nersc-spack-infrastructure

Shahzeb Siddiqui

Aug 03, 2022

CONTENTS

Welcome to NERSC Spack Infrastructure, this project contains the spack configuration for our spack stacks built for NERSC system such as Cori and Perlmutter. We leverage gitlab to automate spack deployments and project is located at https://software.nersc.gov/NERSC/spack-infrastructure. You must have a NERSC account in order to access our system and gitlab server.

There is a push mirror of this repo at https://github.com/NERSC/spack-infrastructure for public consumption.

CHAPTER

ONE

SPACK INFRASTRUCTURE

The spack infrastructure repository contains spack configuration in the form of `spack.yaml` required to build spack stacks on Cori and Perlmutter system. We leverage gitlab to automate software stack deployment which is configured using the .gitlab-ci.yml file. The documentation is available at https://nersc-spack-infrastructure.rtfd.io/

1.1 Spack Configuration

The spack configuration can be found in spack-configs directory with subdirectory for each deployment. Each pipeline can be run if one sets the variable `PIPELINE_NAME` to a unique value in order to run a pipeline. You can check the .gitlab-ci.yml for the gitlab configuration. The pipeline can be run via web interface, if you chose this route, you must set `PIPELINE_NAME` to the appropriate value.

If you want to trigger pipeline via web-interface you will need to define PIPELINE_NAME variable to trigger the appropriate pipeline.

system	status	PIPELINE_NAME	description	spack.yaml
Perlmutter	**IN-PROGRESS**	PERLMUTTER_SPACK_DEVELOP	This spack configuration is based on `spack@develop` branch to see what packages can be built. We expect this pipeline will fail and we are not expected to fix build failure. The main purpose of this project is to build as many packages across all the compilers, mpi, blas providers of interest and see what works. Since we don't know which package works during deployment, we will leverage data from this pipeline to make informed decision what packages should be picked with given compilers. This pipeline is our development and we should use this to experiment new compilers. Note that we won't hardcode versions for packages since we want to build with latest release. However we will hardcode externals depending on how system is configured.	https://software.nersc.gov/NERSC/infrastructure/-/blob/main/spack-configs/perlmutter-spack-develop/spack.yaml
Cori	**IN-PROGRESS**	CORI_SPACK_DEVELOP	This spack configuration will build E4S stack using spack `develop` branch on Cori.	https://software.nersc.gov/NERSC/infrastructure/-/blob/main/spack-configs/cori-spack-develop/spack.yaml
Perlmutter	**IN-PROGRESS**	PERLMUTTER_E4S_2205	This E4S 22.05 configuration will build E4S 22.05 on Perlmutter on scheduled pipeline	https://software.nersc.gov/-/ide/project/NERSC/spack-infrastructure/tree/main/-/spack-configs/perlmutter-e4s-22.05/ci/spack.yaml/
Muller	**IN-PROGRESS**	MULLER_E4S_2205	This E4S 22.05 configuration will build E4S 22.05 on Muller on scheduled pipeline	https://software.nersc.gov/-/ide/project/NERSC/spack-infrastructure/tree/main/-/spack-configs/perlmutter-e4s-22.05/ci/spack.yaml/
Cori	**COMPLETED**	CORI_E4S_2202	E4S 22.02 spack configuration will build E4S/22.02 on Cori using a scheduled pipeline.	https://software.nersc.gov/NERSC/infrastructure/-/blob/main/spack-configs/cori-e4s-22.02/ci/spack.yaml
Gerty	**COMPLETED**	GERTY_E4S_2202	E4S 22.02 spack configuration will build E4S/22.02 on gerty using a scheduled pipeline.	https://software.nersc.gov/NERSC/infrastructure/-/blob/main/spack-configs/cori-e4s-22.02/ci/gerty/spack.yaml
Perlmutter	**COMPLETED**	PERLMUTTER_E4S_2111_DEPLOY	This E4S 21.11 configuration is deployment configuration for E4S/21.11. For more details on this stack see https://docs.nersc.gov/applications/e4s/perlmutter/21.11/	https://software.nersc.gov/NERSC/infrastructure/-/blob/main/spack-configs/perlmutter-e4s-21.11/spack.yaml
Perlmutter	**COMPLETED**	PERLMUTTER_E4S_2111	This spack configuration is used for development for building E4S/21.11 using scheduled pipeline.	https://software.nersc.gov/NERSC/infrastructure/-/blob/main/spack-configs/perlmutter-e4s-21.11/ci/spack.yaml
Muller	**COMPLETED**	MULLER_E4S_2111	This E4S 21.11 configuration was used to build E4S/21.11 on Muller using scheduled pipeline. Once e4s/21.11 was built on Muller we followed up with building the same spack configuration on Perlmutter.	https://software.nersc.gov/NERSC/infrastructure/-/blob/main/spack-

1.2 Running CI Pipelines

This project is configured with several scheduled pipelines that will run at different times.

Currently, we have a shell runner installed on Perlmutter using `e4s` account which is configured with following settings. You can find list of runners and their runner status under Settings > CI/CD > Runners. Please make sure you login to the appropriate hostname when starting the gitlab runner.

System	Runner Name	Hostname
perlmutter	`perlmutter-e4s`	`login10`
cori	`cori-e4s`	`cori06`
muller	`muller-e4s`	`login02`
gerty	`gerty-e4s`	`gert01`

The runner configuration files are located in `~/.gitlab-runner` for user **e4s**.

The production pipelines are triggered via web-interface which requires approval from a project maintainer. Production pipelines should be run when we need to do full redeployment of stack.

1.3 Troubleshooting gitlab runner

You will need to login as `e4s` user via `collabsu` command. This will prompt you for password which is your **NERSC password** for your username not **e4s** user.

```
collabsu e4s
```

Once you are logged in, you can login to the desired system to restart the runner. You can check the runner status by navigating to Settings > CI/CD > Runners. If gitlab runner is down you will need to restart the runner which is located in `$HOME/cron` directory for e4s user.

For instance, to access muller you will need to login to Cori/DTN nodes and run `ssh login.muller.nersc.gov`.

The `gitlab-runner` command should be accessible with e4s user. To register a runner you can run `gitlab-runner register` and follow the prompt. The runner configuration will be written to `~/.gitlab-runner/config.toml` however we recommend you create a separate config.toml or copy the file to separate file. For instance if you want to register a runner for muller you can set `gitlab-runner register -c ~/.gitlab-runner/muller.config.toml` when registering the runner and it will write the runner configuration to `~/.gitlab-runner/muller.config.toml`. For more details regarding runner register please see https://docs.gitlab.com/runner/register/

To restart a runner you can run the script based on runner type

```
# restart gerty runner
bash $HOME/cron/restart-gerty.sh

# restart muller runner
bash $HOME/cron/restart-muller.sh

# restart perlmutter runner
bash $HOME/cron/restart-perlmutter.sh

# restart cori runner
bash $HOME/cron/restart-cori.sh
```

In order to access gerty, you will need to login to data transfer node and then login to gerty as follows

```
ssh dtn01.nersc.gov
collabsu e4s
ssh gerty
```

1.4 Current Challenges

There are several challenges with building spack stack at NERSC which can be summarized as follows

- **System OS + Cray Programming Environment (CPE) changes**: A system upgrade such as change to `glibc` or upgrades in CPE can lead to full software stack rebuild, especially if you have externals set to packages like `cray-mpich`, `cray-libsci` which generally change between versions
- **Incompatibile compilers**: Some packages can't be built with certain compilers (`nvhpc`, `aocc`) which could be due to several factors.
  - An application doesn't have support though it was be added in newer version but you don't have it in your spack release used for deployment
  - Lack of support in spack package recipe or spack-core base including spack-cray detection. This may require getting fix and cherry-pick commit or waiting for new version
  - Spack Cray detection is an important part in build errors including how one specifies externals via `modules` vs `prefix` both could be provided and it requires experimentation. An example of this is trying to get `cray-mpich` external one could set something like this with modules or prefix

```
cray-mpich:
  buildable: false
  externals:
  - spec: cray-mpich@8.1.11 %gcc@9.3.0
    prefix: /opt/cray/pe/mpich/8.1.11/ofi/gnu/9.1
    modules:
    - cray-mpich/8.1.11
    - cudatoolkit/21.9_11.4
```

  - **Spack concretizer** prevent one from chosing a build configration for a spec. This requires a few troubleshooting step but usually boils down to:
    - Read the spack package file `spack edit <package>` for conflicts and try `spack spec` to see concretized spec.
    - Try different version, different compiler, different dependency. Some packages have conflicting variant for instance one can't enable `+openmp` and `+pthread` it is mutually exclusive.

There is a document Spack E4S Issues on Permlutter outlining current issues with spack. If you need access to document please contact **Shahzeb Siddiqui**.

1.5 Contact

If you need elevated privledge or assistance with this project please contact one of the maintainers:

- **Shahzeb Siddiqui (shahzebsiddiqui@lbl.gov)**
- **Erik Palmer (epalmer@lbl.gov)**
- **Justin Cook (JSCook@lbl.gov)**
- E4S Team: **Sameer Shende (sameer@cs.uoregon.edu)**, **Christopher Peyralans (lpeyrala@uoregon.edu)**, **Wyatt Spear (wspear@cs.uoregon.edu)**, **Nicholas Chaimov (nchaimov@paratools.com)**

CHAPTER

TWO

SPACK CONFIGURATION

This page will show all of our spack configuration files (*spack.yaml*) used for our production deployments. The spack configuration located in spack-configs directory organized by each subdirectory.

At NERSC, we are building the Extreme-scale Scientific Software Stack (E4S) which is a collection of open-source products software packages part of spack ecosystem for running scientific applications on high-performance computing (HPC) platforms. We acquire the spack configuration from https://github.com/E4S-Project/e4s upon release with list of specs and reference spack branch in order to build the E4S stack. Please see our E4S documentation at https://docs.nersc.gov/applications/e4s/

2.1 Perlmutter Spack Develop

This spack configuration will build all packages using spack *develop* branch on weekly basis. All specs are specified without any version in order to let spack build the latest package which will evolve over time. This stack can be accessible via `module load e4s/spack-develop`. For more information see https://docs.nersc.gov/applications/e4s/e4s-develop/

```
spack:
  view: false
  config:
    install_tree:
      concretizer: clingo
    build_stage: $CFS/m3503/perlmutter-spack-develop/spack-stage
    misc_cache: $CFS/m3503/perlmutter-spack-develop/misc_cache
  cdash:
    build-group: DOE nightly E4S builds
    url: https://cdash.spack.io
    project: Spack
    site: NERSC - Perlmutter spack@develop
  compilers:
  - compiler:
      spec: gcc@11.2.0
      paths:
        cc: /opt/cray/pe/craype/default/bin/cc
        cxx: /opt/cray/pe/craype/default/bin/CC
        f77: /opt/cray/pe/craype/default/bin/ftn
        fc: /opt/cray/pe/craype/default/bin/ftn
      flags: {}
      operating_system: sles15
      target: any
```

(continues on next page)

(continued from previous page)

```
    modules:
    - PrgEnv-gnu
    - gcc/11.2.0
    - craype-x86-milan
    - libfabric
- compiler:
    spec: gcc@10.3.0
    paths:
      cc: /opt/cray/pe/craype/default/bin/cc
      cxx: /opt/cray/pe/craype/default/bin/CC
      f77: /opt/cray/pe/craype/default/bin/ftn
      fc: /opt/cray/pe/craype/default/bin/ftn
    flags: {}
    operating_system: sles15
    target: any
    modules:
    - PrgEnv-gnu
    - gcc/10.3.0
    - craype-x86-milan
    - libfabric
- compiler:
    spec: cce@13.0.1
    paths:
      cc: /opt/cray/pe/craype/default/bin/cc
      cxx: /opt/cray/pe/craype/default/bin/CC
      f77: /opt/cray/pe/craype/default/bin/ftn
      fc: /opt/cray/pe/craype/default/bin/ftn
    flags: {}
    operating_system: sles15
    target: any
    modules:
    - PrgEnv-cray
    - cce/13.0.1
    - craype-x86-milan
    - libfabric
    environment: {}
    extra_rpaths: []
- compiler:
    spec: nvhpc@21.11
    paths:
      cc: /opt/cray/pe/craype/default/bin/cc
      cxx: /opt/cray/pe/craype/default/bin/CC
      f77: /opt/cray/pe/craype/default/bin/ftn
      fc: /opt/cray/pe/craype/default/bin/ftn
    flags: {}
    operating_system: sles15
    target: any
    modules:
    - PrgEnv-nvidia
    - nvidia/21.11
    - craype-x86-milan
    - libfabric
```

(continues on next page)

(continued from previous page)

```
  definitions:
  - gcc_compilers: ['%gcc@11.2.0']
  - nvhpc_compilers: ['%nvhpc@21.11']
  - cray_compilers: ['%cce@13.0.1']
  - cray_specs:
    - adios2
    - blaspp
    - fftw
    - hdf5
    - kokkos +openmp +wrapper +cuda cuda_arch=80
    - kokkos-kernels +openmp
    - lapackpp
    - openpmd-api
    - papi
    - petsc +openmp +strumpack
    - slepc
    - strumpack ~slate
    - superlu
    - superlu-dist +openmp
  - gcc_specs:
    - adios2
    - amrex +fortran +hypre +openmp +petsc +shared
    - blaspp
    - gasnet
    - hdf5
    - hipace
    - hypre +openmp +superlu-dist
    - kokkos +openmp +wrapper
    - kokkos-kernels +openmp ^kokkos +openmp +wrapper
    - lapackpp
    - llvm +clang +compiler-rt +libcxx +lld +lldb +llvm_dylib +flang ~cuda
    - openpmd-api
    - papi
    - petsc +openmp +strumpack
    - py-openpmd-viewer +numba
    - py-numba
    - py-warpx ^warpx dims=1
    - py-warpx ^warpx dims=2
    - py-warpx ^warpx dims=3
    - py-warpx ^warpx dims=rz
    - raja
    - slepc
    - strumpack ~slate
    - sundials +openmp +hypre
    - superlu
    - superlu-dist +openmp
    - upcxx +gasnet +mpi
    - warpx dims=1
    - warpx dims=2
    - warpx dims=3
    - warpx dims=rz
  - cuda_specs:
```

(continues on next page)

(continued from previous page)

```
    - amrex +cuda cuda_arch=80
    - blaspp +cuda cuda_arch=80
    - hipace compute=cuda
    - hpctoolkit +cuda +cray +mpi
    - hypre +cuda cuda_arch=80
    - kokkos-kernels +openmp +cuda cuda_arch=80 ^kokkos +openmp +wrapper +cuda cuda_
↪arch=80
    - kokkos +openmp +wrapper +cuda cuda_arch=80
    - lapackpp ^blaspp +cuda cuda_arch=80
    - magma@2.6.1+cuda cuda_arch=80
    - mfem@4.3.0+cuda cuda_arch=80
    - petsc +cuda cuda_arch=80
    - py-warpx ^warpx dims=1 compute=cuda
    - py-warpx ^warpx dims=2 compute=cuda
    - py-warpx ^warpx dims=3 compute=cuda
    - py-warpx ^warpx dims=rz compute=cuda
    - qmcpack +cuda cuda_arch=80
    - raja +cuda cuda_arch=80
    - slepc +cuda cuda_arch=80
    - trilinos +amesos +amesos2 +anasazi +aztec +belos +boost +epetra +epetraext +ifpack
      +ifpack2 +intrepid +intrepid2 +isorropia +kokkos +ml +minitensor +muelu +nox
      +piro +phalanx +rol +rythmos +sacado +stk +shards +shylu +stokhos +stratimikos
      +teko +tempus +tpetra +trilinoscouplings +zoltan +zoltan2 +superlu-dist␣
↪gotype=long_long
    - strumpack ~slate +cuda cuda_arch=80
    - slate +cuda cuda_arch=80
    - superlu-dist +openmp +cuda cuda_arch=80
    - sundials +openmp +cuda cuda_arch=80
    - upcxx +gasnet +mpi
    - umpire ~shared +cuda cuda_arch=80
    - upcxx +cuda
    - warpx dims=1 compute=cuda
    - warpx dims=2 compute=cuda
    - warpx dims=3 compute=cuda
    - warpx dims=rz compute=cuda
    - zfp +cuda cuda_arch=80
  - nvhpc_specs:
      #- adios2 failed due to libffi see https://github.com/libffi/libffi/issues/691
    - amrex +cuda cuda_arch=80
    - blaspp +cuda cuda_arch=80
    - hypre +cuda cuda_arch=80
    - kokkos +openmp +wrapper +cuda cuda_arch=80
    - kokkos-kernels +openmp +cuda cuda_arch=80 ^kokkos +openmp +wrapper +cuda cuda_
↪arch=80
    - lapackpp ^blaspp +cuda cuda_arch=80
    - openpmd-api
    - petsc +cuda cuda_arch=80
    - py-numba
    - raja +cuda cuda_arch=80
    - umpire ~shared +cuda cuda_arch=80
    - upcxx +cuda
    - zfp +cuda cuda_arch=80
```

(continues on next page)

(continued from previous page)

```
  - nersc_specs:
    #- amber+openmp requires tarball and license
    # skipping arm-forge for now this requires a license and gets stuck in CI job.
    #- arm-forge
    - abinit +wannier90
    - amdblis
    - amdfftw
    # requested by user INC0176750. See https://github.com/NVIDIA/AMGX/issues/165
    - amgx +cuda cuda_arch=80
    - amdscalapack
    - atompaw
    - berkeleygw
    - boost cxxstd=11
    - boost cxxstd=14
    - boost cxxstd=98
    - cmake
    - dpcpp +openmp
    - eigen
    - elpa
    - fpm
    - lammps
    - llvm-openmp
    - metis
    - mt-metis
    - mumps
    - nccmp
    - nco
    - octave
    - parmetis
    - parallel
    - plumed
    - qmcpack
    - quantum-espresso
    - scotch
    - sparskit
    - superlu-mt
    - wannier90
    - valgrind
    # cuda_arch=80 not supported in spack package yet. See https://github.com/spack/
↪spack/issues/28554
    - cp2k +cuda cuda_arch=70 +elpa +cosma

  specs:
  - matrix:
    - [$cray_specs]
    - [$cray_compilers]
  - matrix:
    - [$gcc_specs]
    - [$gcc_compilers]
  - matrix:
    - [$cuda_specs]
```

(continues on next page)

(continued from previous page)

```
    - [$gcc_compilers]
  - matrix:
    - [$nvhpc_specs]
    - [$nvhpc_compilers]
  - matrix:
    - [$nersc_specs]
    - [$gcc_compilers]

  gitlab-ci:
    enable-artifacts-buildcache: false
    rebuild-index: true
    before_script:
    - git clone ${SPACK_REPO}
    - pushd spack && git checkout ${SPACK_CHECKOUT_VERSION} && popd
    - . "./spack/share/spack/setup-env.sh"
    script:
    - pushd ${SPACK_CONCRETE_ENV_DIR} && spack env activate --without-view -d $CI_
↪PROJECT_DIR/spack-configs/perlmutter-spack-develop
      && popd
    - spack env st
    - spack -d ci rebuild
    after_script:
    - rm -rf $SPACK_ROOT
    service-job-attributes:
      tags: [perlmutter-login21]
      script:
      - echo "End Pipeline"
    mappings:
    - match: [os=sles15]
      runner-attributes:
        tags: [perlmutter-login21]
  packages:
    all:
      compiler: [gcc@11.2.0, gcc@10.3.0, nvhpc@21.11, cce@13.0.1]
      providers:
        blas: [cray-libsci]
        mpi: [cray-mpich]
        fftw-api: [cray-fftw]
    amrex:
      variants: +fortran +hypre +openmp +petsc +shared
    bzip2:
      version: [1.0.6]
      externals:
      - spec: bzip2@1.0.6
        prefix: /usr
    cray-fftw:
      buildable: false
      # cray-fftw module provided in several MODULEPATH, craype-x86-milan modulefile␣
↪sets MODULEPATH to cray-fftw optimized build for milan processor
      externals:
      - spec: cray-fftw@3.3.8.12
        modules:
```

(continues on next page)

(continued from previous page)

```
      - craype-x86-milan
      - cray-fftw/3.3.8.12
  cray-libsci:
    buildable: false
    externals:
    - spec: cray-libsci@21.08.1.2
      modules:
      - cray-libsci/21.08.1.2
  cray-mpich:
    buildable: false
    externals:
    - spec: cray-mpich@8.1.15 %gcc@11.2.0
      prefix: /opt/cray/pe/mpich/8.1.15/ofi/gnu/9.1
      modules:
      - cray-mpich/8.1.15
      - cudatoolkit/11.5
    - spec: cray-mpich@8.1.15 %nvhpc@21.11
      prefix: /opt/cray/pe/mpich/8.1.15/ofi/nvidia/20.7
      modules:
      - cray-mpich/8.1.15
      - cudatoolkit/11.5
    - spec: cray-mpich@8.1.15 %cce@13.0.1
      prefix: /opt/cray/pe/mpich/8.1.15/ofi/cray/10.0
      modules:
      - cray-mpich/8.1.15
      - cudatoolkit/11.5
  cuda:
    buildable: false
    version: [11.5.0]
    externals:
    - spec: cuda@11.5.0
      prefix: /opt/nvidia/hpc_sdk/Linux_x86_64/21.11/cuda/11.5
      modules:
      - cudatoolkit/11.5
  diffutils:
    version: [3.6]
    externals:
    - spec: diffutils@3.6
      prefix: /usr
  findutils:
    version: [4.6.0]
    externals:
    - spec: findutils@4.6.0
      prefix: /usr
  hdf5:
    variants: +fortran +hl +shared api=v18
    version: [1.12.1]
  hypre:
    variants: +openmp +superlu-dist
  git:
    version: [2.26.2]
    buildable: false
```

(continues on next page)

(continued from previous page)

```
    externals:
    - spec: git@2.26.2
      prefix: /usr
  gettext:
    version: [0.19.8.1]
    buildable: false
    externals:
    - spec: gettext@0.19.8.1
      prefix: /usr
  libfabric:
    buildable: false
    variants: fabrics=sockets,tcp,udp,rxm
    externals:
    - spec: libfabric@1.11.0.4.414
      prefix: /opt/cray/libfabric/1.11.0.4.114
      modules:
      - libfabric/1.11.0.4.414
  libunwind:
    variants: +pic +xz
  mercury:
    variants: ~bmi
  mesa:
    variants: ~llvm
  mesa18:
    variants: ~llvm
  m4:
    buildable: false
    externals:
    - spec: m4@1.4.18
      prefix: /usr
  mpich:
    variants: ~wrapperrpath
  ncurses:
    variants: +termlib
    externals:
    - spec: ncurses@6.1
      prefix: /usr
  openssl:
    version: [1.1.0i]
    buildable: false
    externals:
    - spec: openssl@1.1.0i
      prefix: /usr
  openssh:
    version: [7.9p1]
    buildable: false
    externals:
    - spec: openssh@7.9p1
      prefix: /usr
  petsc:
    variants: +openmp +strumpack
  pdsh:
```

(continues on next page)

(continued from previous page)

```
    buildable: false
    externals:
    - spec: pdsh@2.34
      prefix: /usr
  readline:
    version: [7.0]
    buildable: false
    externals:
    - spec: readline@7.0
      prefix: /usr
  slurm:
    buildable: false
    version: [20-11-8-1]
    externals:
    - spec: slurm@20-11-8-1
      prefix: /usr
  superlu-dist:
    variants: +openmp
  strumpack:
    variants: ~slate
  tar:
    version: [1.3]
    buildable: false
    externals:
    - spec: tar@1.30
      prefix: /usr
  tcsh:
    version: [6.20.0]
    buildable: false
    externals:
    - spec: tcsh@6.20.0
      prefix: /usr
  trilinos:
    variants: +amesos +amesos2 +anasazi +aztec +belos +boost +epetra +epetraext
      +ifpack +ifpack2 +intrepid +intrepid2 +isorropia +kokkos +ml +minitensor +muelu
      +nox +piro +phalanx +rol +rythmos +sacado +stk +shards +shylu +stokhos␣
↪+stratimikos
      +teko +tempus +tpetra +trilinoscouplings +zoltan +zoltan2 +superlu-dist␣
↪gotype=long_long
  unzip:
    version: [6.0]
    buildable: false
    externals:
    - spec: unzip@6.0
      prefix: /usr
  util-linux-uuid:
    version: [2.33.1]
    buildable: false
    externals:
    - spec: util-linux-uuid@2.33.1
      prefix: /usr
  xz:
```

(continues on next page)

(continued from previous page)

```
    version: [5.2.3]
    buildable: false
    externals:
    - spec: xz@5.2.3
      prefix: /usr
  zsh:
    version: [5.6]
    buildable: false
    externals:
    - spec: zsh@5.6
      prefix: /usr
```

2.2 Cori Spack Develop

This is the spack configuration for spack `develop` branch for Cori. Similar to Perlmutter, this stack will build all specs unconstrained with version.

```
spack:
  view: false
  config:
    build_stage: $CFS/m3503/spack-stage
    misc_cache: $CFS/m3503/misc_cache
    install_tree:
      concretizer: clingo
  compilers:
  - compiler:
      spec: gcc@11.2.0
      paths:
        cc: /opt/cray/pe/craype/default/bin/cc
        cxx: /opt/cray/pe/craype/default/bin/CC
        f77: /opt/cray/pe/craype/default/bin/ftn
        fc: /opt/cray/pe/craype/default/bin/ftn
      flags: {}
      operating_system: cnl7
      target: any
      modules:
      - PrgEnv-gnu
      - gcc/11.2.0
      - craype-haswell
  - compiler:
      spec: intel@19.1.2.254
      paths:
        cc: /opt/cray/pe/craype/default/bin/cc
        cxx: /opt/cray/pe/craype/default/bin/CC
        f77: /opt/cray/pe/craype/default/bin/ftn
        fc: /opt/cray/pe/craype/default/bin/ftn
      flags: {}
      operating_system: cnl7
      target: any
      modules:
```

(continues on next page)

(continued from previous page)

```
    - PrgEnv-intel
    - intel/19.1.2.254
    - craype-haswell
definitions:
- gcc_compilers: ['%gcc@11.2.0']
- intel_compilers: ['%intel@19.1.2.254']
- gcc_specs:
  - adios2
  - amrex +fortran +hypre +openmp +petsc +shared
  - blaspp
  - fftw
  - gasnet
  - papi
  - hdf5
  - hipace
  - hypre +openmp +superlu-dist
  - kokkos +openmp +wrapper
  - kokkos-kernels +openmp ^kokkos +openmp +wrapper
  - lapackpp
  - petsc +openmp +strumpack
  - raja
  - slepc
  - strumpack ~slate
  - sundials +openmp +hypre
  - superlu
  - superlu-dist +openmp
  - tau +mpi +python
- intel_specs:
  - adios2
  - amrex +fortran +hypre +openmp +petsc +shared
  - blaspp
  - fftw
  - hdf5
  - hipace
  - lapackpp
  - openpmd-api
  - py-openpmd-viewer +numba
  - py-numba
  - py-warpx ^warpx dims=1
  - py-warpx ^warpx dims=2
  - py-warpx ^warpx dims=3
  - py-warpx ^warpx dims=rz
  - tau +mpi +python
  - upcxx
  - warpx dims=1
  - warpx dims=2
  - warpx dims=3
  - warpx dims=rz
- nersc_specs:
  - abinit
  - cdo
  - chapel
```

(continues on next page)

(continued from previous page)

```
    - ffmpeg
    - elpa
    - grads
    - gsl
    - gnuplot
    - gromacs
    - libxc
    - libxsmm +shared
    - libint
    - maven
    - metis
    - mpfr
    - octave
    - openjdk
    - parallel
    - parmetis
    - plumed
    - texlive
    - xerces-c
    - valgrind
    - wannier90

  specs:
  - matrix:
    - [$gcc_specs]
    - [$gcc_compilers]
  - matrix:
    - [$intel_specs]
    - [$intel_compilers]
  - $nersc_specs
  packages:
    all:
      compiler: [intel@19.1.2.254, gcc@11.2.0]
      providers:
        blas: [intel-mkl, cray-libsci]
        mpi: [cray-mpich]
        fftw-api: [cray-fftw]
        scalapack: [intel-mkl, cray-libsci]
    amrex:
      variants: +fortran +hypre +openmp +petsc +shared

    bash:
      buildable: false
      externals:
      - spec: bash@4.4.23
        prefix: /
    bzip2:
      version: [1.0.6]
      externals:
      - spec: bzip2@1.0.6
        prefix: /usr
    coreutils:
```

(continues on next page)

(continued from previous page)

```
    buildable: false
    version: [8.29]
    externals:
    - spec: coreutils@8.29
      prefix: /usr
  cpio:
    buildable: false
    externals:
    - spec: cpio@2.12
      prefix: /
  cray-libsci:
    buildable: false
    version: [20.09.1]
    externals:
    - spec: cray-libsci@20.09.1 %gcc
      prefix: /opt/cray/pe/libsci/20.09.1/gnu/8.1
      modules:
      - cray-libsci/20.09.1
    - spec: cray-libsci@20.09.1 %intel
      prefix: /opt/cray/pe/libsci/20.09.1/intel/16.0
      modules:
      - cray-libsci/20.09.1
  cray-fftw:
    buildable: false
    externals:
    - spec: cray-fftw@3.3.8.4
      modules:
      - cray-fftw/3.3.8.4
  cray-mpich:
    buildable: false
    externals:
    - spec: cray-mpich@7.7.19 %intel
      prefix: /opt/cray/pe/mpt/7.7.19/gni/mpich-intel/16.0
      modules:
      - cray-mpich/7.7.19
    - spec: cray-mpich@7.7.19 %gcc
      prefix: /opt/cray/pe/mpt/7.7.19/gni/mpich-gnu/8.2
      modules:
      - cray-mpich/7.7.19
  curl:
    externals:
    - spec: curl@7.66.0+gssapi+ldap+nghttp2
      prefix: /usr
  diffutils:
    version: [3.6]
    externals:
    - spec: diffutils@3.6
      prefix: /usr
  findutils:
    version: [4.6.0]
    externals:
    - spec: findutils@4.6.0
```

(continues on next page)

(continued from previous page)

```
      prefix: /usr
  hdf5:
    variants: +fortran +hl +shared api=v18
  hypre:
    variants: +openmp +superlu-dist
  git:
    version: [2.26.2]
    buildable: false
    externals:
    - spec: git@2.26.2
      prefix: /usr
  gettext:
    version: [0.19.8.1]
    buildable: false
    externals:
    - spec: gettext@0.19.8.1
      prefix: /usr
  intel-mkl:
    buildable: false
    externals:
    - spec: intel-mkl@19.1.2.254
      modules:
      - intel/19.1.2.254
  libunwind:
    variants: +pic +xz
  mercury:
    variants: ~bmi
  mesa:
    variants: ~llvm
  mesa18:
    variants: ~llvm
  m4:
    buildable: false
    externals:
    - spec: m4@1.4.18
      prefix: /usr
  mpich:
    variants: ~wrapperrpath
  ncurses:
    variants: +termlib
    externals:
    - spec: ncurses@6.1
      prefix: /usr
  openssl:
    version: [1.1.0i]
    buildable: false
    externals:
    - spec: openssl@1.1.0i
      prefix: /usr
  openssh:
    version: [7.6p1]
    buildable: false
```

(continues on next page)

(continued from previous page)

```
    externals:
    - spec: openssh@7.6p1
      prefix: /usr
  petsc:
    variants: +openmp +strumpack
  pdsh:
    buildable: false
    externals:
    - spec: pdsh@2.33
      prefix: /usr
  readline:
    version: [7.0]
    buildable: false
    externals:
    - spec: readline@7.0
      prefix: /usr
  sed:
    buildable: false
    externals:
    - spec: sed@4.4
      prefix: /usr
  slurm:
    buildable: false
    version: [20-11-8-1]
    externals:
    - spec: slurm@20-11-8-1
      prefix: /usr
  superlu-dist:
    variants: +openmp
  strumpack:
    variants: ~slate
  tar:
    version: [1.3]
    buildable: false
    externals:
    - spec: tar@1.30
      prefix: /usr
  tcsh:
    version: [6.20.0]
    buildable: false
    externals:
    - spec: tcsh@6.20.0
      prefix: /usr
  trilinos:
    variants: +amesos +amesos2 +anasazi +aztec +belos +boost +epetra +epetraext
      +ifpack +ifpack2 +intrepid +intrepid2 +isorropia +kokkos +ml +minitensor +muelu
      +nox +piro +phalanx +rol +rythmos +sacado +stk +shards +shylu +stokhos␣
↪+stratimikos
      +teko +tempus +tpetra +trilinoscouplings +zoltan +zoltan2 +superlu-dist␣
↪gotype=long_long
  unzip:
    version: [6.0]
```

(continues on next page)

(continued from previous page)

```
    buildable: false
    externals:
    - spec: unzip@6.0
      prefix: /usr
  util-linux-uuid:
    version: [2.31.1]
    buildable: false
    externals:
    - spec: util-linux-uuid@2.31.1
      prefix: /usr
  xz:
    version: [5.2.3]
    buildable: false
    externals:
    - spec: xz@5.2.3
      prefix: /usr
  zsh:
    version: [5.6]
    buildable: false
    externals:
    - spec: zsh@5.6
      prefix: /usr
```

2.3 Cori E4S 22.02

```
# This is a Spack Environment file.
#
# It describes a set of packages to be installed, along with
# configuration settings.
spack:
  view: false
  config:
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    install_tree:
      concretizer: clingo
      root: /global/common/software/spackecp/cori/e4s-22.02/software
    module_roots:
      tcl: /global/common/software/spackecp/cori/e4s-22.02/modules
  mirrors:
    source_mirror: /global/common/software/spackecp/mirrors/source_mirror
  modules::
    prefix_inspections:
      bin:
        - PATH
      lib:
        - LIBRARY_PATH
        - LD_LIBRARY_PATH
      lib64:
        - LIBRARY_PATH
```

(continues on next page)

(continued from previous page)

```
      - LD_LIBRARY_PATH
    include:
      - C_INCLUDE_PATH
      - CPLUS_INCLUDE_PATH
      - CPATH
    man:
      - MANPATH
    share/man:
      - MANPATH
    share/aclocal:
      - ACLOCAL_PATH
    lib/pkgconfig:
      - PKG_CONFIG_PATH
    lib64/pkgconfig:
      - PKG_CONFIG_PATH
    share/pkgconfig:
      - PKG_CONFIG_PATH
    '':
      - CMAKE_PREFIX_PATH
  enable:
  - tcl
  tcl:
    blacklist_implicits: true
    hash_length: 0
    naming_scheme: '{name}/{version}-{compiler.name}-{compiler.version}'
    all:
      autoload: direct
      conflict:
      - '{name}'
      environment:
        set:
          '{name}_ROOT': '{prefix}'
    darshan-runtime:
      conflict:
      - darshan
    darshan-util:
      conflict:
      - darshan
    projections:
      all: '{name}/{version}-{compiler.name}-{compiler.version}'
      warpx dims=1: '{name}/{version}-{compiler.name}-{compiler.version}-dims1'
      warpx dims=2: '{name}/{version}-{compiler.name}-{compiler.version}-dims2'
      warpx dims=3: '{name}/{version}-{compiler.name}-{compiler.version}-dims3'
compilers:
- compiler:
    spec: gcc@11.2.0
    paths:
      cc: /opt/cray/pe/craype/default/bin/cc
      cxx: /opt/cray/pe/craype/default/bin/CC
      f77: /opt/cray/pe/craype/default/bin/ftn
      fc: /opt/cray/pe/craype/default/bin/ftn
    flags: {}
```

(continues on next page)

(continued from previous page)

```
    operating_system: cnl7
    target: any
    modules:
    - PrgEnv-gnu
    - gcc/11.2.0
    - craype-haswell
- compiler:
    spec: intel@19.1.2.254
    paths:
      cc: /opt/cray/pe/craype/default/bin/cc
      cxx: /opt/cray/pe/craype/default/bin/CC
      f77: /opt/cray/pe/craype/default/bin/ftn
      fc: /opt/cray/pe/craype/default/bin/ftn
    flags: {}
    operating_system: cnl7
    target: any
    modules:
    - PrgEnv-intel
    - intel/19.1.2.254
    - craype-haswell
definitions:
- gcc_compilers: ['%gcc@11.2.0']
- intel_compilers: ['%intel@19.1.2.254']
- gcc_specs:
  - adios2@2.7.1
  - amrex@22.02
  - aml@0.1.0
  - arborx@1.1
  - argobots@1.1
  - axom@0.6.1
  - bolt@2.0
  - caliper@2.7.0
  - chai@2.4.0 ~benchmarks ~tests
  - conduit@0.8.2
  - darshan-runtime@3.3.1
  - darshan-util@3.3.1
  - dyninst@12.0.1
  - faodel@1.2108.1
  - flecsi@1.4.2
  - flit@2.1.0
  - gasnet@2021.9.0
  - ginkgo@1.4.0
  - globalarrays@5.8
  - gotcha@1.0.3
  - hdf5@1.10.7 +fortran +hl +shared
  - hdf5@1.12.1 +fortran +hl +shared
  - hdf5@1.13.0 +fortran +hl +shared
  - heffte@2.2.0 +fftw
  - hpx@1.7.1 networking=mpi
  - hypre@2.24.0
  - kokkos@3.5.00 +openmp +wrapper
  - kokkos-kernels@3.5.00 +openmp ^kokkos@3.5.00 +openmp +wrapper
```

(continues on next page)

(continued from previous page)

```
    - legion@21.03.0
    - libquo@1.3.1
    - libunwind@1.5.0
    - mercury@2.1.0
    - metall@0.17
    - mfem@4.3.0
    - mpark-variant@1.4.0
    - nccmp@1.9.0.1 ^netcdf-c@4.8.1
    - nco@5.0.1
    - netlib-scalapack@2.1.0
    - ninja@1.10.2
    - nvhpc@22.1
    - openpmd-api@0.14.4
    - papi@6.0.0.1
    - papyrus@1.0.1
    - parallel-netcdf@1.12.2
    - parsec@3.0.2012 ~cuda
    - pdt@3.25.1
    - petsc@3.16.4 +openmp
    - pumi@2.2.6
    - qthreads@1.16 scheduler=distrib
    - raja@0.14.0
    - stc@0.9.0
    - strumpack@6.3.0~butterflypack~slate
    - sundials@6.1.1
    - superlu@5.3.0
    - superlu-dist@7.2.0
    - swig@4.0.2
    - sz@2.1.12
    - tasmanian@7.7
    - tau@2.31 +mpi +python
    - turbine@1.3.0
    - umap@2.1.0
    - umpire@6.0.0
    - upcxx@2021.9.0
    - veloc@1.5
    - vtk-m@1.7.1
    - zfp@0.5.5
  #- hpctoolkit@2022.01.15
  #- phist@1.9.5 #Unable to locate cray-libsci headers in /opt/cray/pe/libsci/20.09.1/
↪gnu/8.1/include
  #- mpifileutils@0.11.1 ~xattr # failed to install libcircle Unable to find suitable␣
↪MPI Compiler. Try setting MPICC.
  #- plumed@2.6.3  # Build Failed
  #-precice@2.3.0 # Build failed due to petsc
  #- py-warpx@22.02 ^warpx dims=rz
  #- rempi@1.1.0 failed to find MPICC
  #- slate@2021.05.02 ~cuda # Build failure on blaspp. BLAS++ requires a BLAS library␣
↪and none was found.
  #- scr@3.0rc2  Build failure
  #- trilinos@13.0.1 +amesos +amesos2 +anasazi +aztec +belos +boost +epetra +epetraext␣
↪+ifpack +ifpack2 +intrepid +intrepid2 +isorropia +kokkos +ml +minitensor +muelu +nox␣
```

(continues on next page)

(continued from previous page)

```
↪+piro +phalanx +rol +rythmos +sacado +stk +shards +shylu +stokhos +stratimikos +teko␣
↪+tempus +tpetra +trilinoscouplings +zoltan +zoltan2 +superlu-dist gotype=long_long
    #- unifyfs@0.9.1 # Build failure on dependency mercury
    #- wannier90@3.1.0 #  Error: A PrgEnv-* modulefile must be loaded.
  - intel_specs:
    - adios2@2.7.1
    - arborx@1.1
    - argobots@1.1
    - caliper@2.7.0
    - conduit@0.8.2
    - chai@2.4.0 ~benchmarks ~tests
    - darshan-runtime@3.3.1
    - darshan-util@3.3.1
    - faodel@1.2108.1
    - flecsi@1.4.2
    - flit@2.1.0
    - gasnet@2021.9.0
    - ginkgo@1.4.0
    - globalarrays@5.8
    - gotcha@1.0.3
    - hdf5@1.10.7 +fortran +hl +shared
    - hdf5@1.12.1 +fortran +hl +shared
    - hdf5@1.13.0 +fortran +hl +shared
    - heffte@2.2.0 +fftw
    - hypre@2.24.0
    - kokkos@3.5.00 +openmp +wrapper
    - legion@21.03.0
    - libquo@1.3.1
    - libunwind@1.5.0
    - loki@0.1.7
    - mercury@2.1.0
    - metall@0.17
    - mfem@4.3.0
    - mpark-variant@1.4.0
    - nccmp@1.9.0.1 ^netcdf-c@4.8.1
    - netlib-scalapack@2.1.0
    - ninja@1.10.2
    - openpmd-api@0.14.4
    - papi@6.0.0.1
    - parallel-netcdf@1.12.2
    - parsec@3.0.2012 ~cuda
    - papyrus@1.0.1
    - petsc@3.16.4 +openmp
    - pdt@3.25.1
    - precice@2.3.0
    - pumi@2.2.6
    - qthreads@1.16 scheduler=distrib
    - raja@0.14.0
    - slepc@3.16.2
    - strumpack@6.3.0~butterflypack ~slate
    - sundials@6.1.1
    - superlu@5.3.0
```

(continues on next page)

(continued from previous page)

```
    - superlu-dist@7.2.0
    - swig@4.0.2
    - sz@2.1.12
    - tasmanian@7.7
    - turbine@1.3.0
    - umap@2.1.0
    - umpire@6.0.0
    - upcxx@2021.9.0
    - variorum@0.4.1
    - veloc@1.5
    - vtk-m@1.7.1
    - wannier90@3.1.0
    - warpx dims=1
    - warpx dims=2
    - warpx dims=3
    - zfp@0.5.5
    #- axom@0.6.1 # Build failure in cmake for axom
    #- butterflypack@2.1.0 # Build failure  sed: can't read *.inc: No such file or␣
↪directory
    #- dyninst@12.0.1 # %intel conflict
    # - hpx@1.7.1 networking=mpi # Failed on asio
    #- lammps@20220107 # Build Failure during cmake
    #- kokkos-kernels@3.5.00 +openmp ^kokkos@3.5.00 +openmp +wrapper  # Build failure
    #- plasma@21.8.29 # %intel conflict
    #- phist@1.9.5  # Error: NoHeadersError: Unable to locate cray-libsci headers in /
↪opt/cray/pe/libsci/20.09.1/intel/16.0/include
    #- plumed@2.6.3
    #- rempi@1.1.0  # FAILED to find MPICC
    #- slate@2021.05.02 ~cuda # %intel conflict
    #- scr@3.0rc2   Build failure
    #- trilinos@13.0.1 +amesos +amesos2 +anasazi +aztec +belos +boost +epetra +epetraext␣
↪+ifpack +ifpack2 +intrepid +intrepid2 +isorropia +kokkos +ml +minitensor +muelu +nox␣
↪+piro +phalanx +rol +rythmos +sacado +stk +shards +shylu +stokhos +stratimikos +teko␣
↪+tempus +tpetra +trilinoscouplings +zoltan +zoltan2 +superlu-dist gotype=long_long
    #- warpx dims=rz failed on blaspp

  - nersc_specs:
    - cdo@2.0.3 +curl
    - chapel@1.24.1
    - ffmpeg@4.4.1
    - elpa@2021.11.001
    - grads@2.2.1
    - gsl@2.7
    - gromacs@2021.5
    - libxc@5.1.7
    - libxsmm@1.17 +shared
    - libint@2.6.0
    - nano@4.9
    - maven@3.8.4
    - metis@5.1.0
    - octave@6.4.0
    - openjdk@11.0.12_7
```

(continues on next page)

(continued from previous page)

```
    - parallel@20210922
    - parmetis@4.0.3
    - texlive
    - xerces-c@3.2.3

    #- abinit+openmp failed to install netcdf-fortran
    #- gnuplot build failure on gnuplot
    #- valgrind@3.18.1 Build failure
  specs:
  - matrix:
    - [$gcc_specs]
    - [$gcc_compilers]
  - matrix:
    - [$intel_specs]
    - [$intel_compilers]
  - matrix:
    - [$nersc_specs]
    - [$gcc_compilers]
  packages:
    all:
      compiler: [gcc@11.2.0, intel@19.1.2.254]
      providers:
        blas: [cray-libsci, intel-mkl]
        fftw-api: [cray-fftw]
        mpi: [cray-mpich]
        scalapack: [cray-libsci, intel-mkl]
    amrex:
      variants: +fortran +hypre +openmp +shared
    bash:
      buildable: false
      externals:
      - spec: bash@4.4.23
        prefix: /
    bzip2:
      version: [1.0.6]
      externals:
      - spec: bzip2@1.0.6
        prefix: /usr
    coreutils:
      buildable: false
      version: [8.29]
      externals:
      - spec: coreutils@8.29
        prefix: /usr
    cpio:
      buildable: false
      externals:
      - spec: cpio@2.12
        prefix: /
    cray-libsci:
      buildable: false
      version: [20.09.1]
```

(continues on next page)

(continued from previous page)

```
    externals:
    - spec: cray-libsci@20.09.1 %gcc
      prefix: /opt/cray/pe/libsci/20.09.1/gnu/8.1
      modules:
      - cray-libsci/20.09.1
    - spec: cray-libsci@20.09.1 %intel
      prefix: /opt/cray/pe/libsci/20.09.1/intel/16.0
      modules:
      - cray-libsci/20.09.1
  cray-fftw:
    buildable: false
    externals:
    - spec: cray-fftw@3.3.8.10
      modules:
      - cray-fftw/3.3.8.10
  cray-mpich:
    buildable: false
    externals:
    - spec: cray-mpich@7.7.19 %intel
      prefix: /opt/cray/pe/mpt/7.7.19/gni/mpich-intel/16.0
      modules:
      - cray-mpich/7.7.19
    - spec: cray-mpich@7.7.19 %gcc
      prefix: /opt/cray/pe/mpt/7.7.19/gni/mpich-gnu/8.2
      modules:
      - cray-mpich/7.7.19
  curl:
    externals:
    - spec: curl@7.66.0+gssapi+ldap+nghttp2
      prefix: /usr
  diffutils:
    version: [3.6]
    externals:
    - spec: diffutils@3.6
      prefix: /usr
  elfutils:
    version: [0.168]
    externals:
    - spec: elfutils@0.168
      prefix: /usr
  findutils:
    version: [4.6.0]
    externals:
    - spec: findutils@4.6.0
      prefix: /usr
  hdf5:
    variants: +fortran +hl +shared api=v18
    version: [1.12.1]
    externals:
    - spec: hdf5@1.12.1.1%intel+shared+fortran+hl~mpi
      modules:
      - cray-hdf5/1.12.1.1
```

(continues on next page)

(continued from previous page)

```
    - spec: hdf5@1.12.1.1%intel+shared+fortran+hl+mpi
      modules:
      - cray-hdf5-parallel/1.12.1.1
    - spec: hdf5@1.12.1.1%gcc+shared+fortran+hl~mpi
      modules:
      - cray-hdf5/1.12.1.1
    - spec: hdf5@1.12.1.1%gcc+shared+fortran+hl+mpi
      modules:
      - cray-hdf5-parallel/1.12.1.1
  hypre:
    variants: +openmp +superlu-dist
  gawk:
    buildable: false
    externals:
    - spec: gawk@4.2.1
      prefix: /usr
  git:
    version: [2.26.2]
    buildable: false
    externals:
    - spec: git@2.26.2
      prefix: /usr
  gmake:
    buildable: false
    externals:
    - spec: gmake@4.2.1
      prefix: /usr
  intel-mkl:
    buildable: false
    externals:
    - spec: intel-mkl@19.1.2.254
      modules:
      - intel/19.1.2.254
  krb5:
    buildable: false
    externals:
    - spec: krb5@1.16.3
      prefix: /usr/lib/mit
  libunwind:
    variants: +pic +xz
  mercury:
    variants: ~bmi
  mesa:
    variants: ~llvm
  mesa18:
    variants: ~llvm
  m4:
    buildable: false
    externals:
    - spec: m4@1.4.18
      prefix: /usr
  mpich:
```

(continues on next page)

(continued from previous page)

```
    variants: ~wrapperrpath
  ncurses:
    variants: +termlib
    externals:
    - spec: ncurses@6.1
      prefix: /usr
  netcdf-c:
    version: [4.8.1.1]
    externals:
    - spec: netcdf-c@4.8.1.1~mpi
      modules:
      - cray-netcdf/4.8.1.1
    - spec: netcdf-c@4.8.1.1+mpi
      modules:
      - cray-netcdf-hdf5parallel/4.8.1.1
  openssl:
    buildable: false
    version: [1.1.1d]
    externals:
    - spec: openssl@1.1.1d
      prefix: /usr
  openssh:
    buildable: false
    externals:
    - spec: openssh@8.1p1
      prefix: /usr
  pdsh:
    buildable: false
    externals:
    - spec: pdsh@2.33
      prefix: /usr
  petsc:
    variants: +openmp
  perl:
    version: [5.32.0]
  pkg-config:
    buildable: false
    version: [0.29.2]
    externals:
    - spec: pkg-config@0.29.2
      prefix: /usr
  readline:
    version: [7.0]
    buildable: false
    externals:
    - spec: readline@7.0
      prefix: /usr
  sed:
    buildable: false
    externals:
    - spec: sed@4.4
      prefix: /usr
```

(continues on next page)

(continued from previous page)

```
    slurm:
      buildable: false
      version: [20-11-8-1]
      externals:
      - spec: slurm@20-11-8-1
        prefix: /usr
    superlu-dist:
      variants: +openmp
    strumpack:
      variants: ~slate
    tar:
      version: [1.3]
      buildable: false
      externals:
      - spec: tar@1.30
        prefix: /usr
    tcsh:
      version: [6.20.0]
      buildable: false
      externals:
      - spec: tcsh@6.20.0
        prefix: /usr
    trilinos:
      variants: +amesos +amesos2 +anasazi +aztec +belos +boost +epetra +epetraext
        +ifpack +ifpack2 +intrepid +intrepid2 +isorropia +kokkos +ml +minitensor +muelu
        +nox +piro +phalanx +rol +rythmos +sacado +stk +shards +shylu +stokhos␣
↪+stratimikos
        +teko +tempus +tpetra +trilinoscouplings +zoltan +zoltan2 +superlu-dist␣
↪gotype=long_long
    unzip:
      version: [6.0]
      buildable: false
      externals:
      - spec: unzip@6.0
        prefix: /usr
    util-linux-uuid:
      version: [2.31.1]
      buildable: false
      externals:
      - spec: util-linux-uuid@2.31.1
        prefix: /usr
    zsh:
      version: [5.6]
      buildable: false
      externals:
      - spec: zsh@5.6
        prefix: /usr
```

2.4 Perlmutter E4S 21.11

Shown below the production spack configuration for Perlmutter E4S 21.11. You can access this stack via `module load e4s/21.11-tcl` or `module load e4s/21.11-lmod` on Perlmutter. Please see our user documentation for this stack at https://docs.nersc.gov/applications/e4s/perlmutter/21.11/.

```
# This is a Spack Environment file.
#
# It describes a set of packages to be installed, along with
# configuration settings.
spack:
  view: false
  config:
    build_stage: $CFS/m3503/spack-stage
    misc_cache: $CFS/m3503/misc_cache
    install_tree:
      concretizer: clingo
      root: /global/common/software/spackecp/perlmutter/e4s-21.11/software
    module_roots:
      tcl: /global/common/software/spackecp/perlmutter/e4s-21.11/modules/tcl
      lmod: /global/common/software/spackecp/perlmutter/e4s-21.11/modules/lmod
  modules:
    prefix_inspections:
      include: [C_INCLUDE_PATH, CPLUS_INCLUDE_PATH, CPATH]
      lib: [LIBRARY_PATH, LD_LIBRARY_PATH]
      lib64: [LIBRARY_PATH, LD_LIBRARY_PATH]
    default:
      enable:
      - lmod
      lmod:
        blacklist_implicits: true
        hash_length: 0
        core_compilers:
        - gcc@7.5.0
        hierarchy:
        - mpi
        defaults:
        - gcc
        - nvhpc
        - cray-mpich@8.1.13 %gcc
        - cray-mpich@8.1.13 %nvhpc
        all:
          autoload: direct
          environment:
            set:
              '{name}_ROOT': '{prefix}'
          suffixes:
            ^cuda: cuda
        warpx:
          suffixes:
            warpx dims=2: dims2
            warpx dims=3: dims3
        projections:
```

(continues on next page)

(continued from previous page)

```
        all: '{name}/{version}'
  tcl:
    hash_length: 0
    naming_scheme: '{name}/{version}-{compiler.name}-{compiler.version}'
    blacklist_implicits: true
    all:
      autoload: direct
      conflict:
      - '{name}'
      environment:
        set:
          '{name}_ROOT': '{prefix}'
      suffixes:
        ^cray-mpich: mpi
        ^cuda: cuda
    warpx:
      suffixes:
        warpx dims=2: dims2
        warpx dims=3: dims3
    blacklist:
    - gcc
    - nvhpc
    - cray-mpich
compilers:
- compiler:
    spec: gcc@7.5.0
    paths:
      cc: /usr/bin/gcc
      cxx: /usr/bin/g++
      f77: /usr/bin/gfortran
      fc: /usr/bin/gfortran
    flags: {}
    operating_system: sles15
    target: any
    modules: []
- compiler:
    spec: nvhpc@21.11
    paths:
      cc: /opt/cray/pe/craype/default/bin/cc
      cxx: /opt/cray/pe/craype/default/bin/CC
      f77: /opt/cray/pe/craype/default/bin/ftn
      fc: /opt/cray/pe/craype/default/bin/ftn
    flags: {}
    operating_system: sles15
    target: any
    modules:
    - PrgEnv-nvidia
    - nvidia/21.11
    - craype-x86-milan
    - libfabric
- compiler:
    spec: gcc@11.2.0
```

(continues on next page)

(continued from previous page)

```
    paths:
      cc: cc
      cxx: CC
      f77: ftn
      fc: ftn
    flags: {}
    operating_system: sles15
    target: any
    modules:
    - PrgEnv-gnu
    - gcc/11.2.0
    - craype-x86-milan
    - libfabric
    extra_rpaths: []
definitions:
- gcc_compilers: ['%gcc@11.2.0']
- nvhpc_compilers: ['%nvhpc@21.11']
- compilers: [gcc@11.2.0 %gcc@7.5.0, nvhpc@21.11 %gcc@7.5.0]
- mpis: [cray-mpich@8.1.13 %gcc@11.2.0, cray-mpich@8.1.13 %nvhpc@21.11]
- gcc_specs:
  - adios2@2.7.1
  - amrex@21.11 +fortran +hypre +openmp +petsc +shared
  - conduit@0.7.2
  - dyninst@11.0.1
  - gasnet@2021.9.0
  - globalarrays@5.8
  - hdf5@1.12.1
  - hypre@2.23.0 +openmp +superlu-dist
  - kokkos-kernels@3.4.01 +openmp
  - kokkos@3.4.01 +openmp
  - mercury@2.0.1
  - mfem@4.3.0
  - mpark-variant@1.4.0
  - openpmd-api@0.14.3
  - papi@6.0.0.1
  - papyrus@1.0.2
  - parsec@3.0.2012 ~cuda
  - pdt@3.25.1
  - petsc@3.16.1 +openmp +strumpack
  - qthreads@1.16 scheduler=distrib
  - raja@0.14.0
  - slepc@3.16.0
  - strumpack@6.1.0 ~slate
  - sundials@5.8.0 +openmp +hypre
  - superlu-dist@7.1.1 +openmp
  - superlu@5.3.0
  - swig@4.0.2
  - sz@2.1.12
  - tau +mpi +python
  - trilinos@13.0.1 +amesos +amesos2 +anasazi +aztec +belos +boost +epetra +epetraext␣
↪+ifpack +ifpack2 +intrepid +intrepid2 +isorropia +kokkos +ml +minitensor +muelu +nox␣
↪+piro +phalanx +rol +rythmos +sacado +stk +shards +shylu +stokhos +stratimikos +teko␣
```

(continues on next page)

(continued from previous page)

```
↪+tempus +tpetra +trilinoscouplings +zoltan +zoltan2 +superlu-dist gotype=long_long
    - umap@2.1.0
    - upcxx@2021.9.0 +gasnet +mpi
    #- warpx dims=2
    #- warpx dims=3
  - cuda_specs:
    - hypre@2.23.0+cuda cuda_arch=80
    - kokkos-kernels@3.4.01 +openmp +cuda cuda_arch=80 ^kokkos +openmp +wrapper +cuda␣
↪cuda_arch=80
    - kokkos@3.4.01 +openmp +wrapper +cuda cuda_arch=80
    - mfem@4.3.0+cuda cuda_arch=80
    - petsc@3.16.1 +cuda cuda_arch=80
    - slepc@3.16.0 +cuda cuda_arch=80 ^petsc@3.16.1 +cuda cuda_arch=80
    - umpire@6.0.0 ~shared +cuda cuda_arch=80
    - upcxx@2021.9.0 +cuda
    - zfp@0.5.5 +cuda cuda_arch=80
    - raja@0.14.0+cuda cuda_arch=80 # CUB in your include path is not compatible with␣
↪this release of Thrust
    #- parsec@3.0.2012+cuda cuda_arch=80 # parsec/mca/device/cuda/transfer.c:168:␣
↪multiple definition of `parsec_CUDA_d2h_max_flows'
    #- amrex@21.11 +cuda cuda_arch=80
    #- magma@2.6.1+cuda cuda_arch=80
    #- strumpack@6.1.0 ~slate +cuda cuda_arch=80
    #- slate@2021.05.02 +cuda cuda_arch=80
    #- superlu-dist@7.1.1 +openmp +cuda cuda_arch=80
    #- sundials@5.8.0 +openmp +cuda cuda_arch=80
  - nvhpc_specs:
    - metis@5.1.0
    - umpire@6.0.0 ~shared +cuda cuda_arch=80
    - upcxx@2021.9.0 +cuda
    - zfp@0.5.5 +cuda cuda_arch=80
    #- hypre@2.23.0 +cuda cuda_arch=80
    # unable to install for nvhpc compiler
    #- amrex@21.11 +cuda cuda_arch=80
    #- petsc@3.16.1 +cuda cuda_arch=80
    #- kokkos-kernels@3.4.01 +openmp +wrapper +cuda cuda_arch=80 ^kokkos +openmp␣
↪+wrapper +cuda cuda_arch=80
    #- kokkos@3.4.01 +openmp +wrapper +cuda cuda_arch=80
    #- raja@0.14.0+cuda cuda_arch=80
  - nersc_specs:
    - chapel@1.24.1
    - gsl@2.7
    - fftw@3.3.10
    - nccmp@1.9.0.1
    - netcdf-c@4.8.1
    - netcdf-fortran@4.5.3
    - nco@5.0.1
    - metis@5.1.0
    - parallel-netcdf@1.12.2
    - parmetis@4.0.3
    - gromacs@2021.3
    #- plumed@2.6.3
```

(continues on next page)

(continued from previous page)

```
    #- wannier90@3.1.0
  specs:
  - matrix:
    - [$gcc_specs]
    - [$gcc_compilers]
  - matrix:
    - [$cuda_specs]
    - [$gcc_compilers]
  - matrix:
    - [$nvhpc_specs]
    - [$nvhpc_compilers]
  - $compilers
  - $mpis
  - $nersc_specs
  packages:
    all:
      compiler: [gcc@11.2.0, nvhpc@21.11]
      providers:
        blas: [cray-libsci]
        mpi: [cray-mpich]
    amrex:
      variants: +fortran +hypre +openmp +petsc +shared
    bzip2:
      version: [1.0.6]
      externals:
      - spec: bzip2@1.0.6
        prefix: /usr
    cray-libsci:
      buildable: false
      externals:
      - spec: cray-libsci@21.08.1.2
        modules:
        - cray-libsci/21.08.1.2
    cray-mpich:
      buildable: false
      externals:
      - spec: cray-mpich@8.1.13 %gcc@11.2.0
        prefix: /opt/cray/pe/mpich/8.1.13/ofi/gnu/9.1
        modules:
        - cray-mpich/8.1.13
        - cudatoolkit/11.5
      - spec: cray-mpich@8.1.13 %nvhpc@21.11
        prefix: /opt/cray/pe/mpich/8.1.13/ofi/nvidia/20.7
        modules:
        - cray-mpich/8.1.13
        - cudatoolkit/11.5
    cuda:
      buildable: false
      version: [11.5.0]
      externals:
      - spec: cuda@11.5.0
        prefix: /opt/nvidia/hpc_sdk/Linux_x86_64/21.11/cuda/11.5
```

(continues on next page)

(continued from previous page)

```
      modules:
      - cudatoolkit/11.5
  cub:
    buildable: false
    externals:
    - spec: cub@1.13.1
      prefix: /opt/nvidia/hpc_sdk/Linux_x86_64/21.11/math_libs/11.5
      modules:
      - cudatoolkit/11.5
  curl:
    buildable: false
    externals:
    - spec: curl@7.66.0
      prefix: /usr
  diffutils:
    version: [3.6]
    externals:
    - spec: diffutils@3.6
      prefix: /usr
  findutils:
    version: [4.6.0]
    externals:
    - spec: findutils@4.6.0
      prefix: /usr
  hdf5:
    variants: +fortran +hl +shared api=v18
    version: [1.12.1]
  hypre:
    variants: +openmp +superlu-dist
  gcc:
    buildable: false
    externals:
    - spec: gcc@11.2.0 %gcc@7.5.0
      modules:
      - PrgEnv-gnu
      - gcc/11.2.0
      - craype-x86-milan
      - libfabric
  git:
    version: [2.26.2]
    buildable: false
    externals:
    - spec: git@2.26.2
      prefix: /usr
  libfabric:
    buildable: false
    variants: fabrics=sockets,tcp,udp,rxm
    externals:
    - spec: libfabric@1.11.0.4.75
      prefix: /opt/cray/libfabric/1.11.0.4.75
      modules:
      - libfabric/1.11.0.4.75
```

(continues on next page)

(continued from previous page)

```
    libunwind:
      variants: +pic +xz
    mercury:
      variants: ~bmi
    mesa:
      variants: ~llvm
    mesa18:
      variants: ~llvm
    m4:
      buildable: false
      externals:
      - spec: m4@1.4.18
        prefix: /usr
    mpich:
      variants: ~wrapperrpath
    ncurses:
      variants: +termlib
      externals:
      - spec: ncurses@6.1
        prefix: /usr
    nvhpc:
      buildable: false
      externals:
      - spec: nvhpc@21.11 %gcc@7.5.0
        modules:
        - PrgEnv-nvidia
        - nvidia/21.11
        - craype-x86-milan
        - libfabric
    openssl:
      version: [1.1.0i]
      buildable: false
      externals:
      - spec: openssl@1.1.0i
        prefix: /usr
    openssh:
      version: [7.9p1]
      buildable: false
      externals:
      - spec: openssh@7.9p1
        prefix: /usr
    petsc:
      variants: +openmp +strumpack
    pdsh:
      buildable: false
      externals:
      - spec: pdsh@2.34
        prefix: /usr
    readline:
      version: [7.0]
      buildable: false
      externals:
```

(continues on next page)

(continued from previous page)

```
      - spec: readline@7.0
        prefix: /usr
    slurm:
      buildable: false
      version: [20-11-8-1]
      externals:
      - spec: slurm@20-11-8-1
        prefix: /usr
    superlu-dist:
      variants: +openmp
    strumpack:
      variants: ~slate
    tar:
      version: [1.3]
      buildable: false
      externals:
      - spec: tar@1.30
        prefix: /usr
    trilinos:
      variants: +amesos +amesos2 +anasazi +aztec +belos +boost +epetra +epetraext
        +ifpack +ifpack2 +intrepid +intrepid2 +isorropia +kokkos +ml +minitensor +muelu
        +nox +piro +phalanx +rol +rythmos +sacado +stk +shards +shylu +stokhos␣
↪+stratimikos
        +teko +tempus +tpetra +trilinoscouplings +zoltan +zoltan2 +superlu-dist␣
↪gotype=long_long
    unzip:
      version: [6.0]
      buildable: false
      externals:
      - spec: unzip@6.0
        prefix: /usr
    util-linux-uuid:
      version: [2.33.1]
      buildable: false
      externals:
      - spec: util-linux-uuid@2.33.1
        prefix: /usr
    xz:
      version: [5.2.3]
      buildable: false
      externals:
      - spec: xz@5.2.3
        prefix: /usr
    zsh:
      version: [5.6]
      buildable: false
      externals:
      - spec: zsh@5.6
        prefix: /usr
```

2.5 Cori E4S 21.05

```
spack:
  view: false
  concretization: separately
  config:
    install_tree:
      root: /global/common/software/spackecp/e4s-21.05/software
    module_roots:
      tcl: /global/common/software/spackecp/e4s-21.05/modules/
    build_stage: $tempdir/user/spack-stage
  modules:
    enable:
    - tcl
    tcl:
      blacklist_implicits: true
      hash_length: 0
      naming_scheme: '{name}/{version}-{compiler.name}-{compiler.version}'
      all:
        conflict:
        - '{name}'
        environment:
          set:
            '{name}_ROOT': '{prefix}'
      darshan-runtime:
        conflict:
        - darshan
      darshan-util:
        conflict:
        - darshan
      projections:
        all: '{name}/{version}-{compiler.name}-{compiler.version}'
        py-warpx ^warpx dims=2: '{name}/{version}-dims2'
        py-warpx ^warpx dims=3: '{name}/{version}-dims3'
        py-warpx ^warpx dims=rz: '{name}/{version}-dimsRZ'
        warpx dims=2: '{name}/{version}-dims2'
        warpx dims=3: '{name}/{version}-dims3'
        warpx dims=rz: '{name}/{version}-dimsRZ'
        boost cxxstd=98: '{name}/{version}-cxxstd=98'
        boost cxxstd=17: '{name}/{version}-cxxstd=17'
        kokkos +openmp: '{name}/{version}-openmp'
        kokkos ~openmp: '{name}/{version}'
  mirrors:
    cori-e4s-21.05: https://cache.e4s.io/21.05
  compilers:
  - compiler:
      spec: intel@19.1.3.304
      paths:
        cc: cc
        cxx: CC
        f77: ftn
        fc: ftn
```

(continues on next page)

(continued from previous page)

```
    flags: {}
    operating_system: cnl7
    target: any
    modules:
    - PrgEnv-intel
    - intel/19.1.3.304
    environment: {}
    extra_rpaths: []
packages:
  all:
    compiler:
    - intel@19.1.3.304
    providers:
      blas:
      - openblas
      mpi:
      - mpich
    target:
    - haswell
    variants: +mpi
  slurm:
    buildable: false
    version: [20-02-4-1]
    externals:
    - spec: slurm@20-02-4-1
      prefix: /usr
  mpich:
    buildable: false
    externals:
    - spec: mpich@3.1
      modules:
      - cray-mpich/7.7.10
  autoconf:
    version:
    - '2.69'
  automake:
    version:
    - 1.16.3
  berkeley-db:
    version:
    - 18.1.40
  binutils:
    variants: +ld +gold +headers +libiberty ~nls +plugins
    version:
    - 2.33.1
  boost:
    version:
    - 1.75.0
  bzip2:
    version:
    - 1.0.8
  c-blosc:
```

(continues on next page)

(continued from previous page)

```
    version:
    - 1.21.0
  cmake:
    version:
    - 3.20.2
  curl:
    version:
    - 7.76.0
  diffutils:
    version:
    - 3.7
  elfutils:
    version:
    - 0.182
    variants: +bzip2 ~nls +xz
  expat:
    version:
    - 2.2.10
  findutils:
    version:
    - 4.8.0
  gdbm:
    version:
    - 1.18.1
  gettext:
    version:
    - 0.21
  git:
    version:
    - 2.31.0
  glib:
    version:
    - 2.66.8
  hdf5:
    variants: +fortran +hl +shared
    version:
    - 1.10.7
  help2man:
    version:
    - 1.47.16
  hwloc:
    version:
    - 2.4.1
  json-c:
    version:
    - 0.13.1
  libbsd:
    version:
    - 0.10.0
  libfabric:
    version:
    - 1.12.1
```

(continues on next page)

(continued from previous page)

```
    variants: fabrics=sockets,tcp,udp,rxm
  libiconv:
    version:
    - 1.16
  libsigsegv:
    version:
    - 2.12
  libpciaccess:
    version:
    - 0.16
  libtool:
    version:
    - 2.4.6
  libunwind:
    version:
    - 1.5.0
    variants: +pic +xz
  libxml2:
    version:
    - 2.9.10
  lz4:
    version:
    - 1.9.3
  m4:
    version:
    - 1.4.18
  mesa:
    variants: ~llvm
  mesa18:
    variants: ~llvm
  ncurses:
    version:
    - 6.2
    variants: +termlib
  numactl:
    version:
    - 2.0.14
  openblas:
    version:
    - 0.3.10
    variants: threads=openmp
  perl:
    version:
    - 5.32.0
  pkgconf:
    version:
    - 1.7.3
  python:
    version:
    - 3.8.10
  readline:
    version:
```

(continues on next page)

(continued from previous page)

```
      - 8
    sqlite:
      version:
      - 3.34.0
    tar:
      version:
      - 1.32
    texinfo:
      version:
      - 6.5
    xz:
      version:
      - 5.2.5
      variants: +pic
    zlib:
      version:
      - 1.2.11
    zstd:
      version:
      - 1.4.9

  definitions:
  - cuda_specs:
    - amrex@21.05 +cuda cuda_arch=70
    - axom@0.5.0 +cuda cuda_arch=70 ^umpire~shared
    - caliper@2.5.0 +cuda cuda_arch=70
    - chai@2.3.0 +cuda ~benchmarks ~tests cuda_arch=70 ^umpire~shared
    - ginkgo@1.3.0 +cuda cuda_arch=70
    - hpx@1.6.0 +cuda cuda_arch=70
    - kokkos@3.4.00 +cuda +wrapper cuda_arch=70
    - kokkos-kernels@3.2.00 +cuda cuda_arch=70 ^kokkos +cuda +wrapper cuda_arch=70
    - magma@2.5.4 cuda_arch=70
    - raja@0.13.0 +cuda cuda_arch=70
    - slate@2021.05.02 +cuda cuda_arch=70
    - strumpack@5.1.1 +cuda ~slate cuda_arch=70
    - sundials@5.7.0 +cuda cuda_arch=70
    - superlu-dist@6.4.0 +cuda cuda_arch=70
    - tasmanian@7.5 +cuda cuda_arch=70
    - umpire@4.1.2 +cuda ~shared cuda_arch=70
    - zfp +cuda cuda_arch=70
    #- ascent@0.7.1 +cuda ~shared cuda_arch=70
    #- hypre@2.20.0 +cuda cuda_arch=70
    #- mfem@4.2.0 +cuda cuda_arch=70

  - default_specs:
    - adios2@2.7.1
    - adios@1.13.1
    - aml@0.1.0
    - amrex@21.05
    - arborx@1.0
    - argobots@1.1
    - ascent@0.7.1 ~fortran
```

(continues on next page)

(continued from previous page)

```
    - bolt@2.0
    - cabana@0.3.0
    - caliper@2.5.0
    - chai@2.3.0 ~benchmarks ~tests
    - conduit@0.7.2
    - darshan-runtime@3.3.0
    - darshan-util@3.3.0
    - faodel@1.1906.1
    - flecsi@1.4 +cinch
    - flit@2.1.0
    - gasnet@2021.3.0
    - ginkgo@1.3.0
    - globalarrays@5.8
    - gmp@6.2.1
    - gotcha@1.0.3
    - hdf5@1.10.7
    - hypre@2.20.0
    - kokkos-kernels@3.2.00 +openmp
    - kokkos@3.4.00 +openmp
    - legion@21.03.0
    - libnrm@0.1.0
    - libquo@1.3.1
    - libunwind@1.5.0
    - loki@0.1.7
    - mercury@2.0.1
    - metall@0.13
    - mfem@4.2.0
    - mpark-variant@1.4.0
    - ninja@1.10.2
    - openpmd-api@0.13.4
    - papi@6.0.0.1
    - papyrus@1.0.1
    - parallel-netcdf@1.12.2
    - pdt@3.25.1
    - petsc@3.15.0
    - precice@2.2.1
    - pumi@2.2.5
    - py-libensemble@0.7.2
    - py-petsc4py@3.15.0
    - py-warpx@21.05 ^warpx dims=2
    - py-warpx@21.05 ^warpx dims=3
    - py-warpx@21.05 ^warpx dims=rz
    - qthreads@1.16 scheduler=distrib
    - raja@0.13.0
    - scr@3.0rc1
    - slepc@3.15.0
    - stc@0.9.0
    - strumpack@5.1.1 ~slate
    - sundials@5.7.0
    - superlu-dist@6.4.0
    - superlu@5.2.1
    - swig@4.0.2
```

(continues on next page)

(continued from previous page)

```
    - swig@4.0.2-fortran
    - sz@2.1.11.1
    - tasmanian@7.5
    - tau@2.30.1
    - turbine@1.3.0
    - umap@2.1.0
    - umpire@4.1.2
    - upcxx@2021.3.0
    - zfp@0.5.5

    # Explicit conflicts with Cray -or- Intel compiler (prohibited via package.py)
   #- dyninst@11.0.0
   #- hpctoolkit@2021.03.01
   #- plasma@20.9.20
   #- qt@5.15.2
   #- qwt@6.1.6
   #- slate@2021.05.02 ~cuda

    # Cannot build suite-sparse due to OOM killer
   #- fortrilinos@2.0.0 ^trilinos +nox +superlu-dist +stratimikos
   #- omega-h@9.32.5
   #- trilinos@13.0.1
   #- trilinos@13.0.1 +nox +superlu-dist

    # Failed builds
   #- archer@2.0.0 # llvm@8 fails
   #- axom@0.5.0 # thirdparty/sol/sol.hpp(11408): rvalue ref cannot be bound to an lvalue
   #- heffte@2.0.0 # test/test_units_nompi.cpp(499): error: more than one instance of␣
↪constructor "heffte::box3d::box3d"
   #- hpx@1.6.0 # include/boost/asio/impl/read.hpp(377): no instance of overloaded␣
↪function "hpx::util::detail::bound
   #- mpifileutils@0.11 ~xattr # libcap: _caps_output.gperf:96:53: unknown type name
↪'size_t', libcircle: configure: check if MPI setup correctly
   #- nrm@0.1.0 # py-gevent: configure: compiler doesn't halt on function prototype␣
↪mismatch
   #- py-jupyterhub@1.0.0
   #- rempi@1.1.0 # configure: couldn't find MPI
   #- unifyfs@0.9.1 # configure: couldn't find MPI

  specs:
  - $default_specs
```

2.6 Cori E4S 21.02

```
spack:
  view: false
  concretization: separately
  config:
    install_tree:
      root: /global/common/software/spackecp/e4s-21.02/software
    module_roots:
      tcl: /global/common/software/spackecp/e4s-21.02/modules/
    build_stage: $tempdir/user/spack-stage
  modules:
    enable:
    - tcl
    tcl:
      blacklist_implicits: true
      hash_length: 0
      naming_scheme: '{name}/{version}-{compiler.name}-{compiler.version}'
      all:
        conflict:
        - '{name}'
        environment:
          set:
            '{name}_ROOT': '{prefix}'
      darshan-runtime:
        conflict:
        - 'darshan'
      darshan-util:
        conflict:
        - 'darshan'
      projections:
        all: '{name}/{version}-{compiler.name}-{compiler.version}'
  mirrors:
    cori-e4s-21.02: /global/common/software/spackecp/mirrors/cori-e4s-21.02
  compilers:
  - compiler:
      spec: intel@19.1.2.254
      paths:
        cc: cc
        cxx: CC
        f77: ftn
        fc: ftn
      flags: {}
      operating_system: cnl7
      target: any
      modules:
      - PrgEnv-intel
      - intel/19.1.2.254
      environment: {unset: []}
      extra_rpaths: []
  - compiler:
      spec: gcc@10.1.0
```

(continues on next page)

(continued from previous page)

```
      paths:
        cc: cc
        cxx: CC
        f77: ftn
        fc: ftn
      operating_system: cnl7
      modules:
      - PrgEnv-gnu
      - gcc/10.1.0

  definitions:
  - intel_compiler: ['%intel@19.1.2.254']
  - gcc_compiler: ['%gcc@10.1.0']
  - e4s_intel:
    - adios2@2.7.1 +hdf5
    - aml@0.1.0
    - arborx@0.9-beta +openmp
    - bolt@2.0
    - caliper@2.5.0 +fortran
    - faodel@1.1906.1
    - flecsi@1.4 +cinch +caliper +graphviz +tutorial
    - flit@2.1.0
    - gasnet@2020.3.0 +udp
    - ginkgo@1.3.0
    - gotcha@1.0.3 +test
    - hdf5@1.10.7
    - hypre@2.20.0 +mixedint +superlu-dist +openmp
    - libnrm@0.1.0
    - libquo@1.3.1
    - mercury@2.0.0 +udreg
    - mfem@4.2.0 +examples +gnutls +gslib +lapack +libunwind +openmp +threadsafe +pumi␣
↪+umpire
    - ninja@1.10.2
    - omega-h@9.32.5 ~trilinos
    - openpmd-api@0.13.2
    - papi@6.0.0.1 +example +static_tools +powercap +infiniband
    - papyrus@1.0.1
    - pdt@3.25.1 +pic
    - precice@2.2.0 +python
    - pumi@2.2.5 +fortran
    - qthreads@1.16 ~hwloc
    - raja@0.13.0 +tests
    - slepc@3.14.2
    - strumpack@5.1.1 +shared
    - sundials@5.7.0 +examples-cxx +hypre +klu +lapack
    - superlu@5.2.1
    - superlu-dist@6.4.0 +openmp
    - swig@4.0.2-fortran
    - tasmanian@7.3 +blas +fortran +mpi +python +xsdkflags
    - tau@2.30.1 +mpi ~pdt
    - turbine@1.2.3 +hdf5 +python
    - umap@2.1.0 +tests
```

(continues on next page)

(continued from previous page)

```
    - umpire@4.1.2 +fortran +numa +openmp
    - upcxx@2020.10.0
    - zfp@0.5.5 +aligned +c +fortran +openmp +profile

  - e4s_gcc:
    - darshan-runtime@3.2.1 +slurm
    - darshan-util@3.2.1 +bzip2
    - dyninst@10.2.1
    - legion@20.03.0
    - plasma@20.9.20
    - slate@2020.10.00 ~cuda


    # skipping package
    #  - adios@1.13.1 +bzip2 +fortran +hdf5 +netcdf
    # - kokkos-kernels@3.2.00 +mkl +openmp
    # - kokkos@3.2.00  +compiler_warnings +deprecated_code +examples +hwloc +memkind␣
↪+numactl +openmp +pic +tests
    # - openmpi@4.0.5 +cxx +thread_multiple schedulers=slurm
    # - parallel-netcdf@1.12.1 +burstbuffer
    # - petsc@3.14.4 +X +fftw +jpeg +libpng +libyaml +memkind
    # - py-jupyterhub@1.0.0
    # - py-libensemble@0.7.1 +mpi +nlopt +petsc4py  +scipy
    # - py-petsc4py@3.14.1
    # - trilinos@13.0.1

    # _____________________________ ISSUES TO SOLVE _____________________________
    # issue installing vtkh using intel compiler
    # using gcc compiler ascent has dependency for conduit@develop which not pinned to␣
↪version. There was a build error related to missing HDF5 library
    # - ascent@0.6.0

    # Issue detecting fortran compiler https://cdash.spack.io/viewConfigure.php?
↪buildid=105216. Also issue installing conduit since its tied to 'develop'. Tried using␣
↪conduit@0.7.1 and still failed see https://cdash.spack.io/viewBuildError.php?
↪buildid=105206. Talk to @cyrush at spack slack.
    # - axom@0.4.0 +mfem +python

    # /usr/lib64/gcc/x86_64-suse-linux/7/../../../../x86_64-suse-linux/bin/ld: /usr/lib/
↪libm.so: error adding symbols: file in wrong format see https://cdash.spack.io/
↪buildSummary.php?buildid=104952
    # - adios2@2.7.1 +hdf5 +dataman +dataspaces

    # skipping this version for now 5.7 is the latest version 5.8 doesn't exist in spack␣
↪repo
    # - globalarrays@5.8 +blas +lapack +scalapack

    #  Warning: Linking the shared library libhpcrun.la against the static library see ␣
↪https://cdash.spack.io/viewBuildError.php?buildid=104938
    # - hpctoolkit@2020.08.03 %gcc

    # error: identifier "HPX_SMT_PAUSE" is undefined see https://cdash.spack.io/
```

(continues on next page)

(continued from previous page)

```
↪viewBuildError.php?buildid=105747
    # - hpx@1.6.0 +async_mpi +examples

    # Error building legion with intel compiler https://cdash.spack.io/viewBuildError.
↪php?buildid=105190
    # - legion@20.03.0

    # skip magma because it's a GPU package
    #- magma@2.5.4 cuda_arch=70 ^cuda@10.2.89

    # error with intel compiler:  building dtcmp
    # error with gnu compiler: Could NOT find LibCircle (missing: LibCircle_LIBRARIES
    # - mpifileutils@0.10.1

    # /global/cfs/cdirs/m3503/spack-NSewtxLx/spack-stage/siddiq90/spack-stage-phist-1.9.
↪3-rznbmfuo2mt2erku4rit4peyqxu7iji4/spack-src/fortran_bindings/test/kernels.F90(63):␣
↪catastrophic error: **Internal compiler error: internal abort** Please report this␣
↪error along with the circumstances in which it occurred in a Software Problem Report. ␣
↪Note: File and line given may not be explicit cause of this error. see https://cdash.
↪spack.io/buildSummary.php?buildid=104915
    # - phist@1.9.3


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

    # "%intel@19:" conflicts with "slate" [Does not currently build with icpc >= 2019]
    # - slate@2020.10.00 ^cuda@10.2.89

    # build Error with Intel: error building dtcmp: configure: error: C compiler cannot␣
↪create executables
    # build Error with GCC: make[2]: *** No rule to make target '/global/cfs/cdirs/m3503/
↪spack-qhLmtUlQ/spack_path_placeholder/spack_path_placeholder/spack_path_placeholder/
↪spack_path_placehol/cray-cnl7-haswell/gcc-10.1.0/libyogrt-1.24-
↪6wngjuplxnjjsivzvilwjsp4gwu4ziuj/lib/libyogrt.a', needed by 'examples/test_ckpt_F'. ␣
↪Stop. see https://cdash.spack.io/buildSummary.php?buildid=104889
    # - scr@2.0.0
    # error installing ant Error: JAVA_HOME is not defined correctly. https://software.
↪nersc.gov/NERSC/e4s-2102/-/jobs/87103
    # - stc@0.8.3

    # Issue building sundials with raja support see https://cdash.spack.io/
↪viewBuildError.php?buildid=105455. Not sure if raja support with sundials is␣
↪neccessary.
    # sundials@5.7.0 +examples-cxx +examples-f2003 +f2003 +hypre +klu +lapack +openmp␣
↪+raja +superlu-dist

    # https://cdash.spack.io/viewBuildError.php?buildid=105513
    # - sz@2.1.11.1 +fortran +python +time_compression +random_access +pastri

    # issue building tau with intel see https://cdash.spack.io/viewBuildError.php?
```

(continues on next page)

(continued from previous page)

```
↪buildid=105235 one of the error points to missing `-lpdb` library. Tau has `+pdt`␣
↪enabled by default
    # - tau@2.30.1 +adios2 +gasnet +likwid  +ompt +openmp +mpi  +python +scorep +shmem␣
↪+sqlite

    #  Could NOT find AXL (missing: AXL_LIBRARIES AXL_INCLUDE_DIRS) see https://cdash.
↪spack.io/buildSummary.php?buildid=105476
    # - veloc@1.4

    # issue configure: error: "Couldn't find MPI" see https://cdash.spack.io/
↪viewConfigure.php?buildid=105491
    # issue installing mercury (dependency) for unifyfs with gcc https://cdash.spack.io/
↪buildSummary.php?buildid=105497
    #- unifyfs@0.9.1

  specs:
  - matrix:
    - [$e4s_intel]
    - [$intel_compiler]
  - matrix:
    - [$e4s_gcc]
    - [$gcc_compiler]

  packages:
    all:
      compiler: [intel@19.1.2.254, gcc@10.1.0]
      target: [haswell]
      providers:
        mpi: [mpich]
        mkl: [cray-libsci, intel-mkl]
        blas: [cray-libsci, intel-mkl]
        scalapack: [cray-libsci, intel-mkl]
        pkgconfig: [pkg-config]

    cray-libsci:
      buildable: false
      externals:
      - spec: cray-libsci@19.06.1%intel
        modules:
        - cray-libsci/19.06.1

    fftw:
      buildable: false
      externals:
      - spec: fftw@3.3.8.4%intel
        modules:
        - cray-fftw/3.3.8.4

    hdf5:
      variants: +cxx +debug +fortran +szip +threadsafe +hl

    hwloc:
```

(continues on next page)

(continued from previous page)

```
    buildable: false
    externals:
    - spec: hwloc
      prefix: /usr
  intel-mkl:
    buildable: false
    externals:
    - spec: intel-mkl@19.1.2.254
      modules:
      - intel/19.1.2.254

  mpich:
    buildable: false
    externals:
    - spec: mpich@3.1
      modules:
      - cray-mpich/7.7.10

  netcdf-c:
    buildable: false
    externals:
      - spec: netcdf-c@4.7.4
        modules:
        - cray-netcdf/4.7.4.0

  openssl:
    buildable: false
    externals:
    - spec: openssl@1.1.1g
      prefix: /usr
  # issue installing version 5.32.1 and confirmed 5.32.0 works
  perl:
    version: [5.32.0]

  # disable slate since we can't build with icc >= 19
  strumpack:
    variants: ~slate
```

2.7 Cori E4S 20.10

```
spack:
  concretization: separately
  view: false
  config:
    install_tree: /global/common/software/spackecp/e4s-20.10/software
    build_stage: $tempdir/$user/spack-stage
    module_roots:
      tcl: /global/common/software/spackecp/e4s-20.10/modules/
  mirrors::
    e4s-2020-10: /global/common/software/spackecp/mirrors/e4s-2020-10
```

(continues on next page)

(continued from previous page)

```
  modules:
    enable:
    - tcl
    tcl:
      hash_length: 8
      projections:
        all: '{name}/{version}-{compiler.name}-{compiler.version}'
      all:
        conflict:
        - '{name}'
        filter:
          environment_blacklist: []
        load: []
        environment:
          unset: []
      verbose: false
      whitelist: []
      blacklist: []
      blacklist_implicits: false

  definitions:
  - e4s:
    - adios2@2.6.0
    - aml@0.1.0
    - arborx@0.9-beta +openmp
    - bolt@1.0
    - caliper@2.4.0
    - darshan-runtime@3.2.1 +slurm
    - darshan-util@3.2.1 +bzip2
    - flit@2.1.0
    - gasnet@2020.3.0 +udp
    - ginkgo@1.2.0
    - globalarrays@5.7 +blas +lapack +scalapack
    - gotcha@1.0.3 +test
    - hdf5@1.10.6 +cxx +debug +fortran +szip +threadsafe +hl
    - hypre@2.20.0 +mixedint
    - kokkos-kernels@3.2.00 +mkl +openmp
    - kokkos@3.2.00 +debug +debug_dualview_modify_check +compiler_warnings +examples␣
↪+hwloc +memkind +numactl +openmp +pic +tests
    - libnrm@0.1.0
    - libquo@1.3.1
    - mercury@1.0.1 +udreg
    - mfem@4.1.0 +examples +gnutls +gslib +lapack +libunwind +openmp +threadsafe +pumi␣
↪+umpire
    - ninja@1.10.1
    - openpmd-api@0.12.0
    - papi@6.0.0.1 +example +static_tools
    - parallel-netcdf@1.12.1
    - pdt@3.25.1 +pic
    - petsc@3.14.0
    - pumi@2.2.2 +fortran
    - py-libensemble@0.7.0 +mpi +nlopt +scipy
```

(continues on next page)

(continued from previous page)

```
    - py-petsc4py@3.13.0
    - qthreads@1.14 ~hwloc
    - raja@0.12.1
    - slepc@3.14.0
    - stc@0.8.3
    - sundials@5.4.0 +examples-cxx +examples-f2003 ~examples-f77 +f2003 +klu +openmp␣
↪+hypre +lapack
    - superlu@5.2.1
    - superlu-dist@6.3.1
    - swig@4.0.2
    - sz@2.1.10 +fortran +hdf5 +python +time_compression +random_access +netcdf +pastri
    - tasmanian@7.3 +blas +fortran +mpi +python +xsdkflags
    - turbine@1.2.3 +hdf5 +python
    - umap@2.1.0 +tests
    - umpire@4.0.1 +fortran +numa +openmp
    - upcxx@2020.3.0
    - veloc@1.4
    - zfp@0.5.5


  # - adios@1.13.1 +netcdf +szip +fortran +bzip2  module already installed
  # - ascent@develop skipping package because its on develop
  # - axom@0.3.3 skip build for now, spack ci rebuild issue
  # issue with concretization of dyninst:  "%intel" conflicts with "dyninst" see https://
↪software.nersc.gov/ecp/nersc-e4s/-/jobs/46526
  # - dyninst@10.2.1 +static
  # - faodel@1.1906.1 network=libfabric issue with build https://software.nersc.gov/
↪NERSC/nersc-e4s/-/jobs/60284
  # flesci concretization issue: https://github.com/spack/spack/issues/19292
  # - flecsi@1 +cinch +coverage +doc +doxygen +graphviz +hdf5 +tutorial
  # - hpctoolkit@2020.08.03 +all-static +cray +mpi  # depends on dyninst
  # - hpx@1.5.1 issue with installing boost
  # - legion@20.03.0 failed to build se https://software.nersc.gov/ecp/e4s/
↪facilitypipelines/nersc-e4s/-/jobs/59787
  # - magma@2.5.3 this package requires GPU, this is not applicable for Cori
  # - mpifileutils@0.10.1 +gpfs +lustre # fails on libcircle requires MPICC wrapper see␣
↪https://software.nersc.gov/ecp/e4s/facilitypipelines/nersc-e4s/-/jobs/57907 we could␣
↪install OpenMPI and build this with the wrapper.
  #- openmpi            # skip openmpi
  # - omega-h@9.29.0
  # - papi@6.0.0.1 +example +static_tools   module already installed
  # - phist@1.9.1 see https://software.nersc.gov/NERSC/nersc-e4s/-/jobs/63409
  # concretization issue "%intel" conflicts with "plasma" see https://software.nersc.gov/
↪ecp/nersc-e4s/-/jobs/46533
  # - plasma@20.9.20
  # - precice@2.1.0 issue finding PETSC
  # - py-jupyterhub@1.0.0
  # error building rempi https://software.nersc.gov/ecp/nersc-e4s/-/jobs/32884
  # - rempi@1.1.0
  # - scr@2.0.0  # async_api=CRAY_DW issue finding DATAWARP libraries -- Could NOT find␣
↪DATAWARP (missing: DATAWARP_LIBRARIES DATAWARP_INCLUDE_DIRS) see https://software.
↪nersc.gov/ecp/e4s/facilitypipelines/nersc-e4s/-/jobs/59782
```

(continues on next page)

(continued from previous page)

```
  # - slate@develop package tied to develop skipping this build
  # - strumpack@4.0.0 +shared ~butterflypack ~cuda +count_flops +build_dev_tests +build_
↪tests
  # error building otf2, we can disable tau with otf2 support
  # - tau@2.29 +craycnl +openmp +mpi
  # - trilinos@13.0.0 +debug +float +openmp +pnetcdf +zlib
  # - unifyfs@0.9.0 +hdf5. can't find MPICC see https://software.nersc.gov/NERSC/nersc-
↪e4s/-/jobs/63408

  - arch:
    - '%intel@19.1.2.254 arch=cray-cnl7-haswell'
  specs:
  - matrix:
    - - $e4s
    - - $arch

  compilers:
  - compiler:
      spec: intel@19.1.2.254
      paths:
        cc: cc
        cxx: CC
        f77: ftn
        fc: ftn
      flags: {}
      operating_system: cnl7
      target: any
      modules:
      - PrgEnv-intel
      - intel/19.1.2.254
      environment: {unset: []}
      extra_rpaths: []


  packages:
    all:
      compiler: [intel@19.1.2.254]
      target: [haswell]
      providers:
        mpi: [mpich]
        mkl: [intel-mkl, cray-libsci]
        blas: [intel-mkl, cray-libsci]
        scalapack: [intel-mkl, cray-libsci]
        pkgconfig: [pkg-config]

    berkeley-db:
      version: [18.1.4]

    boost:
      version: [1.74.0]

    bzip2:
```

(continues on next page)

(continued from previous page)

```
    buildable: false
    externals:
    - spec: bzip2
      prefix: /usr

  cmake:
    version: [3.16.5]  # issue with cmake 3.17.3 using 3.16.5 for now see https://
↪github.com/spack/spack/issues/17605

  cray-libsci:
    buildable: false
    externals:
    - spec: cray-libsci@19.06.1%intel
      modules:
      - cray-libsci/19.06.1

  diffutils:
    version: [3.7]

  elfutils:
    version: [0.180]

  expat:
    version: [2.2.9]

  fftw:
    buildable: false
    externals:
    - spec: fftw@3.3.8.4%intel
      modules:
        - cray-fftw/3.3.8.4

  gdbm:
    version: [1.18.1]

  gettext:
    buildable: false
    externals:
    - spec: gettext
      prefix: /usr

  help2man:
    version: [1.47.11]

  hwloc:
    buildable: false
    externals:
    - spec: hwloc
      prefix: /usr

  hypre:
    version: [2.20.0]
```

(continues on next page)

(continued from previous page)

```
  intel-mkl:
    buildable: false
    externals:
    - spec: intel-mkl@19.1.2.254
      modules:
        - intel/19.1.2.254

  libbsd:
    version: [0.10.0]

  libiconv:
    version: [1.16]

  libsigsegv:
    version: [2.12]

  libxml2:
    version: [2.9.10]

  lz4:
    buildable: false
    externals:
    - spec: lz4
      prefix: /usr

  m4:
    buildable: false
    externals:
    - spec: m4
      prefix: /usr

  mpi:
    buildable: false

  mpich:
    buildable: false
    externals:
    - spec: mpich@3.1
      modules:
      - cray-mpich/7.7.10

  openssl:
    buildable: false
    externals:
    - spec: openssl@1.1.1g
      prefix: /usr

  ncurses:
    version: [6.2]

  netcdf:
```

(continues on next page)

(continued from previous page)

```
    buildable: false
    externals:
    - spec: netcdf@4.6.3.2%intel
      modules:
        - cray-netcdf/4.6.3.2

  perl:
    buildable: false
    externals:
    - spec: perl
      prefix: /usr

  petsc:
    version: [3.14.0]

  pdsh: # required for scr
    buildable: false
    externals:
    - spec: pdsh
      prefix: /usr

  pkgconf:
    version: [1.7.3]

  sqlite:
    version: [3.31.1]

  tar:
    buildable: false
    externals:
    - spec: tar
      prefix: /usr

  xz:
    buildable: false
    externals:
    - spec: xz
      prefix: /usr

  zlib:
    version: [1.2.11]
```

CHAPTER

THREE

CONFERENCES

Conference	Talk	Date	Link
SEA Improving Scientific Software Conference 2022	Spack Infrastructure at NERSC	Apr 5th, 2022	PPTX, VIDEO

CHAPTER

FOUR

INDICES AND TABLES

- genindex
- modindex
- search