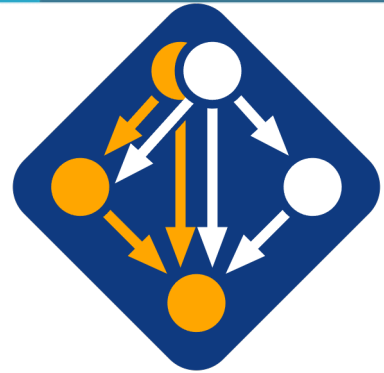




Sandia  
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# Trilinos and TPL Dependencies



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# SEMS modules



- SEMS provides a common environment across **workstations**, **Jenkins nodes**, **cee resources**, and **ascic machines**.
- SEMS is now using **spack(cm)** to build the tpls and modules used by Trilinos and distribute them across the lab
- Spack-cm uses spack environments
  - reproducible builds of compiler toolchains on different platforms
- Leverage spack community for
  - debugging
  - creating reasonable default package configurations
- Trilinos is 1/2 on the spack-cm toolchains.
  - Goal: move the rest over soon

```
jfrye@sems-son-rhel7-tp1-01:~]: module avail

----- /projects/sems/modulefiles/rhel7-x86_64/sems/linux-rhel7-x86_64/compilers -----
sems-clang/11.0.1    sems-clang/14.0.2 (D)    sems-gcc/7.3.0 (D)    sems-gcc/8.3.0    sems-gcc/10.1.0    sems-intel/19.0.5    sems-intel/19.1.2    sems-intel/2021.3 (D)

----- /projects/sems/modulefiles/rhel7-x86_64/sems/linux-rhel7-x86_64/Core -----
sems-anaconda3/2020.07    sems-cmake/3.18.4    sems-cmake/3.23.1 (D)    sems-git-lfs/2.11.0    sems-git/2.37.0 (D)    sems-py-pip/20.2    sems-python/3.9.0
sems-autoconf/2.69    sems-cmake/3.21.1    sems-doxygen/1.8.20    sems-git/2.11.1    sems-metis-int64/5.1.0    sems-python/3.7.9    sems-texlive/20200406
sems-automake/1.16.5    sems-cmake/3.22.4    sems-gdb/9.2    sems-git/2.29.0    sems-ninja/1.10.1    sems-python/3.8.6 (D)    sems-vvtest/1.2.0

----- /projects/sems/modulefiles/rhel7-x86_64/sems/linux-rhel7-x86_64/project-modulefiles -----
Dakota-env    e3sm-env    pyomo-env    sems-dev
```

# SEMS modules hide complexity of the installations with Imod



```
jfrye@sems-son-rhel7-tp1-01: [~]: module avail
```

```
----- /projects/sems/modulefiles/rhel7-x86_64/sems/linux-rhel7-x86_64/compilers -----
sems-clang/11.0.1    sems-clang/14.0.2 (D)    sems-gcc/7.3.0 (D)    sems-gcc/8.3.0    sems-gcc/10.1.0    sems-intel/19.0.5    sems-intel/19.1.2    sems-intel/2021.3 (D)

----- /projects/sems/modulefiles/rhel7-x86_64/sems/linux-rhel7-x86_64/Core -----
sems-anaconda3/2020.07    sems-cmake/3.18.4    sems-cmake/3.23.1 (D)    sems-git-lfs/2.11.0    sems-git/2.37.0 (D)    sems-py-pip/20.2    sems-python/3.9.0
sems-autoconf/2.69    sems-cmake/3.21.1    sems-doxygen/1.8.20    sems-git/2.11.1    sems-metis-int64/5.1.0    sems-python/3.7.9    sems-texlive/20200406
sems-automake/1.16.5    sems-cmake/3.22.4    sems-gdb/9.2    sems-git/2.29.0    sems-ninja/1.10.1    sems-python/3.8.6 (D)    sems-vvtest/1.2.0

----- /projects/sems/modulefiles/rhel7-x86_64/sems/linux-rhel7-x86_64/project-modulefiles -----
Dakota-env    e3sm-env    pyomo-env    sems-dev
```

```
jfrye@sems-son-rhel7-tp1-01: [~]: module load sems-gcc/10.1.0
jfrye@sems-son-rhel7-tp1-01: [~]: module load sems-openmpi/4.0.5
jfrye@sems-son-rhel7-tp1-01: [~]: module avail
```

```
----- /projects/sems/modulefiles/rhel7-x86_64/sems/linux-rhel7-x86_64/openmpi/4.0.5-e64jpc/gcc/10.1.0 -----
sems-cgns/4.1.1    sems-netcdf-c/4.7.3    sems-netcdf-fortran/4.5.3    sems-parmetis-int64/4.0.3    sems-parmetis/4.0.3    sems-scotch-int64/6.0.3    sems-scotch/6.0.3

----- /projects/sems/modulefiles/rhel7-x86_64/sems/linux-rhel7-x86_64/gcc/10.1.0 -----
sems-boost/1.69.0    sems-cuda/10.2.89    sems-gdb/9.2 (D)    sems-metis/5.1.0    sems-nvhpc/22.3    sems-openmpi/4.0.5 (L,D)    sems-superlu/4.3
sems-boost/1.70.0    sems-cuda/11.1.0    sems-gsl/1.16    sems-mpich/3.2.1    sems-openblas/0.3.10    sems-yaml-cpp/0.6.2
sems-boost/1.74.0 (D)    sems-cuda/11.4.2 (D)    sems-metis-int64/5.1.0 (D)    sems-netlib-lapack/3.8.0    sems-openmpi/1.10.7    sems-suite-sparse/5.8.1    sems-zlib/1.2.11

----- /projects/sems/modulefiles/rhel7-x86_64/sems/linux-rhel7-x86_64/compilers -----
sems-clang/11.0.1    sems-clang/14.0.2 (D)    sems-gcc/7.3.0 (D)    sems-gcc/8.3.0    sems-gcc/10.1.0 (L)    sems-intel/19.0.5    sems-intel/19.1.2    sems-intel/2021.3 (D)

----- /projects/sems/modulefiles/rhel7-x86_64/sems/linux-rhel7-x86_64/Core -----
sems-anaconda3/2020.07    sems-cmake/3.18.4    sems-cmake/3.23.1 (D)    sems-git-lfs/2.11.0    sems-git/2.37.0 (D)    sems-py-pip/20.2    sems-python/3.9.0
sems-autoconf/2.69    sems-cmake/3.21.1    sems-doxygen/1.8.20    sems-git/2.11.1    sems-metis-int64/5.1.0    sems-python/3.7.9    sems-texlive/20200406
sems-automake/1.16.5    sems-cmake/3.22.4    sems-gdb/9.2    sems-git/2.29.0    sems-ninja/1.10.1    sems-python/3.8.6 (D)    sems-vvtest/1.2.0

----- /projects/sems/modulefiles/rhel7-x86_64/sems/linux-rhel7-x86_64/project-modulefiles -----
Dakota-env    e3sm-env    pyomo-env    sems-dev
```

# Spack helps generate SEMS modules consistently



- Matches the “look and feel” from the old sems system
- Same process to generate modules for any spack environment by including the spack configuration
  - SEMS nfs resources
  - productions HPC machines
  - testbeds at sandia

```
all:
  conflict:
    - "{name}"
  environment:
    set:
      "{name}_ROOT": "{prefix}"
      "{name}_VERSION": "{version}"
      "{name}_BIN": "{prefix.bin}"
      "{name}_INC": "{prefix.include}"
      "{name}_LIB": "{prefix.lib}"
  projections:
    all: "sems-{name}/{version}"
  verbose: true
```

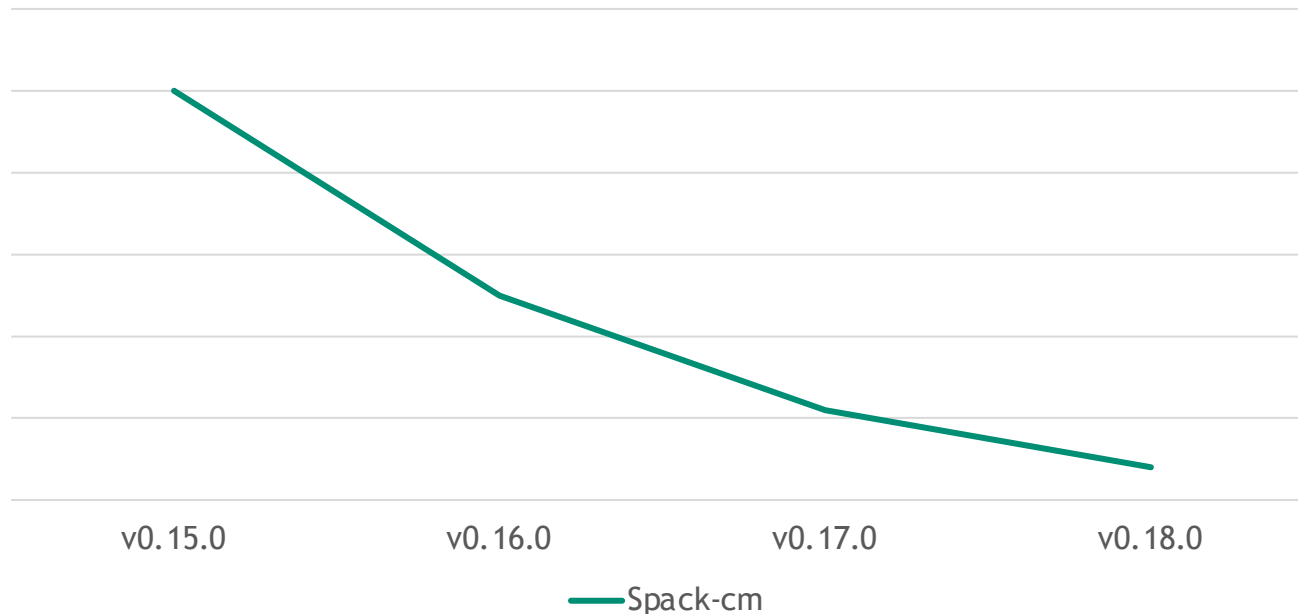
```
setenv("HDF5_ROOT", "/projects/sems/install/rhel7-x86_64/sems/v2/tpl/hdf5/1.10.7/gcc/10.1.0/openmpi/4.0.5/mrkn5gq")
setenv("HDF5_VERSION", "1.10.7")
setenv("HDF5_BIN", "/projects/sems/install/rhel7-x86_64/sems/v2/tpl/hdf5/1.10.7/gcc/10.1.0/openmpi/4.0.5/mrkn5gq/bin")
setenv("HDF5_INC", "/projects/sems/install/rhel7-x86_64/sems/v2/tpl/hdf5/1.10.7/gcc/10.1.0/openmpi/4.0.5/mrkn5gq/include")
setenv("HDF5_LIB", "/projects/sems/install/rhel7-x86_64/sems/v2/tpl/hdf5/1.10.7/gcc/10.1.0/openmpi/4.0.5/mrkn5gq/lib")
```

# What is spack-cm?



- The original goal of spack-cm was to create a tool that would use spack to **replace the original sems install tools** and give a **familiar experience to SEMS TPL users**
- CM = configuration manager. How do we make modular reusable configurations for spack that will recreate the SEMS module experience?
- As spack adds features/resolves bugs spack-cm gets smaller!

spack-cm complexity vs spack release



- Currently a collection of templates used to make spack.yaml files and a script to clean spack state before install
- All project specific configuration (ie SEMS, or HAAPs) is kept in a separate repo and is usable by vanilla spack
- Spack-cm is barely a project anymore 😊



# Next: SEMS + spack + containers



- Targeting delivery of SEMS spack(cm)-built modules in containers
- Currently able to use a container with SEMS modules installed on it to build trinos on
  - trhel8 (podman)
  - my MacBook(docker)
  - testbeds(podman).
- Looking for friendly users to play with containers and provide feedback

SEMS > containers > Container Registry

## Container Registry

5 Image repositories

With the GitLab Container Registry, every project can have its own space to store images. [More information](#)

### Image Repositories



sems/containers/rhel8/spack



1 Tag



sems/containers/rhel8



1 Tag



sems/containers/rhel8/sems-container-rocm5.0



1 Tag



sems/containers/rhel8/sems-continaer-gcc8.5-openmpi-4.1.1-tpetra



1 Tag



sems/containers/rhel8/sems-container-gcc8.5-openmpi-4.1.1



1 Tag



# Live Demo

# Obviously Live Demos don't ever work...



```
jfrye@srrh8cicd01:[~]: podman --version
podman version 4.1.1
jfrye@srrh8cicd01:[~]: which podman
/usr/bin/podman
jfrye@srrh8cicd01:[~]: module avail
lmod has detected the following error: module avail is not possible. MODULEPATH is not set or not set with valid paths.
```

```
[jfrye@srrh8cicd01:[~]: podman run -it cee-gitlab.sandia.gov:4567/sems/containers/docker/rhel8/spack-gcc8.5-openmpi-4.1.1-sems-tpls
[root@d24579b8bd15 /]#
```

```
[root@9808415f1779 /]# module avail

----- /spack/share/spack/lmod/linux-rhel8-x86_64/openmpi/4.1.1-ue2lbi6/gcc/8.5.0 -----
sems-cgns/4.2.0          sems-netcdf-cxx/4.2          sems-parmetis/4.0.3
sems-hdf5/1.10.7        sems-netcdf-fortran/4.5.3    sems-scotch/6.0.3
sems-netcdf-c/4.8.1     sems-parallel-netcdf/1.12.2  sems-superlu-dist/7.1.1

----- /spack/share/spack/lmod/linux-rhel8-x86_64/gcc/8.5.0 -----
sems-boost/1.70.0       sems-ninja/1.10.2           sems-vvtest/1.2.0
sems-cmake/3.21.4       sems-openblas/0.3.18        sems-yaml-cpp/0.6.2
sems-gdb/9.2            sems-openmpi/4.1.1 (L)     sems-zlib/1.2.11
sems-git/2.31.1         sems-suite-sparse/5.8.1
sems-metis/5.1.0        sems-superlu/5.3.0
```



## 9 Obviously Live Demos don't ever work...



```
[root@9808415f1779 /]# module avail

----- /spack/share/spack/lmod/linux-rhel8-x86_64/openmpi/4.1.1-ue2lbi6/gcc/8.5.0 -----
sems-cgns/4.2.0      sems-netcdf-cxx/4.2      sems-parmetis/4.0.3
sems-hdf5/1.10.7    sems-netcdf-fortran/4.5.3  sems-scotch/6.0.3
sems-netcdf-c/4.8.1  sems-parallel-netcdf/1.12.2  sems-superlu-dist/7.1.1

----- /spack/share/spack/lmod/linux-rhel8-x86_64/gcc/8.5.0 -----
sems-boost/1.70.0   sems-ninja/1.10.2      sems-vvtest/1.2.0
sems-cmake/3.21.4   sems-openblas/0.3.18   sems-yaml-cpp/0.6.2
sems-gdb/9.2        sems-openmpi/4.1.1      sems-zlib/1.2.11
sems-git/2.31.1     sems-suite-sparse/5.8.1
sems-metis/5.1.0    sems-superlu/5.3.0
```

```
[root@9808415f1779 /]# module load sems-openmpi/4.1.1
[[root@9808415f1779 /]# mpicc --version
gcc (GCC) 8.5.0 20210514 (Red Hat 8.5.0-4)
Copyright (C) 2018 Free Software Foundation, Inc.
This is free software; see the source for copying conditions. There is NO
warranty; not even for MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.

[[root@9808415f1779 /]# which mpicc
/spack/opt/spack/linux-rhel8-x86_64/gcc-8.5.0/openmpi-4.1.1-ue2lbi6preqaijqgdzohknrwrwzgzg7g/bin/mpicc
```

```
[root@9808415f1779 /]# git clone https://github.com/trilinos/Trilinos.git
Cloning into 'Trilinos'...
remote: Enumerating objects: 1224372, done.
remote: Counting objects: 100% (1079/1079), done.
remote: Compressing objects: 100% (664/664), done.
remote: Total 1224372 (delta 490), reused 947 (delta 407), pack-reused 1223293
Receiving objects: 100% (1224372/1224372), 752.14 MiB | 16.29 MiB/s, done.
Resolving deltas: 100% (927036/927036), done.
Updating files: 100% (52599/52599), done.
```