



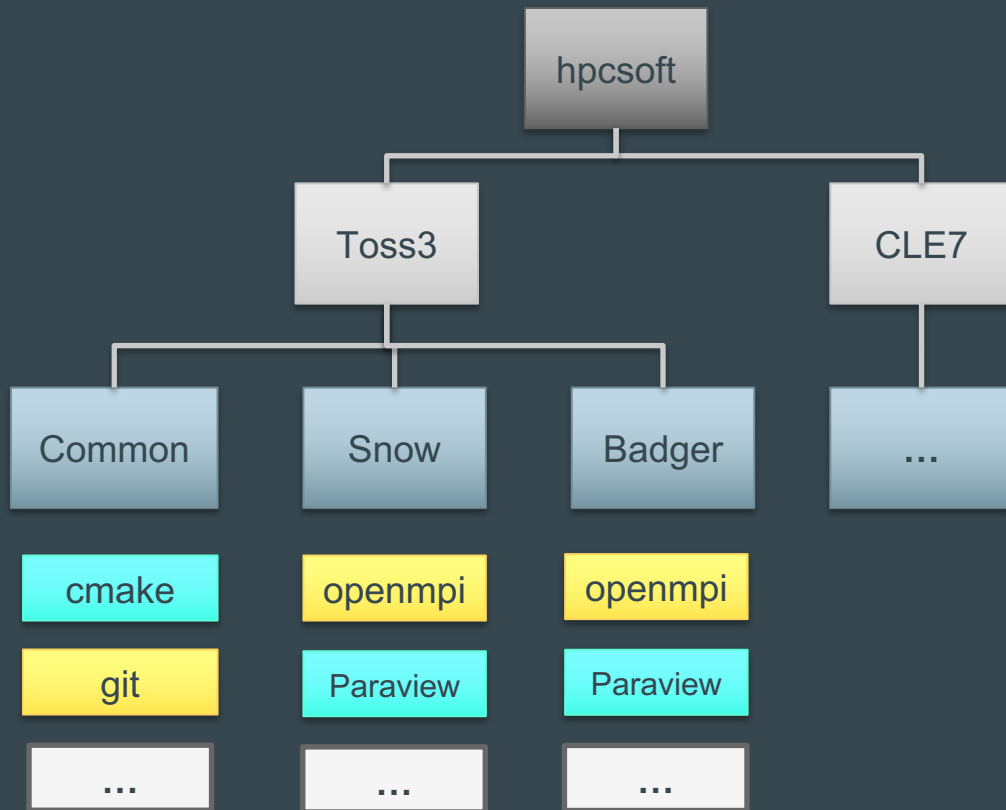
Spack Based Production Programming Environments on Cray Shasta



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Old Deployment Method

Legacy Software Stack

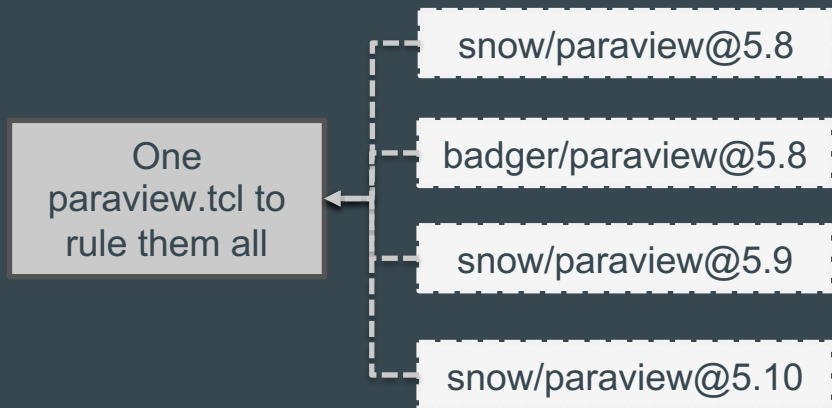


- Per cluster/OS builds
- One owner per product
- Per-product install scripts
- Install areas were a mess
- No Inventory

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

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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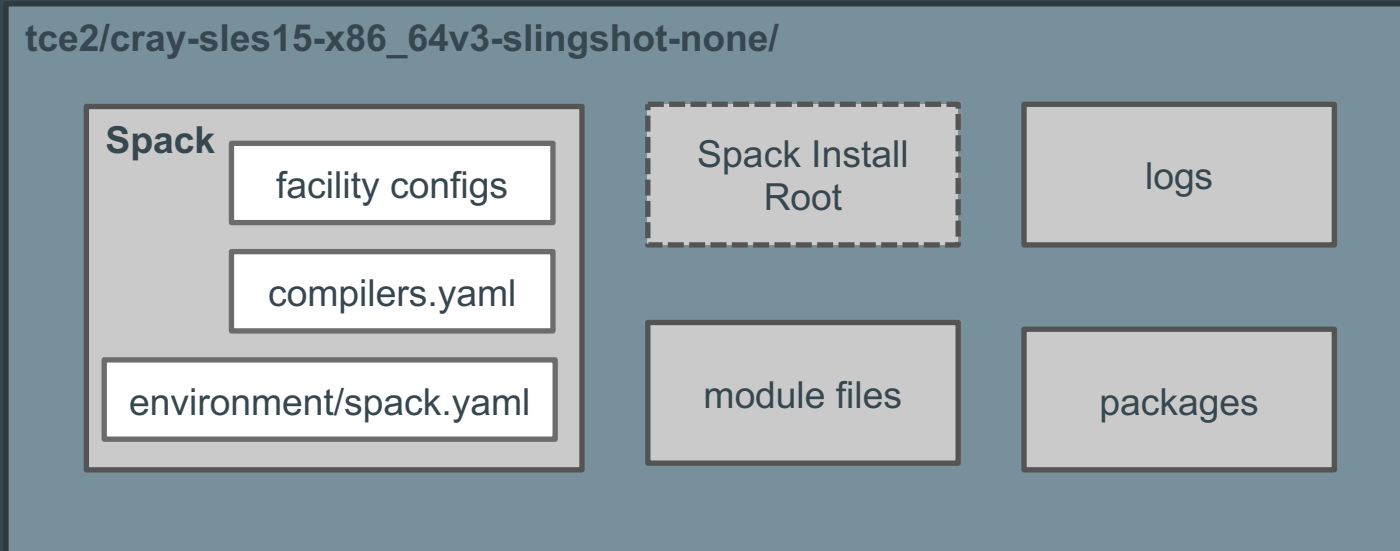
Facility

Environment

Install
Path

Module
Generation

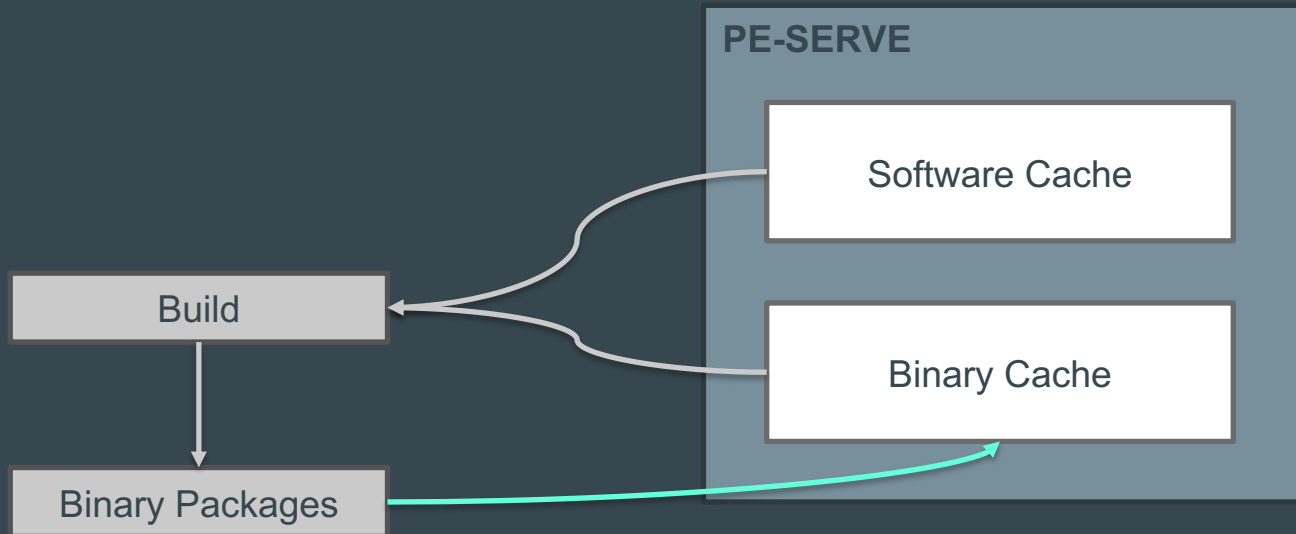
Install Layout



CI



Caching



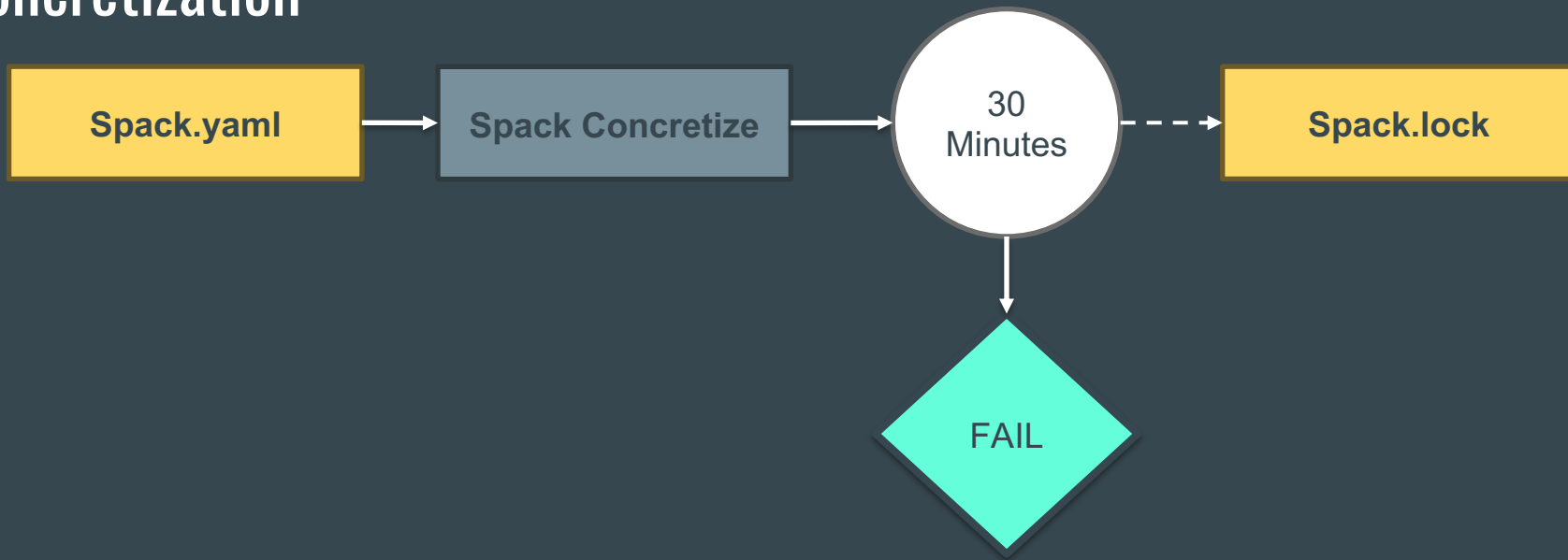
Spack Install just works

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

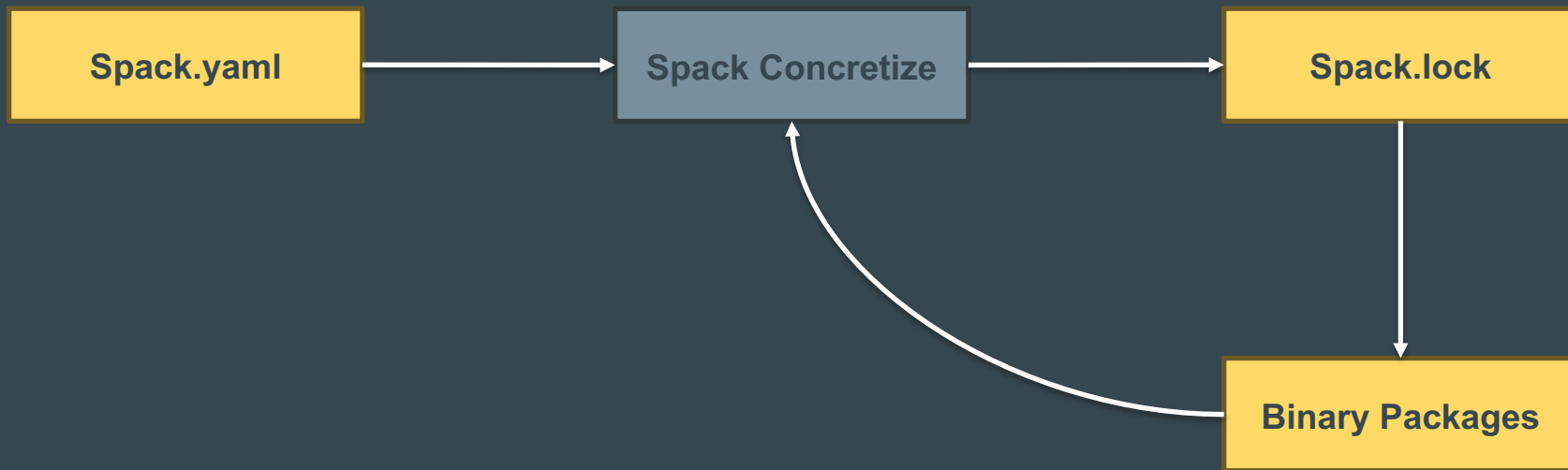
5% of 300 builds is 15 failures

- 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

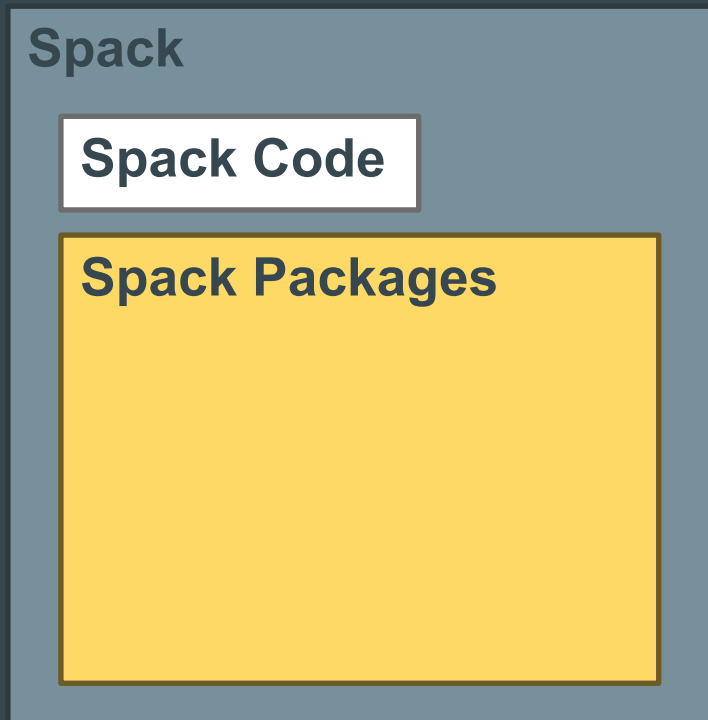


Concretization (reuse)



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

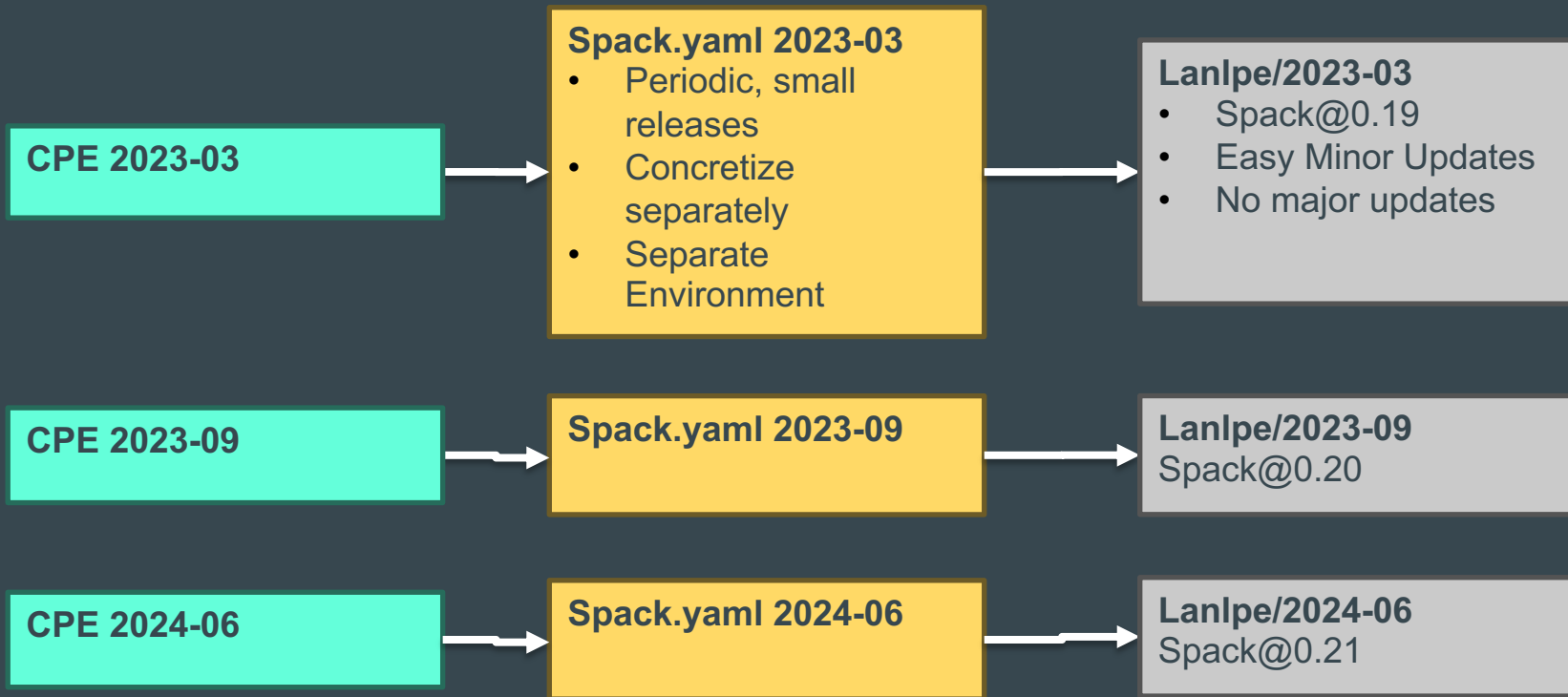
HPE Cray OS (the relevant bits)

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

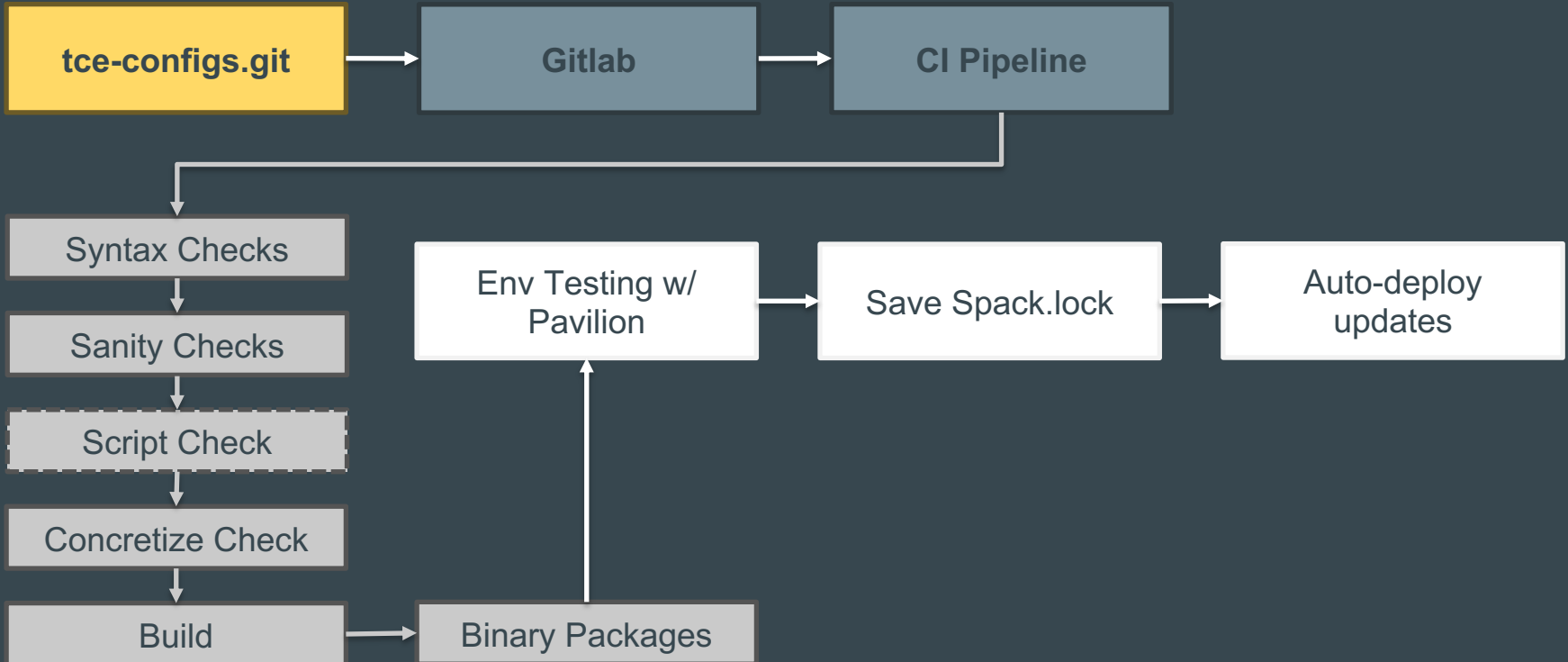
Cray Problems

- 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
- TCE2 Github*
 - <https://github.com/hpc/tce-configs>

* behind current internal gitlab repository