nersc-spack-infrastructure

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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 Project makes use of spack package manager to install spack software stack on NERSC systems. This project contains spack configuration (`spack.yaml`) required to build the spack stacks. The spack stack is based on Extreme-Scale Scientific Software Stack (E4S) where we install spack packages provided by E4S and use the recommended spack branch. We leverage Gitlab CI to automate deployment to ensure reproducible and automated builds. For more details about this project you can see the documentation at https://nersc-spack-infrastructure.rtfd.io

1.1 Software Deployment Overview

The software deployment consist of the following steps

1. Acquire Spack Configuration from E4S project https://github.com/E4S-Project/e4s
2. Create one or more spack configuration files (spack.yaml) with list of E4S packages and integrate spack configuration for NERSC system
3. Create a Gitlab Job to trigger the pipeline for TDS and Deployment system
4. Create a Modulefile as entry point to stack
5. Write User Documentation
6. Share spack configuration with open-source community
7. Send announcement to all NERSC users

1.1.1 Step 1: Acquire Spack Configuration

At NERSC, we plan our software deployment with E4S releases which is typically every 3 months however we perform deployment every 6 months. Once E4S has released the spack configuration we acquire the spack configuration which is typically found in https://github.com/E4S-Project/e4s/tree/master/environments. We also acquire the spack branch used by E4S team as our baseline, this would be documented in the release notes. The name of branch map to the E4S version so version 23.05 will have a branch e4s-23.05.

Next, we copy the packages into our project and create the spack configuration

1.1.2 Step 2: Create Spack Configuration

In this step we create the spack configuration. First we create a sub-directory in *spack-configs* with the naming convention to distinguish E4S version. This typically includes the name of the system such as `cori` or `perlmutter` followed by name of e4s version such as `e4s-23.05`.

```
$ tree -L 1 spack-configs
spack-configs
├── cori-e4s-20.10
├── cori-e4s-21.02
├── cori-e4s-21.05
├── cori-e4s-22.02
├── perlmutter-e4s-21.11
├── perlmutter-e4s-22.05
├── perlmutter-e4s-22.11
├── perlmutter-e4s-23.05
├── perlmutter-spack-develop
└── perlmutter-user-spack

10 directories, 0 files
```

Inside one of the stacks, you will see several sub-directories that are used for defining a sub-stack. These sub-stacks correspond to spack environments. The `prod` directory is used for production deployment to install from the buildcache.

```
$ tree -L 3 spack-configs/perlmutter-e4s-22.11
spack-configs/perlmutter-e4s-22.11
├── cce
│   └── spack.yaml
├── cuda
│   └── spack.yaml
├── definitions.yaml
├── gcc
│   └── spack.yaml
├── nvhpc
│   └── spack.yaml
└── prod
    ├── cce
    │   └── spack.yaml
    ├── cuda
    │   └── spack.yaml
    ├── gcc
    │   └── spack.yaml
    └── nvhpc
        └── spack.yaml

9 directories, 9 files
```

We create a special file named `definitions.yaml` that is used for declaring definitions that is referenced in `spack.yaml`. This file is appended to all spack configuration. We do this to ensure all specs are defined in one place.

During this step, we will create the spack configuration and specify our preferred compilers and package preference. We install software in buildcache so it can be relocated to production path. In order to accomplish this task, we use spack pipelines that uses `spack ci generate` and `spack ci rebuild` to perform parallel pipeline execution. During this step, we determine which packages to install from E4S and add our own packages to comply with our site preference.

1.1.3 Step 3: Create Gitlab Job for Automation

Once spack configuration is written, we create a gitlab job to trigger the pipeline. This can be done by specifying a job in .gitlab-ci.yml.

The gitlab job can be triggered through scheduled pipelines, web-interface, or merge request to the project. A typical gitlab job will look something like this. Shown below is for E4S 23.05 generate job. We make use of gitlab feature named extends which allows us to reuse configuration. The `spack ci generate` command will be the same for each substack. There is two jobs, first is the generate step performed by `spack ci generate` and this triggers the downstream job created by spack.

```
.perlmutter-e4s-23.05-generate:
  stage: generate
  needs: ["perlmutter:check_spack_dependencies"]
  tags: [perlmutter-e4s]
  interruptible: true
  allow_failure: true
  rules:
    - if: ($CI_PIPELINE_SOURCE == "schedule" || $CI_PIPELINE_SOURCE == "web") && (
↪$PIPELINE_NAME == "PERLMUTTER_E4S_23.05")
    - if: ($CI_PIPELINE_SOURCE == "merge_request_event")
      changes:
      - spack-configs/perlmutter-e4s-23.05/$STACK_NAME/spack.yaml
      - spack-configs/perlmutter-e4s-23.05/definitions.yaml
  before_script:
    - *copy_perlmutter_settings
    - *startup_modules
  script:
    - *e4s_23_05_setup
    - cd $CI_PROJECT_DIR/spack-configs/perlmutter-e4s-23.05/$STACK_NAME
    - cat $CI_PROJECT_DIR/spack-configs/perlmutter-e4s-23.05/definitions.yaml >> spack.
↪yaml
    - spack env activate --without-view  .
    - spack env st
    #- spack -d concretize -f | tee $CI_PROJECT_DIR/concretize.log
    - spack -d ci generate --check-index-only --artifacts-root "$CI_PROJECT_DIR/jobs_
↪scratch_dir" --output-file "${CI_PROJECT_DIR}/jobs_scratch_dir/pipeline.yml"
  artifacts:
    paths:
    - ${CI_PROJECT_DIR}/jobs_scratch_dir


perlmutter-e4s-23.05-cce-generate:
  extends: .perlmutter-e4s-23.05-generate
  variables:
    STACK_NAME: cce

perlmutter-e4s-23.05-cce-build:
  stage: build
  needs: ["perlmutter:check_spack_dependencies", "perlmutter-e4s-23.05-cce-generate"]
  allow_failure: true
  rules:
    - if: ($CI_PIPELINE_SOURCE == "schedule" || $CI_PIPELINE_SOURCE == "web") && (
↪$PIPELINE_NAME == "PERLMUTTER_E4S_23.05")
```

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```
    - if: ($CI_PIPELINE_SOURCE == "merge_request_event")
      changes:
      - spack-configs/perlmutter-e4s-23.05/cce/spack.yaml
      - spack-configs/perlmutter-e4s-23.05/definitions.yaml
  trigger:
    include:
      - artifact: jobs_scratch_dir/pipeline.yml
        job: perlmutter-e4s-23.05-cce-generate
    strategy: depend
```

1.1.4 Step 4: Create Modulefile

In this step, we create a modulefile as entry point to software stack and setup `spack`. We do not create spack generated modules for spack packages, instead one is expected to use `spack load`. Shown below are the modulefiles available on NERSC system, they are typically called `e4s/<version>` with a symbolic link to module `spack/e4s-<version>`

```
siddiq90@login37> ml -t av e4s
/global/common/software/nersc/pm-2022.12.0/extra_modulefiles:
e4s/22.05
e4s/22.11
spack/e4s-22.05
spack/e4s-22.11
```

Shown below is the content of our modulefile, the setup is subject to change

```
siddiq90@login37> ml --raw show e4s
-------------------------------------------------------------------------------------------------
↪-------------------------------------------------------------------------------------------------
↪-------------------------------------------------------------------------------------------------
↪---
   /global/common/software/nersc/pm-2022.12.0/extra_modulefiles/e4s/22.11.lua:
-------------------------------------------------------------------------------------------------
↪-------------------------------------------------------------------------------------------------
↪-------------------------------------------------------------------------------------------------
↪---
whatis([[
        The Extreme-scale Scientific Software Stack (E4S) is a collection of open source␣
↪software packages for running scientific applications on high-performance computing␣
↪(HPC) platforms.
        ]])
help([[ The Extreme-scale Scientific Software Stack (E4S) is a community effort to␣
↪provide open source software packages for developing, deploying and running scientific␣
↪applications on high-performance computing (HPC) platforms. E4S provides from-source␣
↪builds and containers of a broad collection of HPC software packages.

References:
  - E4S User Docs: https://e4s.readthedocs.io/en/latest/index.html
  - E4S 22.11 Docs: https://docs.nersc.gov/applications/e4s/perlmutter/22.11/
  - E4S Homepage: https://e4s-project.github.io/
  - E4S GitHub: https://github.com/E4S-Project/e4s
        ]])
```

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```
local root = "/global/common/software/spackecp/perlmutter/e4s-22.11/default/spack"

setenv("SPACK_GNUPGHOME", pathJoin(os.getenv("HOME"), ".gnupg"))
setenv("SPACK_SYSTEM_CONFIG_PATH", "/global/common/software/spackecp/perlmutter/spack_
↪settings")
-- setup spack shell functionality
local shell = myShellType()
if (mode() == "load") then
    local spack_setup = ''
    if (shell == "sh" or shell == "bash" or shell == "zsh") then
         spack_setup = pathJoin(root, "share/spack/setup-env.sh")
    elseif (shell == "csh") then
         spack_setup = pathJoin(root, "share/spack/setup-env.csh")
    elseif (shell == "fish")  then
         spack_setup = pathJoin(root, "share/spack/setup-env.fish")
    end

    -- If we are unable to find spack setup script let's terminate now.
    if not isFile(spack_setup) then
        LmodError("Unable to find spack setup script " .. spack_setup .. "\n")
    end

    execute{cmd="source " .. spack_setup, modeA={"load"}}

    LmodMessage([[
    ------------------------------------------------------------------------------------------
↪------------------
     The Extreme-Scale Scientific Software Stack (E4S) is accessible via the Spack␣
↪package manager.

     In order to access the production stack, you will need to load a spack environment.␣
↪Here are some tips to get started:


     'spack env list' - List all Spack environments
     'spack env activate gcc' - Activate the "gcc" Spack environment
     'spack env status' - Display the active Spack environment
     'spack load amrex' - Load the "amrex" Spack package into your user environment

     For additional support, please refer to the following references:

       NERSC E4S Documentation: https://docs.nersc.gov/applications/e4s/
       E4S Documentation: https://e4s.readthedocs.io
       Spack Documentation: https://spack.readthedocs.io/en/latest/
       Spack Slack: https://spackpm.slack.com


    ------------------------------------------------------------------------------------------
↪------------------
    ]])
-- To remove spack from shell we need to remove a few environment variables, alias and␣
↪remove $SPACK_ROOT/bin from $PATH
```

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```
elseif (mode() == "unload" or mode() == "purge") then
    if (shell == "sh" or shell == "bash" or shell == "zsh") then
      execute{cmd="unset SPACK_ENV",modeA={"unload"}}
      execute{cmd="unset SPACK_ROOT",modeA={"unload"}}
      execute{cmd="unset -f spack",modeA={"unload"}}
    elseif (shell == "csh") then
      execute{cmd="unsetenv SPACK_ENV",modeA={"unload"}}
      execute{cmd="unsetenv SPACK_ROOT",modeA={"unload"}}
      execute{cmd="unalias spack",modeA={"unload"}}
    end

    -- Need to remove $SPACK_ROOT/bin from $PATH which removes the 'spack' command
    remove_path("PATH", pathJoin(root, "bin"))

    -- Remove alias spacktivate. Need to pipe to /dev/null as invalid alias can report␣
↪error to stderr
    execute{cmd="unalias spacktivate > /dev/null",modeA={"unload"}}
end
```

1.1.5 Step 5: User Documentation

User documentation is fundamental to help assist users with using E4S at NERSC. We document every E4S release with its *Release Date* and *End of Support* date along with a documentation page outlining the software stack. Our E4S documentation is available at https://docs.nersc.gov/applications/e4s/. The release date is when documentation is live. We perform this action in conjunction with release of modulefile so that user gain access to software stack.

Upon completion of this task, we are ready to make announcement to our NERSC users

1.1.6 Step 6: Sharing spack configuration with open-source community

In this step, we share our spack configuration with open-source community that may benefit the wider community. We share our spack configuration at https://github.com/spack/spack-configs. In addition, we update the E4S Facility Dashboard that shows all the E4S deployments across all the facilities.

1.1.7 Step 7: Public Announcement

This is the final step of the deployment process, where we make a public announcement in NERSC weekly email, along with various slack channels such as Nersc User Group (NUG), Spack, ECP and E4S slack.

1.2 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 external packages set for 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**.

1.3 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.

You may add the mirror into your spack environment by running:

```
spack mirror add perlmutter-spack-buildcache /global/common/software/spackecp/mirrors/
↪perlmutter-spack-develop
```

Or you can explicitly add the following lines into your spack.yaml

```
mirrors:
  perlmutter-spack-buildcache: file:///global/common/software/spackecp/mirrors/
↪perlmutter-spack-develop
```

Spack Configuration for spack@develop

```
spack:
  view: false
  include:
    - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
    - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree:
      padded_length: 128
  mirrors:
```

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```
    perlmutter-spack-buildcache: file:///global/common/software/spackecp/mirrors/
↪perlmutter-spack-develop
    source_mirror: file:///global/common/software/spackecp/mirrors/source_mirror
  cdash:
    build-group: DOE nightly E4S builds
    url: https://cdash.spack.io
    project: Spack
    site: NERSC - Perlmutter spack@develop

  definitions:
  - gcc_compilers: ['%gcc@11.2.0']
  - nvhpc_compilers: ['%nvhpc@21.11']
  - cray_compilers: ['%cce@13.0.2']
  - cray_specs:
    - adios2
    - fftw
    - hdf5
    - papi
    - petsc +openmp +strumpack
    - superlu
    - superlu-dist +openmp

  - gcc_specs:
    #- adios2
    - hdf5
    #- hypre +openmp +superlu-dist
    - papi
    #- petsc +openmp +strumpack
    - raja
    #- strumpack ~slate
    #- sundials +openmp +hypre
    #- superlu
    #- superlu-dist +openmp

  - cuda_specs:
    - 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
```

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```
    - 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

  - 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
```

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

  gitlab-ci:
    enable-artifacts-buildcache: false
    rebuild-index: true
    before_script:
    - module reset
    - module use /global/common/software/nersc/$(cat /etc/nersc_modules_rev)/extra_
↪modulefiles
    - module load cpu
    - module list
```

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```
    - source setup-env.sh
    - git clone ${SPACK_REPO}
    - pushd spack && git checkout ${SPACK_CHECKOUT_VERSION} && popd
    - . spack/share/spack/setup-env.sh
    - spack --version
    - spack-python --path
    script:
    - cd ${SPACK_CONCRETE_ENV_DIR}
    - spack env activate --without-view -d .
    - spack env st
    - spack -d ci rebuild
    after_script:
    - rm -rf $SPACK_ROOT
    service-job-attributes:
      tags: [perlmutter-e4s]
      script:
      - echo "End Pipeline"
    mappings:
    - match: [os=sles15]
      runner-attributes:
        tags: [perlmutter-e4s]
```

2.2 Perlmutter E4S 23.05

Production Spack Configuration

GCC spack environment

```
spack:
  view: false
  include:
    - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
    - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree: $spack/opt/spack
  concretizer:
    reuse: false
    unify: false
  mirrors:
    perlmutter-e4s-23.05: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪23.05
  specs:
  - matrix:
    - [$gcc_specs]
    - [$gcc_compilers]
  - matrix:
```

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```
    - [$nersc_specs]
    - [$gcc_compilers]
```

CCE Spack Environment

```
spack:
  view: false
  include:
    - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
    - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree: $spack/opt/spack
  concretizer:
    reuse: false
    unify: false
  mirrors:
    perlmutter-e4s-23.05: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪23.05
  specs:
  - matrix:
    - [$cce_specs]
    - [$cce_compilers]
```

NVHPC Spack Environment

```
spack:
  view: false
  include:
    - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
    - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree: $spack/opt/spack
  concretizer:
    reuse: false
    unify: false
  mirrors:
    perlmutter-e4s-23.05: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪23.05
  packages:
    cmake::
      require: '%gcc'
    # build failures with xz %nvhpc so reverting to gcc
    xz::
```

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```
      require: '%gcc'
  specs:
  - matrix:
    - [$nvhpc_specs]
    - [$nvhpc_compilers]
```

CUDA Spack Environment

```
spack:
  view: false
  include:
    - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
    - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree: $spack/opt/spack
  concretizer:
    reuse: false
    unify: false
  mirrors:
    perlmutter-e4s-23.05: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪23.05
  specs:
  - matrix:
    - [$cuda_specs]
    - [$gcc_compilers]
```

DATA Spack Environment

```
spack:
  view: false
  include:
  - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
  - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree: $spack/opt/spack
  concretizer:
    reuse: false
    unify: false
  mirrors:
    perlmutter-e4s-23.05: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪23.05
  specs:
```

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```
    - matrix:
      - [$data_specs]
      - [$gcc_compilers]
```

MATH-LIBS Spack Environment

```
spack:
  view: false
  include:
  - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
  - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree: $spack/opt/spack
  concretizer:
    reuse: false
    unify: false
  mirrors:
    perlmutter-e4s-23.05: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪23.05
  specs:
  - matrix:
    - [$math-libs]
    - [$gcc_compilers]
```

TOOLS Spack Environment

```
spack:
  view: false
  include:
  - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
  - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree: $spack/opt/spack
  concretizer:
    reuse: false
    unify: false
  mirrors:
    perlmutter-e4s-23.05: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪23.05
  specs:
  - matrix:
    - [$tools]
    - [$gcc_compilers]
```

Shown below is the list of definitions that is used for all of our spack environments.

Definitions for Spack Environments

```
definitions:
- cce_compilers: ['%cce@=15.0.0']
- gcc_compilers: ['%gcc@=11.2.0']
- nvhpc_compilers: ['%nvhpc@=22.7']

- cce_specs:
  - fftw
  - hdf5 +fortran +hl +shared
  - hypre
  - kokkos +openmp
  - kokkos-kernels +openmp
  - netcdf-c
  - netcdf-fortran
  - papi
  - petsc
  - slepc
  - sundials
  - superlu
  - superlu-dist

- math-libs:
  - arborx
  - fftw@=3.3.8
  - fftw@=3.3.9
  - fftw@=3.3.10
  - ginkgo
  - heffte
  - hypre
  - intel-mkl
  - openblas
  - petsc
  - phist
  - pumi
  - slate
  - slepc
  - sundials
  - superlu
  - superlu-dist

- data_specs:
  - datatransferkit
  - hdf5
  - hdf5-vol-async
  - hdf5-vol-cache
  - netcdf-c
  - netcdf-fortran
  - parallel-netcdf

  #- hdf5-vol-log Build error
```

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```
  - nvhpc_specs:
    - amrex
    - boost
    - hdf5 ~mpi
    - sundials
    - superlu

    #- superlu-dist
    #- hypre
    #- kokkos
    #- kokkos-kernels
    #- papi   Build failud due to nvc-Error-Unknown switch: -Wno-error


  - cuda_specs:
    - adios2@=2.8.3 +cuda cuda_arch=80 # ecp-data-vis-sdk
    - amrex +cuda cuda_arch=80
    - arborx +cuda cuda_arch=80 ^kokkos +wrapper
    - cabana +cuda ^kokkos +wrapper +cuda_lambda +cuda cuda_arch=80
    - caliper +cuda cuda_arch=80
    - chai ~benchmarks ~tests +cuda cuda_arch=80 ^umpire ~shared
    - cusz +cuda cuda_arch=80
    - flecsi +cuda cuda_arch=80
    - ginkgo +cuda cuda_arch=80
    - heffte +cuda cuda_arch=80
    - hpx max_cpu_count=512 +cuda cuda_arch=80
    - hypre +cuda cuda_arch=80
    - kokkos +wrapper +cuda cuda_arch=80
    - kokkos-kernels +cuda cuda_arch=80 ^kokkos +wrapper +cuda cuda_arch=80
    - lammps +cuda cuda_arch=80
    - legion +cuda cuda_arch=80
    - magma +cuda cuda_arch=80
    - mfem +cuda cuda_arch=80
    - mgard +serial +openmp +timing +unstructured +cuda cuda_arch=80
    - omega-h +cuda cuda_arch=80
    - parsec +cuda cuda_arch=80
    - petsc +cuda cuda_arch=80
    - slate +cuda cuda_arch=80
    - slepc +cuda cuda_arch=80
    - strumpack ~slate +cuda cuda_arch=80
    - sundials +cuda cuda_arch=80
    - superlu-dist +cuda cuda_arch=80
    - tasmanian +cuda cuda_arch=80
    - umpire ~shared +cuda cuda_arch=80
    - zfp +cuda cuda_arch=80

    # - libpressio +bitgrooming +bzip2 +fpzip +hdf5 +libdistributed +lua +openmp +python␣
↪+sz +sz3 +unix +zfp +json +remote +netcdf +cusz +mgard +cuda cuda_arch=80 ^cusz +cuda␣
↪cuda_arch=80    # concretization issue with cuda

    # CUDA NOARCH
```

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```
    - hpctoolkit +cuda
    - papi +cuda
    - tau +mpi +cuda

    #- bricks +cuda
    # - ecp-data-vis-sdk ~rocm +adios2 ~ascent +hdf5 ~paraview ~pnetcdf ~sz +vtkm +zfp␣
↪+cuda cuda_arch=80
    #- raja +cuda cuda_arch=80
  - gcc_specs:
    - alquimia
    - aml
    - amrex
    - arborx
    - argobots
    - bolt
    - boost
    - butterflypack
    - cabana
    - caliper
    - chai ~benchmarks ~tests
    - datatransferkit
    - dyninst ^intel-tbb
    - flecsi
    - flit
    - fortrilinos
    - ginkgo
    - gotcha
    - h5bench
    - hdf5
    - hdf5-vol-async
    - hdf5-vol-cache
    - heffte +fftw
    - hpctoolkit
    - hpx max_cpu_count=512 networking=mpi
    - hypre
    - kokkos +openmp
    - kokkos-kernels +openmp
    - lammps
    - legion
    - libnrm
    - libpressio +bitgrooming +bzip2 ~cuda ~cusz +fpzip +hdf5 +libdistributed +lua␣
↪+openmp +python +sz +sz3 +unix +zfp +json +remote +netcdf
    - libquo
    - libunwind
    - likwid
    - loki
    - mercury
    - metall
    - mfem
    - mgard +serial +openmp +timing +unstructured ~cuda
    - mpark-variant
```

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```
    - nccmp
    - nco
    - netlib-scalapack
    - omega-h
    - openpmd-api
    - papi
    - papyrus
    - parsec ~cuda
    - pdt
    - petsc
    - phist
    - plasma
    - plumed
    - precice
    - pumi
    - py-h5py
    - py-jupyterhub
    - py-libensemble
    - py-petsc4py
    - qthreads scheduler=distrib
    - raja
    - slate ~cuda
    - slepc
    - stc
    - strumpack ~slate
    - sundials
    - superlu
    - superlu-dist
    - swig@4.0.2-fortran
    - sz3
    - tasmanian
    - tau +mpi +python
    - 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
    - turbine
    - umap
    - umpire
    - unifyfs
    - variorum

    # build failures
    # - axom ~mpi
    #- globalarrays
    #- wannier90
    # - rempi
    # - openfoam
    # - mpifileutils ~xattr
    # - lbann
    # - hdf5-vol-log
    # - flux-core
```

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```
      # - ecp-data-vis-sdk ~cuda ~rocm +adios2 +ascent +cinema +darshan +faodel +hdf5 ~
↪paraview +pnetcdf +sz +unifyfs +veloc ~visit +vtkm +zfp # visit: font-util:␣
↪[Makefile:756: install-data-hook] Error 1 share/fonts/X11/cyrillic: failed to write␣
↪cache paraview: ispc: lex.cpp:398:9: error: 'yywrap' macro redefined [-Werror,-Wmacro-
↪redefined]
   # - exaworks
   # - conduit ~mpi

 - nersc_specs:
   - chapel
   - gsl
   - netcdf-c ~mpi
   - netcdf-fortran
   - metis
   - parmetis
   - gromacs
   - cdo
   # trouble building esmf +mpi
   #- ncl ^esmf~mpi
   - ncl
   - nco
   - ncview
   - libxc
   - libcint
   - libint tune=molgw-lmax-7
   - intel-mkl

 - tools:
   - autoconf
   - automake
   - ccache
   - cmake
   - git
   - gmake
   - gawk
   - nano
   - subversion
```

Each spack environment is built in a separate directory using **spack ci** in-order to push specs to buildcache. We have the following spack configuration for each spack environment.

Spack Environments for Spack CI

GCC Spack Environment

```
spack:
  view: false
  include:
  - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
  - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
```

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```
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree:
      padded_length: 128
  concretizer:
    reuse: false
    unify: false
  mirrors:
    perlmutter-e4s-23.05: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪23.05
  ci:
    enable-artifacts-buildcache: false
    rebuild-index: true
    target: gitlab
    pipeline-gen:
    - submapping:
      - match: [os=sles15]
        build-job:
          tags: [perlmutter-e4s]
      match_behavior: first
    - any-job:
        before_script:
        - git clone -c feature.manyFiles=true -b e4s-23.05 $SPACK_REPO
        - . spack/share/spack/setup-env.sh
        - which spack
        - spack --version
    - build-job:
        tags: [perlmutter-e4s]
        before_script:
        - module reset
        - module load cpu cray-pmi
        - module list
        - source setup-env.sh
        - git clone -c feature.manyFiles=true -b e4s-23.05 $SPACK_REPO
        - . spack/share/spack/setup-env.sh
        - which spack
        - spack --version
        - spack-python --path
        script:
        - cd ${SPACK_CONCRETE_ENV_DIR}
        - spack env activate --without-view .
        - spack env st
        - export SPACK_GNUPGHOME=$HOME/.gnupg
        - spack gpg list
        - spack -d ci rebuild
    - reindex-job:
        tags: [perlmutter-e4s]
        script:
        - echo "End Pipeline"
    - noop-job:
        tags: [perlmutter-e4s]
        script:
```

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```
      - echo "End Pipeline"
  specs:
  - matrix:
    - [$gcc_specs]
    - [$gcc_compilers]
  - matrix:
    - [$nersc_specs]
    - [$gcc_compilers]
```

CCE Spack Environment

```
spack:
  view: false
  include:
  - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
  - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree:
      padded_length: 128
  concretizer:
    reuse: false
    unify: false
  mirrors:
    perlmutter-e4s-23.05: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪23.05
  ci:
    enable-artifacts-buildcache: false
    rebuild-index: true
    target: gitlab
    pipeline-gen:
    - submapping:
      - match: [os=sles15]
        build-job:
          tags: [perlmutter-e4s]
      match_behavior: first
    - any-job:
        before_script:
        - git clone -c feature.manyFiles=true -b e4s-23.05 $SPACK_REPO
        - . spack/share/spack/setup-env.sh
        - which spack
        - spack --version
    - build-job:
        tags: [perlmutter-e4s]
        before_script:
        - module reset
        - module load cpu cray-pmi
        - module list
        - source setup-env.sh
```

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```
        - git clone -c feature.manyFiles=true -b e4s-23.05 $SPACK_REPO
        - . spack/share/spack/setup-env.sh
        - which spack
        - spack --version
        - spack-python --path
        script:
        - cd ${SPACK_CONCRETE_ENV_DIR}
        - spack env activate --without-view .
        - spack env st
        - export SPACK_GNUPGHOME=$HOME/.gnupg
        - spack gpg list
        - spack -d ci rebuild
    - reindex-job:
        tags: [perlmutter-e4s]
        script:
        - echo "End Pipeline"
    - noop-job:
        tags: [perlmutter-e4s]
        script:
        - echo "End Pipeline"
  specs:
    - matrix:
      - [$cce_specs]
      - [$cce_compilers]
```

NVHPC Spack Environment

```
spack:
  view: false
  include:
  - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
  - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree:
      padded_length: 128
  concretizer:
    reuse: false
    unify: false
  packages:
    cmake::
      require: '%gcc'
    # build failures with xz %nvhpc so reverting to gcc
    xz::
      require: '%gcc'
  mirrors:
    perlmutter-e4s-23.05: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪23.05
```

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```
  ci:
    enable-artifacts-buildcache: false
    rebuild-index: true
    target: gitlab
    pipeline-gen:
    - submapping:
      - match: [os=sles15]
        build-job:
          tags: [perlmutter-e4s]
      match_behavior: first
    - any-job:
        before_script:
        - git clone -c feature.manyFiles=true -b e4s-23.05 $SPACK_REPO
        - . spack/share/spack/setup-env.sh
        - which spack
        - spack --version
    - build-job:
        tags: [perlmutter-e4s]
        before_script:
        - module reset
        - module load cpu cray-pmi
        - module list
        - source setup-env.sh
        - git clone -c feature.manyFiles=true -b e4s-23.05 $SPACK_REPO
        - . spack/share/spack/setup-env.sh
        - which spack
        - spack --version
        - spack-python --path
        script:
        - cd ${SPACK_CONCRETE_ENV_DIR}
        - spack env activate --without-view .
        - spack env st
        - export SPACK_GNUPGHOME=$HOME/.gnupg
        - spack gpg list
        - spack -d ci rebuild
    - reindex-job:
        tags: [perlmutter-e4s]
        script:
        - echo "End Pipeline"
    - noop-job:
        tags: [perlmutter-e4s]
        script:
        - echo "End Pipeline"
  specs:
    - matrix:
      - [$nvhpc_specs]
      - [$nvhpc_compilers]
```

CUDA Spack Environment

```
spack:
  view: false
```

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```
  include:
  - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
  - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree:
      padded_length: 128
  concretizer:
    reuse: false
    unify: false
  mirrors:
    perlmutter-e4s-23.05: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪23.05
  ci:
    enable-artifacts-buildcache: false
    rebuild-index: true
    target: gitlab
    pipeline-gen:
    - submapping:
      - match: [os=sles15]
        build-job:
          tags: [perlmutter-e4s]
      match_behavior: first
    - any-job:
       before_script:
       - git clone -c feature.manyFiles=true -b e4s-23.05 $SPACK_REPO
       - . spack/share/spack/setup-env.sh
       - which spack
       - spack --version
    - build-job:
        tags: [perlmutter-e4s]
        before_script:
        - module reset
        - module load cpu cray-pmi
        - module list
        - source setup-env.sh
        - git clone -c feature.manyFiles=true -b e4s-23.05 $SPACK_REPO
        - . spack/share/spack/setup-env.sh
        - which spack
        - spack --version
        - spack-python --path
        script:
        - cd ${SPACK_CONCRETE_ENV_DIR}
        - spack env activate --without-view .
        - spack env st
        - export SPACK_GNUPGHOME=$HOME/.gnupg
        - spack gpg list
    - reindex-job:
        tags: [perlmutter-e4s]
```

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```
      script:
      - echo "End Pipeline"
  - noop-job:
      tags: [perlmutter-e4s]
      script:
      - echo "End Pipeline"
specs:
  - matrix:
    - [$cuda_specs]
    - [$gcc_compilers]
```

DATA Spack Environment

```
spack:
  view: false
  include:
  - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
  - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree:
      padded_length: 128
  concretizer:
    reuse: false
    unify: false
  mirrors:
    perlmutter-e4s-23.05: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪23.05
  ci:
    enable-artifacts-buildcache: false
    rebuild-index: true
    target: gitlab
    pipeline-gen:
    - submapping:
      - match: [os=sles15]
        build-job:
          tags: [perlmutter-e4s]
      match_behavior: first
    - any-job:
        before_script:
        - git clone -c feature.manyFiles=true -b e4s-23.05 $SPACK_REPO
        - . spack/share/spack/setup-env.sh
        - which spack
        - spack --version
    - build-job:
        tags: [perlmutter-e4s]
        before_script:
        - module reset
        - module load cpu cray-pmi
```

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```
        - module list
        - source setup-env.sh
        - git clone -c feature.manyFiles=true -b e4s-23.05 $SPACK_REPO
        - . spack/share/spack/setup-env.sh
        - which spack
        - spack --version
        - spack-python --path
        script:
        - cd ${SPACK_CONCRETE_ENV_DIR}
        - spack env activate --without-view .
        - spack env st
        - export SPACK_GNUPGHOME=$HOME/.gnupg
        - spack gpg list
        - spack -d ci rebuild
    - reindex-job:
        tags: [perlmutter-e4s]
        script:
        - echo "End Pipeline"
    - noop-job:
        tags: [perlmutter-e4s]
        script:
        - echo "End Pipeline"
  specs:
    - matrix:
      - [$data_specs]
      - [$gcc_compilers]
```

MATH-LIBS Spack Environment

```
spack:
  view: false
  include:
  - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
  - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree:
      padded_length: 128
  concretizer:
    reuse: false
    unify: false
  mirrors:
    perlmutter-e4s-23.05: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪23.05
  ci:
    enable-artifacts-buildcache: false
    rebuild-index: true
    target: gitlab
    pipeline-gen:
```

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```
    - submapping:
      - match: [os=sles15]
        build-job:
          tags: [perlmutter-e4s]
      match_behavior: first
    - any-job:
        before_script:
        - git clone -c feature.manyFiles=true -b e4s-23.05 $SPACK_REPO
        - . spack/share/spack/setup-env.sh
        - which spack
        - spack --version
    - build-job:
        tags: [perlmutter-e4s]
        before_script:
        - module reset
        - module load cpu cray-pmi
        - module list
        - source setup-env.sh
        - git clone -c feature.manyFiles=true -b e4s-23.05 $SPACK_REPO
        - . spack/share/spack/setup-env.sh
        - which spack
        - spack --version
        - spack-python --path
        script:
        - cd ${SPACK_CONCRETE_ENV_DIR}
        - spack env activate --without-view .
        - spack env st
        - export SPACK_GNUPGHOME=$HOME/.gnupg
        - spack gpg list
        - spack -d ci rebuild
    - reindex-job:
        tags: [perlmutter-e4s]
        script:
        - echo "End Pipeline"
    - noop-job:
        tags: [perlmutter-e4s]
        script:
        - echo "End Pipeline"
  specs:
  - matrix:
    - [$math-libs]
    - [$gcc_compilers]
```

TOOLS Spack Environment

```
spack:
  view: false
  include:
  - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
  - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
```

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```
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree:
      padded_length: 128
  concretizer:
    reuse: false
    unify: false
  mirrors:
    perlmutter-e4s-23.05: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪23.05
  ci:
    enable-artifacts-buildcache: false
    rebuild-index: true
    target: gitlab
    pipeline-gen:
    - submapping:
      - match: [os=sles15]
        build-job:
          tags: [perlmutter-e4s]
      match_behavior: first
    - any-job:
        before_script:
        - git clone -c feature.manyFiles=true -b e4s-23.05 $SPACK_REPO
        - . spack/share/spack/setup-env.sh
        - which spack
        - spack --version
    - build-job:
        tags: [perlmutter-e4s]
        before_script:
        - module reset
        - module load cpu cray-pmi
        - module list
        - source setup-env.sh
        - git clone -c feature.manyFiles=true -b e4s-23.05 $SPACK_REPO
        - . spack/share/spack/setup-env.sh
        - which spack
        - spack --version
        - spack-python --path
        script:
        - cd ${SPACK_CONCRETE_ENV_DIR}
        - spack env activate --without-view .
        - spack env st
        - export SPACK_GNUPGHOME=$HOME/.gnupg
        - spack gpg list
        - spack -d ci rebuild
    - reindex-job:
        tags: [perlmutter-e4s]
        script:
        - echo "End Pipeline"
    - noop-job:
        tags: [perlmutter-e4s]
```

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```
      script:
      - echo "End Pipeline"
  specs:
  - matrix:
    - [$tools]
    - [$gcc_compilers]
```

2.3 Perlmutter E4S 22.11

Production Spack Configuration

GCC spack environment

```
spack:
  view: false
  include:
    - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
    - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree: $spack/opt/spack
  concretizer:
    reuse: false
  mirrors:
    perlmutter-e4s-22.11: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪22.11
  specs:
  - matrix:
    - [$gcc_specs]
    - [$gcc_compilers]
  - matrix:
    - [$utilities]
    - [$gcc_compilers]
  - matrix:
    - [$nersc_specs]
    - [$gcc_compilers]
```

CCE Spack Environment

```
spack:
  view: false
  include:
    - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
    - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
```

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```
    concretizer: clingo
    install_tree: $spack/opt/spack
  concretizer:
    reuse: false
  mirrors:
    perlmutter-e4s-22.11: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪22.11
  specs:
  - matrix:
    - [$cce_specs]
    - [$cce_compilers]
```

NVHPC Spack Environment

```
spack:
  view: false
  include:
    - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
    - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree: $spack/opt/spack
  concretizer:
    reuse: false
  mirrors:
    perlmutter-e4s-22.11: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪22.11
  packages:
    # build failures with xz %nvhpc so reverting to gcc
    xz::
      require: '%gcc'
  specs:
  - matrix:
    - [$nvhpc_specs]
    - [$nvhpc_compilers]
```

CUDA Spack Environment

```
spack:
  view: false
  include:
    - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
    - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree: $spack/opt/spack
```

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```
  concretizer:
    reuse: false
  mirrors:
    perlmutter-e4s-22.11: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪22.11
  specs:
  - matrix:
    - [$cuda_specs]
    - [$gcc_compilers]
```

Shown below is the list of definitions that is used for all of our spack environments.

Definitions for Spack Environments

```
  definitions:
  - cce_compilers: ['%cce@15.0.0']
  - gcc_compilers: ['%gcc@11.2.0']
  - nvhpc_compilers: ['%nvhpc@22.7']

  - gcc_specs:
    - adios2@2.8.3
    - alquimia@1.0.10
    - aml@0.2.0
    - amrex@22.11
    - arborx@1.3
    - argobots@1.1
    - axom@0.7.0
    - bolt@2.0
    - butterflypack@2.2.2
    - cabana@0.5.0
    - caliper@2.8.0
    - chai@2022.03.0 ~benchmarks ~tests
    - conduit@0.8.4 ~blt_find_mpi
    - datatransferkit@3.1-rc3
    - dyninst@12.2.0 ^intel-tbb
    #- ecp-data-vis-sdk@1.0 ~cuda ~rocm +adios2 +ascent +cinema +darshan +faodel +hdf5␣
↪+paraview +pnetcdf +sz +unifyfs +veloc +visit +vtkm +zfp
    - flecsi@1.4.2
    - flit@2.1.0
    - flux-core@0.44.0
    - fortrilinos@2.1.0
    - gasnet@2022.9.0
    - ginkgo@1.4.0
    - globalarrays@5.8
    - gotcha@1.0.4
    - gptune@3.0.0
    - h5bench@1.3
    - hdf5@1.12.2 +fortran +hl +shared
    - hdf5-vol-async@1.3
    - heffte@2.3.0 +fftw
    - hpctoolkit@2022.10.01
    - hpx@1.8.1 networking=mpi
    - hypre@2.26.0
```

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```
    - kokkos@3.7.00 +openmp
    - kokkos-kernels@3.7.00 +openmp
    - lammps@20220623
    - legion@21.03.0
    - libquo@1.3.1
    - libunwind@1.6.2
    - mercury@2.1.0
    - mfem@4.5.0
    - mpark-variant@1.4.0
    #- mpifileutils@0.11.1 ~xattr
    - nccmp@1.9.0.1
    - nco@5.0.1
    - netlib-scalapack@2.2.0
    - openblas@0.3.20 threads=openmp
    - omega-h@9.34.13
    - openpmd-api@0.14.5 ~adios2
    - papi@6.0.0.1
    - papyrus@1.0.2
    - parallel-netcdf@1.12.3
    - parsec@3.0.2209 ~cuda
    - pdt@3.25.1
    - petsc@3.18.1
    - precice@2.5.0
    - pumi@2.2.7
    - py-libensemble@0.9.3
    - py-h5py +mpi
    - py-h5py ~mpi
    - py-petsc4py@3.18.1
    - py-warpx@22.10 ^warpx dims=2
    - py-warpx@22.10 ^warpx dims=3
    - py-warpx@22.10 ^warpx dims=rz
    - qt@5.14.2
    - qthreads@1.16 scheduler=distrib
    - quantum-espresso@7.1
    - raja@2022.03.0
    - slate@2022.07.0 ~cuda
    - slepc@3.18.1
    - strumpack@7.0.1 ~slate
    - sundials@6.4.1
    - superlu@5.3.0
    - superlu-dist@8.1.1
    - tasmanian@7.9
    - tau@2.32 +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 +tempus +tpetra +trilinoscouplings +zoltan +zoltan2 +superlu-dist␣
↪gotype=long_long
    - umap@2.1.0
    - umpire@2022.03.1
    - upcxx@2022.9.0
    - vtk-m@1.9.0
```

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```
    - zfp@0.5.5

    # - bricks@r0.1 build failure
    # - plasma@22.9.29 Could NOT find MKL (missing: MKL_INCLUDE_DIRS MKL_LIBRARIES)
    # - phist@1.11.2 build error
    # - stc@0.9.0 build failure on swig
    # - turbine@1.3.0  failed to build swig
    # - upcxx+gasnet^gasnet@2022.9.2 # see https://software.nersc.gov/NERSC/spack-
↪infrastructure/-/issues/45  Issue with getting checksum for gasnet
     # - visit@3.2.2 ~hdf5
    # - wannier90@3.1.0 Error: Type mismatch between actual argument at (1) and actual␣
↪argument at (2) (COMPLEX(8)/INTEGER(4))../comms.F90:1214:22: 1214 |     call MPI_
↪scatterv(rootglobalarray, counts, displs, MPI_double_precision, &
  - cuda_specs:
    - adios2@2.8.3 +cuda cuda_arch=80   # ecp-data-vis-sdk
    - amrex@22.11 +cuda cuda_arch=80
    - arborx@1.3 +cuda cuda_arch=80 ^kokkos@3.7.00 +wrapper
    - cabana@0.5.0 +cuda ^kokkos@3.7.00 +wrapper +cuda_lambda +cuda cuda_arch=80
    - caliper@2.8.0 +cuda cuda_arch=80
    - chai@2022.03.0 ~benchmarks ~tests +cuda cuda_arch=80 ^umpire@2022.03.1 ~shared
    - cusz@0.3 +cuda cuda_arch=80
    - flecsi@2.1.0 +cuda cuda_arch=80
    - ginkgo@1.4.0 +cuda cuda_arch=80
    - heffte@2.3.0 +cuda cuda_arch=80
    - hpx@1.8.1 +cuda cuda_arch=80
    - hypre@2.26.0 +cuda cuda_arch=80
    - kokkos-kernels@3.7.00 +cuda cuda_arch=80 ^kokkos@3.7.00 +wrapper +cuda cuda_arch=80
    - kokkos@3.7.00 +wrapper +cuda cuda_arch=80
    - mfem@4.5.0 +cuda cuda_arch=80
    - omega-h@9.34.13 +cuda cuda_arch=80
    - petsc@3.18.1 +cuda cuda_arch=80
    - slate@2022.07.0 +cuda cuda_arch=80
    - slepc@3.18.1 +cuda cuda_arch=80
    - strumpack@7.0.1 ~slate +cuda cuda_arch=80
    - sundials@6.4.1 +cuda cuda_arch=80
    - superlu-dist@8.1.1 +cuda cuda_arch=80
    - tasmanian@7.9 +cuda cuda_arch=80
    - umpire@2022.03.1 ~shared +cuda cuda_arch=80
    - vtk-m@1.9.0 +cuda cuda_arch=80    # ecp-data-vis-sdk
    - zfp@0.5.5 +cuda cuda_arch=80      # ecp-data-vis-sdk

    #- ascent@0.8.0 +cuda cuda_arch=80   # unable to build vtk-h -- Could NOT find MPI_C␣
↪(missing: MPI_C_LIB_NAMES) (found version "3.1")
    # - dealii@9.4.0 +cuda cuda_arch=80 # CUDA_LIBRARIES: *** Required variable "CUDA_
↪cusparse_LIBRARY" set to NOTFOUND ***
    #- magma@2.6.2 +cuda cuda_arch=80 # CMake Error: The following variables are used in␣
↪this project, but they are set to NOTFOUND.
    #- raja@2022.03.0 +cuda cuda_arch=80 # error: "RAJA::expt::Register<int32_t,␣
↪RAJA::expt::avx2_register> &(const int32_t &)" contains a vector, which is not␣
↪supported in device code
    #- trilinos@13.4.0 +cuda cuda_arch=80
```

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```
  - nvhpc_specs:
    - hdf5@1.12.2 +fortran +hl +shared
    - kokkos@3.7.00 +openmp
    - kokkos-kernels@3.7.00 +openmp
    - sundials@6.4.1
    - superlu@5.3.0
    #- superlu-dist@8.1.1 # error: this OpenMP construct is not supported in NVIDIA␣
↪subset: The 'taskloop' construct is not supported.

  - cce_specs:
    - fftw@3.3.10
    - hdf5@1.12.2 +fortran +hl +shared
    - hypre@2.26.0
    - kokkos@3.7.00 +openmp
    - kokkos-kernels@3.7.00 +openmp
    - netcdf-c@4.9.0
    - netcdf-fortran@4.6.0
    - sundials@6.4.1
    - superlu@5.3.0
    - superlu-dist@8.1.1

  - nersc_specs:
    - chapel@1.24.1
    - gsl@2.7.1
    - fftw@3.3.10
    - fftw@3.3.9
    - fftw@3.3.8
    - netcdf-c@4.9.0 ~mpi
    - netcdf-fortran@4.6.0
    - metis@5.1.0
    - parmetis@4.0.3
    - gromacs@2022.3
    - cdo
    # trouble building esmf +mpi
    - ncl ^esmf~mpi
    - nco
    - ncview
    - libxc
    - libcint
    - libint tune=molgw-lmax-7
    - intel-mkl
  - utilities:
    - autoconf
    - automake
    - cmake
    - git
    - gmake
    - gawk
    - nano
    - subversion
```

Each spack environment is built in a separate directory using **spack ci** in-order to push specs to buildcache. We have the following spack configuration for each spack environment.

Spack Environments for Spack CI

GCC Spack Environment

```
spack:
  view: false
  include:
    - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
    - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree:
      padded_length: 128
  concretizer:
    reuse: false
  mirrors:
    perlmutter-e4s-22.11: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪22.11
    # source_mirror: file:///global/cfs/cdirs/m3503/mirrors/source_mirror
  gitlab-ci:
    enable-artifacts-buildcache: false
    rebuild-index: true
    before_script:
    - module reset
    - module load cpu cray-pmi
    - module list
    - source setup-env.sh
    - git clone -c feature.manyFiles=true -b e4s-22.11 $SPACK_REPO
    - . spack/share/spack/setup-env.sh
    - which spack
    - spack --version
    - spack-python --path
    script:
    - cd ${SPACK_CONCRETE_ENV_DIR}
    - spack env activate --without-view .
    - spack env st
    - export SPACK_GNUPGHOME=$HOME/.gnupg
    - spack gpg list
    - spack -d ci rebuild
    service-job-attributes:
      tags: [perlmutter-e4s]
      before_script:
        - git clone -b e4s-22.11 $SPACK_REPO
        - . spack/share/spack/setup-env.sh
        - spack --version
        - ls -l /global/common/software/spackecp/mirrors/perlmutter-e4s-22.11/build_
↪cache/_pgp
      script:
      - echo "End Pipeline"
    mappings:
    - match: [os=sles15]
```

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```
      runner-attributes:
        tags: [perlmutter-e4s]
  specs:
  - matrix:
    - [$gcc_specs]
    - [$gcc_compilers]
  - matrix:
    - [$utilities]
    - [$gcc_compilers]
  - matrix:
    - [$nersc_specs]
    - [$gcc_compilers]
```

CCE Spack Environment

```
spack:
  view: false
  include:
    - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
    - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree:
      padded_length: 128
  concretizer:
    reuse: false
  mirrors:
    perlmutter-e4s-22.11: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪22.11
  gitlab-ci:
    enable-artifacts-buildcache: false
    rebuild-index: true
    before_script:
    - module reset
    - module load cpu cray-pmi
    - module list
    - source setup-env.sh
    - git clone -c feature.manyFiles=true -b e4s-22.11 $SPACK_REPO
    - . spack/share/spack/setup-env.sh
    - which spack
    - spack --version
    - spack-python --path
    script:
    - cd ${SPACK_CONCRETE_ENV_DIR}
    - spack env activate --without-view .
    - spack env st
    - export SPACK_GNUPGHOME=$HOME/.gnupg
    - spack gpg list
    - spack -d ci rebuild
```

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```
    service-job-attributes:
      tags: [perlmutter-e4s]
      before_script:
        - git clone -b e4s-22.11 $SPACK_REPO
        - . spack/share/spack/setup-env.sh
        - spack --version
        - ls -l /global/common/software/spackecp/mirrors/perlmutter-e4s-22.11/build_
↪cache/_pgp
      script:
      - echo "End Pipeline"
    mappings:
    - match: [os=sles15]
      runner-attributes:
        tags: [perlmutter-e4s]
  specs:
  - matrix:
    - [$cce_specs]
    - [$cce_compilers]
```

NVHPC Spack Environment

```
spack:
  view: false
  include:
    - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
    - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree:
      padded_length: 128
  concretizer:
    reuse: false
  packages:
    # build failures with xz %nvhpc so reverting to gcc
    xz::
      require: '%gcc'
  mirrors:
    perlmutter-e4s-22.11: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪22.11
  gitlab-ci:
    enable-artifacts-buildcache: false
    rebuild-index: true
    before_script:
    - module reset
    - module load cpu cray-pmi
    - module list
    - source setup-env.sh
    - git clone -c feature.manyFiles=true -b e4s-22.11 $SPACK_REPO
    - . spack/share/spack/setup-env.sh
```

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```
    - which spack
    - spack --version
    - spack-python --path
    script:
    - cd ${SPACK_CONCRETE_ENV_DIR}
    - spack env activate --without-view .
    - spack env st
    - export SPACK_GNUPGHOME=$HOME/.gnupg
    - spack gpg list
    - spack -d ci rebuild
    service-job-attributes:
      tags: [perlmutter-e4s]
      before_script:
        - git clone -b e4s-22.11 $SPACK_REPO
        - . spack/share/spack/setup-env.sh
        - spack --version
        - ls -l /global/common/software/spackecp/mirrors/perlmutter-e4s-22.11/build_
↪cache/_pgp
      script:
      - echo "End Pipeline"
    mappings:
    - match: [os=sles15]
      runner-attributes:
        tags: [perlmutter-e4s]
  specs:
  - matrix:
    - [$nvhpc_specs]
    - [$nvhpc_compilers]
```

CUDA Spack Environment

```
spack:
  view: false
  include:
    - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
    - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree:
      padded_length: 128
  concretizer:
    reuse: false
  mirrors:
    perlmutter-e4s-22.11: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪22.11
    # source_mirror: file:///global/cfs/cdirs/m3503/mirrors/source_mirror
  gitlab-ci:
    enable-artifacts-buildcache: false
    rebuild-index: true
```

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```
    before_script:
    - module reset
    - module load cpu cray-pmi
    - module list
    - source setup-env.sh
    - git clone -c feature.manyFiles=true -b e4s-22.11 $SPACK_REPO
    - . spack/share/spack/setup-env.sh
    - which spack
    - spack --version
    - spack-python --path
    script:
    - cd ${SPACK_CONCRETE_ENV_DIR}
    - spack env activate --without-view .
    - spack env st
    - export SPACK_GNUPGHOME=$HOME/.gnupg
    - spack gpg list
    - spack -d ci rebuild
    service-job-attributes:
      tags: [perlmutter-e4s]
      before_script:
        - git clone -b e4s-22.11 $SPACK_REPO
        - . spack/share/spack/setup-env.sh
        - spack --version
        - ls -l /global/common/software/spackecp/mirrors/perlmutter-e4s-22.11/build_
↪cache/_pgp
      script:
      - echo "End Pipeline"
    mappings:
    - match: [os=sles15]
      runner-attributes:
        tags: [perlmutter-e4s]
  specs:
  - matrix:
    - [$cuda_specs]
    - [$gcc_compilers]
```

2.4 Perlmutter E4S 22.05

Shown below is the production Spack configuration for Perlmutter E4S 22.05. You can access this stack via `module load e4s/22.05` on Perlmutter. Please see our user documentation for this stack at https://docs.nersc.gov/applications/e4s/perlmutter/22.05/.

Production Spack Configuration

GCC spack environment

```
spack:
  view:
    default:
      root: $spack/var/spack/environments/gcc/views/default
      select: ['%gcc']
```

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```
      exclude: ['py-warpx']
      link_type: symlink
      link: roots
      projections:
        all: '{name}/{version}-{compiler.name}-{compiler.version}'
  include:
    - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
    - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree: $spack/opt/spack
  mirrors:
    perlmutter-e4s-22.05: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪22.05
    source_mirror: file:///global/cfs/cdirs/m3503/mirrors/source_mirror
  specs:
  - $nersc_specs
  - $utilities
  - matrix:
    - [$gcc_specs]
    - [$gcc_compilers]
  - matrix:
    - - py-libensemble@0.9.1 ^py-numpy ~blas ~lapack
    - ['%gcc@10.3.0']
```

CCE Spack Environment

```
spack:
  view:
    default:
      root: $spack/var/spack/environments/cce/views/default
      select: ['%cce']
      link_type: symlink
      link: roots
      projections:
        all: '{name}/{version}-{compiler.name}-{compiler.version}'
  include:
    - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
    - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree: $spack/opt/spack
  mirrors:
    perlmutter-e4s-22.05: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪22.05
    source_mirror: file:///global/cfs/cdirs/m3503/mirrors/source_mirror
```

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```
  specs:
  - matrix:
    - [$cce_specs]
    - [$cce_compilers]
```

NVHPC Spack Environment

```
spack:
  view:
    default:
      root: $spack/var/spack/environments/nvhpc/views/default
      select: ['%nvhpc']
      link_type: symlink
      link: roots
      projections:
        all: '{name}/{version}-{compiler.name}-{compiler.version}'
  include:
    - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
    - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree: $spack/opt/spack
  mirrors:
    perlmutter-e4s-22.05: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪22.05
    source_mirror: file:///global/cfs/cdirs/m3503/mirrors/source_mirror
  specs:
  - matrix:
    - [$nvhpc_specs]
    - [$nvhpc_compilers]
```

CUDA Spack Environment

```
spack:
  view:
    default:
      root: $spack/var/spack/environments/cuda/views/default
      select: ['%gcc +cuda']
      link_type: symlink
      link: roots
      projections:
        all: '{name}/{version}-{compiler.name}-{compiler.version}'
  include:
    - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
    - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
```

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```
    concretizer: clingo
    install_tree: $spack/opt/spack
  mirrors:
    perlmutter-e4s-22.05: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪22.05
    source_mirror: file:///global/cfs/cdirs/m3503/mirrors/source_mirror
  specs:
  - matrix:
    - [$cuda_specs]
    - [$gcc_compilers]
```

Shown below is the list of definitions that is used for all of our spack environments.

Definitions for Spack Environments

```
  definitions:
  - cce_compilers: ['%cce@15.0.0']
  - gcc_compilers: ['%gcc@11.2.0']
  - nvhpc_compilers: ['%nvhpc@22.7']
  - gcc_specs:
    - adios2@2.8.0
    - amrex@22.05
    - butterflypack@2.1.1
    - conduit@0.8.3
    - dyninst@12.1.0
    - fortrilinos@2.0.0
    - gasnet@2022.3.0
    - hdf5@1.10.7 +fortran +hl +shared
    - heffte@2.2.0 +fftw
    - hpctoolkit@2022.04.15
    - hpx@1.7.1 networking=mpi
    - hypre@2.24.0
    - kokkos@3.6.00 +openmp
    - kokkos-kernels@3.6.00 +openmp
    - lammps@20220107
    - libquo@1.3.1
    - nccmp@1.9.0.1
    - nco@5.0.1
    - mfem@4.4.0
    - openblas@0.3.20 threads=openmp
    - openpmd-api@0.14.4
    - papi@6.0.0.1
    - parallel-netcdf@1.12.2
    - pdt@3.25.1
    - petsc@3.17.1
    - plasma@21.8.29 ^openblas
    - py-warpx@22.05 ^warpx dims=2 ^openblas
    - py-warpx@22.05 ^warpx dims=3 ^openblas
    - py-warpx@22.05 ^warpx dims=rz ^openblas
    - qthreads@1.16 scheduler=distrib
    - raja@0.14.0
    - slate@2021.05.02 ~cuda
    - slepc@3.17.1
```

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```
    - strumpack@6.3.1 ~slate
    - sundials@6.2.0
    - superlu@5.3.0
    - superlu-dist@7.2.0
    - tasmanian@7.7
    - 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
    - vtk-m@1.7.1
    - upcxx@2022.3.0
    - zfp@0.5.5
    #- ascent@0.8.0     # ascent (DIFFERENT ERROR in ParaTools deployment %gcc@11.2.0)
    #- plumed@2.6.3     # plumed (SAME ERROR in ParaTools deployment %gcc@11.2.0)
    #- variorum@0.4.1   # variorum (SAME ERROR in ParaTools deployment %gcc@11.2.0)
    #- wannier90@3.1.0  # wannier90 (SAME ERROR in ParaTools deployment %gcc@11.2.0)
    # ascent: Could NOT find MPI_C (missing: MPI_C_LIB_NAMES) (found version "3.1")
    # plumed: tools/../../tools/lepton/../../lepton/Operation.h:902:39: error: 'numeric_
↪limits' is not a member of 'std'
    # variorum (1/2): make[2]: *** [variorum/CMakeFiles/variorum.dir/build.make:196:␣
↪variorum/libvariorum.so] Error 1
    # variorum (2/2): /usr/bin/ld: Intel/CMakeFiles/variorum_intel.dir/msr_core.c.o:(.
↪bss+0x0): multiple definition of `g_platform'; CMakeFiles/variorum.dir/config_
↪architecture.c.o:(.bss+0x0): first defined here
    # wannier90: Error: Type mismatch between actual argument at (1) and actual argument␣
↪at (2) (COMPLEX(8)/INTEGER(4)).

  - cuda_specs:
    - adios2@2.8.0 +cuda cuda_arch=80
    - hypre@2.24.0 +cuda cuda_arch=80
    - kokkos@3.6.00 +wrapper +cuda cuda_arch=80
    - kokkos-kernels@3.6.00 +cuda cuda_arch=80 ^kokkos@3.6.00 +wrapper +cuda cuda_arch=80
    - lammps@20220107 +cuda cuda_arch=80 +cuda_mps
    - hpctoolkit@2022.04.15 +cuda +mpi ~papi
    - likwid +cuda
    - papi@6.0.0.1 +cuda
    - petsc@3.17.1+cuda cuda_arch=80
    - raja@0.14.0 +cuda cuda_arch=80
    - slate@2021.05.02 +cuda cuda_arch=80
    - slepc@3.17.1 +cuda cuda_arch=80
    - strumpack@6.3.1 ~slate +cuda cuda_arch=80
    - tau@2.31.1 +mpi +cuda
    - zfp@0.5.5 +cuda cuda_arch=80
    #- heffte@2.2.0 +cuda cuda_arch=80        # heffte (WORKED in ParaTools deployment
↪%gcc@11.2.0)
    #- hpx@1.7.1 +cuda cuda_arch=80           # hpx (WORKED in ParaTools deployment
↪%gcc@11.2.0)
    #- magma@2.6.2 +cuda cuda_arch=80         # magma (WORKED in ParaTools deployment
↪%gcc@11.2.0)
    #- parsec@3.0.2012 +cuda cuda_arch=80     # parsec (SAME ERROR in ParaTools␣
↪deployment %gcc@11.2.0)
```

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```
    #- sundials@6.2.0 +cuda cuda_arch=80      # sundials (WORKED in ParaTools deployment
↪%gcc@11.2.0)
    #- superlu-dist@7.2.0 +cuda cuda_arch=80  # superlu-dist (WORKED in ParaTools␣
↪deployment %gcc@11.2.0)
    #- tasmanian@7.7 +cuda cuda_arch=80       # tasmanian (WORKED in ParaTools␣
↪deployment %gcc@11.2.0)
    #- trilinos@13.2.0 +cuda cuda_arch=80     # trilinos (SAME ERROR in ParaTools␣
↪deployment %gcc@11.2.0)
    #- vtk-m@1.7.1 +cuda cuda_arch=80         # vtk-m (DIFF ERROR in ParaTools␣
↪deployment %gcc@11.2.0)
    # heffte: CMake Error: The following variables are used in this project, but they␣
↪are set to NOTFOUND: CUDA_cufft_LIBRARY
    # hpx: CMake Error: The following variables are used in this project, but they are␣
↪set to NOTFOUND: CUDA_cublas_LIBRARY
    # magma: CMake Error: The following variables are used in this project, but they are␣
↪set to NOTFOUND: CUDA_cublas_LIBRARY
    # parsec: transfer.c:168: multiple definition of `parsec_CUDA_d2h_max_flows';
    # sundials: spack-src/examples/sunmatrix/cusparse/test_sunmatrix_cusparse.cu:167:␣
↪undefined reference to `cusparseCreate'
    # superlu-dist: make[2]: *** No rule to make target '/opt/nvidia/hpc_sdk/Linux_x86_␣
↪64/21.11/cuda/11.5/lib64/libcublas.so', needed by 'SRC/CMakeFiles/superlu_dist.dir/
↪cmake_device_link.o'.
    # tasmanian: CMake Error at /global/cfs/cdirs/m3503/ci-builds/perlmutter/yUW7FC66...␣
↪/Modules/FindPackageHandleStandardArgs.cmake:230 (message): Could NOT find␣
↪TasmanianCudaMathLibs
    # trilinos +cuda: CMake Error at /global/cfs....CMakeTestCXXCompiler.cmake:62␣
↪(message): The C++ compiler "/opt/cray/pe/mpich/8.1.13/ofi/gnu/9.1/bin/mpicxx" is not␣
↪able to compile a simple test program.
    # vtk-m: spack-src/vtkm/internal/brigand.hpp:1061:131: error: expected class-name␣
↪before '{' token struct find<true, false, L1, L2, Ls...> : find<true , F<Ts..., L2>
↪::value, L2, Ls...>

  - cce_specs:
    - adios2@2.8.0
    - hdf5@1.10.7 +fortran +hl +shared

    - kokkos-kernels@3.6.00 +openmp
    - kokkos@3.6.00 +openmp
    - petsc@3.17.1 ~strumpack
    - sundials@6.2.0
    - superlu-dist@7.2.0
    - superlu@5.3.0
    # - hypre@2.24.0 # error in compilation: clang-15: error: unknown argument: '-qsmp=omp
↪'
    #- openblas@0.3.20 threads=openmp   # openblas (SAME ERROR in ParaTools deployment
↪%cce@14.0.0)
    #- strumpack@6.3.1 ~slate           # butterflypack
    # openblas: ftn-2307 ftn: ERROR in command line The "-m" option must be followed by␣
↪0, 1, 2, 3 or 4. ftn-2103 ftn: WARNING in command line.The -W all option is not␣
↪supported or invalid and will be ignored.

  - nvhpc_specs:
```

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```
    - hdf5@1.10.7 +fortran +hl +shared
    - kokkos@3.6.00 +openmp
    - kokkos-kernels@3.6.00 +openmp
    - sundials@6.2.0
    - superlu@5.3.0
    - zfp@0.5.5

    # - raja@0.14.0 +cuda cuda_arch=80 build failure
    # - slate@2021.05.02 +cuda cuda_arch=80
    # - strumpack@6.3.1 ~slate build failure
    # - superlu-dist@7.2.0 NVIDIA subset: The 'taskloop' construct is not supported.

    # ==> Warning: Skipping build of superlu-dist-7.2.0-kmvqtie752awoenzob5pgemabeuzyaiv␣
↪since parmetis-4.0.3-ew3itm7cvpheb7h4e6lmyteghbq7toeo failed
    # ==> Warning: Skipping build of hypre-2.24.0-s2nqxywgft5dfjeps4jgiim6dxvedz3y since␣
↪superlu-dist-7.2.0-kmvqtie752awoenzob5pgemabeuzyaiv failed
    #- hypre@2.24.0 +cuda cuda_arch=80
    # failed to build HDF5 dependency with nvhpc
    #- raja@0.14.0 +cuda cuda_arch=80

  - nersc_specs:
    - ccache@4.5.1
    - cdo
    - gnuplot@5.4.3 +X
    - grads
    - gromacs@2021.5
    - gsl@2.7
    - metis@5.1.0
    - intel-mkl
    - ncl
    - ncview@2.1.8
    - parmetis@4.0.3
    - parallel
    - quantum-espresso@7.0
    - nwchem@7.0.2 ^cray-libsci
  - utilities:
    - autoconf
    - automake
    - cmake
    - git
    - gmake
    - gawk
    - nano
    - subversion
    - xterm
```

Shown below is the list of spack environments that is used for building the stack into buildcache using **spack ci**.

Spack Environments for Spack CI

GCC Spack Environment

```
spack:
```

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```
  include:
    - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
    - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree:
      padded_length: 128
  concretizer:
    reuse: false
  cdash:
    build-group: DOE nightly E4S builds
    url: https://cdash.spack.io
    project: Spack
    site: NERSC - Perlmutter E4S-22.05
  mirrors:
    perlmutter-e4s-22.05: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪22.05
  gitlab-ci:
    enable-artifacts-buildcache: false
    rebuild-index: true
    before_script:
    - module reset
    - module use /global/common/software/nersc/$(cat /etc/nersc_modules_rev)/extra_
↪modulefiles
    - module load cpu
    - module load cray-pmi
    - module list
    - source setup-env.sh
    - git clone --depth=10 -b e4s-22.05 $SPACK_REPO
    - . spack/share/spack/setup-env.sh
    - which spack
    - spack --version
    - spack-python --path
    script:
    - cd ${SPACK_CONCRETE_ENV_DIR}
    - spack env activate --without-view .
    - spack env st
    - export SPACK_GNUPGHOME=$HOME/.gnupg
    - spack gpg list
    - spack -d ci rebuild
    service-job-attributes:
      tags: [perlmutter-e4s]
      before_script:
        - git clone --depth=10 -b e4s-22.05 $SPACK_REPO
        - . spack/share/spack/setup-env.sh
        - spack --version
        - ls -l /global/common/software/spackecp/mirrors/perlmutter-e4s-22.05/build_
↪cache/_pgp
      script:
```

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```
      - echo "End Pipeline"
    mappings:
    - match: [os=sles15]
      runner-attributes:
        tags: [perlmutter-e4s]
  specs:
  - $nersc_specs
  - $utilities
  - matrix:
    - [$gcc_specs]
    - [$gcc_compilers]
  - matrix:
    - - py-libensemble@0.9.1 ^py-numpy ~blas ~lapack
    - ['%gcc@10.3.0']
```

CCE Spack Environment

```
spack:
  include:
    - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
    - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree:
      padded_length: 128
  concretizer:
    reuse: false
  cdash:
    build-group: DOE nightly E4S builds
    url: https://cdash.spack.io
    project: Spack
    site: NERSC - Perlmutter E4S-22.05
  mirrors:
    perlmutter-e4s-22.05: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪22.05
  gitlab-ci:
    enable-artifacts-buildcache: false
    rebuild-index: true
    before_script:
    - module reset
    - module use /global/common/software/nersc/$(cat /etc/nersc_modules_rev)/extra_
↪modulefiles
    - module load cpu
    - module load cray-pmi
    - module list
    - source setup-env.sh
    - git clone --depth=10 -b e4s-22.05 $SPACK_REPO
    - . spack/share/spack/setup-env.sh
    - which spack
```

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```
    - spack --version
    - spack-python --path
    script:
    - cd ${SPACK_CONCRETE_ENV_DIR}
    - spack env activate --without-view .
    - spack env st
    - export SPACK_GNUPGHOME=$HOME/.gnupg
    - spack gpg list
    - spack -d ci rebuild
    service-job-attributes:
      tags: [perlmutter-e4s]
      before_script:
        - git clone --depth=10 -b e4s-22.05 $SPACK_REPO
        - . spack/share/spack/setup-env.sh
        - spack --version
        - ls -l /global/common/software/spackecp/mirrors/perlmutter-e4s-22.05/build_
↪cache/_pgp
      script:
      - echo "End Pipeline"
    mappings:
    - match: [os=sles15]
      runner-attributes:
        tags: [perlmutter-e4s]
  specs:
  - matrix:
    - [$cce_specs]
    - [$cce_compilers]
```

NVHPC Spack Environment

```
spack:
  include:
    - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
    - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree:
      padded_length: 128
  concretizer:
    reuse: false
  cdash:
    build-group: DOE nightly E4S builds
    url: https://cdash.spack.io
    project: Spack
    site: NERSC - Perlmutter E4S-22.05
  mirrors:
    perlmutter-e4s-22.05: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪22.05
```

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```
  gitlab-ci:
    enable-artifacts-buildcache: false
    rebuild-index: true
    before_script:
    - module reset
    - module use /global/common/software/nersc/$(cat /etc/nersc_modules_rev)/extra_
↪modulefiles
    - module load cpu
    - module load cray-pmi
    - module list
    - source setup-env.sh
    - git clone --depth=10 -b e4s-22.05 $SPACK_REPO
    - . spack/share/spack/setup-env.sh
    - which spack
    - spack --version
    - spack-python --path
    script:
    - cd ${SPACK_CONCRETE_ENV_DIR}
    - spack env activate --without-view .
    - spack env st
    - export SPACK_GNUPGHOME=$HOME/.gnupg
    - spack gpg list
    - spack -d ci rebuild
    service-job-attributes:
      tags: [perlmutter-e4s]
      before_script:
        - git clone --depth=10 -b e4s-22.05 $SPACK_REPO
        - . spack/share/spack/setup-env.sh
        - spack --version
        - ls -l /global/common/software/spackecp/mirrors/perlmutter-e4s-22.05/build_
↪cache/_pgp
      script:
      - echo "End Pipeline"
    mappings:
    - match: [os=sles15]
      runner-attributes:
        tags: [perlmutter-e4s]
  specs:
  - matrix:
    - [$nvhpc_specs]
    - [$nvhpc_compilers]
```

CUDA Spack Environment

```
spack:
  include:
    - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
    - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  config:
    concretization: separately
    build_stage: $spack/var/spack/stage
```

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```
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
    install_tree:
      padded_length: 128
  concretizer:
    reuse: false
  cdash:
    build-group: DOE nightly E4S builds
    url: https://cdash.spack.io
    project: Spack
    site: NERSC - Perlmutter E4S-22.05
  mirrors:
    perlmutter-e4s-22.05: file:///global/common/software/spackecp/mirrors/perlmutter-e4s-
↪22.05
  gitlab-ci:
    enable-artifacts-buildcache: false
    rebuild-index: true
    before_script:
    - module reset
    - module use /global/common/software/nersc/$(cat /etc/nersc_modules_rev)/extra_
↪modulefiles
    - module load cpu
    - module load cray-pmi
    - module list
    - source setup-env.sh
    - git clone --depth=10 -b e4s-22.05 $SPACK_REPO
    - . spack/share/spack/setup-env.sh
    - which spack
    - spack --version
    - spack-python --path
    script:
    - cd ${SPACK_CONCRETE_ENV_DIR}
    - spack env activate --without-view .
    - spack env st
    - export SPACK_GNUPGHOME=$HOME/.gnupg
    - spack gpg list
    - spack -d ci rebuild
    service-job-attributes:
      tags: [perlmutter-e4s]
      before_script:
        - git clone --depth=10 -b e4s-22.05 $SPACK_REPO
        - . spack/share/spack/setup-env.sh
        - spack --version
        - ls -l /global/common/software/spackecp/mirrors/perlmutter-e4s-22.05/build_
↪cache/_pgp
      script:
      - echo "End Pipeline"
    mappings:
    - match: [os=sles15]
      runner-attributes:
        tags: [perlmutter-e4s]
  specs:
```

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```
  - matrix:
    - [$cuda_specs]
    - [$gcc_compilers]
```

2.5 Perlmutter E4S 21.11

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

Production Spack Environment

```
# 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: $spack/opt/spack
  include:
    - /global/common/software/spackecp/perlmutter/spack_settings/compilers.yaml
    - /global/common/software/spackecp/perlmutter/spack_settings/packages.yaml
  specs:
  - matrix:
    - [$gcc_specs]
    - [$gcc_compilers]
  - matrix:
    - [$cuda_specs]
    - [$gcc_compilers]
  - $nersc_specs
```

```
  definitions:
  - gcc_compilers: ['%gcc@11.2.0']
  - gcc_specs:
    - adios2@2.7.1
    - amrex@21.11 +fortran +openmp +shared
    - conduit@0.7.2
    - dyninst@11.0.1
    - gasnet@2021.9.0
    - globalarrays@5.8
    - hdf5@1.12.1
    - kokkos-kernels@3.4.01 +openmp
    - kokkos@3.4.01 +openmp
    - mercury@2.0.1
```

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```
    - mpark-variant@1.4.0
    - openpmd-api@0.14.3
    - papi@6.0.0.1
    - papyrus@1.0.2
    - pdt@3.25.1
    - qthreads@1.16 scheduler=distrib
    - raja@0.14.0
    - strumpack@6.1.0 ~slate
    - sundials@5.8.0 +openmp
    - 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␣
↪+tempus +tpetra +trilinoscouplings +zoltan +zoltan2 +superlu-dist gotype=long_long
    - umap@2.1.0
    - upcxx@2021.9.0 +gasnet +mpi
    #- slepc@3.16.0 --dpends on petsc
    #- mfem@4.3.0 --depends on hypre
    #- petsc@3.16.1 +openmp +strumpack --failed to install
    #- hypre@2.23.0 +openmp +superlu-dist --failed to install
    #- parsec@3.0.2012 ~cuda --failed to install
    #- warpx dims=2
    #- warpx dims=3
  - cuda_specs:
    - 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
    - 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
    #- mfem@4.3.0+cuda cuda_arch=80 --depends on hypre
    #- slepc@3.16.0 +cuda cuda_arch=80 ^petsc@3.16.1 +cuda cuda_arch=80 --depends on␣
↪petsc
    #- petsc@3.16.1 +cuda cuda_arch=80 --failed to install
    #- hypre@2.23.0+cuda cuda_arch=80 --failed to install
    #- 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
  - nersc_specs:
    - chapel@1.24.1
    - gsl@2.7
```

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```
    - 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
    #- wannier90@3.1.0
```

2.6 Cori E4S 22.02

Production Spack Environment

```
# 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: file:///global/cfs/cdirs/m3503/mirrors/source_mirror
  modules::
    prefix_inspections:
      bin:
        - PATH
      lib:
        - LIBRARY_PATH
        - LD_LIBRARY_PATH
      lib64:
        - LIBRARY_PATH
        - LD_LIBRARY_PATH
      include:
        - C_INCLUDE_PATH
        - CPLUS_INCLUDE_PATH
        - CPATH
      man:
        - MANPATH
      share/man:
        - MANPATH
```

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```
    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: {}
    operating_system: cnl7
    target: any
    modules:
    - PrgEnv-gnu
    - gcc/11.2.0
    - craype-haswell
- compiler:
    spec: intel@19.1.2.254
    paths:
```

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```
      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
  - 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
```

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```
    - 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␣
↪+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
```

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```
    - 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
    - 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
```

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```
    - 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
    - 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:
```

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```
  - 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]
      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
```

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```
  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
    - 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
```

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```
  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:
    variants: ~wrapperrpath
  ncurses:
    variants: +termlib
    externals:
    - spec: ncurses@6.1
      prefix: /usr
  netcdf-c:
    version: [4.8.1.1]
    externals:
```

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```
    - 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
  slurm:
    buildable: false
    version: [20-11-8-1]
    externals:
    - spec: slurm@20-11-8-1
      prefix: /usr
  superlu-dist:
    variants: +openmp
  strumpack:
```

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```
      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
```

2.7 Cori E4S 21.05

Production Spack Environment

```
spack:
  view: false
  concretization: separately
  config:
    install_tree:
      root: /global/common/software/spackecp/e4s-21.05/software
    module_roots:
```

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```
    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
    flags: {}
    operating_system: cnl7
    target: any
    modules:
    - PrgEnv-intel
    - intel/19.1.3.304
    environment: {}
    extra_rpaths: []
packages:
```

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```
    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:
      version:
      - 1.21.0
    cmake:
      version:
      - 3.20.2
    curl:
      version:
      - 7.76.0
    diffutils:
```

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```
    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
    variants: fabrics=sockets,tcp,udp,rxm
  libiconv:
    version:
    - 1.16
  libsigsegv:
    version:
    - 2.12
  libpciaccess:
    version:
```

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```
    - 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:
    - 8
  sqlite:
    version:
    - 3.34.0
  tar:
    version:
    - 1.32
  texinfo:
    version:
```

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```
    - 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
  - 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
```

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```
    - 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
    - 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
```

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```
    # 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
```

2.8 Cori E4S 21.02

Production Spack Environment

```
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:
```

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```
    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
    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
```

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```
    - 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
    - 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
```

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```
    # - 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/
↪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.
```

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```
↪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?
↪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
```

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```
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:
    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
```

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```
      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
```

2.9 Cori E4S 20.10

Production Spack Environment

```
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
  modules:
    enable:
    - tcl
    tcl:
      hash_length: 8
      projections:
        all: '{name}/{version}-{compiler.name}-{compiler.version}'
      all:
        conflict:
        - '{name}'
        filter:
          environment_blacklist: []
        load: []
```

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```
      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
    - 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
```

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```
    - 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
  # - 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:
```

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```
    - - $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:
      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
```

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```
      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]

  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]
```

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```
  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:
    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:
```

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```
    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

  zlib:
    version: [1.2.11]
```

CHAPTER

THREE

HOW TO GUIDE

3.1 How to setup a schedule pipeline

First go to CI/CD > Schedules and create a schedule pipeline. You should see a similar pipeline for another stack. The schedule pipeline contains a unique variable *PIPELINE_NAME* which is the name of E4S stack to run. The value is all CAPS, so if you want to trigger E4S 23.05 stack for Perlmutter, the value will be *PERLMUTTER_E4S_23.05*. Please make sure the variable *PIPELINE_NAME* matches the one you defined in .gitlab-ci.yml for your job. The pipeline can be run via web interface, if you chose this route, just set *PIPELINE_NAME* to the appropriate value.

The reason why we setup schedule pipeline and web-interface is to allow one to trigger pipeline automatically at schedule interval or trigger pipeline manually such that a commit is not required to trigger pipeline. This is useful when one needs to check if pipeline can rebuild at any given time due to system change.

3.2 How to find available runners

You can find all runners by going to Settings > CI/CD > Runners.

This project is configured with gitlab runner for Perlmutter and Muller using the production account *e4s*. Shown below are the available runners

Table 1: Gitlab Runner by NERSC system

System	Runner Name
Perlmutter	*perlmutter-e4s*
Muller	*muller-e4s*

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

3.3 How to register gitlab runner

We have a script titled *register.sh* that is responsible for registering a gitlab runner. This script will expect a registration token which can be found at Settings > CI/CD > Runners. Shown below is the script used to register the runner on Perlmutter, once you execute the script, you will be prompted for the registration token.

```
e4s:login37> cat ~/register.sh
#!/bin/bash

read -sp "Registration Token?" TOKEN
```

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```
gitlab-runner register \
    --url https://software.nersc.gov \
    --registration-token ${TOKEN} \
        --tag-list ${NERSC_HOST}-${USER} \
    --name "E4S Runner on Perlmutter" \
    --executor custom \
    --custom-config-exec "/global/homes/e/e4s/jacamar/binaries/jacamar-auth" \
    --custom-config-args "-u config --configuration /global/homes/e/e4s/.gitlab-runner/
↪jacamar.toml" \
    --custom-prepare-exec "/global/homes/e/e4s/jacamar/binaries/jacamar-auth" \
    --custom-prepare-args "prepare" \
    --custom-run-exec  "/global/homes/e/e4s/jacamar/binaries/jacamar-auth" \
    --custom-run-args "run" \
    --custom-cleanup-exec "/global/homes/e/e4s/jacamar/binaries/jacamar-auth" \
    --custom-cleanup-args "cleanup --configuration /global/homes/e/e4s/.gitlab-runner/
↪jacamar.toml" \
    --config /global/homes/e/e4s/.gitlab-runner/perlmutter.config.toml
```

CHAPTER

FOUR

SPACK TRAINING

4.1 Goal

The goal of this training is to provide advice for how one can use Spack to install packages and manage a software stack on Perlmutter. We will cover the following topics:

- User Environment
- Defining Compilers in Spack
- Define Package Preference and Externals
- Create a source mirror
- Building CUDA packages
- Generating modulefiles

After completing the training, one can expect to be familiar with the customizations needed for an optimal Spack experience on Perlmutter.

4.2 Pre-Requisite

In order to perform this training, you need a NERSC account and access to Perlmutter. We assume you already have a basic understanding of spack.

4.3 Setup

In order to get started, please Connect to Perlmutter via `ssh`. Once you have access, please clone the following Git repository into your `$HOME` directory.

```
git clone https://github.com/NERSC/spack-infrastructure.git
```

4.4 User Environment

Spack builds can be sensitive to your user environment and any configuration setup in your shell startup files. We recommend you review your startup configuration files. Some things to look out for are the following:

1. Loading or unloading of any modules
2. Activating a Python or Conda environment
3. Any user environment variables such as `$PATH`

Note: We have seen that purging modules (*module purge*) can alter Spack builds and cause most of the Cray programming environment to be removed. For more details see spack/#27124.

When performing Spack builds, we encourage using the default modules. This should look at follows:

```
elvis@login34> module list

Currently Loaded Modules:
  1) craype-x86-milan     4) perftools-base/22.06.0                 7) craype/2.7.16    ␣
↪ 10) cray-libsci/21.08.1.2  13) darshan/3.3.1 (io)
  2) libfabric/1.15.0.0   5) xpmem/2.3.2-2.2_7.5__g93dd7ee.shasta   8) cray-dsmml/0.2.2 ␣
↪ 11) PrgEnv-gnu/8.3.3
  3) craype-network-ofi   6) gcc/11.2.0                             9) cray-mpich/8.1.17␣
↪ 12) xalt/2.10.2

  Where:
   io:  Input/output software
```

In order to setup our environment, let's source the setup script which will create a new Python virtual environment to perform the Spack builds. Please run the following commands:

```
elvis@login34> cd spack-infrastructure/
elvis@login34> source setup-env.sh
Collecting clingo
  Using cached clingo-5.5.2-cp36-cp36m-manylinux_2_17_x86_64.manylinux2014_x86_64.whl (2.
↪2 MB)
Collecting cffi
  Using cached cffi-1.15.1-cp36-cp36m-manylinux_2_5_x86_64.manylinux1_x86_64.whl (402 kB)
Collecting pycparser
  Using cached pycparser-2.21-py2.py3-none-any.whl (118 kB)
Installing collected packages: pycparser, cffi, clingo
Successfully installed cffi-1.15.1 clingo-5.5.2 pycparser-2.21
WARNING: You are using pip version 20.2.3; however, version 21.3.1 is available.
You should consider upgrading via the '/global/homes/e/elvis/spack-infrastructure/spack-
↪pyenv/bin/python3 -m pip install --upgrade pip' command.
/global/homes/e/elvis/spack-infrastructure/spack-pyenv/bin/python
Package    Version
---------- -------
cffi       1.15.1
clingo     5.5.2
pip        20.2.3
pycparser  2.21
```

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```
setuptools 44.1.1
WARNING: You are using pip version 20.2.3; however, version 21.3.1 is available.
You should consider upgrading via the '/global/homes/e/elvis/spack-infrastructure/spack-
↪pyenv/bin/python3 -m pip install --upgrade pip' command.
```

The `setup-env.sh` script will install `clingo` in your Python environment which is typically required by Spack along with a few other configurations relevant for building Spack.

Note: Spack requires clingo in-order to bootstrap clingo however we observed issues where Spack was unable to bootstrap clingo see spack/28315. We found that installing clingo as a Python package addressed the issue.

4.5 Acquiring Spack

Clone the following Spack branch from the Git Repository and source the setup script.

```
git clone -b e4s-22.05 https://github.com/spack/spack.git
source spack/share/spack/setup-env.sh
```

Once you have acquired Spack and sourced the activation script, please run the following commands to ensure your setup is done correctly. We have configured the environment, `SPACK_PYTHON`, to use a Python wrapper in the virtual environment.

```
(spack-pyenv) elvis@login34> spack --version
0.18.0.dev0 (6040c82740449632aa1d6faab08f93f5e4c54615)

(spack-pyenv) elvis@login34> echo $SPACK_PYTHON
/global/homes/e/elvis/spack-infrastructure/spack-pyenv/bin/python

(spack-pyenv) elvis@login34> which python
/global/homes/e/elvis/spack-infrastructure/spack-pyenv/bin/python
```

The command below will pass the full path to the Python interpreter used by Spack, which should be the path set by environment `SPACK_PYTHON`.

```
(spack-pyenv) elvis@login34> spack-python --path
/global/homes/e/elvis/spack-infrastructure/spack-pyenv/bin/python
```

4.6 Creating a Spack Environment

When using Spack, you may be tempted to start installing packages via `spack install` in your Spack instance. Note that it's best you organize your Spack stacks in their own spack environment, similar to how one would organize a Python or Conda environment.

Let's start by creating a Spack environment named *data_viz*, and activating it.

```
spack env create data_viz
spack env activate data_viz
```

Upon completion you should confirm the output of **spack env status** matches the following:

```
(spack-pyenv) elvis@login34> spack env status
==> In environment data_viz
```

Let's navigate to the directory for Spack environment **data_viz**. You will see a file **spack.yaml** that is used to specify your Spack configuration. This includes configuration options such as which compilers to use in your Spack builds.

```
(spack-pyenv) elvis@login34> spack cd -e data_viz
(spack-pyenv) elvis@login34> ls -l
total 1
-rw-rw-r-- 1 elvis elvis 199 Aug  3 19:09 spack.yaml
```

4.7 Defining Compilers

In order to use Spack, one must define a list of compilers in order to build packages. On Perlmutter, we have `gcc/11.2.0` and `cce/13.0.2` compilers available as modulefiles which correspond to the GCC and Cray compiler. In order to specify the compiler definition we must use the corresponding `PrgEnv-*` module.

```
(spack-pyenv) elvis@login34> ml -t av gcc/11.2.0 cce/13.0.2
/opt/cray/pe/lmod/modulefiles/core:
cce/13.0.2
gcc/11.2.0
```

Let's add the following content in *spack.yaml*. Please open the file in your preferred editor and paste the contents. Note that we specify the full path for *cc*, *cxx*, *f77*, and *fc* which should correspond to the Cray wrappers.

```
# This is a Spack Environment file.
#
# It describes a set of packages to be installed, along with
# configuration settings.
spack:
  config:
    view: false
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo

  compilers:
  - compiler:
      spec: gcc@11.2.0
      paths:
        cc: cc
        cxx: CC
        f77: ftn
        fc: ftn
      flags: {}
      operating_system: sles15
      target: any
      modules:
      - PrgEnv-gnu
      - gcc/11.2.0
```

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```
      - craype-x86-milan
      - libfabric
      extra_rpaths: []
  - compiler:
      spec: cce@13.0.2
      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/13.0.2
      - craype-x86-milan
      - libfabric
      environment: {}
      extra_rpaths: []

  # add package specs to the `specs` list
  specs: []
  packages:
    all:
      compiler: [gcc@11.2.0, cce@13.0.2]

  view: true
```

Note: The directory */opt/cray/pe/craype/default* resorts to the default Cray programming environment, `craype`, in this case its 2.7.16 and the *cc* wrapper should be from this corresponding directory.

```
(spack-pyenv) elvis@login34> ls -ld /opt/cray/pe/craype/default
lrwxrwxrwx 1 root root 6 Jun  1 14:56 /opt/cray/pe/craype/default -> 2.7.16

(spack-pyenv) elvis@login34> which cc
/opt/cray/pe/craype/2.7.16/bin/cc
```

On Perlmutter, the *craype/2.7.16* modulefile is responsible for setting the Cray wrappers which is loaded by default as shown below:

```
(spack-pyenv) elvis@login34> ml -t list craype/2.7.16
craype/2.7.16
```

If this modulefile was removed, you will not have access to the Cray wrappers *cc*, *CC* or *ftn* which may result in several errors.

Now let's check all available compilers by running `spack compiler list`

```
(spack-pyenv) elvis@login34> spack compiler list
==> Available compilers
```

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```
-- cce sles15-any ------------------------------------------------
cce@13.0.2

-- gcc sles15-any ------------------------------------------------
gcc@11.2.0
```

4.8 Package Preference

Now let's try to run `spack spec -Il hdf5`, you will notice Spack will try to install all the packages from source, some of which are dependencies that should not be installed but rather set as external packages. For instance, utilities like **openssl**, **bzip2**, **diffutils**, **openmpi**, **openssh** should not be installed from source. We have documented Recommended External Packages for Spack that outlines a list of packages where we recommend using the NERSC system installations.

```
(spack-pyenv) elvis@login34> spack spec -Il hdf5
Input spec
--------------------------------
 -   hdf5

Concretized
--------------------------------
 -   z4dfikd  hdf5@1.12.2%gcc@11.2.0~cxx~fortran~hl~ipo~java+mpi+shared~szip~threadsafe+tools api=default build_type=RelWithDebInfo arch=cray-sles15-zen3
 -   auepzq2      ^cmake@3.23.1%gcc@11.2.0~doc+ncurses+ownlibs~qt build_type=Release arch=cray-sles15-zen3
 -   2t22mc5          ^ncurses@6.2%gcc@11.2.0~symlinks+termlib abi=none arch=cray-sles15-zen3
 -   nugfov2              ^pkgconf@1.8.0%gcc@11.2.0 arch=cray-sles15-zen3
 -   i2r3jpl          ^openssl@1.1.1o%gcc@11.2.0~docs~shared certs=system arch=cray-sles15-zen3
 -   ekj3iat              ^perl@5.34.1%gcc@11.2.0+cpanm+shared+threads arch=cray-sles15-zen3
 -   hafeanv                  ^berkeley-db@18.1.40%gcc@11.2.0+cxx~docs+stl patches=b231fcc arch=cray-sles15-zen3
 -   blbww14                  ^bzip2@1.0.8%gcc@11.2.0~debug~pic+shared arch=cray-sles15-zen3
 -   gvbyw6w                      ^diffutils@3.8%gcc@11.2.0 arch=cray-sles15-zen3
 -   3xwztgy                          ^libiconv@1.16%gcc@11.2.0 libs=shared,static arch=cray-sles15-zen3
 -   bxrz7zm                  ^gdbm@1.19%gcc@11.2.0 arch=cray-sles15-zen3
 -   avhrefq                      ^readline@8.1%gcc@11.2.0 arch=cray-sles15-zen3
 -   ozmcyfj                  ^zlib@1.2.12%gcc@11.2.0+optimize+pic+shared patches=0d38234 arch=cray-sles15-zen3
 -   gdm5qma      ^openmpi@4.1.3%gcc@11.2.0~atomics~cuda~cxx~cxx_exceptions~gpfs~internal-hwloc~java~legacylaunchers~lustre~memchecker~pmi+pmix+romio+rsh~singularity+static+vt+wrapper-rpath fabrics=none schedulers=none arch=cray-sles15-zen3
 -   6rkjosk          ^hwloc@2.7.1%gcc@11.2.0~cairo~cuda~gl~libudev+libxml2~netloc~nvml~opencl+pci~rocm+shared arch=cray-sles15-zen3
 -   oyeiwvg              ^libpciaccess@0.16%gcc@11.2.0 arch=cray-sles15-zen3
 -   56oycjj                  ^libtool@2.4.7%gcc@11.2.0 arch=cray-sles15-zen3
 -   flsruli                      ^m4@1.4.19%gcc@11.2.0+sigsegv patches=9dc5fbd,bfdffa7
```

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```
↪arch=cray-sles15-zen3
 -   wcuq435                          ^libsigsegv@2.13%gcc@11.2.0 arch=cray-sles15-zen3
 -   koitq65                    ^util-macros@1.19.3%gcc@11.2.0 arch=cray-sles15-zen3
 -   u2ai4xj                ^libxml2@2.9.13%gcc@11.2.0~python arch=cray-sles15-zen3
 -   tyswlp4                    ^xz@5.2.5%gcc@11.2.0~pic libs=shared,static arch=cray-
↪sles15-zen3
 -   w2itznc           ^libevent@2.1.12%gcc@11.2.0+openssl arch=cray-sles15-zen3
 -   t4jyphv           ^numactl@2.0.14%gcc@11.2.0 patches=4e1d78c,62fc8a8,ff37630␣
↪arch=cray-sles15-zen3
 -   al4xc7v               ^autoconf@2.69%gcc@11.2.0 patches=35c4492,7793209,a49dd5b␣
↪arch=cray-sles15-zen3
 -   2uxxcnx               ^automake@1.16.5%gcc@11.2.0 arch=cray-sles15-zen3
 -   w5aq2sc           ^openssh@9.0p1%gcc@11.2.0 arch=cray-sles15-zen3
 -   mkoju5b               ^libedit@3.1-20210216%gcc@11.2.0 arch=cray-sles15-zen3
 -   t3wpbom           ^pmix@4.1.2%gcc@11.2.0~docs+pmi_backwards_compatibility~restful␣
↪arch=cray-sles15-zen3
```

Let's try to update our Spack configuration with the external packages as follows:

```yaml
# This is a Spack Environment file.
#
# It describes a set of packages to be installed, along with
# configuration settings.
spack:
  config:
    view: false
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo

  compilers:
  - compiler:
      spec: gcc@11.2.0
      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: []
  - compiler:
      spec: cce@13.0.2
      paths:
        cc: /opt/cray/pe/craype/default/bin/cc
```

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```
      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/13.0.2
    - craype-x86-milan
    - libfabric
    environment: {}
    extra_rpaths: []

# add package specs to the `specs` list
specs: []
packages:
  all:
    compiler: [gcc@11.2.0, cce@13.0.2]
  bzip2:
    version: [1.0.6]
    externals:
    - spec: bzip2@1.0.6
      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
  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
  readline:
    version: [7.0]
    buildable: false
    externals:
    - spec: readline@7.0
      prefix: /usr
```

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```
    tar:
      version: [1.3]
      buildable: false
      externals:
      - spec: tar@1.30
        prefix: /usr
    unzip:
      version: [6.0]
      buildable: false
      externals:
      - spec: unzip@6.0
        prefix: /usr

  view: true
```

Many software packages depend on MPI, BLAS, PMI, and libfabrics, and these packages are typically available on Perlmutter. Shown below is a breakdown of the provider and its corresponding modules typically available on Perlmutter

- MPI: cray-mpich
- BLAS: cray-libsci
- PMI: cray-pmi
- libfabrics: libfabrics

Shown below are the corresponding modules that you should consider when setting up external packages.

```
(spack-pyenv) elvis@login34> ml -d av cray-mpich cray-libsci cray-pmi libfabrics

---------------------------------------------------- Cray Compiler/Network Dependent␣
↪Packages -----------------------------------------------------
   cray-mpich-abi/8.1.17    cray-mpich/8.1.17 (L)

------------------------------------------------------------------ Cray Core Modules -------
↪-------------------------------------------------------
   cray-libsci/21.08.1.2 (L)    cray-pmi-lib/6.0.17    cray-pmi/6.1.3

  Where:
   L:  Module is loaded

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

In Spack, you can use the `spack providers` command to find the corresponding Spack package that maps to the provider. In Spack these are referred to as virtual packages which are a collection of Spack packages that provide the same functionality.

```
(spack-pyenv) elvis@login34> spack providers
Virtual packages:
    D     daal      flame  glu     iconv  jpeg     lua-lang        mkl  mysql-client ␣
↪osmesa  pkgconfig  sycl  unwind  yacc
    awk   elf       fuse   glx     ipp    lapack   luajit          mpe  onedal       ␣
```

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```
↪pbs     rpc        szip  uuid    ziglang
   blas  fftw-api  gl     golang  java   libllvm  mariadb-client  mpi  opencl       ␣
↪pil     scalapack  tbb   xxd
```

For instance, if you want to see all the MPI providers you can run the following. Note that `cray-mpich` is in the list.

```
(spack-pyenv) elvis@login34> spack providers mpi
mpi:
cray-mpich     intel-mpi              mpich@:1.1  mpich          mpt@1:        ␣
↪mvapich2@2.3:  openmpi         spectrum-mpi
cray-mvapich2  intel-oneapi-mpi       mpich@:1.2  mpilander      mpt@3:         mvapich2-
↪gdr   openmpi@1.6.5
fujitsu-mpi    intel-parallel-studio  mpich@:3.1  mpitrampoline  mvapich2      ␣
↪mvapich2x      openmpi@1.7.5:
hpcx-mpi       mpich@:1.0             mpich@:3.2  mpt            mvapich2@2.1:  nvhpc   ␣
↪      openmpi@2.0.0:
```

Now let's try to update our Spack configuration as follows:

```
# This is a Spack Environment file.
#
# It describes a set of packages to be installed, along with
# configuration settings.
spack:
  config:
    view: false
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo

  compilers:
  - compiler:
      spec: gcc@11.2.0
      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: []
  - compiler:
      spec: cce@13.0.2
      paths:
        cc: /opt/cray/pe/craype/default/bin/cc
```

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```
        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/13.0.2
      - craype-x86-milan
      - libfabric
      environment: {}
      extra_rpaths: []

  # add package specs to the `specs` list
  specs: []
  packages:
    all:
      compiler: [gcc@11.2.0, cce@13.0.2]
      providers:
        blas: [cray-libsci]
        mpi: [cray-mpich]
    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@8.1.15 %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 %cce@13.0.2
        prefix: /opt/cray/pe/mpich/8.1.15/ofi/cray/10.0/
        modules:
        - cray-mpich/8.1.15
        - cudatoolkit/11.5
    cray-pmi:
      buildable: false
      externals:
      - spec: cray-pmi@6.1.1
        modules:
        - cray-pmi/6.1.1
```

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```
    diffutils:
      version: [3.6]
      externals:
      - spec: diffutils@3.6
        prefix: /usr
    findutils:
      version: [4.6.0]
      externals:
      - spec: findutils@4.6.0
        prefix: /usr
    libfabric:
      buildable: false
      variants: fabrics=sockets,tcp,udp,rxm
      externals:
      - spec: libfabric@1.11.0.4.114
        prefix: /opt/cray/libfabric/1.11.0.4.114
        modules:
        - libfabric/1.11.0.4.114
    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
    readline:
      version: [7.0]
      buildable: false
      externals:
      - spec: readline@7.0
        prefix: /usr
    tar:
      version: [1.3]
      buildable: false
      externals:
      - spec: tar@1.30
        prefix: /usr
    unzip:
      version: [6.0]
      buildable: false
      externals:
      - spec: unzip@6.0
        prefix: /usr

  view: true
```

Let's try to run `spack spec hypre` and notice that Spack will now use `cray-libsci` and `cray-mpich` as the dependencies, because we have set these packages as externals.

```
(spack-pyenv) elvis@login34> spack spec hypre
Input spec
--------------------------------
hypre@2.24.0

Concretized
--------------------------------
hypre@2.24.0%gcc@11.2.0~complex~cuda~debug+fortran~gptune~int64~internal-superlu~
↪mixedint+mpi~openmp~rocm+shared~superlu-dist~unified-memory arch=cray-sles15-zen3
    ^cray-libsci@21.08.1.2%gcc@11.2.0~mpi~openmp+shared arch=cray-sles15-zen3
    ^cray-mpich@8.1.15%gcc@11.2.0+wrappers arch=cray-sles15-zen3
```

Now let's try to add some packages to our Spack configuration by adding the following lines:

```
# This is a Spack Environment file.
#
# It describes a set of packages to be installed, along with
# configuration settings.
spack:
  config:
    view: false
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
  compilers:
  - compiler:
      spec: gcc@11.2.0
      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: []
  - compiler:
      spec: cce@13.0.2
      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:
```

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```
      - PrgEnv-cray
      - cce/13.0.2
      - craype-x86-milan
      - libfabric
      environment: {}
      extra_rpaths: []
  # add package specs to the `specs` list
  specs:
  - papi %gcc
  - papi %cce
  - hypre %gcc
  - hypre %cce
  - darshan-runtime %gcc
  - darshan-runtime %cce
  packages:
    all:
      compiler: [gcc@11.2.0, cce@13.0.2]
      providers:
        blas: [cray-libsci]
        mpi: [cray-mpich]
    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@8.1.15 %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 %cce@13.0.2
        prefix: /opt/cray/pe/mpich/8.1.15/ofi/cray/10.0/
        modules:
        - cray-mpich/8.1.15
        - cudatoolkit/11.5
    cray-pmi:
      buildable: false
      externals:
      - spec: cray-pmi@6.1.1
        modules:
        - cray-pmi/6.1.1
    diffutils:
      version: [3.6]
```

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```
    externals:
    - spec: diffutils@3.6
      prefix: /usr
  findutils:
    version: [4.6.0]
    externals:
    - spec: findutils@4.6.0
      prefix: /usr
  libfabric:
    buildable: false
    variants: fabrics=sockets,tcp,udp,rxm
    externals:
    - spec: libfabric@1.11.0.4.114
      prefix: /opt/cray/libfabric/1.11.0.4.114
      modules:
      - libfabric/1.11.0.4.114
  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
  readline:
    version: [7.0]
    buildable: false
    externals:
    - spec: readline@7.0
      prefix: /usr
  tar:
    version: [1.3]
    buildable: false
    externals:
    - spec: tar@1.30
      prefix: /usr
  unzip:
    version: [6.0]
    buildable: false
    externals:
    - spec: unzip@6.0
      prefix: /usr
view: true
```

Next, we will concretize the environment, you should see `papi`, `hypre` and `darshan-runtime` built with each compiler.

```
(spack-pyenv) elvis@login34> spack concretize
```

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```
==> Starting concretization pool with 6 processes
==> Environment concretized in 18.58 seconds.
==> Concretized papi%gcc
 -   s2y4nrv  papi@6.0.0.1%gcc@11.2.0~cuda+example~infiniband~lmsensors~nvml~powercap~
↪rapl~rocm~rocm_smi~sde+shared~static_tools arch=cray-sles15-zen3

==> Concretized papi%cce
 -   3aprcx5  papi@6.0.0.1%cce@13.0.2~cuda+example~infiniband~lmsensors~nvml~powercap~
↪rapl~rocm~rocm_smi~sde+shared~static_tools patches=b6d6caa arch=cray-sles15-zen3

==> Concretized hypre%gcc
 -   mbn7bum  hypre@2.24.0%gcc@11.2.0~complex~cuda~debug+fortran~gptune~int64~internal-
↪superlu~mixedint+mpi~openmp~rocm+shared~superlu-dist~unified-memory arch=cray-sles15-
↪zen3
 -   jzbnd6y      ^cray-libsci@21.08.1.2%gcc@11.2.0~mpi~openmp+shared arch=cray-sles15-
↪zen3
 -   3zy6uvs      ^cray-mpich@8.1.15%gcc@11.2.0+wrappers arch=cray-sles15-zen3

==> Concretized hypre%cce
 -   62ofdsf  hypre@2.24.0%cce@13.0.2~complex~cuda~debug+fortran~gptune~int64~internal-
↪superlu~mixedint+mpi~openmp~rocm+shared~superlu-dist~unified-memory arch=cray-sles15-
↪zen3
 -   7uzhxpv      ^cray-libsci@21.08.1.2%cce@13.0.2~mpi~openmp+shared arch=cray-sles15-
↪zen3
 -   tb5uxwe      ^cray-mpich@8.1.15%cce@13.0.2+wrappers arch=cray-sles15-zen3

==> Concretized darshan-runtime%gcc
 -   hkxzwvt  darshan-runtime@3.3.1%gcc@11.2.0~apmpi~apmpi_sync~apxc~hdf5+mpi␣
↪scheduler=NONE arch=cray-sles15-zen3
 -   3zy6uvs      ^cray-mpich@8.1.15%gcc@11.2.0+wrappers arch=cray-sles15-zen3
 -   ozmcyfj      ^zlib@1.2.12%gcc@11.2.0+optimize+pic+shared patches=0d38234 arch=cray-
↪sles15-zen3

==> Concretized darshan-runtime%cce
 -   uj3wa4a  darshan-runtime@3.3.1%cce@13.0.2~apmpi~apmpi_sync~apxc~hdf5+mpi␣
↪scheduler=NONE arch=cray-sles15-zen3
 -   tb5uxwe      ^cray-mpich@8.1.15%cce@13.0.2+wrappers arch=cray-sles15-zen3
 -   e2hl6cx      ^zlib@1.2.12%cce@13.0.2+optimize+pic+shared patches=0d38234 arch=cray-
↪sles15-zen3
```

Let's install all the packages via `spack install`. This would be a good time to get a cup of coffee since it will likely take a few minutes.

```
(spack-pyenv) elvis@login34> spack install
==> Installing environment data_viz
==> Installing papi-6.0.0.1-s2y4nrvu6whr6hhgi63aa3nqwz2d35af
==> No binary for papi-6.0.0.1-s2y4nrvu6whr6hhgi63aa3nqwz2d35af found: installing from␣
↪source
==> Fetching https://mirror.spack.io/_source-cache/archive/3c/
↪3cd7ed50c65b0d21d66e46d0ba34cd171178af4bbf9d94e693915c1aca1e287f.tar.gz
==> No patches needed for papi
==> papi: Executing phase: 'autoreconf'
```

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```
==> papi: Executing phase: 'configure'
==> papi: Executing phase: 'build'
==> papi: Executing phase: 'install'
==> papi: Successfully installed papi-6.0.0.1-s2y4nrvu6whr6hhgi63aa3nqwz2d35af
  Fetch: 1.49s.  Build: 28.94s.  Total: 30.43s.
[+] /global/u1/e/elvis/spack-infrastructure/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/
↪papi-6.0.0.1-s2y4nrvu6whr6hhgi63aa3nqwz2d35af
==> Installing papi-6.0.0.1-3aprcx5klzafe7xt6aq57jx5sequpue2
==> No binary for papi-6.0.0.1-3aprcx5klzafe7xt6aq57jx5sequpue2 found: installing from␣
↪source
==> Using cached archive: /global/u1/e/elvis/spack-infrastructure/spack/var/spack/cache/_
↪source-cache/archive/3c/
↪3cd7ed50c65b0d21d66e46d0ba34cd171178af4bbf9d94e693915c1aca1e287f.tar.gz
==> Applied patch /global/u1/e/elvis/spack-infrastructure/spack/var/spack/repos/builtin/
↪packages/papi/crayftn-fixes.patch
==> papi: Executing phase: 'autoreconf'
==> papi: Executing phase: 'configure'
==> papi: Executing phase: 'build'
==> papi: Executing phase: 'install'
==> papi: Successfully installed papi-6.0.0.1-3aprcx5klzafe7xt6aq57jx5sequpue2
  Fetch: 0.01s.  Build: 28.94s.  Total: 28.95s.
[+] /global/u1/e/elvis/spack-infrastructure/spack/opt/spack/cray-sles15-zen3/cce-13.0.2/
↪papi-6.0.0.1-3aprcx5klzafe7xt6aq57jx5sequpue2
==> cray-libsci@21.08.1.2 : has external module in ['cray-libsci/21.08.1.2']
[+] /opt/cray/pe/libsci/21.08.1.2/GNU/9.1/x86_64 (external cray-libsci-21.08.1.2-
↪jzbnd6ycupy2ycs5jiavwyvkxv3rpuru)
==> cray-mpich@8.1.15 : has external module in ['cray-mpich/8.1.15', 'cudatoolkit/11.5']
[+] /opt/cray/pe/mpich/8.1.15/ofi/gnu/9.1 (external cray-mpich-8.1.15-
↪3zy6uvszbd5a3rniq2xd2v5a3d27qstw)
==> cray-libsci@21.08.1.2 : has external module in ['cray-libsci/21.08.1.2']
[+] /opt/cray/pe/libsci/21.08.1.2/CRAY/9.0/x86_64 (external cray-libsci-21.08.1.2-
↪7uzhxpvoka7ixfxs44354dkishquwyhq)
==> cray-mpich@8.1.15 : has external module in ['cray-mpich/8.1.15', 'cudatoolkit/11.5']
[+] /opt/cray/pe/mpich/8.1.15/ofi/cray/10.0/ (external cray-mpich-8.1.15-
↪tb5uxwezfzx4xth7azefyrhzlvf7koqb)
==> Installing zlib-1.2.12-ozmcyfjfv7i5gjjgklfsh43h67vzsuc5
==> No binary for zlib-1.2.12-ozmcyfjfv7i5gjjgklfsh43h67vzsuc5 found: installing from␣
↪source
==> Fetching https://mirror.spack.io/_source-cache/archive/91/
↪91844808532e5ce316b3c010929493c0244f3d37593afd6de04f71821d5136d9.tar.gz
==> Applied patch /global/u1/e/elvis/spack-infrastructure/spack/var/spack/repos/builtin/
↪packages/zlib/configure-cc.patch
==> zlib: Executing phase: 'install'
==> zlib: Successfully installed zlib-1.2.12-ozmcyfjfv7i5gjjgklfsh43h67vzsuc5
  Fetch: 0.62s.  Build: 2.10s.  Total: 2.72s.
[+] /global/u1/e/elvis/spack-infrastructure/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/
↪zlib-1.2.12-ozmcyfjfv7i5gjjgklfsh43h67vzsuc5
==> Installing zlib-1.2.12-e2hl6cxmzbg5psoh5upqmqqltjftc3pb
==> No binary for zlib-1.2.12-e2hl6cxmzbg5psoh5upqmqqltjftc3pb found: installing from␣
↪source
==> Using cached archive: /global/u1/e/elvis/spack-infrastructure/spack/var/spack/cache/_
↪source-cache/archive/91/
```

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```
↪91844808532e5ce316b3c010929493c0244f3d37593afd6de04f71821d5136d9.tar.gz
==> Applied patch /global/u1/e/elvis/spack-infrastructure/spack/var/spack/repos/builtin/
↪packages/zlib/configure-cc.patch
==> zlib: Executing phase: 'install'
==> zlib: Successfully installed zlib-1.2.12-e2hl6cxmzbg5psoh5upqmqqltjftc3pb
  Fetch: 0.00s.  Build: 2.45s.  Total: 2.45s.
[+] /global/u1/e/elvis/spack-infrastructure/spack/opt/spack/cray-sles15-zen3/cce-13.0.2/
↪zlib-1.2.12-e2hl6cxmzbg5psoh5upqmqqltjftc3pb
==> Installing hypre-2.24.0-mbn7bumcoqmjhf5y2sm3hnr64vml4dvf
==> No binary for hypre-2.24.0-mbn7bumcoqmjhf5y2sm3hnr64vml4dvf found: installing from␣
↪source
==> Fetching https://mirror.spack.io/_source-cache/archive/f4/
↪f480e61fc25bf533fc201fdf79ec440be79bb8117650627d1f25151e8be2fdb5.tar.gz
==> No patches needed for hypre
==> hypre: Executing phase: 'autoreconf'
==> hypre: Executing phase: 'configure'
==> hypre: Executing phase: 'build'
==> hypre: Executing phase: 'install'
==> hypre: Successfully installed hypre-2.24.0-mbn7bumcoqmjhf5y2sm3hnr64vml4dvf
  Fetch: 0.77s.  Build: 37.43s.  Total: 38.20s.
[+] /global/u1/e/elvis/spack-infrastructure/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/
↪hypre-2.24.0-mbn7bumcoqmjhf5y2sm3hnr64vml4dvf
==> Installing hypre-2.24.0-62ofdsfxckay53ewpiidg4nlamhnzq3b
==> No binary for hypre-2.24.0-62ofdsfxckay53ewpiidg4nlamhnzq3b found: installing from␣
↪source
==> Using cached archive: /global/u1/e/elvis/spack-infrastructure/spack/var/spack/cache/_
↪source-cache/archive/f4/
↪f480e61fc25bf533fc201fdf79ec440be79bb8117650627d1f25151e8be2fdb5.tar.gz
==> No patches needed for hypre
==> hypre: Executing phase: 'autoreconf'
==> hypre: Executing phase: 'configure'
==> hypre: Executing phase: 'build'
==> hypre: Executing phase: 'install'
==> hypre: Successfully installed hypre-2.24.0-62ofdsfxckay53ewpiidg4nlamhnzq3b
  Fetch: 0.01s.  Build: 1m 5.86s.  Total: 1m 5.87s.
[+] /global/u1/e/elvis/spack-infrastructure/spack/opt/spack/cray-sles15-zen3/cce-13.0.2/
↪hypre-2.24.0-62ofdsfxckay53ewpiidg4nlamhnzq3b
==> Installing darshan-runtime-3.3.1-hkxzwvtw5rlmsvwt4irwnxxuwzwbuzoj
==> No binary for darshan-runtime-3.3.1-hkxzwvtw5rlmsvwt4irwnxxuwzwbuzoj found:␣
↪installing from source
==> Fetching https://mirror.spack.io/_source-cache/archive/28/
↪281d871335977d0592a49d053df93d68ce1840f6fdec27fea7a59586a84395f7.tar.gz
==> No patches needed for darshan-runtime
==> darshan-runtime: Executing phase: 'autoreconf'
==> darshan-runtime: Executing phase: 'configure'
==> darshan-runtime: Executing phase: 'build'
==> darshan-runtime: Executing phase: 'install'
==> darshan-runtime: Successfully installed darshan-runtime-3.3.1-
↪hkxzwvtw5rlmsvwt4irwnxxuwzwbuzoj
  Fetch: 1.07s.  Build: 9.24s.  Total: 10.31s.
[+] /global/u1/e/elvis/spack-infrastructure/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/
↪darshan-runtime-3.3.1-hkxzwvtw5rlmsvwt4irwnxxuwzwbuzoj
```

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```
==> Installing darshan-runtime-3.3.1-uj3wa4au7kphj52syka4w3dxiadosagh
==> No binary for darshan-runtime-3.3.1-uj3wa4au7kphj52syka4w3dxiadosagh found:␣
↪installing from source
==> Using cached archive: /global/u1/e/elvis/spack-infrastructure/spack/var/spack/cache/_
↪source-cache/archive/28/
↪281d871335977d0592a49d053df93d68ce1840f6fdec27fea7a59586a84395f7.tar.gz
==> No patches needed for darshan-runtime
==> darshan-runtime: Executing phase: 'autoreconf'
==> darshan-runtime: Executing phase: 'configure'
==> darshan-runtime: Executing phase: 'build'
==> darshan-runtime: Executing phase: 'install'
==> darshan-runtime: Successfully installed darshan-runtime-3.3.1-
↪uj3wa4au7kphj52syka4w3dxiadosagh
  Fetch: 0.01s.  Build: 9.58s.  Total: 9.58s.
[+] /global/u1/e/elvis/spack-infrastructure/spack/opt/spack/cray-sles15-zen3/cce-13.0.2/
↪darshan-runtime-3.3.1-uj3wa4au7kphj52syka4w3dxiadosagh
==> Updating view at /global/u1/e/elvis/spack-infrastructure/spack/var/spack/
↪environments/data_viz/.spack-env/view
==> Warning: Skipping external package: cray-libsci@21.08.1.2%gcc@11.2.0~mpi~
↪openmp+shared arch=cray-sles15-zen3/jzbnd6y
==> Warning: Skipping external package: cray-mpich@8.1.15%gcc@11.2.0+wrappers arch=cray-
↪sles15-zen3/3zy6uvs
==> Warning: Skipping external package: cray-libsci@21.08.1.2%cce@13.0.2~mpi~
↪openmp+shared arch=cray-sles15-zen3/7uzhxpv
==> Warning: Skipping external package: cray-mpich@8.1.15%cce@13.0.2+wrappers arch=cray-
↪sles15-zen3/tb5uxwe
==> Error: 178 fatal error(s) when merging prefixes:
    `/global/u1/e/elvis/spack-infrastructure/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/
↪papi-6.0.0.1-s2y4nrvu6whr6hhgi63aa3nqwz2d35af/.spack/archived-files/src/removed_la_
↪files.txt` and `/global/u1/e/elvis/spack-infrastructure/spack/opt/spack/cray-sles15-
↪zen3/cce-13.0.2/papi-6.0.0.1-3aprcx5klzafe7xt6aq57jx5sequpue2/.spack/archived-files/
↪src/removed_la_files.txt` both project to `.spack/papi/archived-files/src/removed_la_
↪files.txt`
    `/global/u1/e/elvis/spack-infrastructure/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/
↪papi-6.0.0.1-s2y4nrvu6whr6hhgi63aa3nqwz2d35af/.spack/install_environment.json` and `/
↪global/u1/e/elvis/spack-infrastructure/spack/opt/spack/cray-sles15-zen3/cce-13.0.2/
↪papi-6.0.0.1-3aprcx5klzafe7xt6aq57jx5sequpue2/.spack/install_environment.json` both␣
↪project to `.spack/papi/install_environment.json`
    `/global/u1/e/elvis/spack-infrastructure/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/
↪papi-6.0.0.1-s2y4nrvu6whr6hhgi63aa3nqwz2d35af/.spack/install_manifest.json` and `/
↪global/u1/e/elvis/spack-infrastructure/spack/opt/spack/cray-sles15-zen3/cce-13.0.2/
↪papi-6.0.0.1-3aprcx5klzafe7xt6aq57jx5sequpue2/.spack/install_manifest.json` both␣
↪project to `.spack/papi/install_manifest.json`
```

Upon completion you can run `spack find` to see all installed packages.

```
(spack-pyenv) elvis@login34> spack find
==> In environment data_viz
==> Root specs
-- no arch / cce -------------------------------------------------
darshan-runtime%cce  hypre%cce  papi%cce
```

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```
-- no arch / gcc -------------------------------------------------
darshan-runtime%gcc  hypre%gcc  papi%gcc

==> 12 installed packages
-- cray-sles15-zen3 / cce@13.0.2 ---------------------------------
cray-libsci@21.08.1.2  cray-mpich@8.1.15  darshan-runtime@3.3.1  hypre@2.24.0  papi@6.0.
↪0.1  zlib@1.2.12

-- cray-sles15-zen3 / gcc@11.2.0 ---------------------------------
cray-libsci@21.08.1.2  cray-mpich@8.1.15  darshan-runtime@3.3.1  hypre@2.24.0  papi@6.0.
↪0.1  zlib@1.2.12
```

4.9 Defining a Source Mirror

You may have noticed Spack will fetch tarballs from the web when installing packages and this can be time-consuming when downloading large tarballs. It is a good idea to store tarballs on the filesystem once and then let Spack use them for any Spack builds. You should have one location where tarballs. Let's run the following command:

```
(spack-pyenv) elvis@login34> spack mirror create -d $CI_PROJECT_DIR/spack_mirror -a
==> Adding package cray-libsci@21.08.1.2 to mirror
==> Adding package cray-libsci@21.08.1.2 to mirror
==> Adding package cray-mpich@8.1.15 to mirror
==> Adding package cray-mpich@8.1.15 to mirror
==> Adding package darshan-runtime@3.3.1 to mirror
==> Using cached archive: /global/u1/e/elvis/spack-infrastructure/spack/var/spack/cache/_
↪source-cache/archive/28/
↪281d871335977d0592a49d053df93d68ce1840f6fdec27fea7a59586a84395f7.tar.gz
==> Adding package darshan-runtime@3.3.1 to mirror
==> Adding package hypre@2.24.0 to mirror
==> Using cached archive: /global/u1/e/elvis/spack-infrastructure/spack/var/spack/cache/_
↪source-cache/archive/f4/
↪f480e61fc25bf533fc201fdf79ec440be79bb8117650627d1f25151e8be2fdb5.tar.gz
==> Adding package hypre@2.24.0 to mirror
==> Adding package papi@6.0.0.1 to mirror
==> Using cached archive: /global/u1/e/elvis/spack-infrastructure/spack/var/spack/cache/_
↪source-cache/archive/3c/
↪3cd7ed50c65b0d21d66e46d0ba34cd171178af4bbf9d94e693915c1aca1e287f.tar.gz
==> Fetching https://mirror.spack.io/_source-cache/archive/64/
↪64c57b3ad4026255238cc495df6abfacc41de391a0af497c27d0ac819444a1f8
==> Adding package papi@6.0.0.1 to mirror
==> Adding package zlib@1.2.12 to mirror
==> Using cached archive: /global/u1/e/elvis/spack-infrastructure/spack/var/spack/cache/_
↪source-cache/archive/91/
↪91844808532e5ce316b3c010929493c0244f3d37593afd6de04f71821d5136d9.tar.gz
==> Adding package zlib@1.2.12 to mirror
==> Successfully created mirror in file:///global/homes/e/elvis/spack-infrastructure/
↪spack_mirror
  Archive stats:
    4    already present
    4    added
```

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```
    0    failed to fetch.
```

If you inspect the directory you will notice the tarballs are present in this directory.

```
(spack-pyenv) elvis@login34> ls -l $CI_PROJECT_DIR/spack_mirror/*
/global/homes/e/elvis/spack-infrastructure/spack_mirror/darshan-runtime:
total 1
lrwxrwxrwx 1 elvis elvis 99 Aug  4 08:28 darshan-runtime-3.3.1.tar.gz -> ../_source-
↪cache/archive/28/281d871335977d0592a49d053df93d68ce1840f6fdec27fea7a59586a84395f7.tar.
↪gz

/global/homes/e/elvis/spack-infrastructure/spack_mirror/hypre:
total 1
lrwxrwxrwx 1 elvis elvis 99 Aug  4 08:28 hypre-2.24.0.tar.gz -> ../_source-cache/archive/
↪f4/f480e61fc25bf533fc201fdf79ec440be79bb8117650627d1f25151e8be2fdb5.tar.gz

/global/homes/e/elvis/spack-infrastructure/spack_mirror/papi:
total 2
lrwxrwxrwx 1 elvis elvis 99 Aug  4 08:28 papi-6.0.0.1.tar.gz -> ../_source-cache/archive/
↪3c/3cd7ed50c65b0d21d66e46d0ba34cd171178af4bbf9d94e693915c1aca1e287f.tar.gz
lrwxrwxrwx 1 elvis elvis 92 Aug  4 08:28 raw-64c57b3 -> ../_source-cache/archive/64/
↪64c57b3ad4026255238cc495df6abfacc41de391a0af497c27d0ac819444a1f8

/global/homes/e/elvis/spack-infrastructure/spack_mirror/_source-cache:
total 1
drwxrwxr-x 7 elvis elvis 512 Aug  4 08:28 archive

/global/homes/e/elvis/spack-infrastructure/spack_mirror/zlib:
total 1
lrwxrwxrwx 1 elvis elvis 99 Aug  4 08:28 zlib-1.2.12.tar.gz -> ../_source-cache/archive/
↪91/91844808532e5ce316b3c010929493c0244f3d37593afd6de04f71821d5136d9.tar.gz
```

4.10 Building CUDA Packages

On Perlmutter, the standalone CUDA package is available by loading the following modulefile:

```
(spack-pyenv) elvis@login34> ml -t av cudatoolkit
/opt/cray/pe/lmod/modulefiles/core:
cudatoolkit/11.5
cudatoolkit/11.7
```

NVIDIA provides CUDA as part of the NVHPC compiler which is installed on Perlmutter and accessible via the `nvhpc` modulefile.

```
(spack-pyenv) elvis@login34> ml -t av nvhpc
/opt/cray/pe/lmod/modulefiles/mix_compilers:
nvhpc-mixed/21.11
nvhpc-mixed/22.5
/opt/cray/pe/lmod/modulefiles/core:
nvhpc/21.11
nvhpc/22.5
```

The root of `nvhpc/21.11` is available at `/opt/nvidia/hpc_sdk/Linux_x86_64/21.11`. You can see content of this modulefile by running `module show nvhpc/21.11` and inspecting the modulefile. Shown below is the directory structure for root of NVHPC stack.

```
(spack-pyenv) elvis@login34> ls -l /opt/nvidia/hpc_sdk/Linux_x86_64/21.11
total 0
drwxr-xr-x  2 root root  72 Aug  1 07:03 cmake
drwxrwxr-x  6 root root 144 Aug  1 07:07 comm_libs
drwxrwxr-x 14 root root 235 Aug  1 07:07 compilers
drwxrwxr-x  3 root root  78 Aug  1 07:07 cuda
drwxrwxr-x 11 root root 205 Aug  1 07:05 examples
drwxrwxr-x  3 root root  55 Aug  1 07:07 math_libs
drwxrwxr-x  4 root root  71 Aug  1 07:07 profilers
drwxrwxr-x  6 root root  90 Aug  1 07:03 REDIST
```

`cuda/11.5` is installed in following directory, which can be activated by loading the `cudatoolkit/11.5` modulefile.

```
(spack-pyenv) elvis@login34> ls -l /opt/nvidia/hpc_sdk/Linux_x86_64/21.11/cuda/11.5
total 65
drwxrwxr-x 3 root root   335 Aug  1 07:04 bin
drwxrwxr-x 4 root root   385 Aug  1 07:04 compute-sanitizer
-rw-r--r-- 1 root root   160 Dec  8  2021 DOCS
-rw-r--r-- 1 root root 61727 Dec  8  2021 EULA.txt
drwxrwxr-x 4 root root    44 Aug  1 07:04 extras
lrwxrwxrwx 1 root root    28 Dec  8  2021 include -> targets/x86_64-linux/include
lrwxrwxrwx 1 root root    24 Dec  8  2021 lib64 -> targets/x86_64-linux/lib
drwxrwxr-x 7 root root   242 Aug  1 07:04 libnvvp
drwxrwxr-x 3 root root    30 Aug  1 07:04 nvml
drwxrwxr-x 7 root root   106 Aug  1 07:04 nvvm
drwxrwxr-x 7 root root    94 Aug  1 07:04 nvvm-prev
-rw-r--r-- 1 root root   524 Dec  8  2021 README
drwxrwxr-x 3 root root    26 Aug  1 07:04 share
drwxrwxr-x 3 root root    35 Aug  1 07:04 targets
drwxrwxr-x 2 root root    52 Aug  1 07:05 tools
-rw-r--r-- 1 root root  2669 Dec  8  2021 version.json
```

We can confirm the `nvcc` compiler provided by CUDA is available in this directory along with the `libcudart.so` (CUDA Runtime) library

```
(spack-pyenv) elvis@login34> /opt/nvidia/hpc_sdk/Linux_x86_64/21.11/cuda/11.5/bin/nvcc --
↪version
nvcc: NVIDIA (R) Cuda compiler driver
Copyright (c) 2005-2021 NVIDIA Corporation
Built on Thu_Nov_18_09:45:30_PST_2021
Cuda compilation tools, release 11.5, V11.5.119
Build cuda_11.5.r11.5/compiler.30672275_0

(spack-pyenv) elvis@login34> ls /opt/nvidia/hpc_sdk/Linux_x86_64/21.11/cuda/11.5/lib64/
↪libcudart.so
/opt/nvidia/hpc_sdk/Linux_x86_64/21.11/cuda/11.5/lib64/libcudart.so
```

Let's define our CUDA package preference in our Spack configuration. To illustrate, we will install `papi` with the spec `papi +cuda %gcc`. This indicates that we want PAPI installed with CUDA support using the GCC compiler. Please copy the following content in your `spack.yaml`.

```yaml
# This is a Spack Environment file.
#
# It describes a set of packages to be installed, along with
# configuration settings.
spack:
  config:
    view: false
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
  compilers:
  - compiler:
      spec: gcc@11.2.0
      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: []
  - compiler:
      spec: cce@13.0.2
      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/13.0.2
      - craype-x86-milan
      - libfabric
      environment: {}
      extra_rpaths: []

  # add package specs to the `specs` list
  specs:
  - papi %gcc
  - papi %cce
  - hypre %gcc
  - hypre %cce
  - darshan-runtime %gcc
```

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```
  - darshan-runtime %cce
  - papi +cuda %gcc
packages:
  all:
    compiler: [gcc@11.2.0, cce@13.0.2]
    providers:
      blas: [cray-libsci]
      mpi: [cray-mpich]
  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@8.1.15 %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 %cce@13.0.2
      prefix: /opt/cray/pe/mpich/8.1.15/ofi/cray/10.0/
      modules:
      - cray-mpich/8.1.15
      - cudatoolkit/11.5
  cray-pmi:
    buildable: false
    externals:
    - spec: cray-pmi@6.1.1
      modules:
      - cray-pmi/6.1.1
  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:
```

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```
      version: [4.6.0]
      externals:
      - spec: findutils@4.6.0
        prefix: /usr
    libfabric:
      buildable: false
      variants: fabrics=sockets,tcp,udp,rxm
      externals:
      - spec: libfabric@1.11.0.4.114
        prefix: /opt/cray/libfabric/1.11.0.4.114
        modules:
        - libfabric/1.11.0.4.114
    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
    readline:
      version: [7.0]
      buildable: false
      externals:
      - spec: readline@7.0
        prefix: /usr
    tar:
      version: [1.3]
      buildable: false
      externals:
      - spec: tar@1.30
        prefix: /usr
    unzip:
      version: [6.0]
      buildable: false
      externals:
      - spec: unzip@6.0
        prefix: /usr
  view: true
```

Now let's try to install.

```
(spack-pyenv) elvis@login34> spack install
==> Installing environment data_viz
==> cuda@11.5.0 : has external module in ['cudatoolkit/11.5']
[+] /opt/nvidia/hpc_sdk/Linux_x86_64/21.11/cuda/11.5 (external cuda-11.5.0-
↪puekfe32hbj72iftffa3etecesmlqwqg)
==> Installing papi-6.0.0.1-x43djbqgyb64susljh3vu4czlqapbyie
```

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```
==> No binary for papi-6.0.0.1-x43djbqgyb64susljh3vu4czlqapbyie found: installing from␣
↪source
==> Using cached archive: /global/u1/e/elvis/spack-infrastructure/spack/var/spack/cache/_
↪source-cache/archive/3c/
↪3cd7ed50c65b0d21d66e46d0ba34cd171178af4bbf9d94e693915c1aca1e287f.tar.gz
==> No patches needed for papi
==> papi: Executing phase: 'autoreconf'
==> papi: Executing phase: 'configure'
==> papi: Executing phase: 'build'
==> papi: Executing phase: 'install'
==> papi: Successfully installed papi-6.0.0.1-x43djbqgyb64susljh3vu4czlqapbyie
  Fetch: 0.01s.  Build: 4m 46.76s.  Total: 4m 46.76s.
[+] /global/u1/e/elvis/spack-infrastructure/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/
↪papi-6.0.0.1-x43djbqgyb64susljh3vu4czlqapbyie
==> Updating view at /global/u1/e/elvis/spack-infrastructure/spack/var/spack/
↪environments/data_viz/.spack-env/view
==> Warning: Skipping external package: cray-libsci@21.08.1.2%gcc@11.2.0~mpi~
↪openmp+shared arch=cray-sles15-zen3/jzbnd6y
==> Warning: Skipping external package: cray-mpich@8.1.15%gcc@11.2.0+wrappers arch=cray-
↪sles15-zen3/3zy6uvs
==> Warning: Skipping external package: cray-libsci@21.08.1.2%cce@13.0.2~mpi~
↪openmp+shared arch=cray-sles15-zen3/7uzhxpv
==> Warning: Skipping external package: cray-mpich@8.1.15%cce@13.0.2+wrappers arch=cray-
↪sles15-zen3/tb5uxwe
==> Warning: Skipping external package: cuda@11.5.0%gcc@11.2.0~allow-unsupported-
↪compilers~dev arch=cray-sles15-zen3/puekfe3
==> Error: 193 fatal error(s) when merging prefixes:
    `/global/u1/e/elvis/spack-infrastructure/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/
↪papi-6.0.0.1-s2y4nrvu6whr6hhgi63aa3nqwz2d35af/.spack/archived-files/src/removed_la_
↪files.txt` and `/global/u1/e/elvis/spack-infrastructure/spack/opt/spack/cray-sles15-
↪zen3/cce-13.0.2/papi-6.0.0.1-3aprcx5klzafe7xt6aq57jx5sequpue2/.spack/archived-files/
↪src/removed_la_files.txt` both project to `.spack/papi/archived-files/src/removed_la_
↪files.txt`
    `/global/u1/e/elvis/spack-infrastructure/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/
↪papi-6.0.0.1-s2y4nrvu6whr6hhgi63aa3nqwz2d35af/.spack/install_environment.json` and `/
↪global/u1/e/elvis/spack-infrastructure/spack/opt/spack/cray-sles15-zen3/cce-13.0.2/
↪papi-6.0.0.1-3aprcx5klzafe7xt6aq57jx5sequpue2/.spack/install_environment.json` both␣
↪project to `.spack/papi/install_environment.json`
    `/global/u1/e/elvis/spack-infrastructure/spack/opt/spack/cray-sles15-zen3/gcc-11.2.0/
↪papi-6.0.0.1-s2y4nrvu6whr6hhgi63aa3nqwz2d35af/.spack/install_manifest.json` and `/
↪global/u1/e/elvis/spack-infrastructure/spack/opt/spack/cray-sles15-zen3/cce-13.0.2/
↪papi-6.0.0.1-3aprcx5klzafe7xt6aq57jx5sequpue2/.spack/install_manifest.json` both␣
↪project to `.spack/papi/install_manifest.json`
```

4.11 Generating Modulefiles

In this section we let Spack generate modulefiles for the Spack packages we installed. Perlmutter is using Lmod as the module system which supports both `tcl` and `lua` modules. You may want to refer to Modules for more information.

```
(spack-pyenv) elvis@login34> module --version

Modules based on Lua: Version 8.3.1  2020-02-16 19:46 :z
    by Robert McLay mclay@tacc.utexas.edu
```

For this training we will cover how to generate `tcl` modules in a flat hierarchy. To get started, let's add the following to our Spack configuration:

```
# This is a Spack Environment file.
#
# It describes a set of packages to be installed, along with
# configuration settings.
spack:
  config:
    view: false
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
  compilers:
  - compiler:
      spec: gcc@11.2.0
      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: []
  - compiler:
      spec: cce@13.0.2
      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
```

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```
    - cce/13.0.2
    - craype-x86-milan
    - libfabric
    environment: {}
    extra_rpaths: []

# add package specs to the `specs` list
specs:
- papi %gcc
- papi %cce
- hypre %gcc
- hypre %cce
- darshan-runtime %gcc
- darshan-runtime %cce
- papi +cuda %gcc
packages:
  all:
    compiler: [gcc@11.2.0, cce@13.0.2]
    providers:
      blas: [cray-libsci]
      mpi: [cray-mpich]
  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@8.1.15 %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 %cce@13.0.2
      prefix: /opt/cray/pe/mpich/8.1.15/ofi/cray/10.0/
      modules:
      - cray-mpich/8.1.15
      - cudatoolkit/11.5
  cray-pmi:
    buildable: false
    externals:
    - spec: cray-pmi@6.1.1
      modules:
      - cray-pmi/6.1.1
  cuda:
```

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```
      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
    libfabric:
      buildable: false
      variants: fabrics=sockets,tcp,udp,rxm
      externals:
      - spec: libfabric@1.11.0.4.114
        prefix: /opt/cray/libfabric/1.11.0.4.114
        modules:
        - libfabric/1.11.0.4.114
    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
    readline:
      version: [7.0]
      buildable: false
      externals:
      - spec: readline@7.0
        prefix: /usr
    tar:
      version: [1.3]
      buildable: false
      externals:
      - spec: tar@1.30
        prefix: /usr
    unzip:
      version: [6.0]
      buildable: false
```

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```
    externals:
    - spec: unzip@6.0
      prefix: /usr
  modules:
    default:
      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}'
          suffixes:
            ^cuda: cuda

  view: true
```

The `blacklist_implicits: true` will ignore module generation for dependencies which is useful when you are building a large software stack, you don't want an explosion of modulefiles for utilities that you would never use. The `hash_length: 0` will avoid adding hash characters at end of modulefile, the `naming_scheme` will instruct Spack how to format the modulefiles being written on the file-system. Now let's generate the modulefiles. It is generally a good idea to run this in debug mode to understand how files are being generated. The `spack module tcl refresh` command will generate `tcl` modules, it is good idea to specify `--delete-tree -y` which will delete the root of module tree and `-y` will accept confirmation. In the output take note of where modulefiles are being written. You will see a list of specs as `BLACKLISTED_AS_IMPLICIT` which are specs that will not generate modulefiles

```
(spack-pyenv) elvis@login34> spack -d module tcl refresh --delete-tree -y
==> [2022-08-04-09:42:35.558437] Reading config file /global/u1/e/elvis/spack-
↪infrastructure/spack/etc/spack/defaults/config.yaml
==> [2022-08-04-09:42:35.708144] Reading config file /global/u1/e/elvis/spack-
↪infrastructure/spack/var/spack/environments/data_viz/spack.yaml
==> [2022-08-04-09:42:35.767338] Using environment 'data_viz'
==> [2022-08-04-09:42:35.968497] Imported module from built-in commands
==> [2022-08-04-09:42:35.975354] Imported module from built-in commands
==> [2022-08-04-09:42:35.991742] Reading config file /global/u1/e/elvis/spack-
↪infrastructure/spack/etc/spack/defaults/bootstrap.yaml
==> [2022-08-04-09:42:36.044748] DATABASE LOCK TIMEOUT: 3s
==> [2022-08-04-09:42:36.044959] PACKAGE LOCK TIMEOUT: No timeout
==> [2022-08-04-09:42:36.161175] Reading config file /global/u1/e/elvis/spack-
↪infrastructure/spack/etc/spack/defaults/repos.yaml
==> [2022-08-04-09:42:36.634555] Reading config file /global/u1/e/elvis/spack-
↪infrastructure/spack/etc/spack/defaults/modules.yaml
==> [2022-08-04-09:42:36.691668] Reading config file /global/u1/e/elvis/spack-
↪infrastructure/spack/etc/spack/defaults/cray/modules.yaml
==> [2022-08-04-09:42:38.077573]    BLACKLISTED_AS_IMPLICIT : cray-libsci@21.08.1.2
↪%cce@13.0.2~mpi~openmp+shared arch=cray-sles15-zen3/7uzhxpv
```

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```
==> [2022-08-04-09:42:38.079387]    BLACKLISTED_AS_IMPLICIT : cray-libsci@21.08.1.2
↪%gcc@11.2.0~mpi~openmp+shared arch=cray-sles15-zen3/jzbnd6y
==> [2022-08-04-09:42:38.081189]    BLACKLISTED_AS_IMPLICIT : cray-mpich@8.1.15%cce@13.0.
↪2+wrappers arch=cray-sles15-zen3/tb5uxwe
==> [2022-08-04-09:42:38.082661]    BLACKLISTED_AS_IMPLICIT : cray-mpich@8.1.15%gcc@11.2.
↪0+wrappers arch=cray-sles15-zen3/3zy6uvs
==> [2022-08-04-09:42:38.084601]    BLACKLISTED_AS_IMPLICIT : cuda@11.5.0%gcc@11.2.0~
↪allow-unsupported-compilers~dev arch=cray-sles15-zen3/puekfe3
==> [2022-08-04-09:42:38.097284]    BLACKLISTED_AS_IMPLICIT : zlib@1.2.12%cce@13.0.
↪2+optimize+pic+shared patches=0d38234 arch=cray-sles15-zen3/e2hl6cx
==> [2022-08-04-09:42:38.099494]    BLACKLISTED_AS_IMPLICIT : zlib@1.2.12%gcc@11.2.
↪0+optimize+pic+shared patches=0d38234 arch=cray-sles15-zen3/ozmcyfj
==> [2022-08-04-09:44:22.697989] Regenerating tcl module files
==> [2022-08-04-09:44:22.872234]    WRITE: darshan-runtime@3.3.1%cce@13.0.2~apmpi~apmpi_
↪sync~apxc~hdf5+mpi scheduler=NONE arch=cray-sles15-zen3/uj3wa4a [/global/u1/e/elvis/
↪spack-infrastructure/spack/share/spack/modules/cray-sles15-zen3/darshan-runtime/3.3.1-
↪cce-13.0.2]
==> [2022-08-04-09:44:23.696894] Module name: cce/13.0.2
==> [2022-08-04-09:44:23.697138] Package directory variable prefix: CCE
==> [2022-08-04-09:44:23.959854] Module name: cce/13.0.2
==> [2022-08-04-09:44:23.960027] Package directory variable prefix: CCE
==> [2022-08-04-09:44:24.183730] Module name: cce/13.0.2
==> [2022-08-04-09:44:24.183920] Package directory variable prefix: CCE
==> [2022-08-04-09:44:24.810258] Module name: cce/13.0.2
==> [2022-08-04-09:44:24.810473] Package directory variable prefix: CCE
==> [2022-08-04-09:44:25.037930] Module name: cce/13.0.2
==> [2022-08-04-09:44:25.038163] Package directory variable prefix: CCE
==> [2022-08-04-09:44:25.052737]    BLACKLISTED_AS_IMPLICIT : cray-mpich@8.1.15%cce@13.0.
↪2+wrappers arch=cray-sles15-zen3/tb5uxwe
==> [2022-08-04-09:44:25.056012]    BLACKLISTED_AS_IMPLICIT : zlib@1.2.12%cce@13.0.
↪2+optimize+pic+shared patches=0d38234 arch=cray-sles15-zen3/e2hl6cx
==> [2022-08-04-09:44:25.060927] Reading config file /global/u1/e/elvis/spack-
↪infrastructure/spack/etc/spack/defaults/packages.yaml
==> [2022-08-04-09:44:25.113314]    WRITE: darshan-runtime@3.3.1%gcc@11.2.0~apmpi~apmpi_
↪sync~apxc~hdf5+mpi scheduler=NONE arch=cray-sles15-zen3/hkxzwvt [/global/u1/e/elvis/
↪spack-infrastructure/spack/share/spack/modules/cray-sles15-zen3/darshan-runtime/3.3.1-
↪gcc-11.2.0]
==> [2022-08-04-09:44:25.219719]    BLACKLISTED_AS_IMPLICIT : cray-mpich@8.1.15%gcc@11.2.
↪0+wrappers arch=cray-sles15-zen3/3zy6uvs
==> [2022-08-04-09:44:25.222960]    BLACKLISTED_AS_IMPLICIT : zlib@1.2.12%gcc@11.2.
↪0+optimize+pic+shared patches=0d38234 arch=cray-sles15-zen3/ozmcyfj
==> [2022-08-04-09:44:25.258546]    WRITE: hypre@2.24.0%cce@13.0.2~complex~cuda~
↪debug+fortran~gptune~int64~internal-superlu~mixedint+mpi~openmp~rocm+shared~superlu-
↪dist~unified-memory arch=cray-sles15-zen3/62ofdsf [/global/u1/e/elvis/spack-
↪infrastructure/spack/share/spack/modules/cray-sles15-zen3/hypre/2.24.0-cce-13.0.2]
==> [2022-08-04-09:44:25.550468] Module name: cce/13.0.2
==> [2022-08-04-09:44:25.550681] Package directory variable prefix: CCE
==> [2022-08-04-09:44:25.785678] Module name: cce/13.0.2
==> [2022-08-04-09:44:25.785853] Package directory variable prefix: CCE
==> [2022-08-04-09:44:25.995944] Module name: cce/13.0.2
==> [2022-08-04-09:44:25.996162] Package directory variable prefix: CCE
==> [2022-08-04-09:44:26.212011] Module name: cce/13.0.2
```

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```
==> [2022-08-04-09:44:26.212283] Package directory variable prefix: CCE
==> [2022-08-04-09:44:26.225681]    BLACKLISTED_AS_IMPLICIT : cray-libsci@21.08.1.2
↪%cce@13.0.2~mpi~openmp+shared arch=cray-sles15-zen3/7uzhxpv
==> [2022-08-04-09:44:26.230079]    BLACKLISTED_AS_IMPLICIT : cray-mpich@8.1.15%cce@13.0.
↪2+wrappers arch=cray-sles15-zen3/tb5uxwe
==> [2022-08-04-09:44:26.238876]    WRITE: hypre@2.24.0%gcc@11.2.0~complex~cuda~
↪debug+fortran~gptune~int64~internal-superlu~mixedint+mpi~openmp~rocm+shared~superlu-
↪dist~unified-memory arch=cray-sles15-zen3/mbn7bum [/global/u1/e/elvis/spack-
↪infrastructure/spack/share/spack/modules/cray-sles15-zen3/hypre/2.24.0-gcc-11.2.0]
==> [2022-08-04-09:44:26.385208]    BLACKLISTED_AS_IMPLICIT : cray-libsci@21.08.1.2
↪%gcc@11.2.0~mpi~openmp+shared arch=cray-sles15-zen3/jzbnd6y
==> [2022-08-04-09:44:26.388329]    BLACKLISTED_AS_IMPLICIT : cray-mpich@8.1.15%gcc@11.2.
↪0+wrappers arch=cray-sles15-zen3/3zy6uvs
==> [2022-08-04-09:44:26.398423]    WRITE: papi@6.0.0.1%cce@13.0.2~cuda+example~
↪infiniband~lmsensors~nvml~powercap~rapl~rocm~rocm_smi~sde+shared~static_tools␣
↪patches=b6d6caa arch=cray-sles15-zen3/3aprcx5 [/global/u1/e/elvis/spack-infrastructure/
↪spack/share/spack/modules/cray-sles15-zen3/papi/6.0.0.1-cce-13.0.2]
==> [2022-08-04-09:44:26.749919] Module name: cce/13.0.2
==> [2022-08-04-09:44:26.750092] Package directory variable prefix: CCE
==> [2022-08-04-09:44:26.762459]    WRITE: papi@6.0.0.1%gcc@11.2.0~cuda+example~
↪infiniband~lmsensors~nvml~powercap~rapl~rocm~rocm_smi~sde+shared~static_tools␣
↪arch=cray-sles15-zen3/s2y4nrv [/global/u1/e/elvis/spack-infrastructure/spack/share/
↪spack/modules/cray-sles15-zen3/papi/6.0.0.1-gcc-11.2.0]
==> [2022-08-04-09:44:26.897249]    WRITE: papi@6.0.0.1%gcc@11.2.0+cuda+example~
↪infiniband~lmsensors~nvml~powercap~rapl~rocm~rocm_smi~sde+shared~static_tools␣
↪arch=cray-sles15-zen3/x43djbq [/global/u1/e/elvis/spack-infrastructure/spack/share/
↪spack/modules/cray-sles15-zen3/papi/6.0.0.1-gcc-11.2.0-cuda]
==> [2022-08-04-09:44:27.240985] Module name: gcc/11.2.0
==> [2022-08-04-09:44:27.241199] Package directory variable prefix: GCC
==> [2022-08-04-09:44:27.316093]    BLACKLISTED_AS_IMPLICIT : cuda@11.5.0%gcc@11.2.0~
↪allow-unsupported-compilers~dev arch=cray-sles15-zen3/puekfe3
```

Spack will generate the modulefiles, in its default location **$SPACK_ROOT/share/spack/modules** which is organized by architecture (*spack arch*) as shown below:

```
(spack-pyenv) elvis@login34> ls $SPACK_ROOT/share/spack/modules/$(spack arch)/*
/global/homes/e/elvis/spack-infrastructure/spack/share/spack/modules/cray-sles15-zen3/
↪darshan-runtime:
3.3.1-cce-13.0.2  3.3.1-gcc-11.2.0

/global/homes/e/elvis/spack-infrastructure/spack/share/spack/modules/cray-sles15-zen3/
↪hypre:
2.24.0-cce-13.0.2  2.24.0-gcc-11.2.0

/global/homes/e/elvis/spack-infrastructure/spack/share/spack/modules/cray-sles15-zen3/
↪papi:
6.0.0.1-cce-13.0.2  6.0.0.1-gcc-11.2.0  6.0.0.1-gcc-11.2.0-cuda
```

Let's change the directory path such that modulefiles are not inside Spack's root directory and they are easy to remember. For this exercise let's generate the modulefiles in your `$HOME/spack-infrastructure/modules` directory.

```
# This is a Spack Environment file.
```

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```
#
# It describes a set of packages to be installed, along with
# configuration settings.
spack:
  config:
    view: false
    concretization: separately
    build_stage: $spack/var/spack/stage
    misc_cache: $spack/var/spack/misc_cache
    concretizer: clingo
  compilers:
  - compiler:
      spec: gcc@11.2.0
      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: []
  - compiler:
      spec: cce@13.0.2
      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/13.0.2
      - craype-x86-milan
      - libfabric
      environment: {}
      extra_rpaths: []

  # add package specs to the `specs` list
  specs:
  - papi %gcc
  - papi %cce
  - hypre %gcc
  - hypre %cce
  - darshan-runtime %gcc
```

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```
  - darshan-runtime %cce
  - papi +cuda %gcc
  packages:
    all:
      compiler: [gcc@11.2.0, cce@13.0.2]
      providers:
        blas: [cray-libsci]
        mpi: [cray-mpich]
    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@8.1.15 %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 %cce@13.0.2
        prefix: /opt/cray/pe/mpich/8.1.15/ofi/cray/10.0/
        modules:
        - cray-mpich/8.1.15
        - cudatoolkit/11.5
    cray-pmi:
      buildable: false
      externals:
      - spec: cray-pmi@6.1.1
        modules:
        - cray-pmi/6.1.1
    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:
```

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```
      version: [4.6.0]
      externals:
      - spec: findutils@4.6.0
        prefix: /usr
    libfabric:
      buildable: false
      variants: fabrics=sockets,tcp,udp,rxm
      externals:
      - spec: libfabric@1.11.0.4.114
        prefix: /opt/cray/libfabric/1.11.0.4.114
        modules:
        - libfabric/1.11.0.4.114
    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
    readline:
      version: [7.0]
      buildable: false
      externals:
      - spec: readline@7.0
        prefix: /usr
    tar:
      version: [1.3]
      buildable: false
      externals:
      - spec: tar@1.30
        prefix: /usr
    unzip:
      version: [6.0]
      buildable: false
      externals:
      - spec: unzip@6.0
        prefix: /usr
  modules:
    default:
      enable:
      - tcl
      roots:
        tcl: /global/homes/e/elvis/spack-infrastructure/modules
      tcl:
        blacklist_implicits: true
        hash_length: 0
        naming_scheme: '{name}/{version}-{compiler.name}-{compiler.version}'
```

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```
      all:
        autoload: direct
        conflict:
        - '{name}'
        environment:
          set:
            '{name}_ROOT': '{prefix}'
        suffixes:
          ^cuda: cuda

  view: true
```

Now you will see the modulefiles are written in `$HOME/spack-infrastructure/modules`.

```
(spack-pyenv) elvis@login34> spack -d module tcl refresh --delete-tree -y
==> [2022-08-04-09:53:00.452047] Reading config file /global/u1/e/elvis/spack-
↪infrastructure/spack/etc/spack/defaults/config.yaml
==> [2022-08-04-09:53:00.563502] Reading config file /global/u1/e/elvis/spack-
↪infrastructure/spack/var/spack/environments/data_viz/spack.yaml
==> [2022-08-04-09:53:00.617365] Using environment 'data_viz'
==> [2022-08-04-09:53:00.625951] Imported module from built-in commands
==> [2022-08-04-09:53:00.632039] Imported module from built-in commands
==> [2022-08-04-09:53:00.637512] Reading config file /global/u1/e/elvis/spack-
↪infrastructure/spack/etc/spack/defaults/bootstrap.yaml
==> [2022-08-04-09:53:00.654001] DATABASE LOCK TIMEOUT: 3s
==> [2022-08-04-09:53:00.654065] PACKAGE LOCK TIMEOUT: No timeout
==> [2022-08-04-09:53:00.657750] Reading config file /global/u1/e/elvis/spack-
↪infrastructure/spack/etc/spack/defaults/repos.yaml
==> [2022-08-04-09:53:00.670487] Reading config file /global/u1/e/elvis/spack-
↪infrastructure/spack/etc/spack/defaults/modules.yaml
==> [2022-08-04-09:53:00.687615] Reading config file /global/u1/e/elvis/spack-
↪infrastructure/spack/etc/spack/defaults/cray/modules.yaml
==> [2022-08-04-09:53:00.891563]    BLACKLISTED_AS_IMPLICIT : cray-libsci@21.08.1.2
↪%cce@13.0.2~mpi~openmp+shared arch=cray-sles15-zen3/7uzhxpv
==> [2022-08-04-09:53:00.892858]    BLACKLISTED_AS_IMPLICIT : cray-libsci@21.08.1.2
↪%gcc@11.2.0~mpi~openmp+shared arch=cray-sles15-zen3/jzbnd6y
==> [2022-08-04-09:53:00.894129]    BLACKLISTED_AS_IMPLICIT : cray-mpich@8.1.15%cce@13.0.
↪2+wrappers arch=cray-sles15-zen3/tb5uxwe
==> [2022-08-04-09:53:00.895334]    BLACKLISTED_AS_IMPLICIT : cray-mpich@8.1.15%gcc@11.2.
↪0+wrappers arch=cray-sles15-zen3/3zy6uvs
==> [2022-08-04-09:53:00.896502]    BLACKLISTED_AS_IMPLICIT : cuda@11.5.0%gcc@11.2.0~
↪allow-unsupported-compilers~dev arch=cray-sles15-zen3/puekfe3
==> [2022-08-04-09:53:00.904007]    BLACKLISTED_AS_IMPLICIT : zlib@1.2.12%cce@13.0.
↪2+optimize+pic+shared patches=0d38234 arch=cray-sles15-zen3/e2hl6cx
==> [2022-08-04-09:53:00.905394]    BLACKLISTED_AS_IMPLICIT : zlib@1.2.12%gcc@11.2.
↪0+optimize+pic+shared patches=0d38234 arch=cray-sles15-zen3/ozmcyfj
==> [2022-08-04-09:53:03.555915] Regenerating tcl module files
==> [2022-08-04-09:53:03.577058]    WRITE: darshan-runtime@3.3.1%cce@13.0.2~apmpi~apmpi_
↪sync~apxc~hdf5+mpi scheduler=NONE arch=cray-sles15-zen3/uj3wa4a [/global/homes/e/elvis/
↪spack-infrastructure/modules/cray-sles15-zen3/darshan-runtime/3.3.1-cce-13.0.2]
==> [2022-08-04-09:53:04.003818] Module name: cce/13.0.2
==> [2022-08-04-09:53:04.004044] Package directory variable prefix: CCE
```

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```
==> [2022-08-04-09:53:04.248393] Module name: cce/13.0.2
==> [2022-08-04-09:53:04.248675] Package directory variable prefix: CCE
==> [2022-08-04-09:53:04.484157] Module name: cce/13.0.2
==> [2022-08-04-09:53:04.484420] Package directory variable prefix: CCE
==> [2022-08-04-09:53:04.766465] Module name: cce/13.0.2
==> [2022-08-04-09:53:04.766692] Package directory variable prefix: CCE
==> [2022-08-04-09:53:05.024080] Module name: cce/13.0.2
==> [2022-08-04-09:53:05.024335] Package directory variable prefix: CCE
==> [2022-08-04-09:53:05.043781]    BLACKLISTED_AS_IMPLICIT : cray-mpich@8.1.15%cce@13.0.
↪2+wrappers arch=cray-sles15-zen3/tb5uxwe
==> [2022-08-04-09:53:05.048836]    BLACKLISTED_AS_IMPLICIT : zlib@1.2.12%cce@13.0.
↪2+optimize+pic+shared patches=0d38234 arch=cray-sles15-zen3/e2hl6cx
==> [2022-08-04-09:53:05.055298] Reading config file /global/u1/e/elvis/spack-
↪infrastructure/spack/etc/spack/defaults/packages.yaml
==> [2022-08-04-09:53:05.111091]    WRITE: darshan-runtime@3.3.1%gcc@11.2.0~apmpi~apmpi_
↪sync~apxc~hdf5+mpi scheduler=NONE arch=cray-sles15-zen3/hkxzwvt [/global/homes/e/elvis/
↪spack-infrastructure/modules/cray-sles15-zen3/darshan-runtime/3.3.1-gcc-11.2.0]
==> [2022-08-04-09:53:05.161578]    BLACKLISTED_AS_IMPLICIT : cray-mpich@8.1.15%gcc@11.2.
↪0+wrappers arch=cray-sles15-zen3/3zy6uvs
==> [2022-08-04-09:53:05.164707]    BLACKLISTED_AS_IMPLICIT : zlib@1.2.12%gcc@11.2.
↪0+optimize+pic+shared patches=0d38234 arch=cray-sles15-zen3/ozmcyfj
==> [2022-08-04-09:53:05.171012]    WRITE: hypre@2.24.0%cce@13.0.2~complex~cuda~
↪debug+fortran~gptune~int64~internal-superlu~mixedint+mpi~openmp~rocm+shared~superlu-
↪dist~unified-memory arch=cray-sles15-zen3/62ofdsf [/global/homes/e/elvis/spack-
↪infrastructure/modules/cray-sles15-zen3/hypre/2.24.0-cce-13.0.2]
==> [2022-08-04-09:53:05.469562] Module name: cce/13.0.2
==> [2022-08-04-09:53:05.469791] Package directory variable prefix: CCE
==> [2022-08-04-09:53:05.767046] Module name: cce/13.0.2
==> [2022-08-04-09:53:05.767239] Package directory variable prefix: CCE
==> [2022-08-04-09:53:06.050449] Module name: cce/13.0.2
==> [2022-08-04-09:53:06.050663] Package directory variable prefix: CCE
==> [2022-08-04-09:53:06.295722] Module name: cce/13.0.2
==> [2022-08-04-09:53:06.295923] Package directory variable prefix: CCE
==> [2022-08-04-09:53:06.307895]    BLACKLISTED_AS_IMPLICIT : cray-libsci@21.08.1.2
↪%cce@13.0.2~mpi~openmp+shared arch=cray-sles15-zen3/7uzhxpv
==> [2022-08-04-09:53:06.313024]    BLACKLISTED_AS_IMPLICIT : cray-mpich@8.1.15%cce@13.0.
↪2+wrappers arch=cray-sles15-zen3/tb5uxwe
==> [2022-08-04-09:53:06.321590]    WRITE: hypre@2.24.0%gcc@11.2.0~complex~cuda~
↪debug+fortran~gptune~int64~internal-superlu~mixedint+mpi~openmp~rocm+shared~superlu-
↪dist~unified-memory arch=cray-sles15-zen3/mbn7bum [/global/homes/e/elvis/spack-
↪infrastructure/modules/cray-sles15-zen3/hypre/2.24.0-gcc-11.2.0]
==> [2022-08-04-09:53:06.366559]    BLACKLISTED_AS_IMPLICIT : cray-libsci@21.08.1.2
↪%gcc@11.2.0~mpi~openmp+shared arch=cray-sles15-zen3/jzbnd6y
==> [2022-08-04-09:53:06.369882]    BLACKLISTED_AS_IMPLICIT : cray-mpich@8.1.15%gcc@11.2.
↪0+wrappers arch=cray-sles15-zen3/3zy6uvs
==> [2022-08-04-09:53:06.377335]    WRITE: papi@6.0.0.1%cce@13.0.2~cuda+example~
↪infiniband~lmsensors~nvml~powercap~rapl~rocm~rocm_smi~sde+shared~static_tools␣
↪patches=b6d6caa arch=cray-sles15-zen3/3aprcx5 [/global/homes/e/elvis/spack-
↪infrastructure/modules/cray-sles15-zen3/papi/6.0.0.1-cce-13.0.2]
==> [2022-08-04-09:53:06.656390] Module name: cce/13.0.2
==> [2022-08-04-09:53:06.656565] Package directory variable prefix: CCE
==> [2022-08-04-09:53:06.670466]    WRITE: papi@6.0.0.1%gcc@11.2.0~cuda+example~
```

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```
↪infiniband~lmsensors~nvml~powercap~rapl~rocm~rocm_smi~sde+shared~static_tools␣
↪arch=cray-sles15-zen3/s2y4nrv [/global/homes/e/elvis/spack-infrastructure/modules/cray-
↪sles15-zen3/papi/6.0.0.1-gcc-11.2.0]
==> [2022-08-04-09:53:06.719655]    WRITE: papi@6.0.0.1%gcc@11.2.0+cuda+example~
↪infiniband~lmsensors~nvml~powercap~rapl~rocm~rocm_smi~sde+shared~static_tools␣
↪arch=cray-sles15-zen3/x43djbq [/global/homes/e/elvis/spack-infrastructure/modules/cray-
↪sles15-zen3/papi/6.0.0.1-gcc-11.2.0-cuda]
==> [2022-08-04-09:53:07.034250] Module name: gcc/11.2.0
==> [2022-08-04-09:53:07.034531] Package directory variable prefix: GCC
==> [2022-08-04-09:53:07.055549]    BLACKLISTED_AS_IMPLICIT : cuda@11.5.0%gcc@11.2.0~
↪allow-unsupported-compilers~dev arch=cray-sles15-zen3/puekfe3
```

We can see that Spack has generated the modulefiles in the format of `{name}/{version}-{compiler.name}-{compiler.version}`. For example, the `-cuda` suffix was added for the PAPI module that has CUDA-enabled features.

```
(spack-pyenv) elvis@login34> ls -l $CI_PROJECT_DIR/modules/$(spack arch)/*
/global/homes/e/elvis/spack-infrastructure/modules/cray-sles15-zen3/darshan-runtime:
total 8
-rw-r--r-- 1 elvis elvis 2245 Aug  4 09:53 3.3.1-cce-13.0.2
-rw-r--r-- 1 elvis elvis 2243 Aug  4 09:53 3.3.1-gcc-11.2.0

/global/homes/e/elvis/spack-infrastructure/modules/cray-sles15-zen3/hypre:
total 8
-rw-r--r-- 1 elvis elvis 1951 Aug  4 09:53 2.24.0-cce-13.0.2
-rw-r--r-- 1 elvis elvis 1943 Aug  4 09:53 2.24.0-gcc-11.2.0

/global/homes/e/elvis/spack-infrastructure/modules/cray-sles15-zen3/papi:
total 12
-rw-r--r-- 1 elvis elvis 2441 Aug  4 09:53 6.0.0.1-cce-13.0.2
-rw-r--r-- 1 elvis elvis 2425 Aug  4 09:53 6.0.0.1-gcc-11.2.0
-rw-r--r-- 1 elvis elvis 2503 Aug  4 09:53 6.0.0.1-gcc-11.2.0-cuda
```

We can add this directory to `MODULEPATH` by running the following:

```
(spack-pyenv) elvis@login34> module use $CI_PROJECT_DIR/modules/$(spack arch)
```

Next, if we run `ml av` we will see the modules generated from Spack that correspond to the installed Spack packages.

```
(spack-pyenv) elvis@login34> ml av

---------------------------------- /global/homes/e/elvis/spack-infrastructure/modules/
↪cray-sles15-zen3 -----------------------------------
   darshan-runtime/3.3.1-cce-13.0.2        hypre/2.24.0-cce-13.0.2        papi/6.0.0.1-
↪cce-13.0.2         papi/6.0.0.1-gcc-11.2.0
   darshan-runtime/3.3.1-gcc-11.2.0 (D)    hypre/2.24.0-gcc-11.2.0 (D)    papi/6.0.0.1-
↪gcc-11.2.0-cuda
```

This concludes the Spack training.

CHAPTER

FIVE

ADMINISTRATION GUIDE

This page holds documentation for the processes that support the development, deployment and continuous integration activities of Spack infrastructure at NERSC.

5.1 Login Access

You can access Cori and Perlmutter, for more details see Connecting to NERSC. If either system is down you can access data transfer nodes (`dtn[01-04].nersc.gov`) and then access the appropriate system. Please check out the NERSC MOTD at https://www.nersc.gov/live-status/motd/ for live updates to system.

In order to access TDS systems like `muller` or `gerty` you will need to access one of the systems (cori, perlmutter, dtn) and then run the following:

```
ssh dtn01.nersc.gov
ssh gerty
```

It is probably a good idea to run `usgrsu` once you are in the correct login node otherwise you may be prompted for a password for the `e4s` user.

The `e4s` user is a collaboration account which is a shared account used for spack deployments. You will need to login as `e4s` user via `usgrsu` command or use `sshproxy` to get 24hr credential and then **ssh** as the collaboration account. This will prompt you for a password which is your **NERSC password** for your username not **e4s** user.

Only members part of *c_e4s* unix group have access to use the collaboration account. You can run the following to see list of users that belong to the group. If you don't belong to this group and should be part of this group, please send a ticket at https://help.nersc.gov

```
getent group c_e4s
```

5.2 Production Software Stack

The spack stack is installed on shared filesystem at `/global/common/software/spackecp`. The project space has a quota limit for space and inode count. To check for the quota space please run the following

```
cfsquota /global/common/software/spackecp
```

The production installation of e4s stack on Perlmutter is stored in sub-directory *perlmutter* with a version for each stack as follows

```
(spack-pyenv) e4s:login22> ls -ld /global/common/software/spackecp/perlmutter/e4s-*
drwxrwsr-x+ 8 e4s spackecp 512 Jun  6 10:09 /global/common/software/spackecp/perlmutter/
↪e4s-21.11
drwxrwsr-x+ 9 e4s spackecp 512 Jan 12 07:34 /global/common/software/spackecp/perlmutter/
↪e4s-22.05
drwxrwsr-x+ 5 e4s spackecp 512 Mar 28 10:24 /global/common/software/spackecp/perlmutter/
↪e4s-22.11
```

Within the installation you will see several subdirectories which contain a unique identified from the CI job. The *default* is a symbolic link to the active production stack

```
(spack-pyenv) e4s:login22> ls -l /global/common/software/spackecp/perlmutter/e4s-22.11/
total 4
drwxrwsr-x+ 3 e4s spackecp 512 Mar  6 14:40 82028
drwxrwsr-x+ 3 e4s spackecp 512 Mar 28 10:16 82069
drwxrwsr-x+ 3 e4s spackecp 512 Mar 28 08:34 83104
lrwxrwxrwx  1 e4s spackecp   5 Mar 28 10:24 default -> 83104
```

We have one modulefile per e4s stack, they are named as `e4s/<version>` with a symobolic link `spack/e4s-<version>`. In the modulefile you will see path to root installation of spack. As we can see from example below, the root of spack is located in `/global/common/software/spackecp/perlmutter/e4s-22.11/default/spack`

```
(spack-pyenv) e4s:login22> module --redirect --raw show e4s/22.11 | grep root
local root = "/global/common/software/spackecp/perlmutter/e4s-22.11/default/spack"
         spack_setup = pathJoin(root, "share/spack/setup-env.sh")
         spack_setup = pathJoin(root, "share/spack/setup-env.csh")
         spack_setup = pathJoin(root, "share/spack/setup-env.fish")
   remove_path("PATH", pathJoin(root, "bin"))

(spack-pyenv) e4s:login22> ls -l /global/common/software/spackecp/perlmutter/e4s-22.11/
↪default/spack
total 100
drwxrwsr-x+ 2 e4s spackecp   512 Mar 28 08:54 bin
-rw-rw-r--  1 e4s spackecp 55695 Mar 28 08:35 CHANGELOG.md
-rw-rw-r--  1 e4s spackecp  1941 Mar 28 08:35 CITATION.cff
-rw-rw-r--  1 e4s spackecp  3262 Mar 28 08:35 COPYRIGHT
drwxrwsr-x+ 3 e4s spackecp   512 Mar 28 08:35 etc
drwxrwsr-x+ 3 e4s spackecp   512 Mar 28 08:35 lib
-rw-rw-r--  1 e4s spackecp 11358 Mar 28 08:35 LICENSE-APACHE
-rw-rw-r--  1 e4s spackecp  1107 Mar 28 08:35 LICENSE-MIT
-rw-rw-r--  1 e4s spackecp  1167 Mar 28 08:35 NOTICE
drwxrwsr-x+ 3 e4s spackecp   512 Mar 28 08:35 opt
-rw-rw-r--  1 e4s spackecp  2946 Mar 28 08:35 pyproject.toml
-rw-rw-r--  1 e4s spackecp   764 Mar 28 08:35 pytest.ini
-rw-rw-r--  1 e4s spackecp  6522 Mar 28 08:35 README.md
-rw-rw-r--  1 e4s spackecp   699 Mar 28 08:35 SECURITY.md
drwxrwsr-x+ 3 e4s spackecp   512 Mar 28 08:35 share
drwxrwsr-x+ 3 e4s spackecp   512 Mar 28 08:35 var
```

5.2.1 Changing Production stack within a release

To change the production path you will need to change the *default* symbolic link to the latest run. First navigate to the directory where you have the production installation. For example, lets change to the root of *e4s-22.11* and remove the symbolic link

```
cd  /global/common/software/spackecp/perlmutter/e4s-22.11/
unlink default
```

Next create a symbolic link to the new directory

```
ln -s <DIRECTORY_ID> default
```

5.3 Troubleshooting GitLab Runner

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 the GitLab runner is down you will need to restart the runner. To check the status of the runner you can do the following, if you see the following message this means the runner is active and running.

```
 perlmutter-e4s.service - Gitlab runner for e4s runner on perlmutter
  Loaded: loaded (/global/homes/e/e4s/.config/systemd/user/perlmutter-e4s.service;␣
↪enabled; vendor preset: disabled)
  Active: active (running) since Mon 2023-06-05 10:36:39 PDT; 23h ago
Main PID: 140477 (gitlab-runner)
   Tasks: 47 (limit: 39321)
  Memory: 11.9G
     CPU: 1d 5h 43min 43.685s
  CGroup: /user.slice/user-93315.slice/user@93315.service/app.slice/perlmutter-e4s.
↪service
          └─ 140477 /global/homes/e/e4s/jacamar/gitlab-runner run -c /global/homes/e/e4s/
↪.gitlab-runner/perlmutter.config.toml
```

If the runner is not active you can restart this by running

```
systemctl --user restart perlmutter-e4s
```

The systemd service files are used for managing the gitlab runners. These files are the following

```
(spack-pyenv) e4s:login22> ls -l ~/.config/systemd/user/*.service
-rw-rw-r-- 1 e4s e4s 326 May  9 07:32 /global/homes/e/e4s/.config/systemd/user/muller-
↪e4s.service
-rw-rw-r-- 1 e4s e4s 334 May  9 07:30 /global/homes/e/e4s/.config/systemd/user/
↪perlmutter-e4s.service
```

The `gitlab-runner` command should be accessible via the 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 location. 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 registration please see https://docs.gitlab.com/runner/register/.

Sometimes you may see unexpected results during CI jobs if you made changes to the GitLab configuration and you have multiple GitLab-runner processes running on different nodes. Therefore, we recommend you use `pdsh` to search

for all process across all nodes to find the process and then terminate it. The command below will search for the gitlab-runner process for service *perlmutter-e4s* across all Perlmutter login nodes.

```
pdsh -w login[01-40] systemctl --user status perlmutter-e4s 2>&1 < /dev/null
```

5.4 Jacamar

The GitLab runnners are using Jacamar CI, there should be a `jacamar.toml` file in the following location:

```
e4s:login27> ls -l ~/.gitlab-runner/jacamar.toml
-rw-rw-r-- 1 e4s e4s 758 Aug 11 08:57 /global/homes/e/e4s/.gitlab-runner/jacamar.toml
```

Any updates to the Jacamar configuration are applied to runner and there is no need to restart GitLab runner.

The binaries `jacamar` and `jacamar-auth` are located in the following location, if we need to upgrade Jacamar we should place them in this location,

```
e4s:login27> ls -l ~/jacamar/binaries/
total 15684
-rwxr-xr-x 1 e4s e4s 6283264 Jul  7 15:50 jacamar
-rwxr-xr-x 1 e4s e4s 9773296 Jul  7 15:50 jacamar-auth
```

5.5 Test for NERSC System Changes

NERSC uses ReFrame to test system health after maintenance. In order to ensure the earliest possible notification of system changes that will affect E4S builds, a test has been added. This test can be found at https://gitlab.nersc.gov/nersc/consulting/reframe-at-nersc/reframe-nersc-tests.

CHAPTER

SIX

CONTRIBUTING GUIDE

This guide will discuss how one can contribute back to this project. First, you will need to clone this repository locally.

```
git clone https://software.nersc.gov/NERSC/spack-infrastructure.git
```

You will need to setup a Personal Access Token in order to clone via HTTPS since git over ssh is disabled.

The typical contribution process will be as follows:

```
git checkout -b <featureX>
git add <file1> <file2> ... <fileN>
git commit -m "COMMIT MESSAGE"
git push
```

Please create a feature branch, add the files that need to be changed, commit and push your changes. Next create a merge request to main branch.

If you want to reproduce the steps in the CI, we encourage you review the .gitlab-ci.yml and run the instructions to recreate the environment.

Once you clone this repo locally, you can source the setup-env.sh script.

```
cd spack-infrastructure
source setup-env.sh
```

This script will create a python environment where you can perform spack builds. This script will set `CI_PROJECT_DIR` to root of spack-infrastructure project.

```
(spack-pyenv) siddiq90@login31> echo $CI_PROJECT_DIR
/global/homes/s/siddiq90/gitrepos/software.nersc.gov/spack-infrastructure
```

6.1 Troubleshooting CI builds

First you will need to review the pipeline build in https://software.nersc.gov/NERSC/spack-infrastructure/-/pipelines and login as `e4s` user on the appropriate system. At top of pipeline you will see location where project was cloned typically this would be in **$CFS/m3503**. The content would look something like

```
Reinitialized existing Git repository in /global/cfs/cdirs/m3503/ci/oGV2kxLA/0/NERSC/
↪spack-infrastructure/.git/
```

You will need to navigate to the directory and then repeat the steps specified in `.gitlab-ci.yml` to reproduce the issue.

6.2 How to add a new E4S stack

All spack configuration are stored in spack-configs, so if you want to add a new spack configuration please create a new directory to store your spack configuration. You can use the directory format `<site>-e4s-<e4s version>` to map a E4S release to a particular system so `cori-e4s-22.02` refers to E4S 22.02 release built for Cori.

You will need to create one or more gitlab job in `.gitlab-ci.yml` to ensure gitlab can run the pipeline. We recommend you create a scheduled pipeline in order to run job on a scheduled basis. The scheduled pipeline must define name `PIPELINE_NAME` with name of gitlab job to run.

The production pipelines should not run via scheduled pipeline, instead they should be run manually via web interface. The production pipeline should only be run when one need to redeploy the entire stack due to rebuild.

6.3 Building User Documentation

The documentation is built using sphinx and hosted on readthedocs. We have enabled Preview Documentation from Pull Requests. When a pull request or push event occurs, the documentation will be rebuilt and hosted. This allows us to preview the changes during the review process.

If you want to build documentation locally, use the following steps:

1. Create a python virtual environment and activate the environment

```
python3 -m venv $HOME/nersc-spack
source $HOME/nersc-spack/bin/activate
```

2. Install the dependencies

```
pip install -r docs/requirement.txt
```

3. Build the documentation

```
cd docs
make clean
make html
```

Shown below is a typical build for documentation

```
(nersc-spack)  ~/Documents/github/spack-infrastructure/docs/ [update_contributing_
↪guide*] make clean
Removing everything under '_build'...
(nersc-spack)  ~/Documents/github/spack-infrastructure/docs/ [update_contributing_
↪guide*] make html
Running Sphinx v5.1.1
making output directory... done
myst v0.18.0: MdParserConfig(commonmark_only=False, gfm_only=False, enable_extensions=[],
↪ disable_syntax=[], all_links_external=False, url_schemes=('http', 'https', 'mailto',
↪'ftp'), ref_domains=None, highlight_code_blocks=True, number_code_blocks=[], title_to_
↪header=False, heading_anchors=None, heading_slug_func=None, footnote_transition=True,␣
↪words_per_minute=200, sub_delimiters=('{', '}'), linkify_fuzzy_links=True, dmath_allow_
↪labels=True, dmath_allow_space=True, dmath_allow_digits=True, dmath_double_
↪inline=False, update_mathjax=True, mathjax_classes='tex2jax_process|mathjax_
↪process|math|output_area')
building [mo]: targets for 0 po files that are out of date
```

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```
building [html]: targets for 3 source files that are out of date
updating environment: [new config] 3 added, 0 changed, 0 removed
reading sources... [100%] spack_configs
looking for now-outdated files... none found
pickling environment... done
checking consistency... done
preparing documents... done
writing output... [100%] spack_configs
generating indices... genindex done
writing additional pages... search done
copying static files... done
copying extra files... done
dumping search index in English (code: en)... done
dumping object inventory... done
build succeeded.

The HTML pages are in _build/html.
```

The documentation page can be accessible by opening the file `_build/html/index.html` in your browser. Alternatively you can use the `open` command from your terminal

```
open _build/html/index.html
```

Sphinx will read a configuration file, conf.py, when building the documentation

Please refer to the Configuration section of the Sphinx documentation for more details.

CHAPTER

SEVEN

CONFERENCES

Conference	Talk	Date	Link
SEA Improving Scientific Software Conference 2022	Spack Infrastructure at NERSC	Apr 5th, 2022	PPTX, VIDEO
HPC Software Summit	NERSC Spack Infrastructure	Aug 17th, 2022	PDF
E4S at NERSC 2022	NERSC Spack Infrastructure	Aug 25th, 2022	PDF

CHAPTER

EIGHT

INDICES AND TABLES

- genindex
- modindex
- search