OAK RIDGE National Laboratory

National Center for Computational Sciences Software Provisioning (NSP)

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Systems Acceptance & User Environment

Oak Ridge National Laboratory

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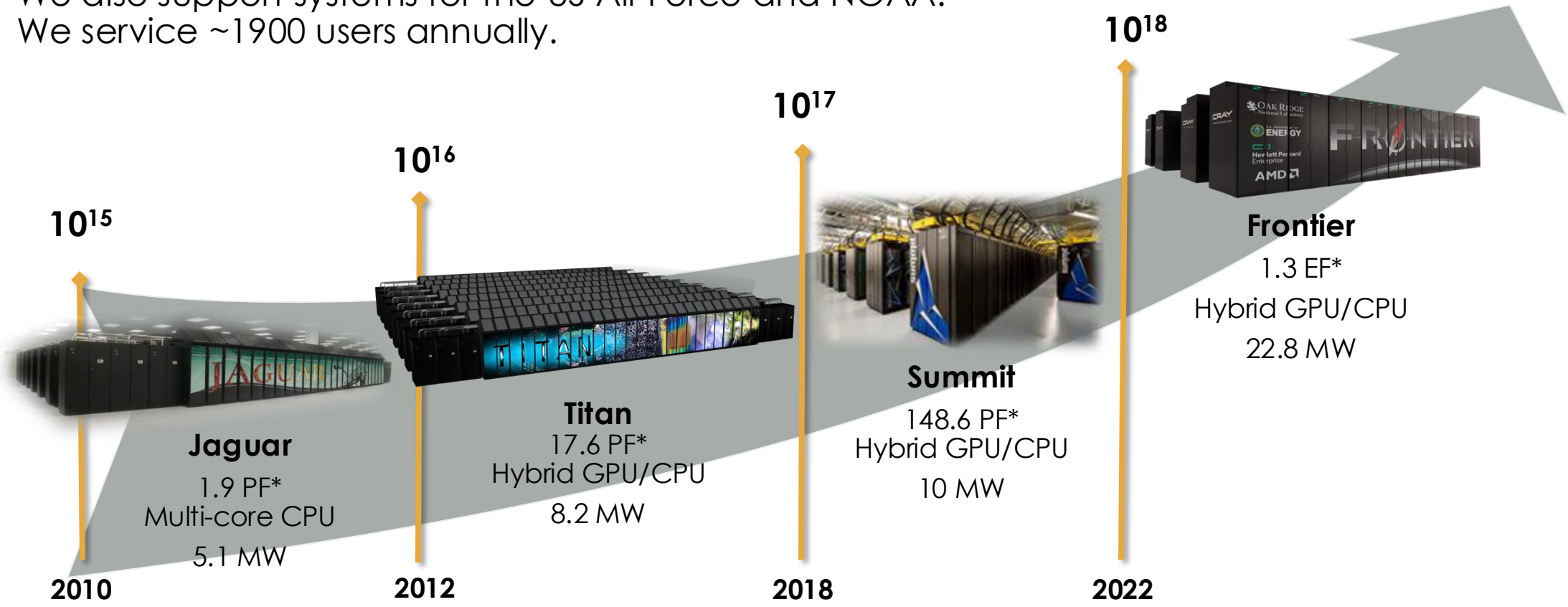
HPC History at NCCS

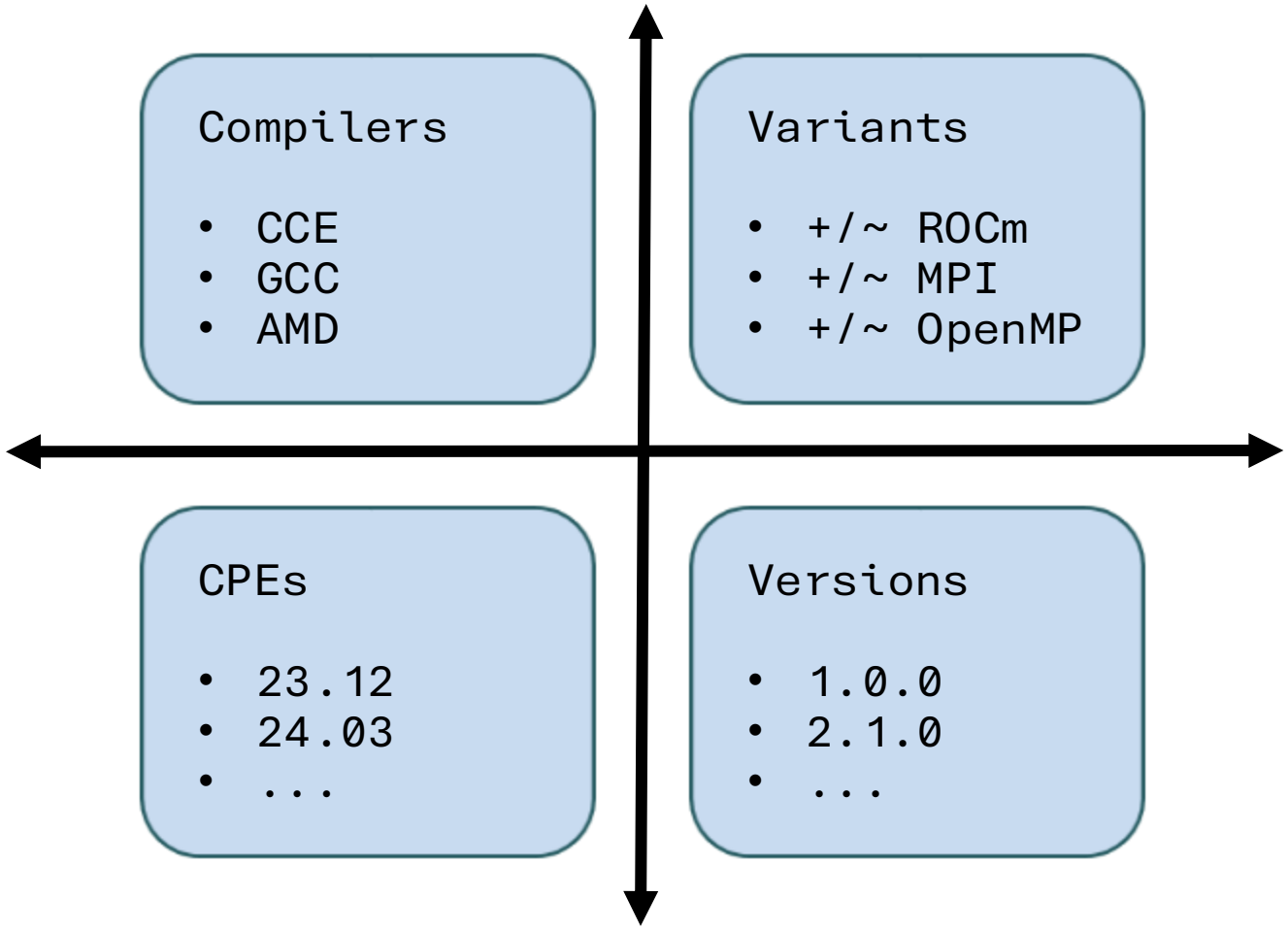
- NCCS host the Oak Ridge Leadership Computing Facility (OLCF) which provides leadership scale computing resources for open science.
- We also support systems for the US Air Force and NOAA.
- We service ~1900 users annually.



* Latest available TOP500 double-precision HPL achieved performance

Software Stack Complexity on Frontier

- Recent projects such as ECP*/E4S* have dramatically increased the amount of available software for large scale computing.
- We maintain a stack of around ~100 packages.
- All these factors combine to create a software stack of combinatorial complexity.



*Exascale Computing Project (ECP)
*Extreme-Scale Scientific Software Stack (E4S)

Difficulties in Deploying Software

Integrating Site and Vendor Modules

- Module files for compilers, MPI and GPU libraries are managed by Cray PE.
- The paths that Spack generates for modules are practically random because of hashes.
- Spack does not support "non-virtual" specs (like ROCm) in the module hierarchy.

Managing Environments in Spack

- Multiple CPE version on the machine at the same time can lead to a BIG spack.yaml file (e.g 1800+ lines).
- Managing transitions to new versions of Spack can cause an environment to become messy.

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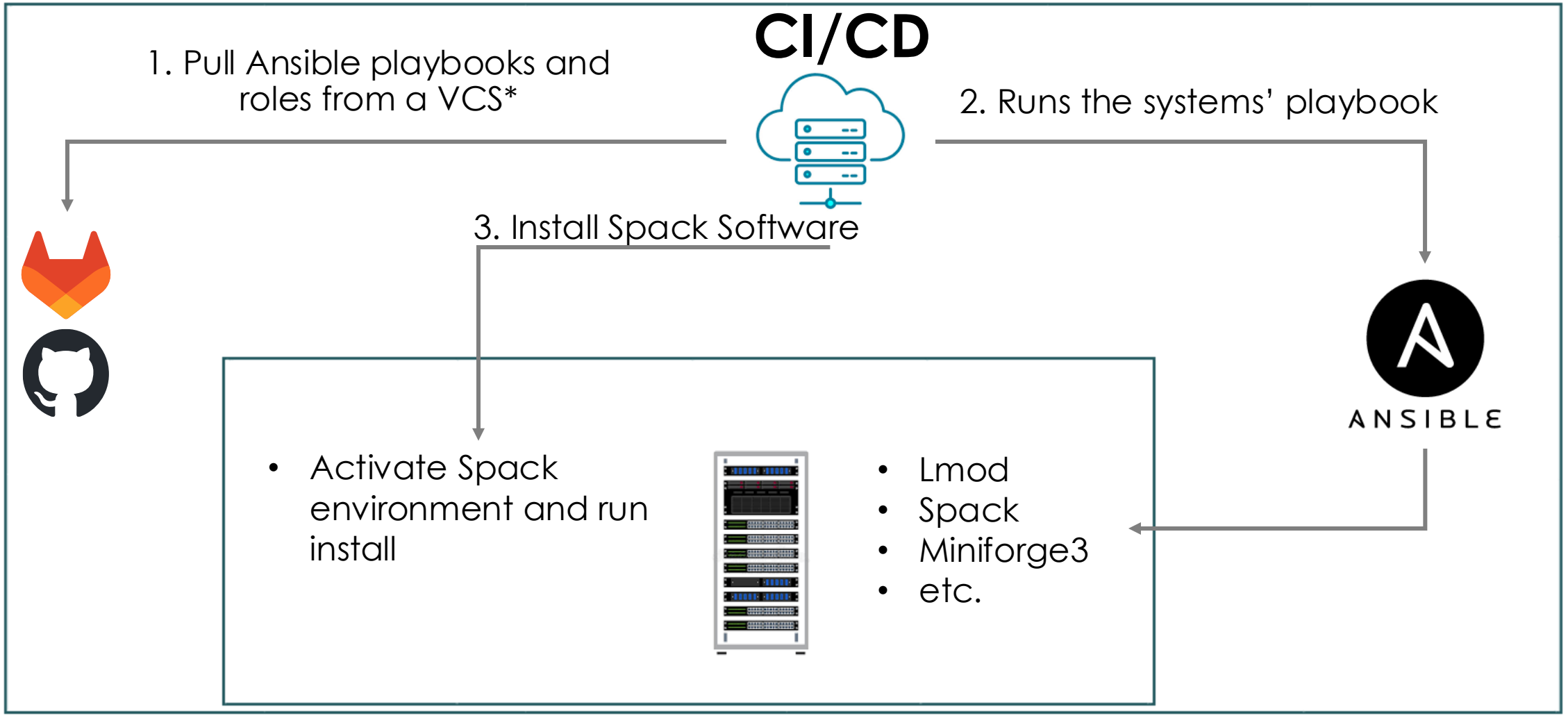
What is NSP?

- A collection of tools and strategies for software stacks.
  - Trackable
  - Reproducible
- Tools:
  - Ansible
  - Spack
  - Lmod
- Strategies:
  - Breaking the software stack into multiple templated Spack environments.
  - Configuring Spack to create custom projections for our module files.
  - Using Lmod hooks to integrate CPE and site modules.

NSP Workflow



*Version Control System

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Ansible Roles and Configuration

NSP Ansible Roles
(Public)

Ansible Playbooks for NCCS Systems
(Private)

```
.
├── ansible.cfg
├── spack
│   ├── defaults
│   ├── meta
│   ├── tasks
│   └── templates
├── lmod
│   ├── defaults
│   ├── meta
│   ├── tasks
│   └── templates
...
```

```
.
├── ansible.cfg -> roles/ansible.cfg
├── odo
│   ├── files
│   ├── playbook.yaml
│   └── spack
├── frontier
│   ├── files
│   ├── init
│   ├── lmod
│   ├── playbook.yaml
│   └── spack
├── README.md
└── roles (.gitmodules)
```


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NSP Ansible Roles

- Install/configure the respective piece of software.
- We ensure that these roles follow certain guidelines such as uniform install prefixes.
- We maintain a variety of roles in ansible.
  - Spack
  - Lmod
  - GCC
  - Miniforge3
  - …

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The Spack & Lmod Roles

Spack

- Clones and patches a version(s) of Spack.
- Renders templated Spack environments.
- Renders a templated help script called "***spacktivate***."
  - Selects the correct version of spack and activates the requested environment.

Lmod

- Implements a hook to dynamically add paths to ***MODULEPATH*** based on the currently loaded modules.
- Implements a custom ***spider*** to show all available Spack built software.
- Logs module usage to an HTTP API end point.

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Templating Spack Environments

```
cray_dyninst: 12.3.4
cray_fftw: 3.3.10.9
cray_hdf5: 1.14.3.3
cray_hdf5_parallel: 1.14.3.3
cray_mrnet: 5.1.4
```

+

```
packages:
  cray-dyninst:
    buildable: false
    externals:
     - spec: cray-dyninst@{{ cray_dyninst }}
       modules:
         - cray-dyninst/{{ cray_dyninst }}
  cray-fftw:
    buildable: false
    externals:
      - spec: cray-fftw@{{ cray_fftw }}
        modules:
          - cray-fftw/{{ cray_fftw }}
```

=

```
packages:
  cray-dyninst:
    buildable: false
    externals:
      - spec: cray-dyninst@12.3.4
        modules:
          - cray-dyninst/12.3.4
  cray-fftw:
    buildable: false
    externals:
      -  spec: cray-fftw@3.3.18.9
        modules:
          - cray-fftw/3.3.18.9
```


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Module Projections

- A module ***projection*** is simply the path to the module file.
  - Built with ***gcc/14.2.0***: /.../gcc-14.2.0/hdf5/1.14.5.lua
  - Built with ***llvm/19.1.1***: /.../llvm-19.1.1/hdf5/1.14.5.lua
- We call this changing part of the projection the ***hierarchy***.
- We generally have three components in our hierarchy.
  - Compiler
  - MPI
  - GPU
- Example: /.../cray-mpich-8.1.31/rocm-6.2.4/cce-18.0.1/amrex/24.05.lua

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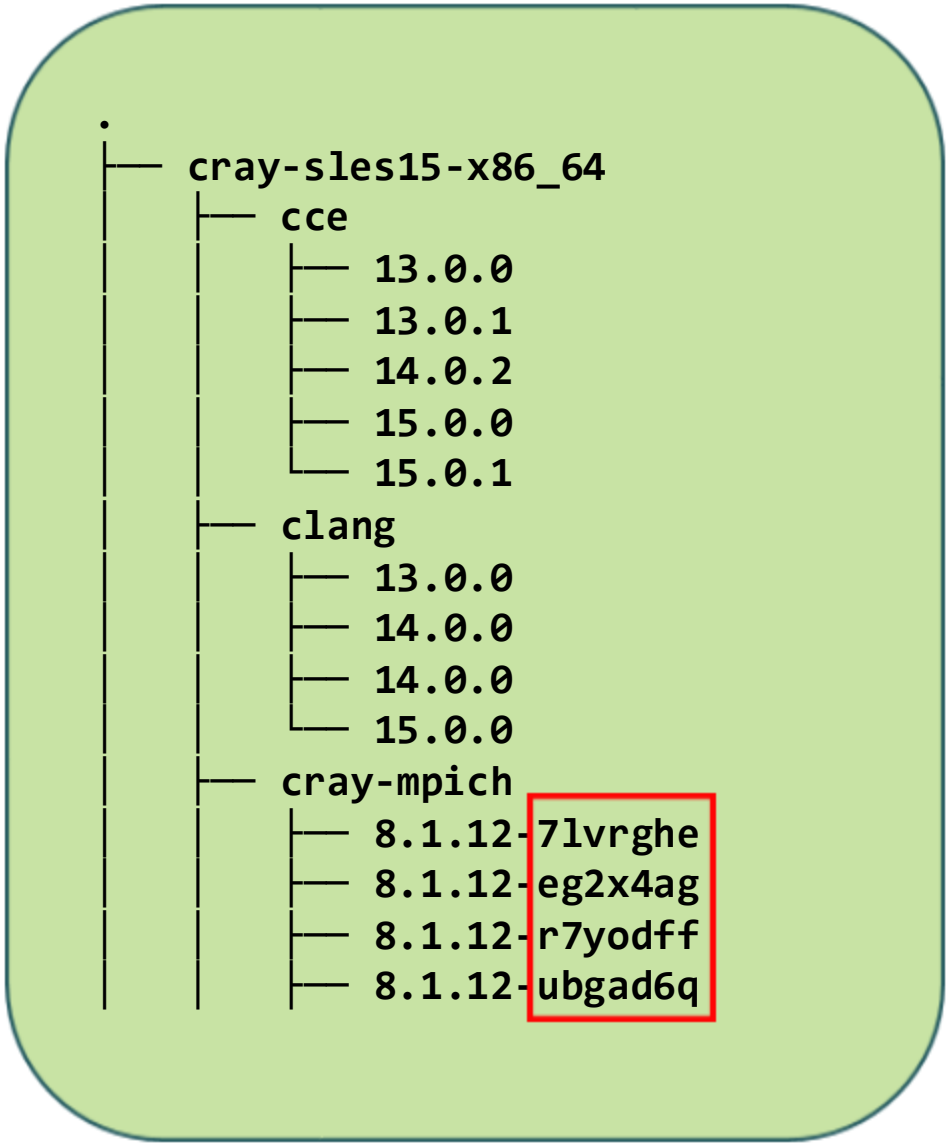
Default Module Projections with Spack

- Spack adds hashes to the module projections (sometimes multiple hashes for the same version of a package).
- Because Spack doesn't generate our cray-mpich modules, all these paths must be added manually as patches to the CPE module files.
- Spack's hierarchy only supports "virtual" packages which excludes ROCm from the hierachy.



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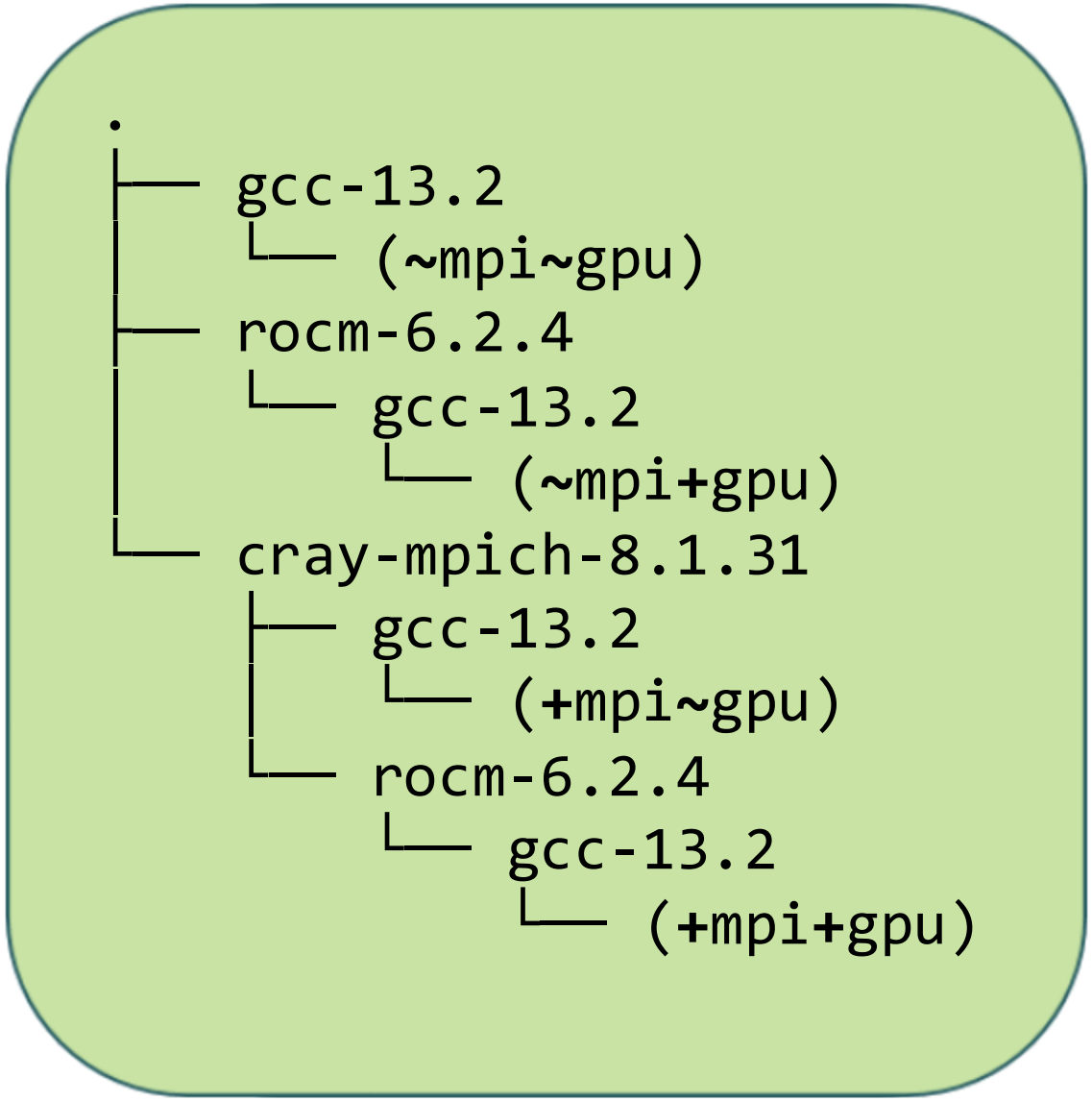
NSP Projections

- NO hashes.
- Paths to modules do not have to be known ahead of time. They can be dynamically constructed.
- ROCm is in the hierarchy.



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Configuring Spack Projections

```
arch_folder: false
lmod:
  all:
    autoload: none
    exclude_implicits: true
  hash_length: 0
  hierarchy:: [ ]
  projections:
    ^llvm-amdgpu ^mpi: "{^mpi.name}-{^mpi.version}/rocm-{^llvm-amdgpu.version}/..."
    ^llvm-amdgpu: "rocm-{^llvm-amdgpu.version}/{compiler.name}..."
    ^mpi: "{^mpi.name}-{^mpi.version}/{compiler.name}-{compiler.version}/..."
    all: "{compiler.name}-{compiler.version}/{name}/{version}"
```


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Lmod Hooks

- A ***hook*** is a function that is called at a specific point in Lmod's execution (e.g. the ***load*** hook is called whenever a module is loaded).
- Hooks are stored in a file called ***SitePackage.lua***.

```
local Hook = require("Hook")

function my_hook(t)
    -- do something
end

Hook.register("load", my_hook)
```

- The location of this file can be set with ***LMOD_PACKAGE_PATH***.

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Configuring the NSP Hook

- The NSP hook watches for changes in modules and add/removes paths to Spack built modules based on the provided path projections.

```
NSP_LMOD_spack_modules: "{{ path to spack modules }}"
NSP_LMOD_hierarchy:
    compiler:
        members: [ 'cce', 'amd', 'gcc-native' ]
        paths:
            - { path: '|compiler.name|-|compiler.version|', weight: 20 }
            - { path: '|mpi.name|-|mpi.version|/|compiler.name|-|compiler.version|', weight: 30 }
            - { path: '|gpu.name|-|gpu.version|/|compiler.name|-|compiler.version|', weight: 40 }
    gpu:
        members: [ 'rocm' ]
        paths:
        ...
    mpi:
        members: [ 'cray-mpich' ]
        ...
NSP_LMOD_nv_mappings:
    # '%s' substitutes in the value provided by the module
    amd/6.2.4: { name: 'rocmcc', version: '%s' }
    gcc-native/13.2: { name: 'gcc', version: '%s' }
```


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Integrating Spack Modules into `module spider`

- Dynamic additions to ***MODULEPATH*** do not allow Lmod to track ***ALL*** available modules.
- We wrote a custom spider command integrated into Lmod (via a Hook).
  - Uses the default spider method to generate a cache of all non-Spack installed software.
  - Crawls our Spack installed software to generate an additional cache.
  - Combines the two caches and prints out the requested info to the user.

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NSP Take Aways

- Ansible
  - Template configuration files (especially Spack config files).
  - Track changes to system playbooks through version control.
  - Dramatically improves the ease of reproducing a software stack!
- Spack
  - Break software stacks into multiple environments.
  - Leverage projections to create a custom module layout.
- Lmod
  - Use hooks to create a responsive module environment integrating site and vendor modules.

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Questions?

- GitHub: https://github.com/olcf/nccs-software-provisioning
- Docs: https://olcf.github.io/nccs-software-provisioning
- Email: rentschleraj@ornl.gov

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