Multi-package development at Fermilab with Spack

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Spack adoption at Fermilab

Spack is the **s**upercomputing **pack**age manager.

- It has gained widespread traction across the HPC community and within HEP
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- Constraints on effort to maintain Fermilab-specific package manager
- Take advantage of technology provided by the broader computing community
- Engage and influence the broader computing community

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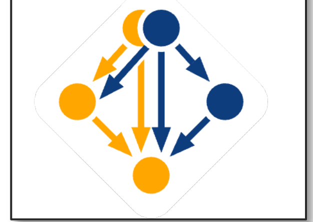

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Fermilab progress in the last few years:

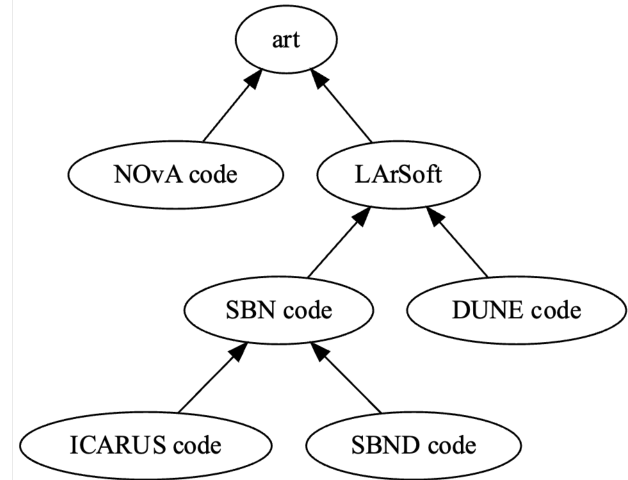
- Proof-of-principle installation of all offline code for DUNE, Mu2e, etc.
- Joined Spack's technical steering committee
- Establishing process for layered releases/environments of Fermilab-supported software
- Created solution for building CMake packages together in a Spack context

Developing multiple repositories together

Many experiments at Fermilab share software.

It is common for an experiment to develop their own code at the same time as adjusting a piece of shared software.

Simplified dependency graph



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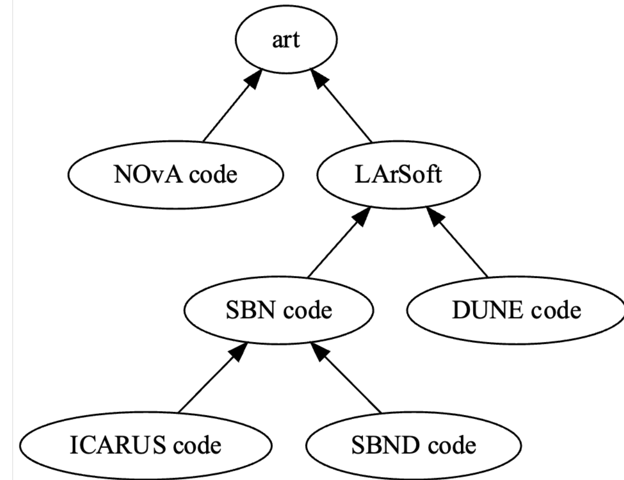
Most of these bodies of software are CMake packages, which can often be built together as a larger CMake project.

For the past decade, this has been done at Fermilab with the **m**ulti-**r**epository **b**uild (MRB) system.



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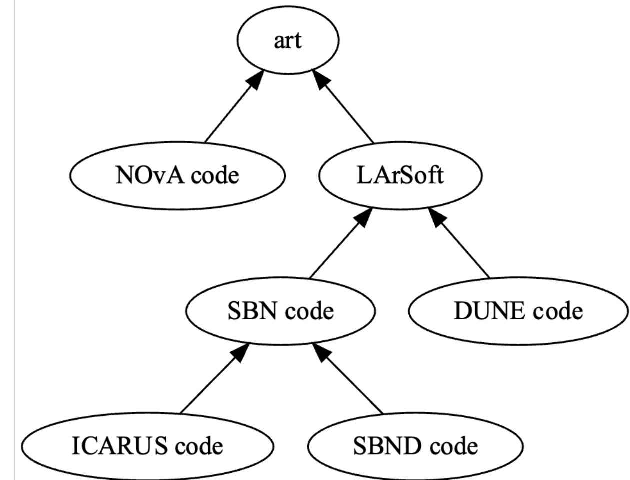

As successful as MRB has been in building repositories in concert, it relies heavily on Fermilab's home-grown package management system (UPS).

Fermilab is pursuing a Spack-based approach for developing multiple repositories.

Code development using Spack

Fermilab has tried different approaches for replacing MRB:

1. FNAL-created `spack dev` extension

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   Well-integrated with Spack installations

   Supports development of any Spack package

   More Spack expertise required of users, and substantial inefficiencies in incremental builds

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3. FNAL-created `spack mpd` (MPD) extension https://github.com/FNALssi/spack-mpd

   Allows users to develop CMake packages **in concert** with Spack-provided software

   Tailored for iterative algorithm development

   Try to give a familiar feel to MRB…but *not too* familiar

Desired features of MPD

Spack interactions

- Minimize user’s required knowledge of Spack
- Take advantage of packages installed in upstream Spack instances/environments
- Directly support the installation of dependencies
  - This was not feasible with UPS
  - Must avoid rebuilding dependencies with existing installations

Usability

- Easy to setup an MPD development session
- Easy to switch between my MPD projects
  - Avoid reliance on environment variables
- Easy to list which MPD projects are available to you

Spack MPD commands

```
$ spack mpd -h
usage: spack mpd [-hV] SUBCOMMAND ...

develop multiple packages using Spack for external software

positional arguments:
  SUBCOMMAND
    build (b)             build repositories
    clear                 clear selected MPD project
    git-clone (g, clone)
                          clone git repositories
    deploy (d)            deploy developed packages
    init                  initialize MPD on this system
    install (i)           install built repositories
    list (ls)             list MPD projects
    new-project (n, newDev)
                          create MPD development area
    refresh               refresh project
    rm-project (rm)       remove MPD project
    select                select MPD project
    status                current MPD status
    test (t)              build and run tests
    zap (z)               delete everything in your build and/or install areas

optional arguments:
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Commands that establish a user environment for developing a given project.

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Initialization
Once per Spack instance

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Development workflow

Create new project

```
$ spack mpd new-project --name my-art-devel -T my-art-devel -E gcc-14-1 cxxstd=20 %gcc@14

==> Creating project: my-art-devel

Using build area: /scratch/knoepfel/my-art-devel/build
Using local area: /scratch/knoepfel/my-art-devel/local
Using sources area: /scratch/knoepfel/my-art-devel/srcs

==> You can clone repositories for development by invoking

  spack mpd git-clone --suite <suite name>

  (or type 'spack mpd git-clone --help' for more options)
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Fermilab

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  (or type 'spack mpd git-clone --help' for more options)
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Clone repositories

```
$ spack mpd git-clone --fork cetlib cetlib-except hep-concurrency

==> Cloning and forking:

  cetlib .................. done    (cloned, added fork knoepfel/cetlib)
  cetlib-except ........... done    (cloned, created fork knoepfel/cetlib-except)
  hep-concurrency ......... done    (cloned, created fork knoepfel/hep-concurrency)

==> You may now invoke:

  spack mpd refresh
```

Development workflow

Refresh project

Concretization *is when Spack looks for a set of package specifications that satisfy dependency requirements.*

```
$ spack mpd refresh

==> Refreshing project: my-art-devel

...

==> Concretizing project (this may take a few minutes)
==> Environment my-art-devel has been created
==> Updating view at /scratch/knoepfel/spack/var/.../my-art-devel/.spack-env/view
==> Concretization complete
```


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Development workflow

Refresh project

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The ***installation*** *step installs only the* ***dependencies*** *of the packages being developed.*

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==> Ready to install MPD project my-art-devel

==> Would you like to continue with installation? [Y/n]
==> Specify number of cores to use (default is 12)
==> Installing my-art-devel
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==> Concretization complete

==> Ready to install MPD project my-art-devel

==> Would you like to continue with installation? [Y/n]
==> Specify number of cores to use (default is 12)
==> Installing my-art-devel
[+] /usr (external glibc-2.34-hjl43avhawltutkgujn2ns3577kjowlq)

...

[+] /scratch/knoepfel/spack/.../intel-tbb-2021.9.0-gtkaoizm5i4m6goy7rptg7v3i5q2jrg7

==> MPD project my-art-devel has been installed.  To load it, invoke:

  spack env activate my-art-devel
```

Development workflow

Activate environment
Build

```
$ spack env activate my-art-devel
$ spack mpd build -G Ninja -j12
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CMake configuration

```
==> Configuring with command:

cmake --preset default /scratch/knoepfel/my-art-devel/srcs ...

Preset CMake variables:

  CMAKE_BUILD_TYPE:STRING="RelWithDebInfo"
  ...

-- Found TBB: /.../lib64/cmake/TBB/TBBConfig.cmake (found version "2021.9.0")
-- The C compiler identification is GNU 14.1.0
...
-- Configuring done (2.2s)
-- Generating done (0.2s)
-- Build files have been written to: /home/knoepfel/scratch/my-art-devel/build
```

Build

```
==> Building with command:

cmake --build /scratch/knoepfel/my-art-devel/build -- -j12

[0/2] Re-checking globbed directories...
[278/278] Linking CXX executable cetlib/bin/ntuple_t
```

Development workflow

Test

```
$ spack mpd test -j12

==> Testing with command:

ctest --test-dir /scratch/knoepfel/my-art-devel/build -j12

Internal ctest changing into directory: /home/knoepfel/scratch/my-art-devel/build
Test project /home/knoepfel/scratch/my-art-devel/build
        Start   1: coded_exception_test
        Start   2: demangle_t
        Start   3: exception_collector_test
        Start   4: exception_test
        Start   5: exception_category_matcher_t
        Start   6: exception_message_matcher_t
        Start   7: exception_bad_append_t
        Start   8: runThreadSafeOutputFileStream_t.sh
        Start   9: assert_only_one_thread_test
        Start  10: serial_task_queue_chain_t
        Start  11: serial_task_queue_t
        Start  12: waiting_task_list_t
  1/100 Test   #1: coded_exception_test .........................   Passed    0.01 sec
...
100/100 Test  #55: cpu_timer_test ...............................   Passed    0.55 sec

100% tests passed, 0 tests failed out of 100
```


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Helper commands

Status

```
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==> Selected project: my-art-devel
    Environment status: active
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List projects available to me

```
$ spack mpd ls

==> Existing MPD projects:

      Project name        Environment    Deployed environment
      ----------------    -----------    --------------------
      art-devel           (none)         (none)
      meld-devel          installed      (none)
   ▶  my-art-devel        active         (none)
      my-larsoft-devel    created        (none)
   ◀  test-devel          (none)         (none)
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Selected in this shell

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Switch MPD Projects

```
$ spack mpd select test-devel
==> Warning: Project test-devel selected in another shell.  Use with caution.
```


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Caveats

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  The recipe does not need to be part of the Spack mainline repository.

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  Spack forms an environment of *dependencies* used for building the repositories.

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- **Minimize use of environment variables**

  Spack recipes can (and do) set environment variables during the build and run stages. But when building that code outside of Spack, those variables need to be set in a different way.

  Best to find alternatives to environment variables

  Better insulates each MPD project from each other

Conclusions

- Fermilab is switching from its custom package manager to Spack.
- Multi-package development with Spack will be achieved with the MPD extension.
- MPD is ready for beta-testing.

  Pull requests and bug reports at https://github.com/FNALssi/spack-mpd are welcome.

Thanks for your time.

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