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NERSC



- National Energy Research Scientific Computing Center (NERSC) is scientific computing facility as part of the <u>Office of Science</u> in the <u>U.S Department of Energy</u>
- At NERSC we support up to 8000+ users that span a wide range of disciplines including climate modeling, simulation of universe, high energy physics experiments, protein simulation, and many more.
- NERSC most recent supercomputer called <u>Perlmutter</u> is named after astrophysicist <u>Saul Perlmutter</u> for his Nobel Prize in Physics for discovering the rate of expansion of the universe









- <u>Perlmutter</u> is a HPE Cray Shasta platform composed of CPU-only and GPU accelerated nodes.
- The system will be delivered in two phases
- The system contains 1536 GPU accelerated nodes with NVIDIA A100 GPUs and 3072 CPU-only nodes powered with AMD EPYC Milan CPUs
- Perlmutter is currently ranked #7 on the <u>Top500 list</u> with a peak performance of <u>PFlop/s</u> 75 PFlop/s





Perlmutter - HPE Cray EX235n, AMD EPYC 7763 64C	761,856	70.87	93.75	2,589
2.45GHz, NVIDIA A100 SXM4 40 GB, Slingshot-10, HPE				
DOE/SC/LBNL/NERSC				
United States				





stack



We recently published a technical report <u>Software Deployment Process at NERSC: Deploying the Extreme-scale Scientific Software Stack (E4S) Using Spack at the National Energy Research Scientific Computing Center (NERSC)</u>

that outlines our software deployment process.

- We are working with MVAPICH2 team to enable MPI support for Perlmutter when building the spack stack.
- Currently we are building the spack stack with cray-mpich which works for building most of the stack, however some spack packages don't build hence we will try to build remainder of packages with mvapich2gdr

Office of Science

MPI Support

We are working with the <u>MVAPICH2</u> team from Ohio State University to experiment with **mvapich2** as an MPI provider for building the E4S stack on Perlmutter. The mvapich2-gdr is an optimized version of mvapich that takes advantage of GPU Direct RDMA technology to improve inter-node data movement on NVIDIA GPUs which is relevant for Perlmutter since we support NVIDIA A100 GPUs. Currently, we are using cray-mpich as our MPI provider which is available on our system but we have run into build errors with certain packages which expect mpi wrapper *mpicc* instead of cc. We plan on using cray-mpich as the MPI provider for building the stack and introduce **mvapich2** for building a subset of packages for future e4s release. The collaboration between the E4S and the NERSC teams has helped install MVAPICH2 and 87 packages with 575 total installed specs from E4S 22.02 as shown in the figures below. These packages use mvapich2-gdr configured with SLURM and CUDA 11.5 on Perlmutter. The total time for installation of these packages was less than one day! The E4S packages may be accessed using the module or spack commands as shown below.

ameer@perlmutter:login21:~> module use /global/common/software/spackecp/perlmutter/mvapich2/modulefile ameer@perlmutter:login21:~> module avail e4s/22.02

```
/global/common/software/spackecp/perlmutter/myapich2/modulefiles
   eds/22.02 (D)
   D: Default Module
 Use "module spider" to find all possible modules and extensions
      "module keyword keyl key2 ..." to search for all possible modules matching any of the "keys"
  ameergperlmutter:login21:~> module load e4s
Lood is automatically replacing "nvidia/21.11" with "occ/10.3.8"
Due to MODILEPATH changes, the following have been reloaded
  1) cray-mpich/8.1.13
 sameer@merlmutter:lonin21:se snack find
 > 575 installed packages
                                  heffte82.2.8
                                                                     nlohnann-ison@3.18.5
                                                                                                       py-jupyter-client07.0.6
                                                                                                                                           py-setuptools-scm06.3.7
                                 heffte32.2.8
hpctoolkits2822.81.1
                                                                     nrm00.1.8
numact102.8.14
                                                                                                       py-jupyter-client@7.8.6
                                                                                                                                           py-setuptools-scm-git-archive@1.1
                                                                                                        py-jupyter-core=4.
                                                                                                                                            py-six01.16.4
                                                                      nyhpce22.
                                                                                                       py-jupyter-packaging1120.
py-jupyter-packaging700.7
                                                                                                                                           py-sniffigel.2.0
                                   pctoolkit@2022.01.1
                                                                      orega-h@.34.
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 louisia
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                                                                      openblasce.3
openidk011.0
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py-jupyter-telemetry20.1.
                                                                                                                                            w_tables83.6
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                                  hylac#2
                                                                      opennoi01.
                                                                                                        py-jupyterlabml.2.
                                                                                                                                              -terminado
                                                                                                       py-jupyterlab-servere2.6.0
py-jupyterlab-widgetse1.0.
                                                                                                                                              -threadpoolctlm3.0.0
                                                                      opennp184
                                                                                                                                           nu-tonles
                                  hypres2.23.
                                                                      openped-apine.14.
                                                                                                        py-kiwisplyer@1.3.
                                                                                                                                             -tomlig1
 aroobots
 arpack-ng03.8.0
                                  hypres2.24.
hypres2.24.
                                                                      opensshed.
openssle1.
                                                                                                        py-lazy-object-proxy@1.4.3
py-lhsmdug1.1
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                                  incutoroto@2.
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 sutoconf-arch
                                  intel-tbb0
                                                                                                                                            py-traitlets
 automakem1.16.
                                  intel-xedo12.4
                                                                     pagmo202.18.0
                                                                                                       py-markupsafe=2.
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                                  jansson@2,13,1
                                                                      pap105.0.0.
                                                                                                        ov-matolotlibe3.5
                                                                                                                                           py-typing-extensions01.
                                                                                                        py-matplotlib@3.
                                                                                                                                            py-urllib381.26.0
                                  1500-C00-1
                                                                      papid5.0.8.
                                                                                                        py-matplotlib-inlines8.1.2
                                                                     papyrus@1.0.1
parallel-netcdf@1
 berkeley-db818.1.4
                                   (boroto)]
                                                                                                       py-mistune .
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                                  kin-apin2.
                                                                      naraview25.10.1
                                                                                                        ny-markad.e.
                                                                                                                                           no-warman22.4
                                  kokkos3.5.
                                                                      parmetise4.0.3
parsec@3.8.2012
                                                                                                                                           py-warpos22.02
py-warpos22.02
py-wcwidthe0.2
                                                                                                        y-mpi4py33.1
 blaspp@2021.04.03
                                                                                                        ov-mol4ov
blaspo@2821.84.81
                                  kokkosa)
                                                                      pereas. de
                                                                                                        ny-msonackill.
                                                                                                                                           py-websocket-client01.2.1
 blasppm2821.84.8
                                                                                                                                           py-wheelp0.37.
```

FIGURE 23. How to access e4s/22.02 stack built with myapich2-gdr



Perlmutter



 We have modulefiles for mvapich2 on shared filesystem, one must add the directory to MODULEPATH since we don't expose these modules to all users

* ~/ module use /global/cfs/cdirs/m3896/shared/modulefiles
* ~/ module av

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

mvapich2/3.0a





builds



- We have noticed a few spack packages fail to build with cray-mpich due to proper support with cray compilers.
- Some packages expect MPI wrappers such as mpicc but on Cray we expect to use cray wrappers cc, CC, ftn when invoking MPI programs

configure: error: Failed to find C MPI Wrapper. see https://cdash.spack.io/buildSummary.php?buildid=104940
- rempi@1.1.0

#- mpifileutils@0.11.1 ~xattr # failed to install libcircle Unable to find suitable MPI Compiler. Try setting MPICC.





Perlmutter



- MVAPICH2 3.0a supports SLURM and Slingshot 11 network interfaces on both CPU and GPU nodes of Perlmutter
- To use MVAPICH2:
 - module use /global/cfs/cdirs/m3896/shared/modulefiles
 - module load mvapich2/3.0a
 - Use mpicc, mpicxx, mpif90 as compilers
 - mpicc foo.c -o foo
 - \circ $\,$ Use srun to launch the binary
 - srun -n 4 ./foo





Building E4S on Perlmutter



- The Extreme-scale Scientific Software Stack (E4S) is installed on Perlmutter using the mvapich2/3.0a module.
- For more details regarding this deployment, please refer to E4S documentation page <u>https://e4s.readthedocs.io/en/latest/deployment.</u> <u>html#perlmutter</u>
 - module use /global/cfs/cdirs/m3896/shared/modulefiles
 - module avail e4s
 - e4s/22.05/mvapich2-3.0a ...
- **ENERGY** of Older load e4s/22.05/mvapich2-3.0a Science dule avail



MVAPICH2/3.0a



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 -----

.0.1 py-warpx/22.05-dims3
py-warpx/22.05-dimsRZ (D)
.34.1 scr/3.0rc2
pi/0.14.4 slate/2021.05.02-cuda80-openmp
.0.2 slate/2021.05.02-openmp (D)
0.2012 slepc/3.17.1-cuda80
7.1-cuda80 slepc/3.17.1 (D)
7.1 (D) strumpack/6.3.1-openmp
.4.0 sundials/6.2.0
7 tasmanian/7.7-openmp
sci/1.7.0 tau/2.31.1-cuda
emble/0.9.1 veloc/1.5
py/3.17.1
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

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		<pre>mpark-variant/1.4.0</pre>		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		





MVAPICH2



/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-kif4mquqvtlh4cybnqifuux4fn3ivrtd 1: adios2 2: aml /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/myapich2-3.0a/spack/opt/spack/crav-sles15-zen3/gcc-11.2.0/aml-0.1.0-5gdli3ickdtb27gg6p2kopfpdoxmui3t /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/qcc-11.2.0/amrex-22.05-ft3rksivlgipgauadvsh7axuis4iza6m 3: amrex 4: arborx /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/crav-sles15-zen3/gcc-11.2.0/arborx-1.2-tc4i6d3k6piplycwtmv6shbg2wba4tbp 5: archer /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/crav-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-nsmph2wbkrus4zx4jemebzhabx7ggr7y /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 7: axom 8: bolt /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/crav-sles15-zen3/gcc-11.2.0/bolt-2.0-7hf4fziabmplai7hrvhps5cozunhvmvv 9: butterflypack /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/crav-sles15-zen3/gcc-11.2.0/butterflvpack-2.1.1-ooghg5wo5xszwmojoew4g74rscnzwmsg 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-l2bj6kvhvuxd3xabnrv3p272ogq2b65v 11: caliper /qlobal/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/crav-sles15-zen3/acc-11.2.0/caliper-2.7.0-svgn26f3u7gha5626zeftyf2mbrkkpis /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/crav-sles15-zen3/gcc-11.2.0/chai-2.4.0-w6sv4m7r4r2hxawg63vrw5i55aikxggx 12: chai 13: 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/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-isf6lagpcman3gr73lk64d5jaacngw3j 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-bhhseffdpfpuewy53ztrrgrv5k3vsnl2 20: fortrilinos /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/fortrilinos-2.0.0-zlzgmevcesulgwzidlgwm2juplvgs4kg 21: gasnet /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/crav-sles15-zen3/acc-11.2.0/gasnet-2022.3.0-bwmz3brgu4ogcttgs6ibkeztmxvgtxim 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-gvk5kjo3gpgzxlsompg27ddbjd3irjtd 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-rhohgdk3vg3icaoxtn6g46wia3zl3bwp 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-s2xkdnmdusbrxwuhssavgrcsh7rnhucn 25: aptune /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/crav-sles15-zen3/gcc-11.2.0/gptune-3.0.0-k4g6zkfhkctseol46lvbhek54ulwgrw6 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-bubavnl5ec5lmfxd3ck3g4jtjtym7fsk 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-wgagrclzssnki6agtmcrpgsr2jvkutjl 28: hpx /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/crav-sles15-zen3/gcc-11.2.0/hpx-1.7.1-xuw726mdztobnu7api6jowdhgcr6zgz4 29: hypre 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(contd.)



39: mpark-variant /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/crav-sles15-zen3/gcc-11.2.0/mpark-variant-1.4.0-uvr4bft4rni7i254ctevurkikuv36z6x /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/crav-sles15-zen3/gcc-11.2.0/nccmp-1.9.0.1-pwidebixx7bk4glw573b4lekifybuk5g 40: nccmp /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/crav-sles15-zen3/gcc-11.2.0/nco-5.0.1-dtzaouk2bid2kgvijzgodu773x75sgvi 41: nco 42: netlib-scalapack /global/cfs/cdirs/m3896/shared/ParaTools/E4S/22.05/mvapich2-3.0a/spack/opt/spack/crav-sles15-zen3/gcc-11.2.0/netlib-scalapack-2.2.0-dhiu327cln5fgl3dimva2g56sudvuvve 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-0.1.0-7dphpnstxxwwtvaifatne2vm25sva5ok 44: omega-h 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MVAPICH2



- We have developed a test to run the OSU benchmark for the mvapich2 installation.
- Test are run via <u>buildtest</u>, an HPC testing framework that will automate build and execution of test

buildspecs:
<pre>mvapich2_mpi_omb_tests:</pre>
type: script
executor: perlmutter.slurm.debug
description: Run OSU microbenchmarks
tags: [gpu, mpi]
sbatch: ["-N 2", "-t 5" , "-G 4", "-C gpu", "-A m3503_g"]
run:
<pre>module use /global/cfs/cdirs/m3896/shared/modulefiles</pre>
module load mvapich2/3.0a
srun -n 2 osu_latency
srun -n 2 osu_bw
srun -n 2 osu bibw

 Test results are pushed to CDASH via buildtest

Test: myapich2 mpi or	mb tests (Passed)	# OSU MPI Bi-Directional Bandwidth Test v5.9		
Build: gpu (perlmutter)	on 2022-08-18 05:09:31	# Size	Bandwidth (MB/s)	
Labels: mpi, gpu		1	2.37	
compiler		2	4.80	
description	Run OSU microbenchmarks	4	9.65	
endtime	2022/08/17 22:10:32	8	19.13	
hostname	login27	16	38.54	
starttime	022/08/17 22:09:31	32	76.35	
user	e4s	64	154.04	
Return Code	0	128	306.16	
Test ID	4dcd3df7-1101-4943-b370-2d8c88c84c88	256	556.54	
build script	/oloba/c5k/cdim/m3503/buildtest/nuns/perfmutter check/2022-08-17/perfmutterslum debuu/mvapich2-omb/mvapich2-mpi omb tests/4dcd3df7/mvapich2 mpi omb tests build sh	512	1092.87	
buildenv	Aloha/cfs/cdir/m3503/buildtest/mus/perimiter_check/2022-08-17/perimitersium_debuu/mvanich2-omb/mvanich2_mpi omb_tests/ddcd3df7/build-envtxt	1024	2189.58	
command	nashonrnonrofileo nipefali myanich? mi omb tests built sh	2048	4386.47	
errfile	Anichal/ds/cr/im/m3830/hite/thest/mes/nedmitter_check/2020_08-17/nedmitter_slum dehuu/mvanich2-omh/mvanich2 mpi_omh_tests/ador/3017/mvanich2 mpi_omh_tests err	4096	8648.64	
executor		8192	15222.25	
id.	permanenter and the second s	16384	23030.97	
lognath	noouoon////ins/m3602/ci.data.dir/sixidin00/static/00185001/NERSC/Jniikitast.naren/huikitast/inmoinnen/huikitas	32768	28904.61	
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- NERSC will provide support for the vendor MPI (cray-mpich), on the contrary NERSC users will experiment with any MPI provider they have access to including OpenMPI, MVAPICH2, MPICH which can be troubling since we don't have proper support for any other MPI
- MVAPICH2-GDR is promising, considering it provides support with Slurm and Slingshot 11
- With sufficient testing, we can provide user with documentation on how to use MVAPICH2-GDR on Perlmutter
 - Performance comparison between cray-mpich and MVAPICH2-GDR
- MVAPICH2-GDR can provide user to experiment with spack build instead of being locked into cray-mpich, we have seen several spack packages fail to recognize MPI wrappers.



