cjmkyyxukbvoxg56ugmpqmcnlp6x7ebr
99: warpx           /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/warpx-22.02-6cv6qr45lyyg3z2ym625wx2i7okqwe3l
100: zfp            /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/zfp-0.5.5-cmhh4bkpgptkbhyg6g4s4csjuamh6525
```

E4S 22.02 Release: full featured GPU image, LLVM DOE image

- Full featured images
  - ppc64le and x86_64
  - Docker and Singularity
- LLVM DOE E4S image

E4S 22.02 Release: GPU, ppc64le for Docker Containers

- 100 E4S Products
- Support for GPUs
  - ppc64le and x86_64

% docker pull ecpe4s/e4s-gpu

E4S 22.02 bare-metal installation
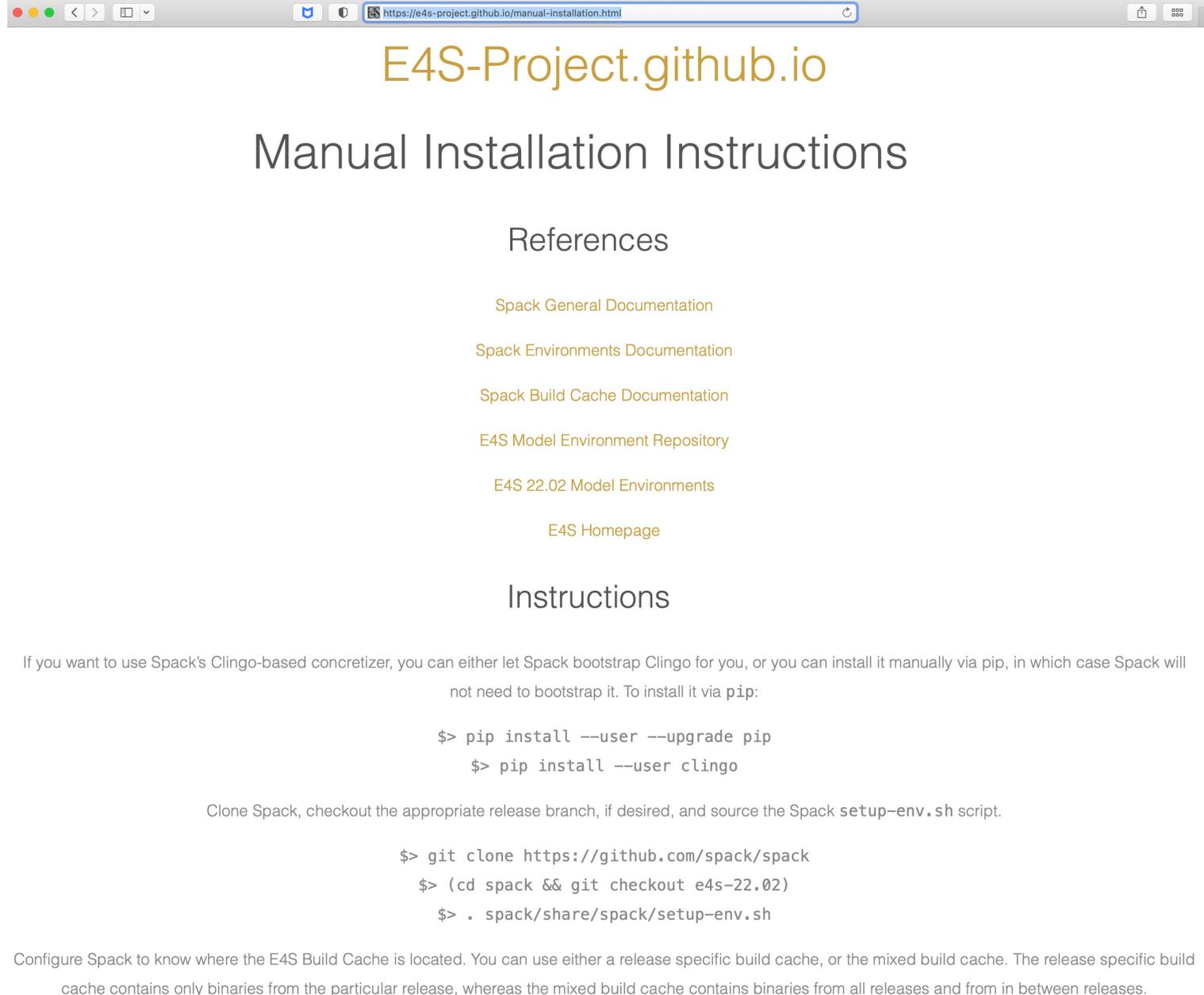
E4S-Project.github.io

Manual Installation Instructions

References

Spack General Documentation

Spack Environments Documentation

Spack Build Cache Documentation

E4S Model Environment Repository

E4S 22.02 Model Environments

E4S Homepage

Instructions

If you want to use Spack's Clingo-based concretizer, you can either let Spack bootstrap Clingo for you, or you can install it manually via pip, in which case Spack will not need to bootstrap it. To install it via `pip`:

```
$> pip install --user --upgrade pip
$> pip install --user clingo
```

Clone Spack, checkout the appropriate release branch, if desired, and source the Spack `setup-env.sh` script.

```
$> git clone https://github.com/spack/spack
$> (cd spack && git checkout e4s-22.02)
$> . spack/share/spack/setup-env.sh
```

Configure Spack to know where the E4S Build Cache is located. You can use either a release specific build cache, or the mixed build cache. The release specific build cache contains only binaries from the particular release, whereas the mixed build cache contains binaries from all releases and from in between releases.

E4S 22.02 bare-metal Spack installation environments on GitHub

```
 8    packages:
 9      all:
10        compiler:
11        - gcc@9.3.0
12        providers:
13          blas:
14          - openblas
15          mpi:
16          - mpich
17        target:
18        - x86_64
19        variants: +mpi
20      binutils:
21        variants: +ld +gold +headers +libiberty ~nls
22        version:
23        - 2.36.1
24      cuda:
25        version:
26        - 11.4.2
27      doxygen:
28        version:
29        - 1.8.20
30      elfutils:
31        variants: +bzip2 ~nls +xz
32      hdf5:
33        variants: +fortran +hl +shared
34        version:
35        - 1.10.7
36      libfabric:
37        variants: fabrics=sockets,tcp,udp,rxm
38      libunwind:
39        variants: +pic +xz
40      mesa:
41        variants: ~llvm
42      mesa18:
43        variants: ~llvm
44      mpich:
45        variants: ~wrapperrpath
46      ncurses:
47        variants: +termlib
48      openblas:
49        variants: threads=openmp
50      python:
51        version:
52        - 3.8.12
53      trilinos:
54        variants: +amesos +amesos2 +anasazi +aztec +belos +boost +epetra +epetraext
55          +ifpack +ifpack2 +intrepid +intrepid2 +isorropia +kokkos +ml +minitensor +muelu
56          +nox +piro +phalanx +rol +rythmos +sacado +stk +shards +shylu +stokhos +stratimikos
57          +teko +tempus +tpetra +trilinoscouplings +zoltan +zoltan2 +superlu-dist gotype=long_long
```

spack.yaml

E4S 22.02 bare-metal installation spack.yaml recipe

Browser URL: https://github.com/E4S-Project/e4s/blob/master/environments/22.02/spack-x86_64.yaml

```
174      - cuda_specs:
175        - amrex@22.02 +cuda cuda_arch=80
176        - caliper@2.7.0 +cuda cuda_arch=80
177        - chai@2.4.0 ~benchmarks ~tests +cuda cuda_arch=80 ^umpire@6.0.0 ~shared
178        - flecsi@2.1.0 +cuda cuda_arch=80
179        - flux-core@0.35.0 +cuda # not CudaPackage
180        - ginkgo@1.4.0 +cuda cuda_arch=80
181        - heffte@2.2.0 +cuda cuda_arch=80
182        - hpctoolkit@2022.01.15 +cuda # not CudaPackage
183        - hpx@1.7.1 +cuda cuda_arch=80
184        - hypre@2.24.0 +cuda cuda_arch=80
185        - kokkos-kernels@3.5.00 +cuda cuda_arch=80 ^kokkos@3.5.00 +wrapper +cuda cuda_arch=80
186        - kokkos@3.5.00 +wrapper +cuda cuda_arch=80
187        - magma@2.6.1 +cuda cuda_arch=80
188        - mfem@4.3.0 +cuda cuda_arch=80
189        - openmpi@4.1.2 +cuda # not CudaPackage
190        - papi@6.0.0.1 +cuda # not CudaPackage
191        - parsec@3.0.2012 +cuda cuda_arch=80
192        - petsc@3.16.4 +cuda cuda_arch=80
193        - raja@0.14.0 +cuda cuda_arch=80
194        - slate@2021.05.02 +cuda cuda_arch=80
195        - slepc@3.16.2 +cuda cuda_arch=80
196        - strumpack@6.3.0 ~slate +cuda cuda_arch=80
197        - sundials@6.1.1 +cuda cuda_arch=80
198        - superlu-dist@7.2.0 +cuda cuda_arch=80
199        - tasmanian@7.7 +cuda cuda_arch=80
200        - trilinos@13.2.0 +cuda cuda_arch=80
201        - umpire@6.0.0 ~shared +cuda cuda_arch=80
202        - vtk-m@1.7.1 +cuda cuda_arch=80
203        - zfp@0.5.5 +cuda cuda_arch=80
204      #- arborx@1.1 +cuda # not CudaPackage
205      #- ascent@0.7.1 ~shared +cuda cuda_arch=80
206      #- axom@0.6.1 +cuda cuda_arch=80 ^umpire ~shared
207      #- cabana@0.4.0 +cuda # not CudaPackage
208      #- dealii@9.3.2 +cuda cuda_arch=80 # gmsh
209      #- legion@21.03.0 +cuda cuda_arch=80
210      #- llvm@13.0.0 +cuda cuda_arch=80
211      #- paraview@5.10.0 +cuda cuda_arch=80
212      #- upcxx@2021.9.0 +cuda # not CudaPackage, needs driver
213
214      - rocm_specs:
215        - amrex@22.02 +rocm amdgpu_target=gfx908
216        - chai@2.4.0 ~benchmarks +rocm amdgpu_target=gfx908
217        - ginkgo@1.4.0 +rocm amdgpu_target=gfx908
218        - heffte@2.2.0 +rocm amdgpu_target=gfx908
219        - hpx@1.7.1 +rocm amdgpu_target=gfx908
220        - kokkos@3.5.00 +rocm amdgpu_target=gfx908
221        - magma@2.6.1 ~cuda +rocm amdgpu_target=gfx908
222        - mfem@4.3.0 +rocm amdgpu_target=gfx908
223        - petsc@3.16.4 +rocm amdgpu_target=gfx908
224        - raja@0.14.0 ~openmp +rocm amdgpu_target=gfx908
225        - slate@2021.05.02 +rocm amdgpu_target=gfx908
226        - slepc@3.16.2 +rocm amdgpu_target=gfx908 ^petsc +rocm amdgpu_target=gfx908
227        - strumpack@6.3.0 ~slate +rocm amdgpu_target=gfx908
```

- E4S products built with CUDA for A100
- Built with ROCm for MI100 and MI250X
- Built with oneAPI

ECP EXASCALE COMPUTING PROJECT

E4S: Spack build cache at U. Oregon to speed up installation

- 80,000+ binaries
- S3 mirror
- No need to build from source code!

- https://oaciss.uoregon.edu/e4s/inventory.html

E4S base container images for x86_64, ppc64le, and aarch64

Minimal Spack

X86_64 and PPC64LE

This image contains a minimal setup for using Spack 0.17.1, including Clingo concretizer and GNU compilers.

ecpe4s/ubuntu18.04-spack 🐳 docker

e4s-ubuntu18.04-spack-x86_64.sif Ⓢ mirror 1 Ⓢ mirror 2

e4s-ubuntu18.04-spack-ppc64le.sif Ⓢ mirror 1 Ⓢ mirror 2

GPU Base Images

These images come with MPICH, CMake, and the relevant GPU SDK -- either ROCM, NVIDIA CUDA Toolkit and NVHPC, or Intel OneAPI -- available as LMOD modules

NVIDIA Multi-Arch (X86_64, PPC64LE, AARCH64)	ROCM X86_64	Intel OneAPI X86_64
ecpe4s/e4s-base-cuda:22.02 🐳 docker	ecpe4s/e4s-base-rocm:22.02 🐳 docker	ecpe4s/e4s-base-oneapi:22.02 🐳 docker
e4s-x86_64-cuda-x86.sif Ⓢ mirror 1 Ⓢ mirror 2	e4s-x86_64-rocm.sif Ⓢ mirror 1 Ⓢ mirror 2	e4s-x86_64-oneapi.sif Ⓢ mirror 1 Ⓢ mirror 2
e4s-aarch64-cuda.sif Ⓢ mirror 1 Ⓢ mirror 2		
e4s-ppc64le-cuda.sif Ⓢ mirror 1 Ⓢ mirror 2		

Continuous Integration Images

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

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

X86_64	PPC64LE
ecpe4s/rhel7-runner-x86_64 🐳 docker GitHub	ecpe4s/rhel7-runner-ppc64le 🐳 docker GitHub
ecpe4s/rhel8-runner-x86_64 🐳 docker GitHub	ecpe4s/rhel8-runner-ppc64le 🐳 docker GitHub
ecpe4s/ubuntu18.04-runner-x86_64 🐳 docker GitHub	ecpe4s/ubuntu18.04-runner-ppc64le 🐳 docker GitHub
ecpe4s/ubuntu20.04-runner-x86_64 🐳 docker GitHub	ecpe4s/ubuntu20.04-runner-ppc64le 🐳 docker GitHub

- Hub.docker.com
- ecpe4s
- Platforms:
  - x86_64
  - ppc64le
  - aarch64
- GPU runtimes:
  - Cuda
  - ROCm
  - oneAPI
- Singularity images
- Miminal Spack image

Minimal Spack base image on Dockerhub

- Create custom container images
- 1M+ downloads!

E4S 22.02 AWS cloud, CI, and custom images

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

Continuous Integration Images

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

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

X86_64	PPC64LE
ecpe4s/rhel7-runner-x86_64 docker GitHub	ecpe4s/rhel7-runner-ppc64le docker GitHub
ecpe4s/rhel8-runner-x86_64 docker GitHub	ecpe4s/rhel8-runner-ppc64le docker GitHub
ecpe4s/ubuntu18.04-runner-x86_64 docker GitHub	ecpe4s/ubuntu18.04-runner-ppc64le docker GitHub
ecpe4s/ubuntu20.04-runner-x86_64 docker GitHub	ecpe4s/ubuntu20.04-runner-ppc64le docker GitHub

Custom Images

ecpe4s/ubuntu1804_aarch64_waggle docker GitHub

ecpe4s/superlu_sc docker GitHub

E4S Facility Deployment

NERSC

OLCF

AWS EC2 Image

The E4S 22.02 release is also available on AWS as an EC2 AMI with ID ami-0b25a3c02556d434e. in the US-West-2 (Oregon) region.

17

E4S 22.02 AWS image: US-West2 (OR) ami-0b25a3c02556d434e

E4S 22.02 AWS
- Intel oneAPI
- CUDA
- NVHPC
- ROCm
- AWS DCV
- Spack Build Cache
- ECP: Nalu-Wind
- OpenFOAM
- ParaView
- VisIt
- TAU
- Docker
- Shifter
- Charliecloud
- E4S Singularity…

Thank you

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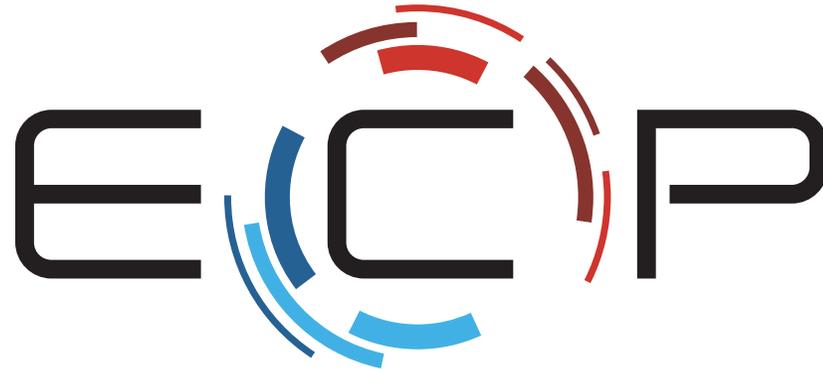
Thank you to all collaborators in the ECP and broader computational science communities. The work discussed in this presentation represents creative contributions of many people who are passionately working toward next-generation computational science.