Spack Driven Software Development and Spack-Manager

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EXASCALE COMPUTING PROJECT

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Overview

- Spack Overview
- Introduction to Spack Develop
- Overview of Spack Develop API
- Making it simpler with Spack-Manager

This presentation will just be a simple overview to highlight capabilities.

ECP: Funding Statement

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Spack: Package Manager++

- Package manager focused on HPC applications
- Spack has many attractive features:
  - Complex package and environment configurations
  - Embedded tribal HPC knowledge
  - A unique, scalable, multicomponent development tool (spack develop)
- Spec:
  - trilinos@develop+fortran build_type=Release %gcc@10.3.0
- Environment:
  - Constrain what software is available and gets built (pyenv, conda, etc)

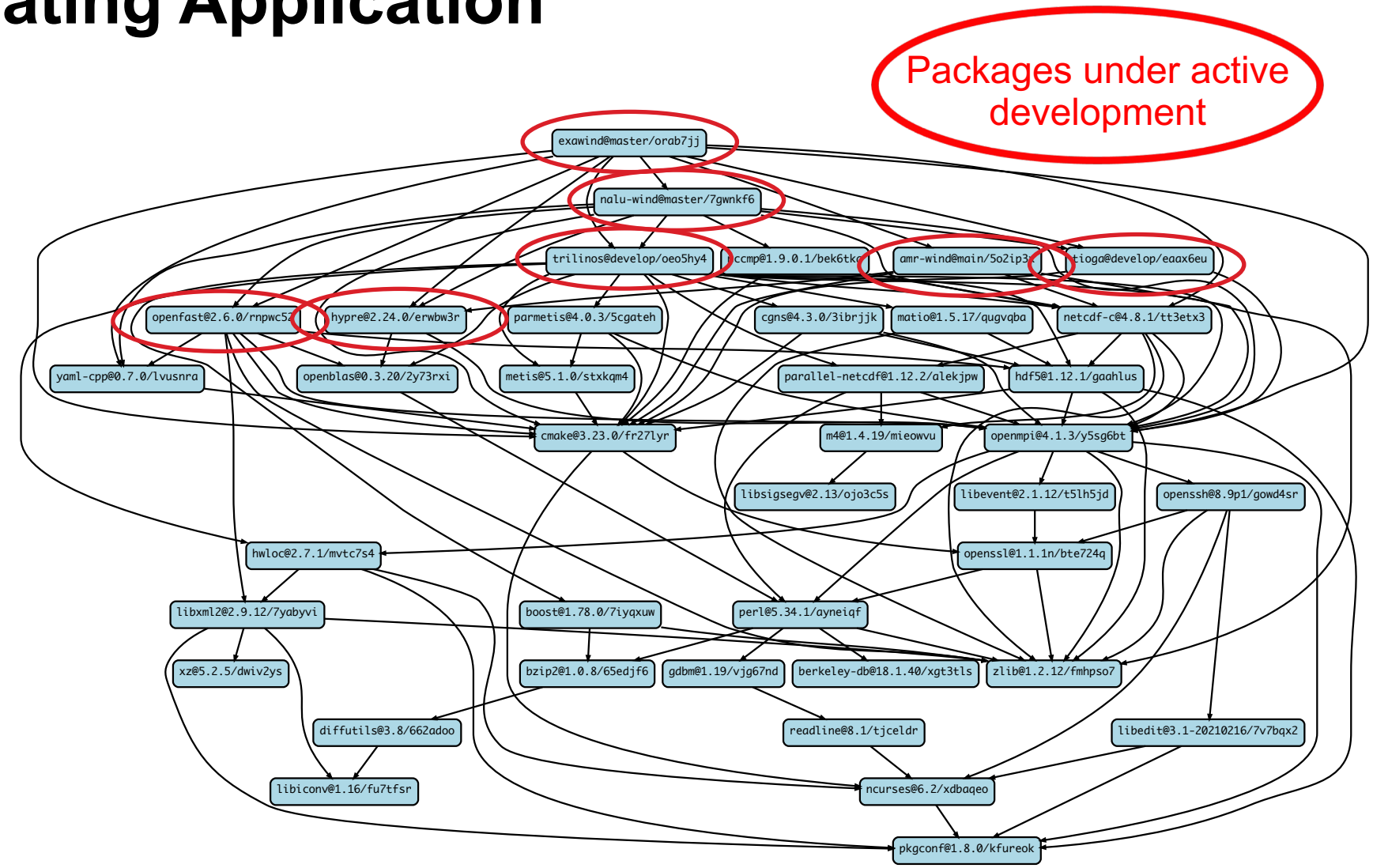
```
# This is a Spack Environment file.
#
# It describes a set of packages to be
installed, along with
# configuration settings.
spack:
  specs:
  - nalu-wind
  - trilinos@develop
  view: false
  develop:
    nalu-wind:
      spec: nalu-wind@master
    trilinos:
      spec: trilinos@develop
```

Root specs

Develop specs

ExaWind: A Motivating Application

- ExaWind software stack:
  - Combine two loosely coupled CFD codes with entirely different software stacks (Trilinos and AMReX)
  - Living on the develop branch of multiple dependencies
  - Project is actively supporting development of 7+ software packages in the stack (CPU+GPU)
- Challenges:
  - Building
  - Developing
  - Testing
  - Deploying



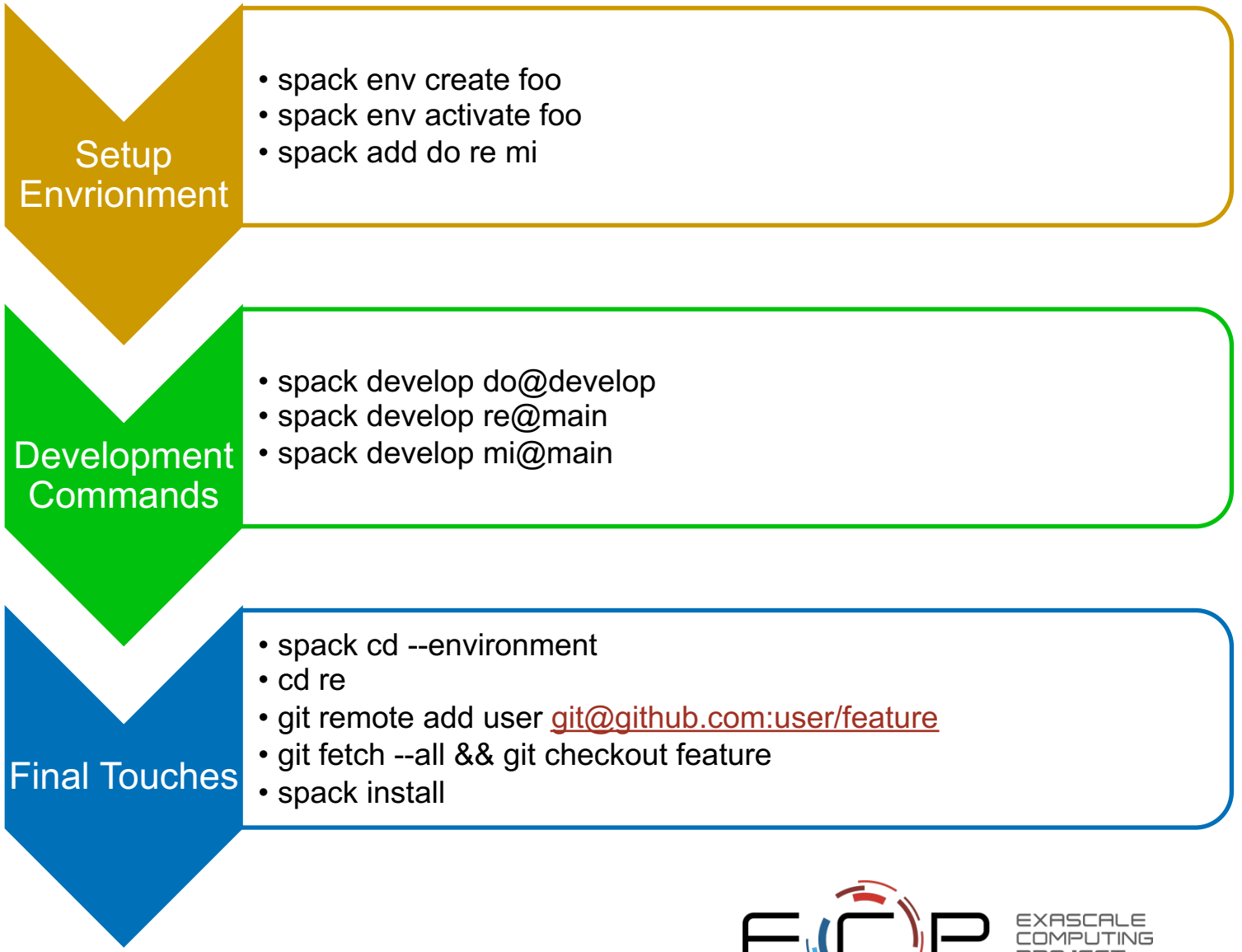
Spack Develop

- In a spack environment *develop specs* can be added
- Develop specs are
  - If DAG_spec.satisfies(develop_spec)
    - Do a build from the users source code rather than from spack's staging procedure
    - Perform incremental builds based on timestamp of files in the source directory
- Allows for arbitrary development of packages in the DAG
  - Dependencies will get automatically rebuilt
- Allows for multiple builds from the same source
  - Cuda and Non-Cuda builds from the same source code at the same time
  - DAG level parallelism is available in builds

```
# In this configuration you will get
# 4 develop builds: cuda and non-cuda
# nalu-wind and trilinos coming from
# the same sources
spack:
  specs:
  - nalu-wind +cuda cuda_arch=70
  - nalu-wind ~cuda
  view: false
  develop:
    nalu-wind:
      spec: nalu-wind@master
    trilinos:
      spec: trilinos@develop
```

Development Environment API

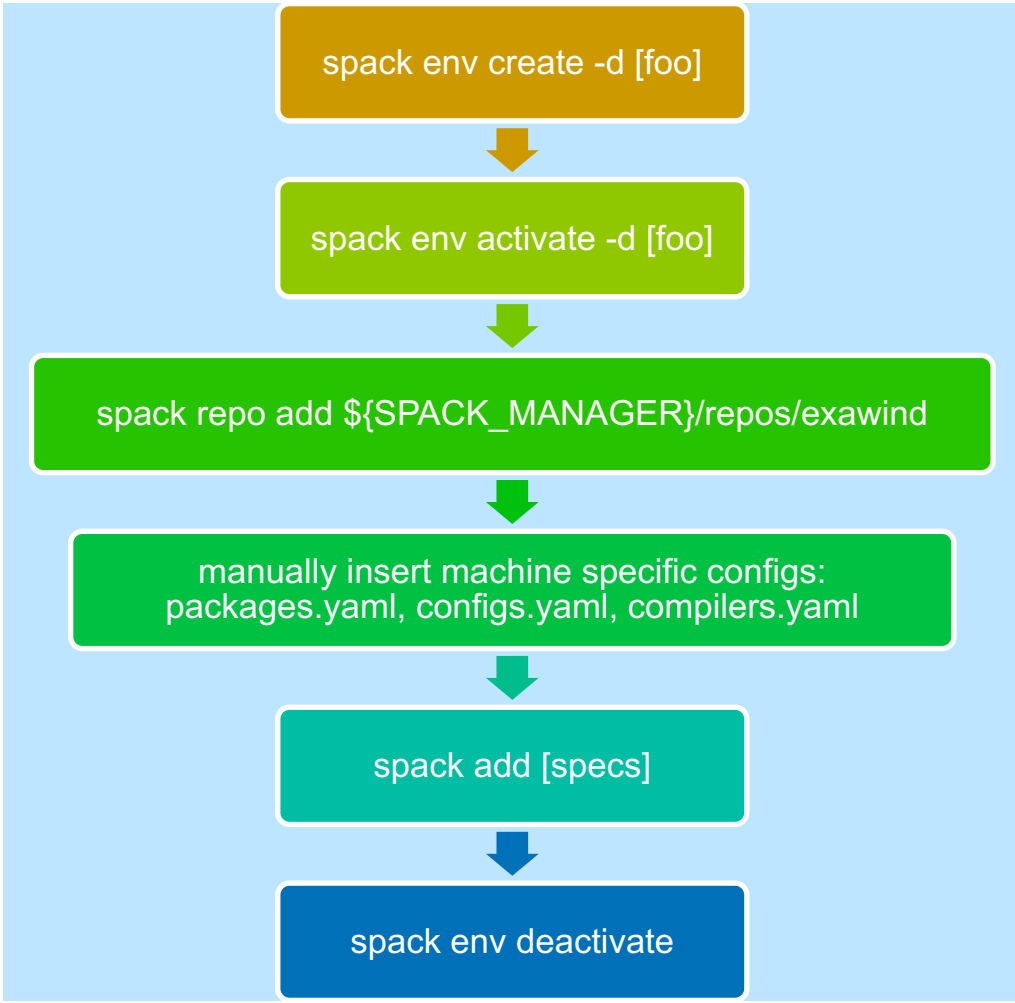
- Utilize develop feature
  - Create environment
  - Tag the specs/packages you wish to develop
  - Make sure the source code is correct (several ways to do this)
  - Install
- To develop
  - Make code changes
  - Spack install (incremental build)



Spack-Manager: API Reduction

- Spack-Manager:
  - Embed machine specific natively
  - Reduce the API for using spack develop
- Utilize Spack API's to write Spack extensions
  - Environment curation
  - All of our scripts serve to reduce the end user API
  - Can be replicated through core Spack commands and a little manual intervention
- A core example of this is:
  - find-machine + create-env
    - find-machine: a utility that allows custom python scripts to identify the current machine
    - create-env: uses find-machine and stored configs to automate platform specific environments

spack manager create-env –d [foo] –s [specs]



What does it look like?

spack manager create-env --spec exawind amr-wind nalu-wind

spack.yaml

```yaml
spack:
  include: [include.yaml]
  concretization: together
  view: false
  specs: [exawind, amr-wind, nalu-wind]
```

include.yaml

```yaml
repos:
- $spack/../repos/exawind
packages:
  hypre:
    variants: +shared
    version: [develop]
  all:
    target: [x86_64]
    compiler: [apple-clang, gcc, clang]
    providers:
      mpi: [mpich, openmpi]
      blas: [netlib-lapack]
      lapack: [netlib-lapack]
    variants: build_type=Release +mpi
  boost:
    version: [1.76.0]
    variants: cxxstd=14
  hdf5:
    version: [1.10.7]
    variants: +cxx+hl
  netcdf-c:
    version: [4.7.4]
    variants: +parallel-netcdf maxdims=65536 maxvars=524288
  openfast:
    version: [master]
    variants: +cxx
  parallel-netcdf:
    version: [1.12.2]
  tioga:
    version: [develop]
  yaml-cpp:
    version: [0.6.3]
  trilinos:
    version: [develop]
    variants: ~adios2~alloptpkgs~amesos+amesos2~anasazi~aztec+belos+boost~chaco~complex~debug~dtk~epetra~epetraext+exodus+explicit_template_instantiation~float+fortran~fortrilinos+glm+gtest+hdf5~hypre~ifpack+ifpack2~intrepid~intrepid2~isorropia+kokkos~mesquite+metis~minitensor~ml+mpi+muelu~mumps~nox~openmp~phalanx~piro~python~rol~rythmos~sacado+shards~shylu+stk~stratimikos~suite-sparse~superlu~superlu-dist~teko~tempus+teuchos+tpetra+uvm~x11~xsdkflags+zlib+zoltan+zoltan2
      gotype=long cxxstd=14 build_type=Release
config:
  mirrors:
    e4s: https://cache.e4s.io
  source_cache: ~/.spack/downloads
  misc_cache: $spack/../.cache
  build_stage:
  - $spack/../stage
  concretizer: clingo
```

Onboarding Developers

- Conflict: 1 command build vs a learning curve
  - Made significant efforts to reduce the API
- Ask developers to learn 3 things about Spack:
  - How to query the API for help i.e. --help and spack info
  - How to read and write a Spack spec
  - What the major steps in the Spack build process are
- Learn to speak the basics of the language

I [..] was able to install Exawind using Spack fairly easily as a new hire. I have definitely had a good experience so far
- Ilker Topcuoglu (NREL)

I have to type a whole 12 characters to compile just 2 different codes with a zillion dependencies to debug my code
- Ganesh Vijayakumar (NREL)

Spack Manager and Spack have saved me an incredible amount of time and headache, providing an intuitive framework that ensures dependency resolution and repeatable, shareable, self-documenting builds.
- Nate deVelder (SNL)

Pros and Cons of Spack Driven Development

Pros

- Spack is already solving the dependency issues
- Spack is scalable
  - DAG parallelism
    - HPC Case study: 3 compiler configurations for ExaWind
      - 1.5 hours with DAG parallelism
      - 4.5+ hours without
- Spack is configurable
  - +cuda and ~cuda in same environment (DAG parallel)
- Spack is extendable
- Spack is testable
- Simplified and unified API dramatically reduces Dev-Ops workload

Cons

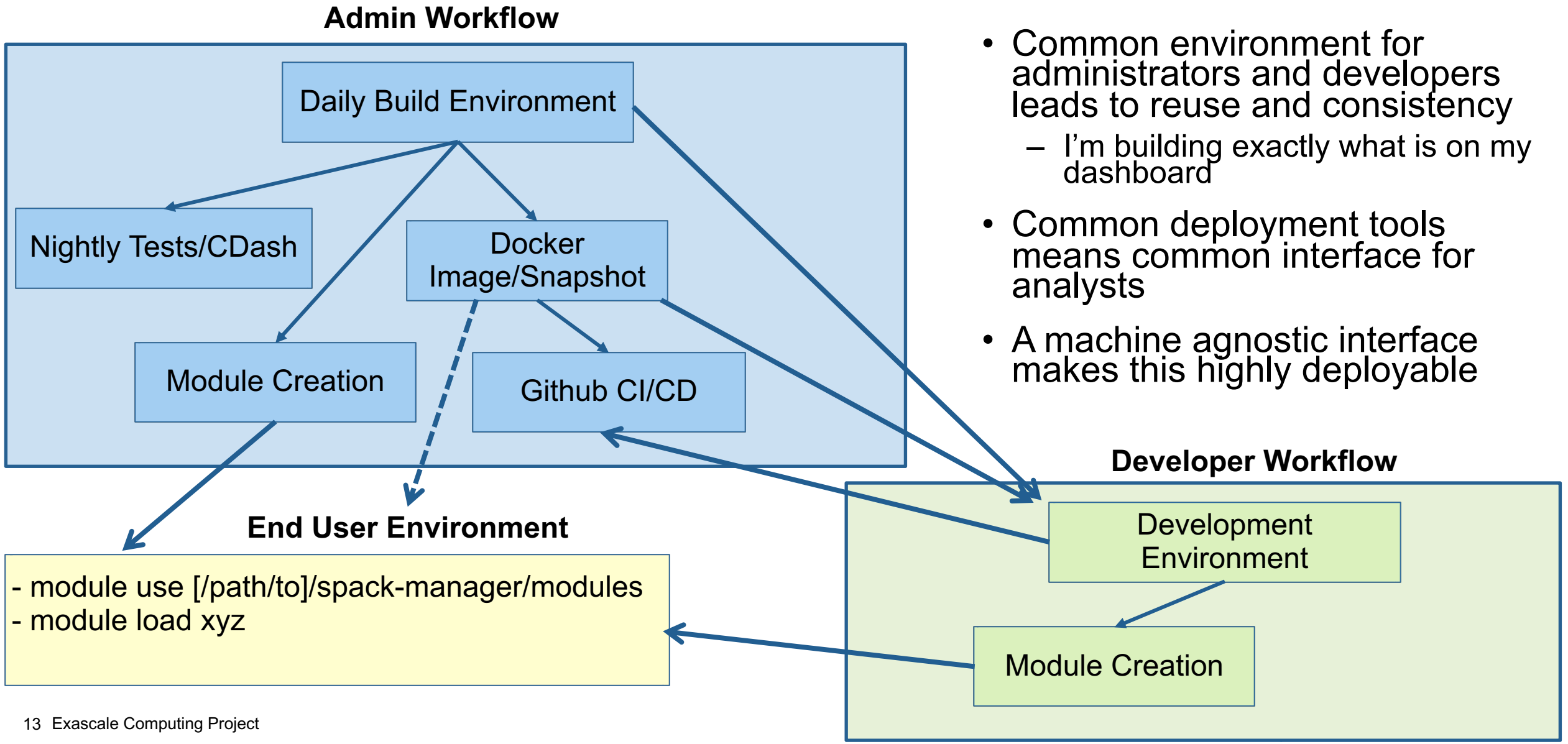
- Spack can be overwhelming
  - 3-5 ways to do just about everything
- Spack build process has some quirks
  - Hash based issues and confusion
  - Bootstrapping and occasional ssl issues
- Spack data management and logs make developers uncomfortable
  - spack-build-[hash]
  - spack cd -b [package]
- Spack still has some optimization to do
  - spack install is a too big of a hammer for incremental builds

Conclusions

- Spack is taking on a lot of challenges in the HPC software space
  - Not everything is perfect, but the progress is rapid
  - We can help make it better!
- Very happy with Spack as the driver for development on ExaWind
  - Unified API dramatically reduces infrastructure needs
  - Gives developers the tools to customize their own environments
- Cons can be mitigated with education and light scripts
- Spack-Manager is a tool for managing and reducing the Spack API with a particular emphasis on development
  - We'd love to have more Trilinos developers test it out

Supplementary Slides

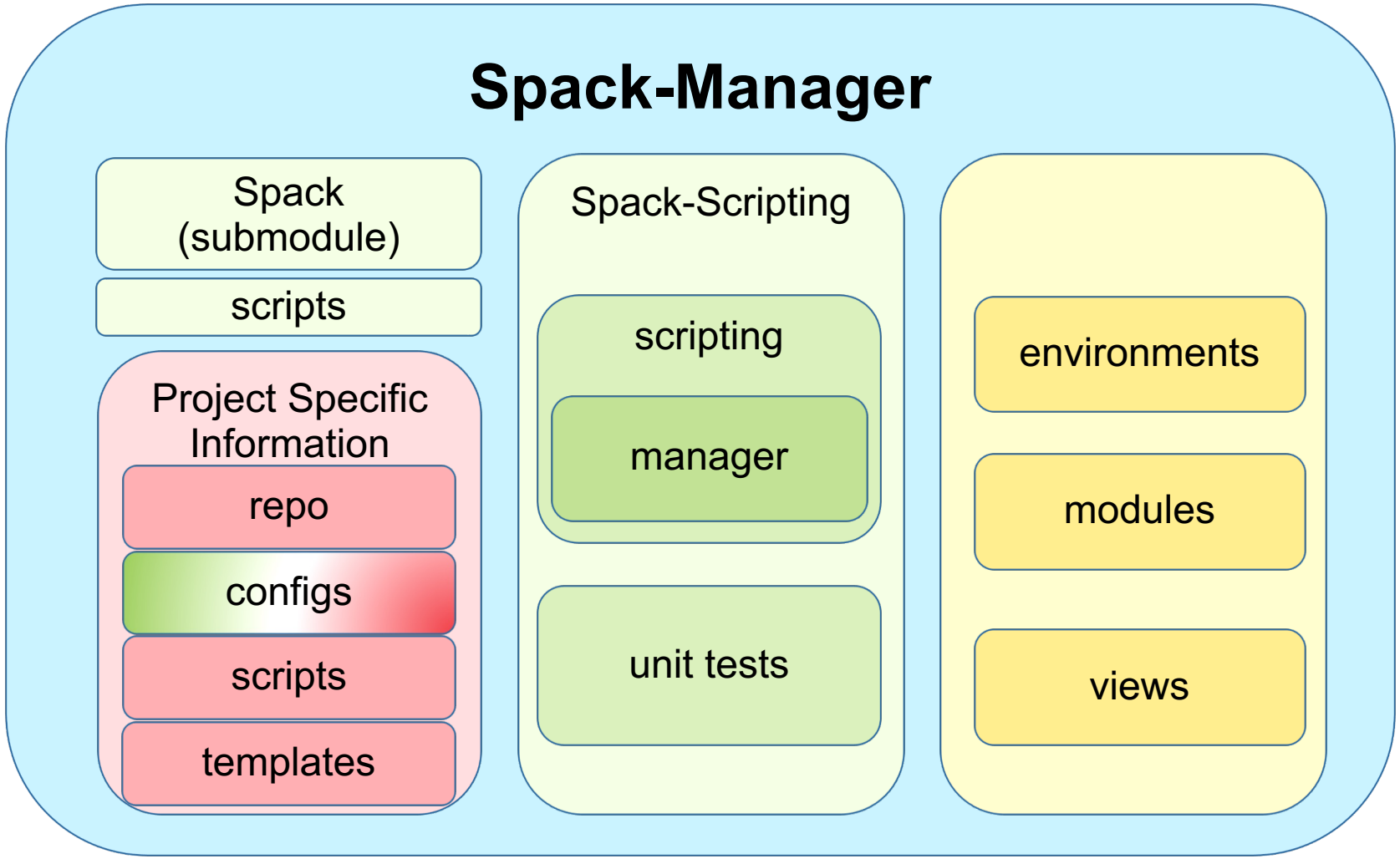
The Vision: Unified Tooling and Environments



- Common environment for administrators and developers leads to reuse and consistency
  - I'm building exactly what is on my dashboard
- Common deployment tools means common interface for analysts
- A machine agnostic interface makes this highly deployable

Spack-Manager Layout

- Spack-Manager
  - Project agnostics code/scripts
    - Tooling and testing
  - Pre-configured locations
  - Project specific information
    - Customize packages
    - Create machine specific implementations
    - Add machine specific templates



Bash ”quick-commands”

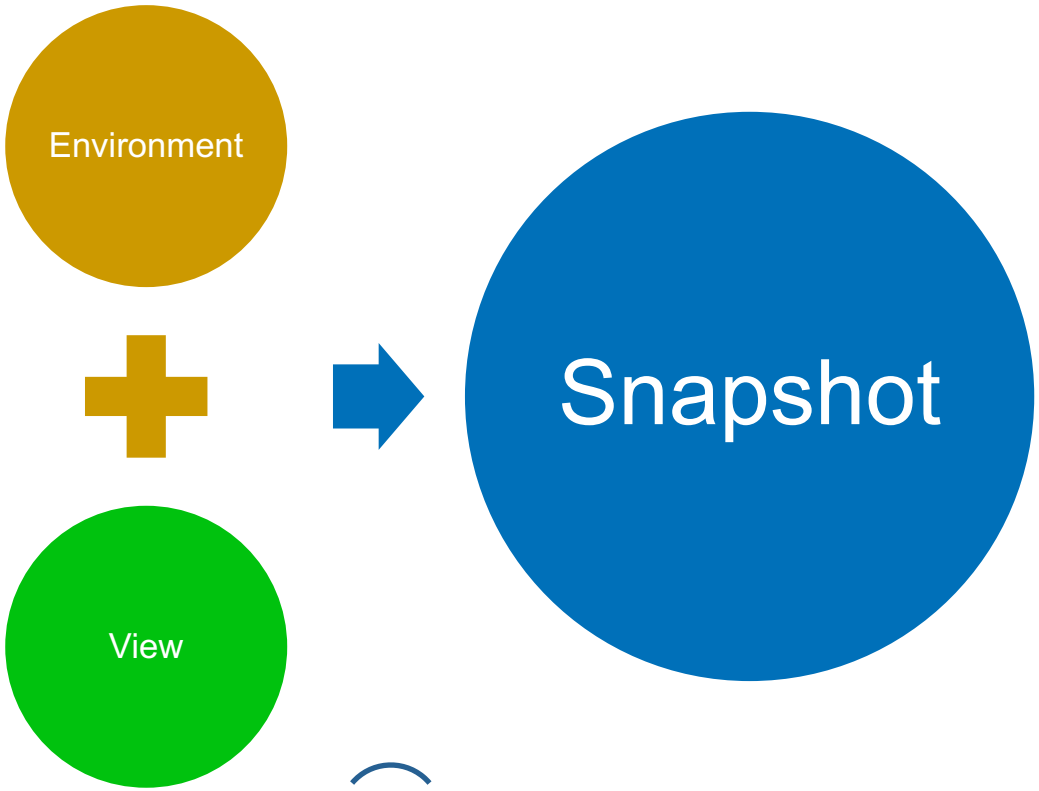
- Wrap the functionality of basic setup and development commands together
- Common features:
  - Shell source Spack/Spack-Manager
  - Create an anonymous Spack environment
  - Activate the created environment
- Development specific assumptions:
  - All concrete spec’s are intended as develop specs ([name]@[version])
  - Anything not pre-cloned should be fetched via spack develop

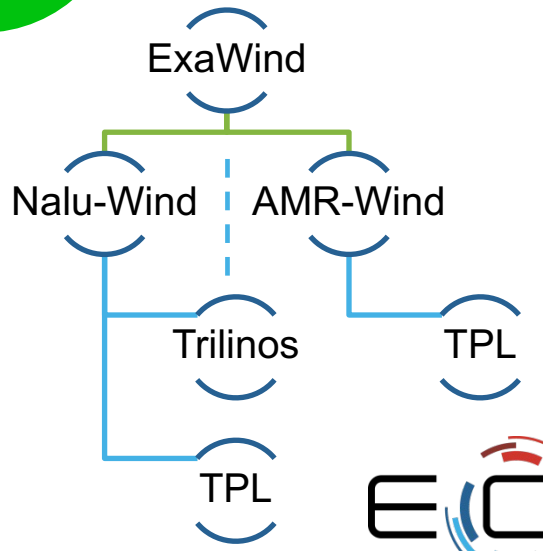
Step	quick-create	quick-create-dev	quick-develop
spack-start	x	x	x
Create an environment	x	x	x
Activate an environment	x	x	x
Add root specs	x	x	x
Add develop specs		x	x
Add externals			x
Concretize and install			

- quick-create-dev --spec do@develop re@main mi@main

Externals: Re-Using Binaries

- Spack has several different ways to reuse binaries
  - Upstreams
  - Binary Caches
  - --reuse
  - Externals
- First 3 rely directly on the concertizer to make the “best” decision
- Development workflow often wants specific binaries
- Created a way to auto generate externals in an externals.yaml file
- “Snapshots” are time-dated versions of the software installed on each system

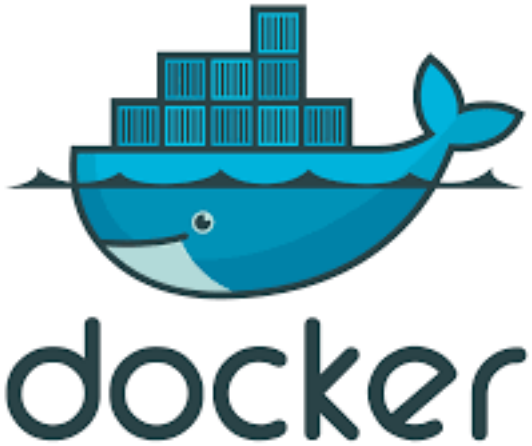




Containers

- Partnered with E4S to create nightly containers
- Software provenance preserved through history of containers on Docker Hub
- Infrastructure makes containerization trivial
  - E4S added 4 lines to their base Ubuntu docker configuration
- With externals + container we can drive our CI for every package through 1 image
- Developers can download image and have same environment on laptops

GitHub Actions




```yaml
CPU:
  #needs: Formatting
  runs-on: ubuntu-latest
  container:
    image: ecpe4s/exawind-snapshot
    env:
        SPACK_MANAGER: /spack-manager
        E4S_MACHINE: true
  steps:
    - name: Cancel previous runs
      uses: styfle/cancel-workflow-action@0.6.0
      with:
        access_token: ${{github.token}}
    - name: Clone
      uses: actions/checkout@v3
      with:
        submodules: true
    - name: Tests
      working-directory: /spack-manager/environments/exawind
      run: |
        /bin/bash -c " \
          source ${SPACK_MANAGER}/start.sh && \
          ln -s ${GITHUB_WORKSPACE} nalu-wind && \
          source ${SPACK_MANAGER}/start.sh && \
          quick-develop -s nalu-wind@master && \
          spack install && \
          spack cd -b nalu-wind && \
          spack build-env nalu-wind ctest -j $(nproc) -L unit --output-on-failure \
        "
```