

E4S Training

E4S at NERSC 2022 workshop:

<https://www.nersc.gov/users/training/events/e4s-at-nersc-2022/>
1:30pm – 2:15pm PT, Thursday, August 25, 2022

https://e4s.io/talks/E4S_at_NERSC_Shende_2.pptx

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Deployment of E4S at facilities: NERSC

- Update E4S for supporting Slingshot 11 upgrade on Perlmutter.
- Create Spack recipes for deployment of E4S on Perlmutter at NERSC using system compilers, runtime systems (MPI) and SLURM aware MPI (mvapich2) and vendor specific libraries.
- Validate deployment of packages on Perlmutter.
- Coordinate transfer of Spack recipes to the HI team (Shahzeb Siddiqui) for deployment and for GitLab Buildtest CI testing.
- **Perlmutter** module use `/global/cfs/cdirs/m3896/shared/modulefiles`
 - mvapich2/3.0a
 - PrgEnv-gnu
 - NOTE: `/global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/[mvapich2-3.0a,PrgEnv-gnu]/` has `spack.yaml` file for the builds.
 - `./start-spack.sh`
 - `./module-use.sh`; module avail;

Using E4S 22.05 on Perlmutter: Update for Slingshot 11

Using bare-metal installation using MPI with support for SLURM and Slingshot 11 network adapter:

```
module use /global/cfs/cdirs/m3896/shared/modulefiles
```

```
> module avail e4s
```

```
/global/cfs/cdirs/m3896/shared/modulefiles
```

```
e4s/22.05/mvapich2-3.0a    e4s/22.05/PrgEnv-gnu (D)
```

```
> module load e4s/22.05/mvapich2-3.0a
```

```
> which mpicc
```

```
/global/cfs/cdirs/m3896/shared/opt/mvapich2/mvapich2-3.0a/install-slurm/bin/mpicc
```

- GPU (GDR), SLURM, and Slingshot aware MPI

E4S 22.05 on Perlmutter using Slingshot 11 and SLURM with MPI

```
sameer@perlmutter:login24:~> module avail
```

```
----- /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a-slurm/spack/share/spack/lmod/cray-sles15-x86_64/mvapich2/3.0a-es35auw/Core -----
adios/1.13.1                fortrilinos/2.0.0                nccmp/1.9.0.1                    py-warpx/22.05-dims3
adios2/2.8.0-cuda80         globalarrays/5.8                 nco/5.0.1                        py-warpx/22.05-dimsRZ            (D)
adios2/2.8.0                (D) hdf5/1.10.7                   omega-h/9.34.1                   scr/3.0rc2
amrex/22.05                 heffte/2.2.0-cuda80             openpmd-api/0.14.4               slate/2021.05.02-cuda80-openmp
arborx/1.2                  heffte/2.2.0                    (D) papyrus/1.0.2                   slate/2021.05.02-openmp         (D)
axom/0.6.1-openmp          hpx/1.7.1-cuda80                parsec/3.0.2012                  slepc/3.17.1-cuda80
butterflypack/2.1.1        hpx/1.7.1                       (D) petsc/3.17.1-cuda80            slepc/3.17.1                    (D)
cabana/0.4.0               hypre/2.24.0                    petsc/3.17.1                    (D) strumpack/6.3.1-openmp
caliper/2.7.0-cuda80       kokkos-kernels/3.6.00-cuda80    precice/2.4.0                   sundials/6.2.0
caliper/2.7.0              (D) lammps/20220107-openmp          pumi/2.2.7                      tasmanian/7.7-openmp
darshan-runtime/3.3.1      libquo/1.3.1                    py-cinemasci/1.7.0              tau/2.31.1-cuda
datatransferkit/3.1-rc3    mercury/2.1.0                   py-libensemble/0.9.1            veloc/1.5
dyninst/12.1.0-openmp     metall/0.20                      py-petsc4py/3.17.1
faodel/1.2108.1           mfem/4.4.0                      py-warpx/22.05-dims2

----- /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a-slurm/spack/share/spack/lmod/cray-sles15-x86_64/openmpi/4.1.3-gw3a4bv/Core -----
gptune/3.0.0

----- /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a-slurm/spack/share/spack/lmod/cray-sles15-x86_64/Core -----
aml/0.1.0                   flux-core/0.38.0-cuda            legion/21.03.0-cuda80-cuda       plasma/21.8.29
archer/2.0.0               flux-core/0.38.0                (D) legion/21.03.0                 (D) py-jupyterhub/1.4.1
argobots/1.1               gasnet/2022.3.0                 magma/2.6.2-cuda80              qthreads/1.16
bolt/2.0                   ginkgo/1.4.0-cuda80-openmp      mpark-variant/1.4.0            raja/0.14.0-cuda80-openmp
chai/2.4.0                 ginkgo/1.4.0-openmp            (D) mvapich2/3.0a                  (D) superlu/5.3.0
charliecloud/0.26         gmp/6.2.1                       nrm/0.1.0                      swig/4.0.2-fortran
cmake/3.23.1              (D) gotcha/1.0.3                   nvhpc/22.3                      umap/2.1.0
darshan-util/3.3.1        kokkos-kernels/3.6.00-openmp (D) papi/6.0.0.1-cuda              zfp/0.5.5-cuda80
flit/2.1.0                kokkos/3.6.00-openmp            pdt/3.25.1
```


E4S 22.05 on Perlmutter using Slingshot 11 and SLURM with MPI

```
1: adios2 /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/adios2-2.8.0-kif4mquqyt1h4cybngifuux4fn3ivrted
2: aml /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/aml-0.1.0-5gd1j3ickdtb27qq6p2kopfpdioxm3t
3: amrex /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/amrex-22.05-ft3rksivlgipqauadvsh7gxuis4izq6m
4: arborx /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/arborx-1.2-tc4i6d3k6piplycwmt6shbq2wba4tbp
5: archer /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/archer-2.0.0-pa33i3csxzhlsd5t5nfcw64taxxrw7tx
6: argobots /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/argobots-1.1-nsmph2wbkrus4zx4jemebzhabx7qgr7y
7: axom /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/axom-0.6.1-gdjebwss54lr2capdigtrhh5zt6xd4u3
8: bolt /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/bolt-2.0-7hf4fziabmplaj7hryhps5cozunhyv
9: butterflypack /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/butterflypack-2.1.1-ooghq5wo5xszwmojow4g74rscnzwm5g
10: cabana /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/cabana-0.4.0-l2bj6kvhvud3xabnrv3p272oqq2b65v
11: caliper /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/caliper-2.7.0-svgn26f3u7qha5626zefy2mbrkkpis
12: chai /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/chai-2.4.0-w6sv4m7r4r2hxawg63yrw5j55aikxqxx
13: charliecloud /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/charliecloud-0.26-czgnnskv4k7rjfcjxv3ndy62lwk44skb
14: conduit /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/conduit-0.8.3-wkjkgnso3xztj63gg3heb3kp72btef
15: darshan-runtime /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/darshan-runtime-3.3.1-44lbnty4ftucbf7gowla26ztvdkovxvt
16: datatransferkit /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/datatransferkit-3.1-rc3-ivroc2m2xowtjvtyqoj5a5rk6o6tuec7
17: dyninst /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/dyninst-12.1.0-wickbpnlxl6iztkpnnigte4jtiiych
18: faodel /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/faodel-1.2108.1-isf6laqpcman3qr73lk64d5jaacngw3j
19: flit /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/flit-2.1.0-bhhseffdpfuewy53ztrrrrv5k3vsnl2
20: fortilinos /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/fortilinos-2.0.0-zlzmeycesulqwidlgwm2juplygs4kg
21: gasnet /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/gasnet-2022.3.0-bwmz3brqu4oqcttgs6ibkeztxyqtxjm
22: ginkgo /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/ginkgo-1.4.0-qvk5kj03gpqzlsompq27dobj3irjtd
23: globalarrays /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/globalarrays-5.8-rhohqdk3vg3icaoxtn6q46wia3z13bwp
24: gotcha /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/gotcha-1.0.3-s2xkdnmdusbrxwuhssqvgrcsh7rnhucn
25: gptune /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/gptune-3.0.0-k4q6zkfhkctseol46lvbhek54ulwgrw6
26: hdf5 /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/hdf5-1.12.2-bubavn15ec5lmfxd3ck3g4jtjym7fsk
27: heffte /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/heffte-2.2.0-wgagrclzssnki6aqtmcrcpqr2jvktj1
28: hpx /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/hpx-1.7.1-xuw726mdztobnu7api6jowdhgrc6zgz4
29: hypre /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/hypre-2.24.0-2okdvy7gxn1htwnvum2uvo3ntjmwhr
30: kokkos /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/kokkos-3.6.00-7eud56psz6e63twkwkoi2722f7n645vl
31: kokkos-kernels /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/kokkos-kernels-3.6.00-lcqcx55m2chvnyizpfboscsivhialepe
32: lammps /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/lammps-20220107-uk7x4i2eio4yvgwk5e4rxws5coerrvpz
33: legion /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/legion-21.03.0-53f3b6ytkfwl5fnux5y3uka3bl5cshr
34: libquo /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/libquo-1.3.1-5ju66szpfrwprkdb6o2lwhhkitrnwy5v
35: magma /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/magma-2.6.2-zwuh6mm62fc5oe6ypvkmgajbizz4hkzq
36: mercury /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/mercury-2.1.0-leykx65oexkkj6xh4fnt5glmqz7tcho
37: metall /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/metall-0.20-ncgmfczomrownqbgxvinm4tz5exdfa7s
38: mfem /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/mfem-4.4.0-iyvynznmxdoxacwoynhfz5ru2clxvwe
```


E4S 22.05 on Perlmutter using Slingshot 11 and SLURM with MPI

```
39: mpark-variant /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/mpark-variant-1.4.0-uvr4bft4rni7i254ctevurkikuv36z6x
40: nccmp /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/nccmp-1.9.0.1-pwjdebjxx7bk4glw573b4lekjfybuk5g
41: nco /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/nco-5.0.1-dtzaouk2bid2kqyijzqodu773x75sqvj
42: netlib-scalapack /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/netlib-scalapack-2.2.0-dhiu327cLn5fqL3djmya2q56sudyuyve
43: nrm /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/nrm-0.1.0-7dphpnstxxwvtvqjfqtn2vm25syq5ok
44: omega-h /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/omega-h-9.34.1-mpoe4zlgqnls7hpavj6quk62luzom5lw
45: openmpi /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/openmpi-4.1.3-gw3a4bvon2tyeg55baui7pvedk45c42
46: openpmd-api /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/openpmd-api-0.14.4-dx3hlgzye2mdfuvlfouvjwggkhkdzodgn
47: papi /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/papi-6.0.0.1-o5pxe7ejjzala2y5bwreiv6utoldk4mz
48: papyrus /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/papyrus-1.0.2-twr7purknxy6ympux6xdqnfmlau5l5rq
49: parsec /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/parsec-3.0.2012-vuxyi7v3czbng3vicfoyd4uj5s53he6n
50: pdt /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/pdt-3.25.1-4wzbsadvu6upir6eowsqbymg2op3a5j
51: petsc /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/petsc-3.17.1-v5gxr3udlpadu6b24s5mdf73xfmynw
52: plasma /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/plasma-21.8.29-6wzczv2jqnn23s7gc2ujfxq3yvzy4ckb
53: precice /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/precice-2.4.0-v7wscgidow3wlmn4chqgxo4kgjdhrqn
54: pumi /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/pumi-2.2.7-ff2gzmwq5b4l7uvtfxcqechbdfbf2edf
55: py-cinemasci /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/py-cinemasci-1.7.0-j7sbb2inxr5piawm2wy4uhb4jfrbesf
56: py-jupyterhub /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/py-jupyterhub-1.4.1-jsyxh242wzampidb5r355lx7bd4tixwb
57: py-libensemble /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/py-libensemble-0.9.1-ppigxh7jxsypypqilgt2vje4m3x3zy
58: qthreads /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/qthreads-1.16-s32g45lb5o62o7fmlkcyb4rrzvp6pug
59: raja /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/raja-0.14.0-ztcuu26vls3eibwdi6pfxw22qryfluki
60: scr /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/scr-3.0rc2-s3cjkoco7bok3bqz44sjt54qwikzh7v
61: slate /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/slate-2021.05.02-wkdnnguku4cicegrntu4pu4p5j5u7o3b5
62: slepc /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/slepc-3.17.1-t5dplaiot4kzutfmoegqpnka5voxw2n
63: strumpack /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/strumpack-6.3.1-vdjhqejektmzxu3kr2dnpj7anc32om6
64: sundials /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/sundials-6.2.0-dn7ff7ianhsyvu7g2ybegqbfeapipteg
65: superlu-dist /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/superlu-dist-7.2.0-h2asqfgihip3kws2clrfz3yzkzqnv5p
66: swig /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/swig-4.0.2-fortran-orersnc6ghyazliftwa6qvk2lhttpcxe
67: sz /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/sz-2.1.12-dkedzkkzozqrrhlazcwruso67icas3nc
68: tasmanian /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/tasmanian-7.7-55rvccldbg53cwkprl2ybedxqvkvxf
69: tau /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/tau-2.31.1-x75mktmyggs6ew5mqs7em4mvaauivgq3
70: trilinos /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/trilinos-13.0.1-yft4mfqzoyqaulh3mqbmc2jcmjswrpw
71: umap /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/umap-2.1.0-5ryuhm3tefsqtfiv3dayyegjexob2d
72: umpire /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/umpire-6.0.0-4wkonl77m7w53j554ak7juwxu26fbhrv
73: veloc /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/veloc-1.5-3zk6uqg36fu7ctmqnrroof2bnykz3mr
74: zfp /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/zfp-0.5.5-jha3y22e7gajahbmt6qfwlq3fwvtie3
```

Using E4S 22.05 on Perlmutter

Using bare-metal installation using Cray mpich with PrgEnv-gnu:

```
module use /global/cfs/cdirs/m3896/shared/modulefiles
```

```
> module avail e4s
```

```
----- /global/cfs/cdirs/m3896/shared/modulefiles -----
```

```
e4s/22.05/mvapich2-3.0a    e4s/22.05/PrgEnv-gnu
```

```
> module load e4s/22.05/PrgEnv-gnu
```

```
> module list
```

- GPU (GDR), SLURM, and Slingshot aware MPI

E4S 22.05 on Perlmutter using PrgEnv-gnu

```
sameer@perlmutter:login37:~> module avail e4s  
  
----- /global/common/software/ner/sc/pm-2022.05.0/extra_modulefiles -----  
e4s/spack-develop e4s/21.11-lmod e4s/21.11-tcl e4s/22.05 (L,D) spack/e4s-22.02 (D)
```

Where:

L: Module is loaded
D: Default Module

Use "module spider" to find all possible modules and extensions.
Use "module keyword key1 key2 ..." to search for all possible modules matching any of the "keys".

```
sameer@perlmutter:login37:~> module load e4s/22.05  
sameer@perlmutter:login37:~> which spack  
/global/common/software/spackecp/perlmutter/e4s-22.05/spack/bin/spack  
sameer@perlmutter:login37:~> spack find | more  
==> In environment e4s  
==> Root specs  
-- no arch / cce@13.0.2 -----  
adios2@2.8.0%cce@13.0.2  
hdf5@1.10.7%cce@13.0.2 +fortran+hl+shared  
hypre@2.24.0%cce@13.0.2  
kokkos@3.6.0%cce@13.0.2 +openmp  
kokkos-kernels@3.6.0%cce@13.0.2 +openmp  
petsc@3.17.1%cce@13.0.2 ~strumpack  
slepc@3.17.1%cce@13.0.2  
sundials@6.2.0%cce@13.0.2  
superlu@5.3.0%cce@13.0.2  
superlu-dist@7.2.0%cce@13.0.2  
  
-- no arch / gcc@11.2.0 -----  
adios2@2.8.0%gcc@11.2.0  
adios2@2.8.0%gcc@11.2.0 +cuda cuda_arch=80  
amrex@22.05%gcc@11.2.0  
butterflypack@2.1.1%gcc@11.2.0  
cdo%gcc@11.2.0  
conduit@0.8.3%gcc@11.2.0  
dyninst@12.1.0%gcc@11.2.0  
fortrilinos@2.0.0%gcc@11.2.0  
gasnet@2022.3.0%gcc@11.2.0  
gnuplot@5.4.3%gcc@11.2.0 +X  
grads%gcc@11.2.0  
gromacs@2021.5%gcc@11.2.0  
gsl@2.7%gcc@11.2.0  
hdf5@1.10.7%gcc@11.2.0 +fortran+hl+shared  
heffte@2.2.0%gcc@11.2.0 +fftw  
hpctoolkit@2022.04.15%gcc@11.2.0
```


Perlmutter @ NERSC: E4S 22.05 with SLURM and gcc@11.2.0

```
1: adios2 /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/adios2-2.8.0-kif4mquqyt1h4cybngifux4fn3ivrt
2: aml /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/aml-0.1.0-5gd1j3ickdtb27qq6p2kopfpdoxmui3t
3: amrex /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/amrex-22.05-ft3rksivlgipqauadvsh7gxuis4izq6m
4: arborx /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/arborx-1.2-tc4i6d3k6piplycwtmy6shbq2wba4tbp
5: archer /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/archer-2.0.0-pa33i3csxzhlsd5t5nfcw64taxxr77x
6: argobots /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/argobots-1.1-nsmph2wbkruz4zx4jemebzhabx7qgr7y
7: axom /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/axom-0.6.1-gdjebwss54lr2capdigtrhh5zt6xd4u3
8: bolt /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/bolt-2.0-7hf4fziabmplaj7hryhps5cozunhyv
9: butterflypack /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/butterflypack-2.1.1-ooghq5wo5xszwmojow4g74rscnzwmgs
10: cabana /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/cabana-0.4.0-l2bj6kvhvudx3abnr3p272oqq2b65v
11: caliper /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/caliper-2.7.0-svgn26f3u7qha5626zefy2mbrkkpis
12: chai /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/chai-2.4.0-w6sv4m7r4r2hxawg63yrw5j55aikxqxx
13: charliecloud /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/charliecloud-0.26-czgnnskv4k7rjfcjxv3ndy62lwk44skb
14: conduit /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/conduit-0.8.3-wkjkgso3xztj63gg3heby3kp72btef
15: darshan-runtime /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/darshan-runtime-3.3.1-44lbnty4ftucbf7gowla26ztvdkovxvt
16: datatransferkit /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/datatransferkit-3.1-rc3-ivroc2m2xowtjvtyqoj5a5rk6o6tuec7
17: dyninst /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/dyninst-12.1.0-wickbpnlxl6iztkpnnigte4jtiiych
18: faodel /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/faodel-1.2108.1-isf6laqpcman3qr73lk64d5jaacngw3j
19: flit /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/flit-2.1.0-bhhseffdpfuewy53ztrrrvr5k3vsnl2
20: fortilinos /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/fortilinos-2.0.0-zlzmeycesulqwidlgwm2juplygs4kg
21: gasnet /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/gasnet-2022.3.0-bwmz3brqu4oqcttgs6ibkeztxyqtxjm
22: ginkgo /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/ginkgo-1.4.0-qvk5kj03gpqzlsompq27ddb3irjtd
23: globalarrays /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/globalarrays-5.8-rhohqdk3vg3icaoxtn6q46wia3z13bwp
24: gotcha /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/gotcha-1.0.3-s2xkdnmdusbrxwuhssqvgrcsh7rnhucn
25: gptune /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/gptune-3.0.0-k4q6zkfhkctseol46lvbhek54ulwgrw6
26: hdf5 /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/hdf5-1.12.2-bubavn15ec5lmfxd3ck3g4jtjym7fsk
27: heffte /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/heffte-2.2.0-wgagrclzssnki6aqtmcrcpqr2jvkutjl
28: hpx /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/hpx-1.7.1-xuw726mdztobnu7api6jowdhgrc6zgz4
29: hypre /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/hypre-2.24.0-2okdvy7gxn1htwnvum2uvo3ntjmwhr
30: kokkos /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/kokkos-3.6.00-7eud56psz6e63wkwkoi2722f7n645vl
31: kokkos-kernels /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/kokkos-kernels-3.6.00-lcqcx55m2chvnyizpfboscsivhialepe
32: lammps /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/lammps-20220107-uk7x4i2eio4yvgwk5e4rxws5coerrvpz
33: legion /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/legion-21.03.0-53f3b6ytkfwl5fnux5y23uka3bl5cshr
34: libquo /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/libquo-1.3.1-5ju66szpfrwprkdb6o2lwhhkitrnwy5v
35: magma /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/magma-2.6.2-zwuh6mm62fc5oe6ypvkmgaibizz4hkzq
36: mercury /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/mercury-2.1.0-leykx65oexkkj6xh4fnt5glmqz7tcho
37: metall /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/metall-0.20-ncgmfczomrownqbgxvinm4tz5exdfa7s
38: mfem /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/mfem-4.4.0-iyvynznmxdoxacwoynhfbz5ru2clxvwe
```


Perlmutter @ NERSC: E4S 22.05 with SLURM and gcc@11.2.0

```
39: mpark-variant /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/mpark-variant-1.4.0-uvr4bft4rni7i254ctevurkikuv36z6x
40: nccmp /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/nccmp-1.9.0.1-pwjdebjxx7bk4glw573b4lekjfybuk5g
41: nco /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/nco-5.0.1-dtzaouk2bid2kqyijzqodu773x75sqvj
42: netlib-scalapack /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/netlib-scalapack-2.2.0-dhiu327cLn5fql3djmya2q56sudyuyve
43: nrm /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/nrm-0.1.0-7dphpnstxxwvtvqjfqtn2vm25syq5ok
44: omega-h /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/omega-h-9.34.1-mpoe4zlgqnls7hpavj6quk62luzom5lw
45: openmpi /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/openmpi-4.1.3-gw3a4bvon2tyeg55baui7pvedk45c42
46: openpmd-api /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/openpmd-api-0.14.4-dx3hlgzye2mdfuvlfouvjwggkhdzodgn
47: papi /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/papi-6.0.0.1-o5pxe7ejjzala2y5bwreiv6utoldk4mz
48: papyrus /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/papyrus-1.0.2-twr7purknxy6ympux6xdqnfmlau5l5rq
49: parsec /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/parsec-3.0.2012-vuxyi7v3czbng3vicfoyd4uj5s53he6n
50: pdt /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/pdt-3.25.1-4wzbsadvu6upir6eowsqbymg2op3a5j
51: petsc /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/petsc-3.17.1-v5gxr3udlpadu6b24sy5mdf73xfmynw
52: plasma /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/plasma-21.8.29-6wzczv2jqnn23s7gc2ujfxq3yvzy4ckb
53: precice /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/precice-2.4.0-v7wscgidow3wlmn4chqgxiow4kgjdhrqn
54: pumi /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/pumi-2.2.7-ff2gzmwq5b4l7uvtfxcqechbdfbf2edf
55: py-cinemasci /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/py-cinemasci-1.7.0-j7sbb2inxr5piawm2wy4uhb4jfrbesf
56: py-jupyterhub /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/py-jupyterhub-1.4.1-jsyxh242wzampidb5r355lx7bd4tixwb
57: py-libensemble /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/py-libensemble-0.9.1-ppigxh7jxsypypqilgt2vje4m3x3zy
58: qthreads /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/qthreads-1.16-s32g45lb5o62o7fmlkcyb4rrzvp6pug
59: raja /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/raja-0.14.0-ztcuu26vls3eibwidi6pfxw22qryfluki
60: scr /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/scr-3.0rc2-s3cjkoco7bok3bqz44sjt54quwikzh7v
61: slate /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/slate-2021.05.02-wkdnnguku4cicegrntu4pu4p5j5u7o3b5
62: slepc /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/slepc-3.17.1-t5dplaiot4kzutfmoegqpnka5voxw2n
63: strumpack /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/strumpack-6.3.1-vdjhqejektmzxu3kr2dnpj7anc32om6
64: sundials /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/sundials-6.2.0-dn7ff7ianhsyvu7g2ybegqbfeapipteg
65: superlu-dist /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/superlu-dist-7.2.0-h2asqfgihip3kws2clrfz3yzkzqnv5p
66: swig /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/swig-4.0.2-fortran-orersnc6ghyazliftwa6qvk2lhttpcxe
67: sz /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/sz-2.1.12-dkedzkkzozqqrhlazcwrusoa67icas3nc
68: tasmanian /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/tasmanian-7.7-55rvccldbg53cwkprl2ybedxqvkvxf
69: tau /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/tau-2.31.1-x75mktmygqs6ew5mqs7em4mvaauivgq3
70: trilinos /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/trilinos-13.0.1-yft4mfqzoyqaulh3mqbmc2jcmjswrpw
71: umap /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/umap-2.1.0-5ryuhm3tefsqtfiv3dayyegjexob2d
72: umpire /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/umpire-6.0.0-4wkonl77m7w53j554ak7juwxu26fbhrv
73: veloc /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/veloc-1.5-3zk6uqg36fu7ctmqnrroof2bnykz3mr
74: zfp /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/zfp-0.5.5-jha3y22e7gajahbmt6qfwlq3fwvtie3
```


Perlmutter @ NERSC: E4S 22.05 with PrgEnv-gnu

```
1: adios2 /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/adios2-2.8.0-ebqgj4m7gva7iiulnloq2qfq2zj75wot
2: aml /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/aml-0.1.0-5gdlj3ickdtb27qq6p2kopfpdouxm3t
3: amrex /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/amrex-22.05-rkmj3qh35wjczpsggz2kmiks5zvliooj
4: arborx /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/arborx-1.2-dzq55sq43ukm47m6tmqpwfjt5ccdp37
5: archer /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/archer-2.0.0-pa33i3csxzhlsd5t5nfcw64tksrxw7tx
6: argobots /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/argobots-1.1-nsmph2wbkrs4zx4jemebzhabx7qgr7y
7: axom /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/axom-0.6.1-arx3rdkr6dcwtntmbzvuyqej3363qpm
8: bolt /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/bolt-2.0-7hf4fziabmplaj7hryhps5cozunhymv
9: butterflypack /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/butterflypack-2.1.1-n5jtjakqydw43iw5eb44qber623nmx3
10: cabana /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/cabana-0.4.0-ywmbdzwhmfsq4ozmaneglmhr5q6ap5v3
11: caliper /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/caliper-2.7.0-tenxvf32vmze54krfcuo5onpploexkdo
12: chai /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/chai-2.4.0-aclkr5ozpze3utmoaehmw64tksrxw7tx
13: charliecloud /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/charliecloud-0.26-czgnnsvk4k7rjfcjxv3ndy62lwk44skb
14: conduit /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/conduit-0.8.3-dinrfzrgynaiodrske75dv3fdo7oyvno
15: darshan-runtime /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/darshan-runtime-3.3.1-imunxqtyb2b33h6ragdwj2wpcwtowvcp
16: datatransferkit /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/datatransferkit-3.1-rc3-oom6wpuwop4fmuhc7gdwhtojzihu6f4
17: dyninst /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/dyninst-12.1.0-7cz2lmh7lsh27llesnxelehs4xb4ji2l
18: faodel /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/faodel-1.2108.1-e4gshfews4qmgec5vwkqv3tkfsmvfti6
19: flecsi /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/flecsi-1.4.2-mp3xmyaqwa5yjerhem77n2z7rsesjio
20: flit /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/flit-2.1.0-bhhseffdpfpuewy53ztrrrqv5k3vsnl2
21: flux-sched /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/flux-sched-0.22.0-fvp6nkzgaaxgh5ticecxegfa5pc2jou
22: fortrilinos /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/fortrilinos-2.0.0-i4onp4upkkvd3rojcioueqs2crttlqa
23: gasnet /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/gasnet-2022.3.0-bwmz3brqu4oqctts6ibkeztmxyqtxjm
24: ginkgo /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/ginkgo-1.4.0-qvk5kjo3gpqzxlsompq27ddbjd3irjtd
25: globalarrays /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/globalarrays-5.8-7fcamxiwkukxhmr4zuhm7dfdgnwpp2xj
26: gotcha /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/gotcha-1.0.3-s2xkdnmdusbrxwuhssqvgrcsh7rnhucn
27: gptune /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/gptune-3.0.0-k4q6zkfhkctseol46lvbhek54ulwgrw6
28: hdf5 /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/hdf5-1.12.2-nhriei2p4726tu72qalywexiza7hi6jw
29: heffte /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/heffte-2.2.0-xrarvwygout4cm4ydp37swbvxvwn41
30: hpctoolkit /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/hpctoolkit-2022.04.15-ixt7dgumm32e3zuxgbztvisgho6z2h5f
31: hpx /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/hpx-1.7.1-cdmjvsvgg26p72tb3kbcktlag4a66kmw
32: hypre /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/hypre-2.24.0-loubbk3bpbk6lnz53g6setwmx4pqsyx6
33: kokkos /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/kokkos-3.6.00-yq47xesrwau5hkvizotendpdc7rnhucn
34: kokkos-kernels /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/kokkos-kernels-3.6.00-vxyxliujcemrwbkg22jhm3kohbpbz6bxx
35: lammps /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/lammps-20220107-dm2c3slvgxprezhazhdm5swe64yelxh
36: legion /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/legion-21.03.0-53f3b6ytkfw15fnux5y3uka3b15cshr
37: libquo /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/libquo-1.3.1-fl2s7e6im2fhajouta5xxkkp7w2pek6i
38: magma /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/magma-2.6.2-zwuh6mm62fc50e6ypvkmgajbizz4hkzq
39: mercury /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/mercury-2.1.0-nhzjaqz556sldnrog2dag5vdpqc627u
40: metall /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/metall-0.20-skcxyx6dq5r61fypnsywmxg5v7ed6h73
41: mfem /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/mfem-4.4.0-lxsd7oqkkfkgqyglcvfrq235d6ain7yn
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Perlmutter @ NERSC: E4S 22.05 with PrgEnv-gnu

```
42: mpark-variant /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/mpark-variant-1.4.0-uvr4bft4rni7i254ctevurkikuv36z6x
43: mpifileutils /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/mpifileutils-0.11.1-zs6fdx5wxdpuoilaajtj47rrtqckj2z4
44: nccmp /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/nccmp-1.9.0.1-mfryg4t3s46zrshzvu4l27gqeabhlmq
45: nco /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/nco-5.0.1-tk7gnyokee7zip6kp3vr46fx2vawak36
46: netlib-scalapack /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/netlib-scalapack-2.2.0-dhiu327c1n5fq13djmya2q56sudyuyve
47: nrm /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/nrm-0.1.0-7dphpnstxxwvtvqjftne2vm25syq50k
48: omega-h /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/omega-h-9.34.1-bc76qpjlaqn4ttohy6fgav5u7v2zrqfy
49: openmpi /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/openmpi-4.1.3-gw3a4bvon2tyeg55baui7pvedk45c42
50: openpmd-api /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/openpmd-api-0.14.4-m6ohwjdwzjsytqf4spkvk2ygmrlrx4ns
51: papi /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/papi-6.0.0.1-o5pxe7ejjzala2y5bwreiv6uto1dk4mz
52: papyrus /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/papyrus-1.0.2-ggjpndneiuvoizfwkiqlhedwjxje47w
53: parallel-netcdf /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/parallel-netcdf-1.12.2-zwbammyyjjbfunvurlbh3g7qvmq3mmkn
54: parsec /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/parsec-3.0.2012-xyu7xpkvn2c7hrx7vysha4da2cduwrgf
55: pdt /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/pdt-3.25.1-4wzbsadvu6upir6eowsqbymg2op3a5j
56: petsc /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/petsc-3.17.1-u7tsfkjnw3onz7fojsbywagkezuzyrss
57: phist /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/phist-1.9.5-lq76cw473chjmuvevsjnhwfdmldcdwdq
58: plasma /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/plasma-21.8.29-6wzczv2jqnn23s7gc2ujfxq3yvzy4ckb
59: precice /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/precice-2.4.0-v2gv4iluyrsbuzhpq5b5446puffbpel6
60: pumi /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/pumi-2.2.7-wr6bm21fpybzxw3sufv3m4irdbjjevt7
61: py-cinemasci /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/py-cinemasci-1.7.0-rucnpuzn73dvwxzcsld13vf2a2utqp
62: py-jupyterhub /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/py-jupyterhub-1.4.1-jsyxh242wzampidb5r3551x7bd4tixwb
63: py-libensemble /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/py-libensemble-0.9.1-c7orlmyeeivswieqv5ybtbdk3u
64: qthreads /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/qthreads-1.16-s32g451b5o62o7fmlkcyb4rrzvp6pug
65: raja /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/raja-0.14.0-ztcuu26vls3eibwdi6pfxw22qryfluki
66: scr /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/scr-3.0rc2-td5ivq6fxy44z1g7cziasvd7sog4efp
67: slate /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/slate-2021.05.02-3qu12vtqh24ixhwjg3xxznjluua6qa5r
68: slepc /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/slepc-3.17.1-mbijafs75iqzjaft6nj31bqcjz6aa5p
69: stc /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/stc-0.9.0-sm5urbkhheg4rxnqof4bjf4j4yzgdneoc
70: strumpack /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/strumpack-6.3.1-iapp37z5vat2tyejpv5zynflbhqhs2n
71: sundials /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/sundials-6.2.0-kn5wm4foklvkm6oj6d4riyt275ygi5ul
72: superlu-dist /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/superlu-dist-7.2.0-bsd63xtzha3klfkgm3wqk1blc4swkinu
73: swig /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/swig-4.0.2-fortran-orersnc6ghyaz1lftwa6qv2lhttpcxe
74: sz /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/sz-2.1.12-dkedzzkzoghrlazcwrusoa67icas3nc
75: tasmanian /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/tasmanian-1.7-vizyvcrrjtsqyd2epn6fjebkzjhtpbwp
76: tau /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/tau-2.31.1-icww2pa2es56isc4gzgjmcnj5tbehujj
77: trilinos /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/trilinos-13.0.1-rhk32i353nr3dyivvgf3y3g6kuhc4uk1r
78: umap /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/umap-2.1.0-5ryuhmh3tefsqtffiv3dayyegjexob2d
79: umpire /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/umpire-6.0.0-birc3ndlvj5ds6poer2djbreduxipxg
80: veloc /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/veloc-1.5-45ipct3s3i3htlbp6dg7sraipoz4pruh
81: zfp /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/PrgEnv-gnu/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/zfp-0.5.5-jha3y22e7gajahbmut6qfwl3fylvwie3
```

Container deployment at NERSC on Perlmutter

- Using Shifter container images for 22.05 (base and full featured)

- `shifterimg images | grep e4s | grep 22.05`

- `perlmutter docker READY cd20a7d2c5 2022-06-14T06:59:30 ecpe4s/e4s-base-cuda:22.05`

- `perlmutter docker READY 7832c93f11 2022-06-14T07:53:07 ecpe4s/e4s-cuda:22.05`

- `shifter --image=ecpe4s/e4s-cuda:22.05 /bin/bash --rcfile /etc/bashrc`

E4S 22.05 container deployment on Perlmutter using Shifter

```
sameer@perlmutter:login19:~> shifter --image=ecpe4s/e4s-base-cuda:22.05 /bin/bash --rcfile /etc/bashrc

Inactive Modules:
  1) PrgEnv-gnu          3) cray-libsci        5) craype             7) craype-x86-milan  9) libfabric          11) xpmem
  2) cray-dsmml         4) cray-mpich         6) craype-network-ofi 8) gcc               10) perftools-base
```

Lmod is automatically replacing "cray-mpich/8.1.15" with "mpich/4.0.2".

```
((base) sameer@login19:~$ cat /etc/os-release
NAME="Ubuntu"
VERSION="20.04.4 LTS (Focal Fossa)"
ID=ubuntu
ID_LIKE=debian
PRETTY_NAME="Ubuntu 20.04.4 LTS"
VERSION_ID="20.04"
HOME_URL="https://www.ubuntu.com/"
SUPPORT_URL="https://help.ubuntu.com/"
BUG_REPORT_URL="https://bugs.launchpad.net/ubuntu/"
PRIVACY_POLICY_URL="https://www.ubuntu.com/legal/terms-and-policies/privacy-policy"
VERSION_CODENAME=focal
UBUNTU_CODENAME=focal
```

```
((base) sameer@login19:~$ nvidia-smi
Tue Jun 14 07:23:04 2022

+-----+
| NVIDIA-SMI 470.103.01   Driver Version: 470.103.01   CUDA Version: 11.5   |
+-----+
| 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          | 00000000:03:00.0 Off |           0          |
| N/A   39C    P0     38W / 250W |  0MiB / 40536MiB |           0%    Default |
|                                           Disabled      |
+-----+-----+

+-----+
| Processes:
| GPU   GI    CI          PID    Type    Process name                        GPU Memory
|      ID    ID                                     |              Usage
+-----+-----+
| No running processes found
+-----+

```

```
((base) sameer@login19:~$ spack find
==> 21 installed packages
-- linux-ubuntu20.04-x86_64 / gcc@9.4.0 -----
cmake@3.23.1  libfabric@1.14.1  libxml2@2.9.13  lua-luafilesystem@1_8_0  ncurses@6.2  readline@8.1  xz@5.2.5
curl@7.83.0  libiconv@1.16  lmod@8.7.2  lua-luaposix@35.0  nvhpc@22.3  tcl@8.6.12  yaksa@0.2
hwloc@2.7.1  libpciaccess@0.16  lua@5.3.5  mpich@4.0.2  openssl@1.1.1o  unzip@6.0  zlib@1.2.12
((base) sameer@login19:~$ which mpicc
/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mpich-4.0.2-ssbmd2ccbzxkxk7fzr1lekupe23rokw2/bin/mpicc
```

- E4S containers
- Accessing A100 GPUs
- CUDA 11.5



E4S 22.05 packages built with support for A100 GPUs in a container

```
sameer@perlmutter:login19:~> shifterimg images | grep e4s | grep :22.05
perlmutter docker      READY   cd20a7d2c5   2022-06-14T06:59:30   ecpe4s/e4s-base-cuda:22.05
perlmutter docker      READY   7832c93f11   2022-06-14T07:53:07   ecpe4s/e4s-cuda:22.05
sameer@perlmutter:login19:~> shifter --image=ecpe4s/e4s-cuda:22.05 /bin/bash --rcfile /etc/bashrc
```

```
Inactive Modules:
  1) PrgEnv-gnu      3) cray-libsci     5) craype          7) craype-x86-milan  9) libfabric        11) xpmem
  2) cray-dsmml     4) cray-mpich      6) craype-network-ofi  8) gcc              10) perftools-base
```

Lmod is automatically replacing "cray-mpich/8.1.15" with "mpich/4.0.2".

```
(base) sameer@login19:~$ grep Ubuntu /etc/os-release
NAME="Ubuntu"
PRETTY_NAME="Ubuntu 20.04.4 LTS"
(base) sameer@login19:~$ nvidia-smi
Tue Jun 14 08:39:09 2022
```

NVIDIA-SMI 470.103.01 Driver Version: 470.103.01 CUDA Version: 11.5									
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:C3:00.0	Off					0
N/A	41C	P0	38W / 250W	0MiB / 40536MiB	0%	Default	Disabled		

```
Processes:
```

GPU	GI	CI	PID	Type	Process name	GPU Memory Usage
ID	ID					
No running processes found						

```
(base) sameer@login19:~$ which mpicc
/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mpich-4.0.2-ssbmd2ccbzxkxk7fzrlekupe23rokw2/bin/mpicc
```

```
(base) sameer@login19:~$ spack find +cuda cuda_arch=80
==> 27 installed packages
```

```
-- linux-ubuntu20.04-x86_64 / gcc@9.4.0 -----
adios2@2.8.0      camp@0.2.2      heffte@2.2.0   kokkos@3.6.00   magma@2.6.2     petsc@3.17.1   slepc@3.17.1   superlu-dist@7.2.0  umpire@6.0.0
arborx@1.2       chai@2.4.0      hpv@1.7.1      kokkos@3.6.00   mfem@4.4.0      raja@0.14.0    strumpack@6.3.1  tasmanian@7.7      vtk-m@1.7.1
caliper@2.7.0    ginkgo@1.4.0    hypre@2.24.0   kokkos-kernels@3.6.00  parsec@3.0.2012  slate@2021.05.02  sundials@6.2.0  trilinos@13.2.0    zfp@0.5.5
```

```
(base) sameer@login19:~$ 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.config.list_physical_devices('GPU')
[PhysicalDevice(name='/physical_device:GPU:0', device_type='GPU')]
>>>
(base) sameer@login19:~$ █
```

- AI/ML
- HPC

Running MPI applications on other systems

- Applications built with MPI in the E4S container can replace the MPI in the container with the system MPI!
- This allows fast inter-node communication using the native interconnect.
- Application and data are external to the E4S container.
- Programming models, compilers, runtime libraries, and tools are inside the container.
- We can replace MPI using the MPICH ABI and Wi4MPI compatibility layer.
- Goal: Build an MPI binary once and run it un-modified on all HPC Linux x86_64 clusters!

e4s-cl: A tool to simplify the launch of MPI jobs in E4S containers

- E4S containers support replacement of MPI libraries using MPICH ABI compatibility layer and Wi4MPI [CEA] for OpenMPI replacement.
- Applications binaries built using E4S can be launched with Singularity using MPI library substitution for efficient inter-node communications.
- e4s-cl is a new tool that simplifies the launch and MPI replacement.

```
- e4s-cl init --backend [docker|singularity|shifter] --image <file> --source <startup_cmds.sh>
- e4s-cl srun -n <N> <command>
```

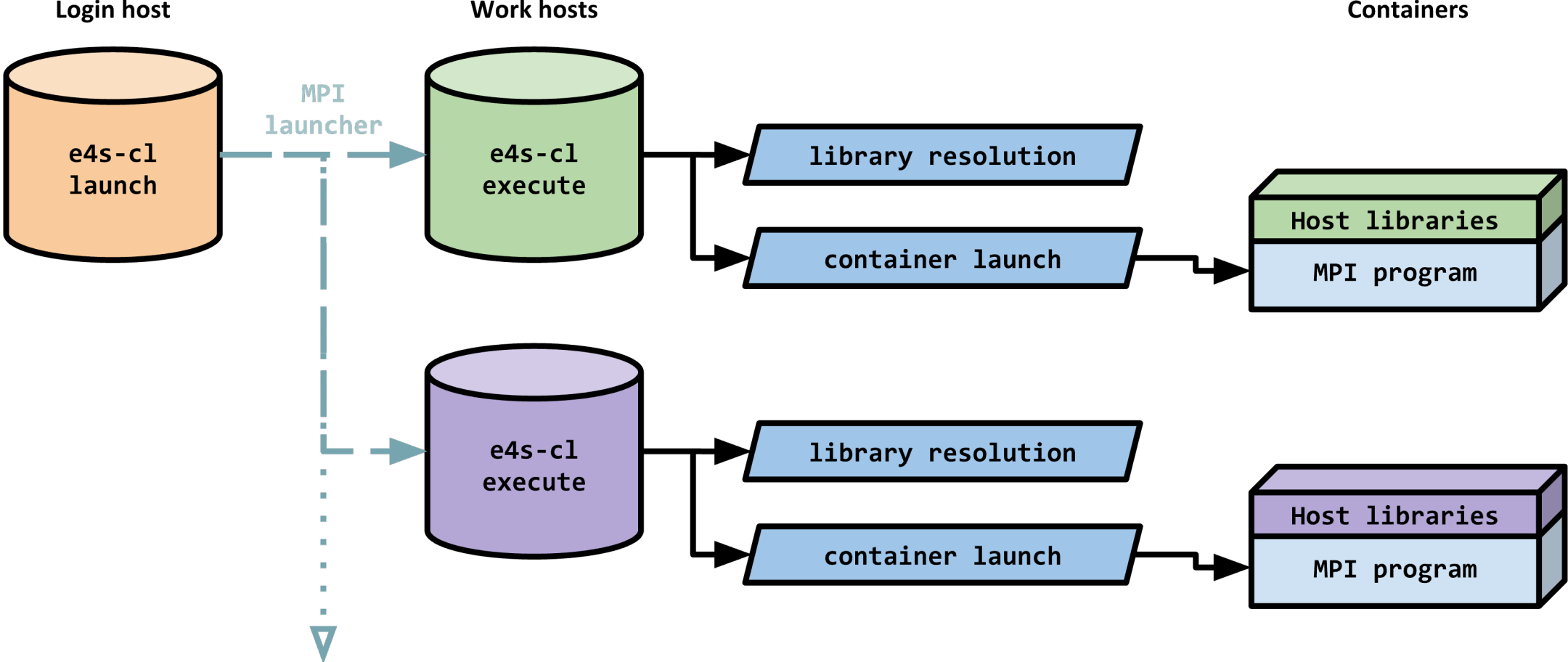
- Usage:

```
module load cray-mpich-abi
e4s-cl init --backend shifter --image --image=ecpe4s/e4s-cuda:22.05 --source ~/source.sh
cat ~/source.sh
  . /spack/share/spack/setup-env.sh
  spack load trilinos+cuda cuda_arch=80
e4s-cl srun -n 4 ./a.out
```

Running an e4s-cl example on Perlmutter: Zoltan from Trilinos

- Allocate two nodes using your account id and use your account id for the run_e4s-cl.sh file:
 - `wget https://e4s.io/tar/e4s_tests.tgz; tar xf e4s_tests.tgz ; cd e4s_tests; cat README`
 - `salloc --nodes 2 --qos interactive --time 01:00:00 --constraint gpu --gpus 4 --account=m3896_g`
 - `shifter --image=ecpe4s/e4s-cuda:22.05 -E /bin/bash --rcfile /etc/bashrc`
 - `cd Zoltan; cat README`
 - `./compile.sh`
 - `exit`
 - `./run_e4s-cl.sh`
 - `cat ./run_e4s-cl.sh`
- See other examples in e4s_tests

e4s-cl Container Launcher



Acknowledgment



“This research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of two U.S. Department of Energy organizations (Office of Science and the National Nuclear Security Administration) responsible for the planning and preparation of a capable exascale ecosystem, including software, applications, hardware, advanced system engineering, and early testbed platforms, in support of the nation’s exascale computing imperative.”

