



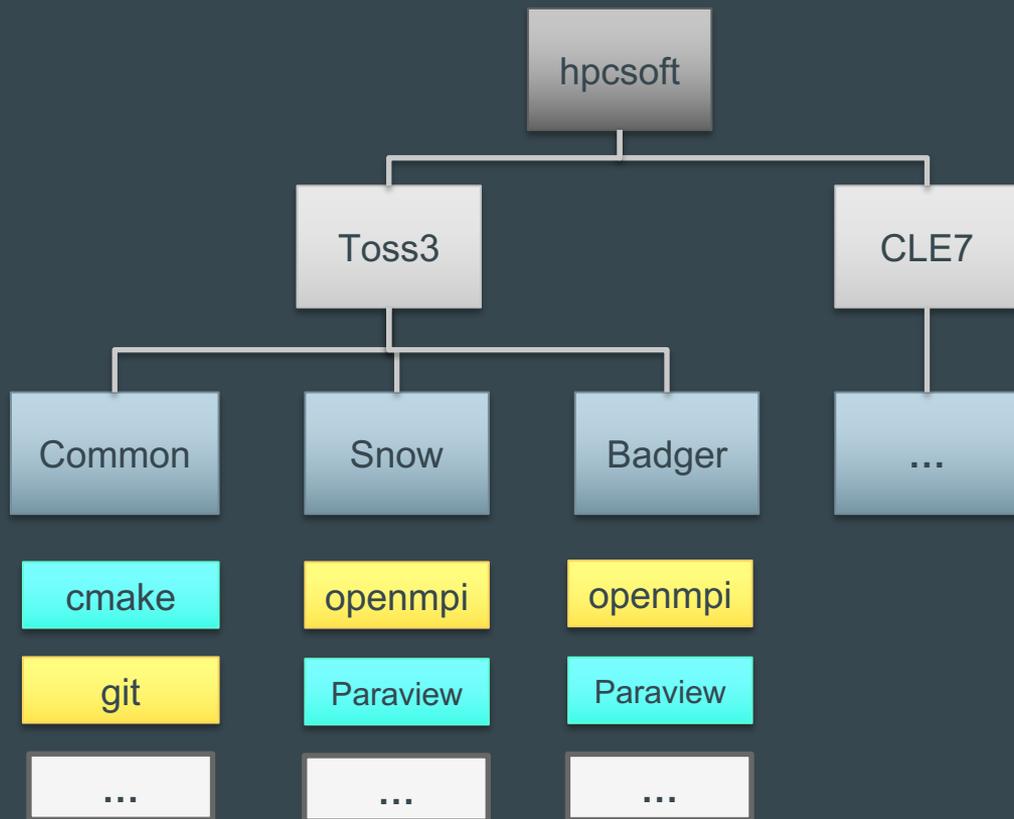
# Spack Based Production Programming Environments on Cray Shasta



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# Old Deployment Method

# Legacy Software Stack

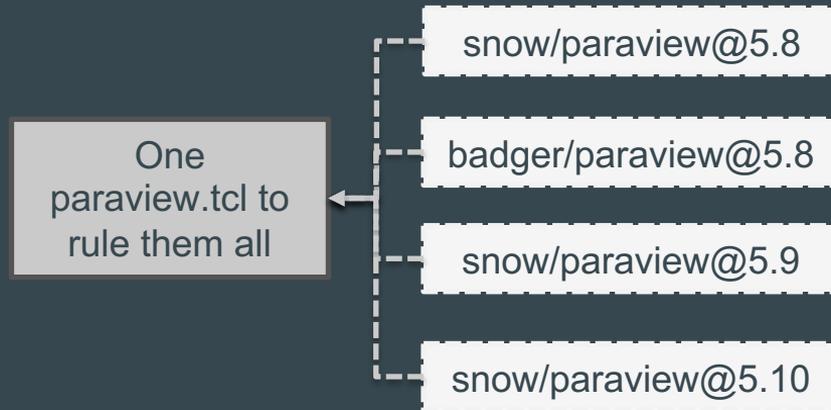


- Per cluster/OS builds
- One owner per product
- Per-product install scripts
- Install areas were a mess
- No Inventory

Paul Managed

Shivam Managed

# Legacy Software Management



# Needs software deployment system

- Build from source against system dependencies
  - One common install 'language'
  - Eliminate 'siloing'
  - Long Term Support – *Life of the machine*
  - Shared installs where possible
- Install from Inventory
- Reproducibility
- Combinatorial Installs
- Auto-generate module files
- Efficient
- Save FTE Hours



*# Spack Has Entered The Chat*

[spack.readthedocs.io](https://spack.readthedocs.io)

# Spack (in no particular order)

- Non-privileged package management tool
- Large HPC focused package library
- Uses YAML for config files
- Widespread adoption

# TCE2 (process.sh)

```
./bin/process.sh  
-f lanl  
-e cray-sles15-x86_64_v3-slingshot-none  
-i /usr/projects/hpcsoft/tce/23-03  
-m
```

# TCE2 (process.sh)

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./bin/process.sh
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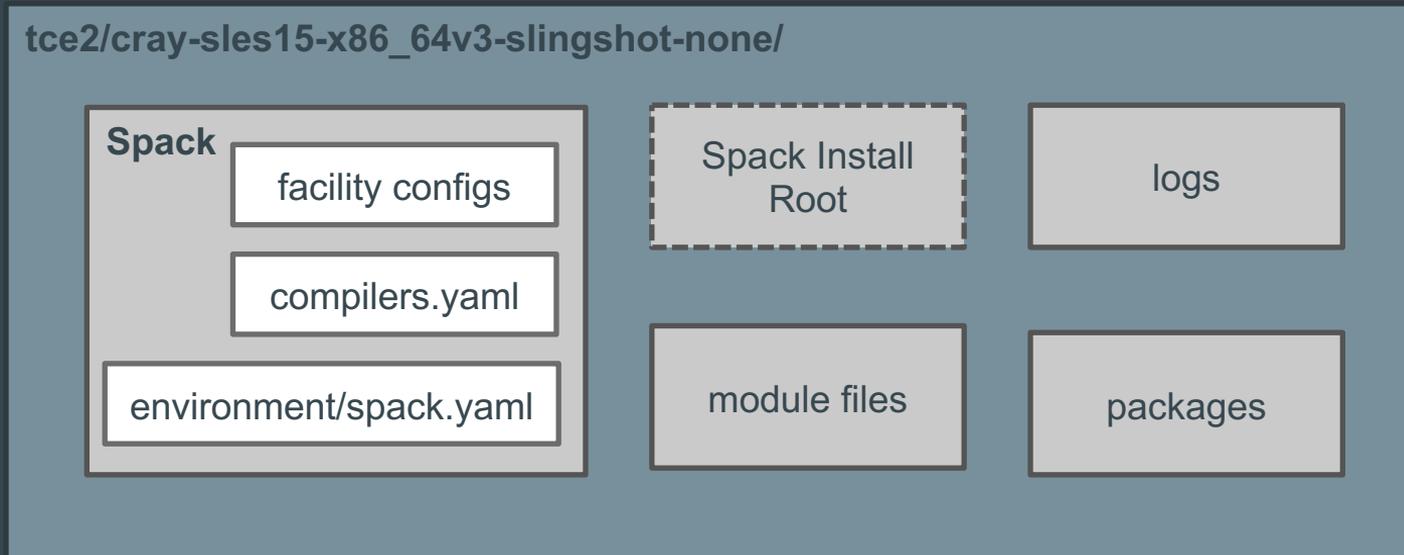
Facility

Environment

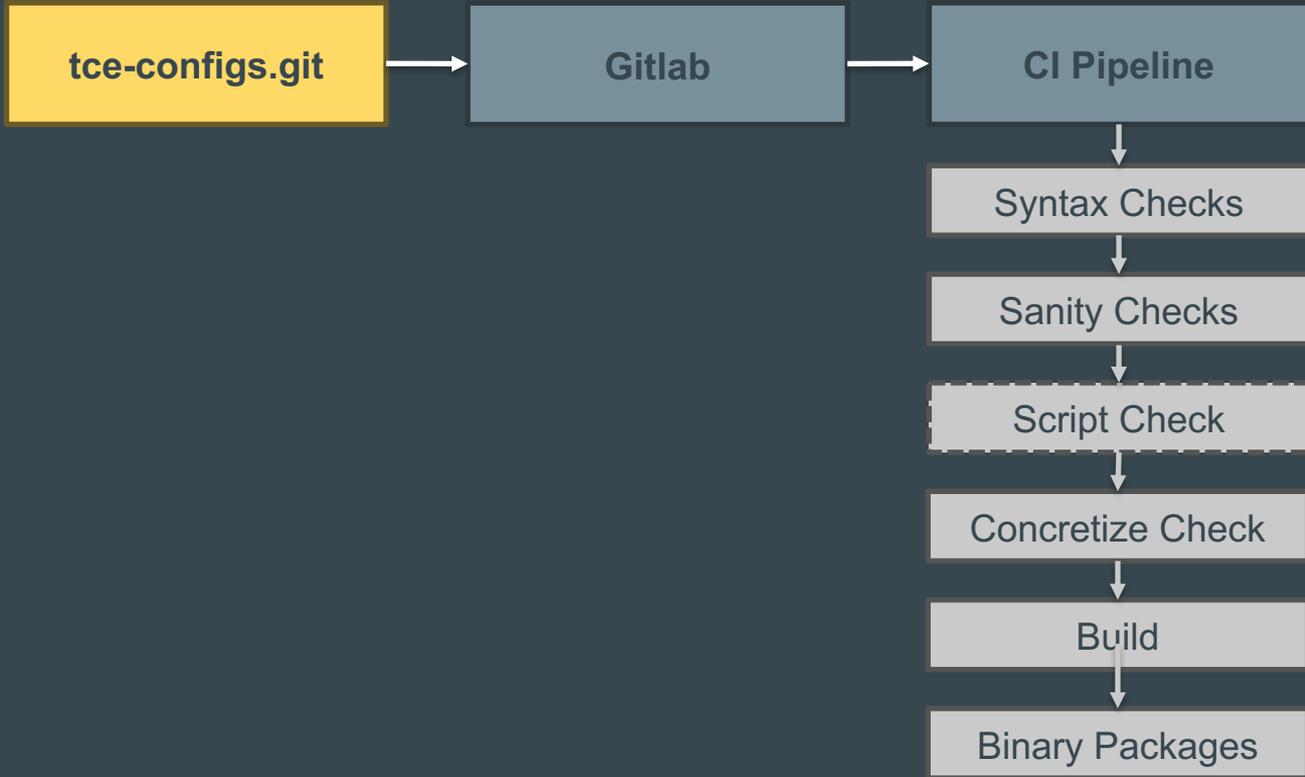
Install  
Path

Module  
Generation

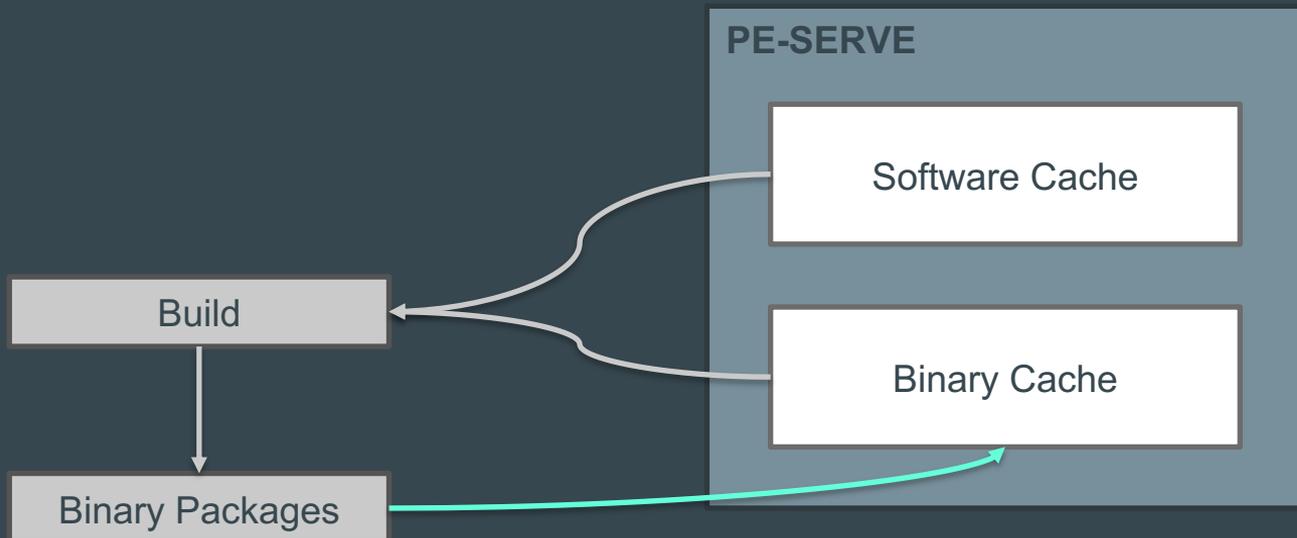
# Install Layout



# CI



# Caching



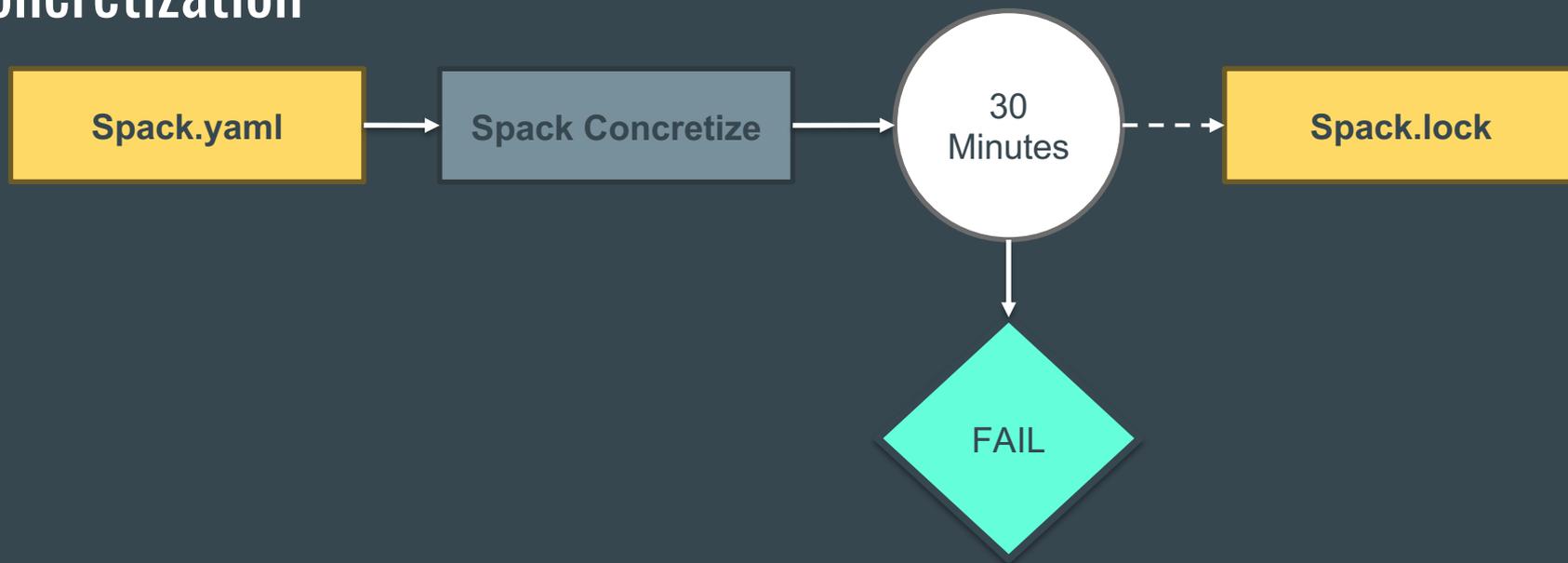
# Spack Install just works

- ‘spack install foo’
  - Given access to source
  - And able to bootstrap
- Well, 95% of the time.

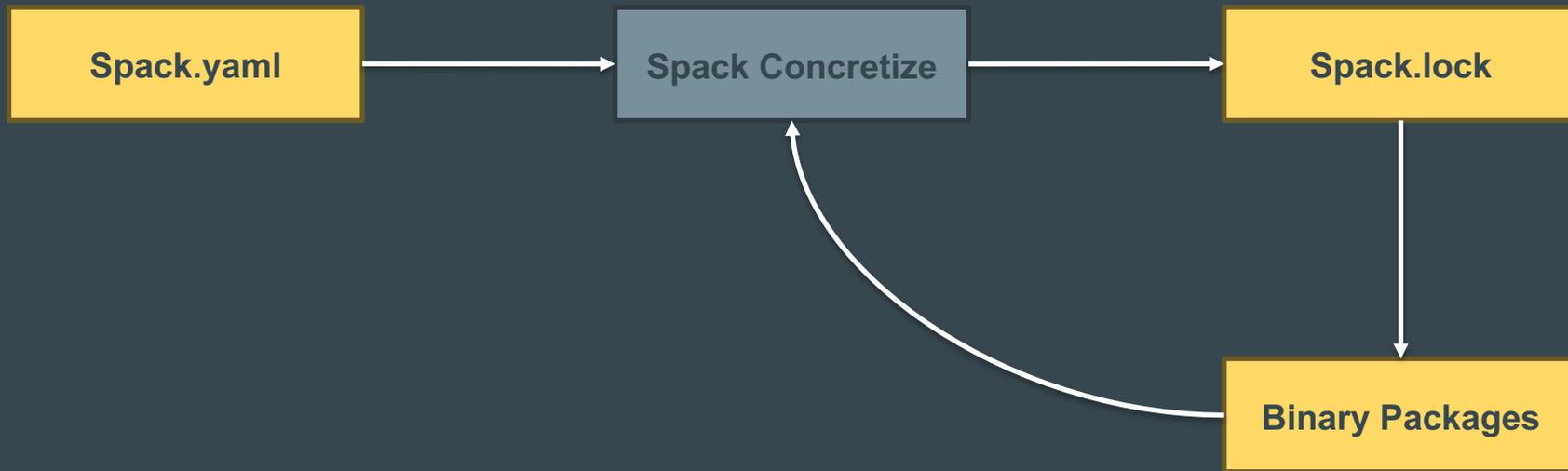
# 5% of 300 builds is 15 failures

- What then?
  - `spack build-env mypackage bash`
    - Play around in the build environment
- BUT...
  - There is no ‘mypackage’ spec
  - It’s really ‘`mypackage@5.1.2%gcc@10.2.0 ^somedep%gcc@10.2.0 ^somevariant ~othervariant ...`’
    - As defined by the `spack.yaml`
    - With no way to concisely express it.
- So really, it’s
  - `pushd /tmp/bob/spack-stage/spack-stage-mypackage-91827341234/`
  - `source spack-build-env.txt spack-build-env-mods.txt`
  - Then debug.

# Concretization

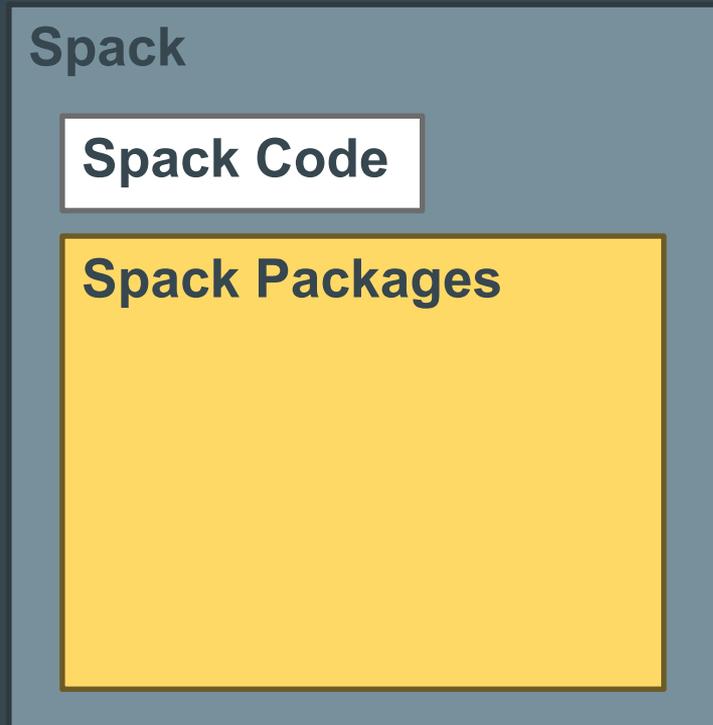


# Concretization (reuse)



# Spack Version Upgrades

- Code upgrades
  - Mostly fine
  - Largely retains backwards compatibility
  - Generally makes things better.
- Package upgrades
  - No compatibility guarantees
    - Variant changes
    - Paradigm changes
  - New Bugs
  - New dependencies
  - Generally a nightmare



# Release Model Options

## Monolithic Spack.yaml

- All new software added to one continuous version
- Spack concretization times grow unchecked
- Massive amount of issues switching Spack Versions

## Spack.yaml 2023-03

- Periodic, small releases
- Concretize separately
- Separate Environment

## Spack.yaml 2023-09

## Spack.yaml 2024-03

## Merged Environment

- Shared Spack
- Shared Installs



**Hewlett Packard**  
Enterprise

*# HPE Cray OS Has Entered The Chat*

[www.hpe.com](http://www.hpe.com)

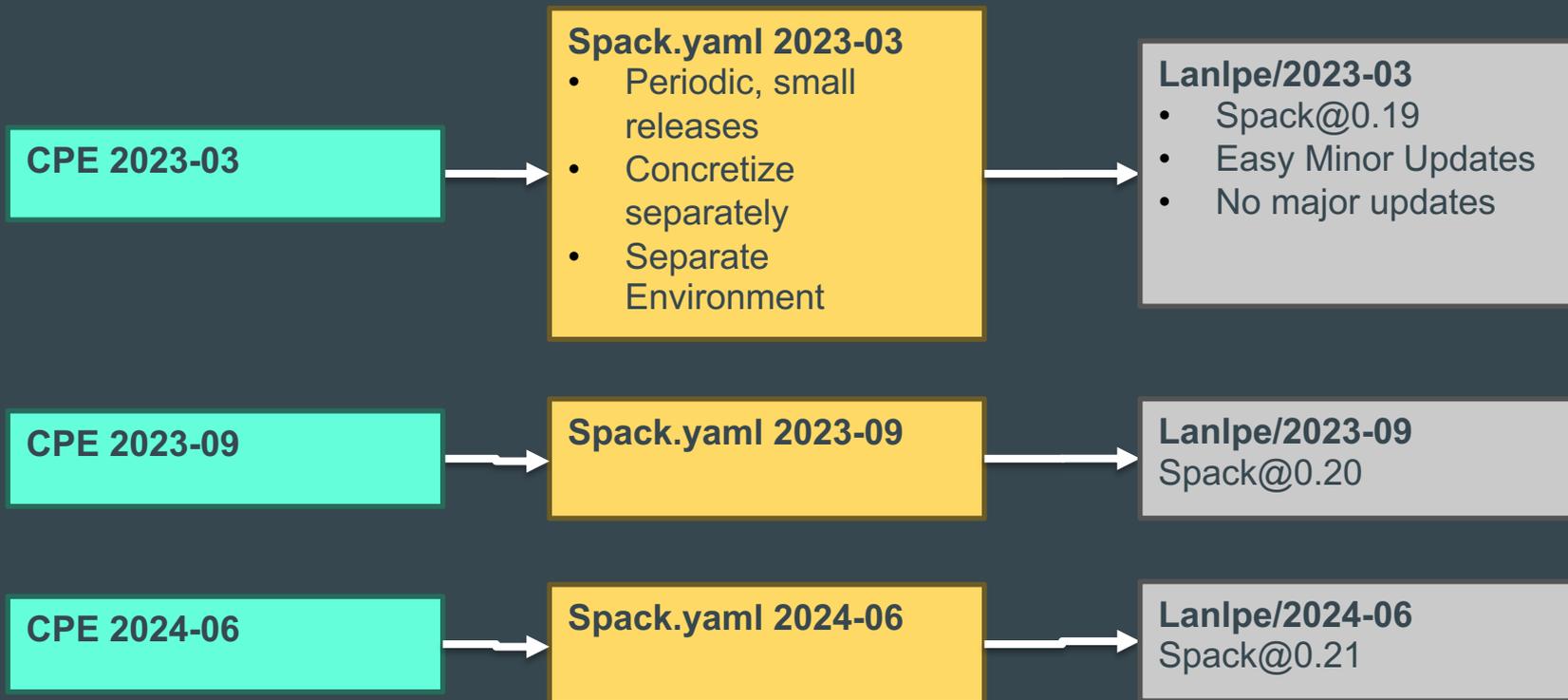
# HPE Cray OS (the relevant bits)

- HPE Cray Programming Environment
  - Communication/scientific/IO libraries
  - Compiling/programming environments
  - Performance analysis tools
  - Debuggers

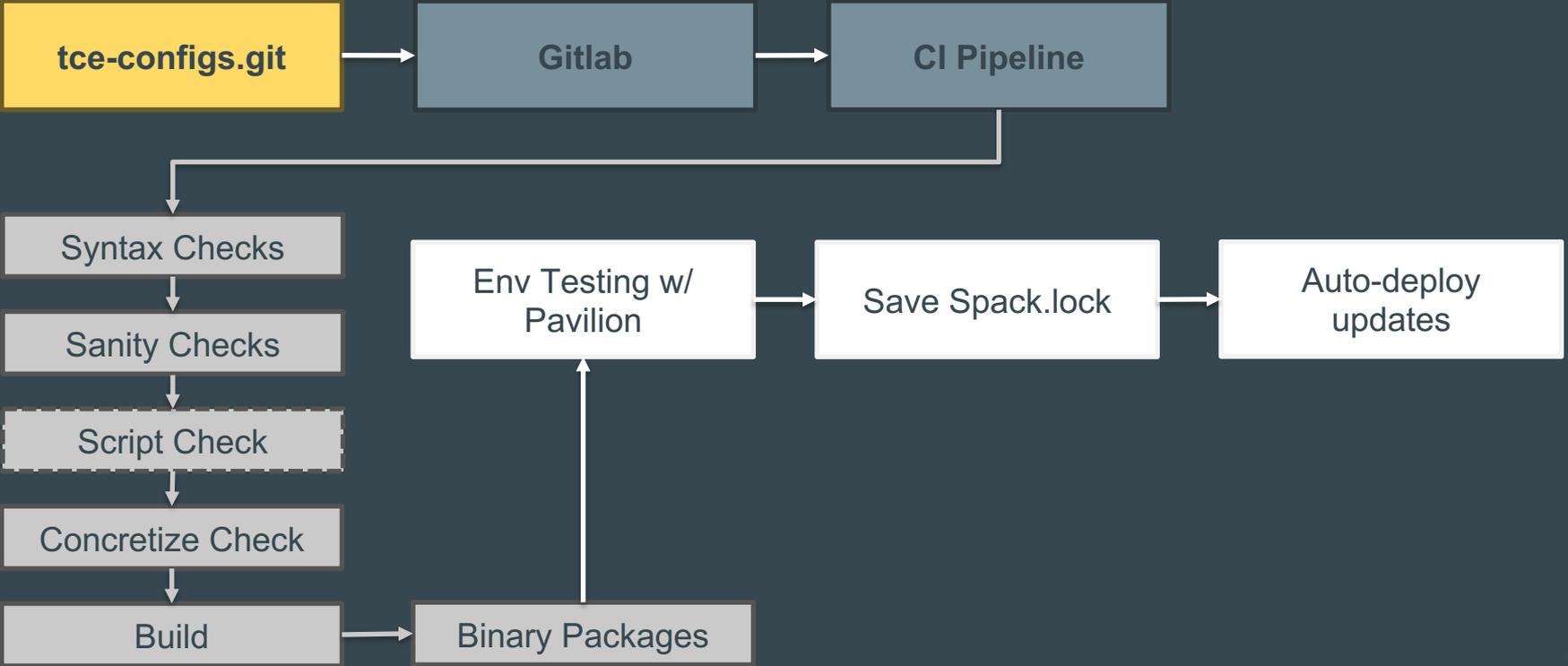
# Cray Problems

- Spack and hierarchical Lmod don't get along
  - 'spack compiler find' doesn't quite work
  - Externals based on modulefile *REALLY* don't work.
- Fixes to Cray Issues take many months.
  - Take longer to figure out (without cray-mpich source)
  - Ticket turnaround time
  - Fixes then wait on next CPE release
  - Or worse, the next CSM install

# TCE2 on Cray Release Model



# Next Steps



# Conclusion

- Spack conversion has been costly
- Upgrades are worth it
  - Team structure – anyone can add new/support packages
  - Modernized Infrastructure
  - Can support more for users
    - New Cray clusters require more software support

# Acknowledgements

- Nick Sly
  - Most of the original TCE2 work
  - Generally great guy
- LLNL Spack Team
  - Greg Becker especially
- Jen Green
  - Abandoned us to our fates

# Citations

- Spack Documentation
  - <https://spack.readthedocs.io/en/latest/>
- HPE Cray OS Software
  - [https://www.hpe.com/psnow/doc/a50002722enw?jumpid=in\\_lit-psnow-red](https://www.hpe.com/psnow/doc/a50002722enw?jumpid=in_lit-psnow-red)
- TCE2 Github\*
  - <https://github.com/hpc/tce-configs>

\* behind current internal gitlab repository