Towards Reproducible Research on CyberGISX with Lmod and Easybuild

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Gateways 2021
October 19-21, 2021

CyberGISX

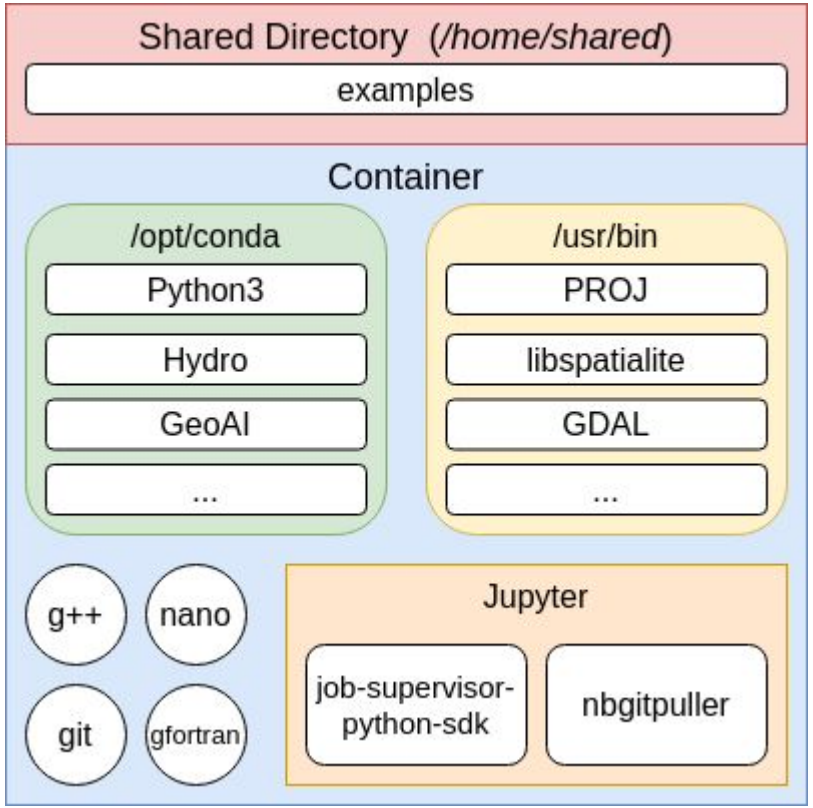
CyberGISX is a Jupyter-based science gateway targeted at the GeoSciences.

https://cybergisxhub.cigi.illinois.edu/

Our Previous Solution

Everything in one container

7.66GB compressed
22.4GB uncompressed



Updating our Compute Environment

Any kind of update or upgrade to our compute environment:

- Led to a rebuild/reinstall of some proportion of the software
- Old versions of software are no longer available in our compute environment.

Binder

Binder could alleviate some of the problem, but:

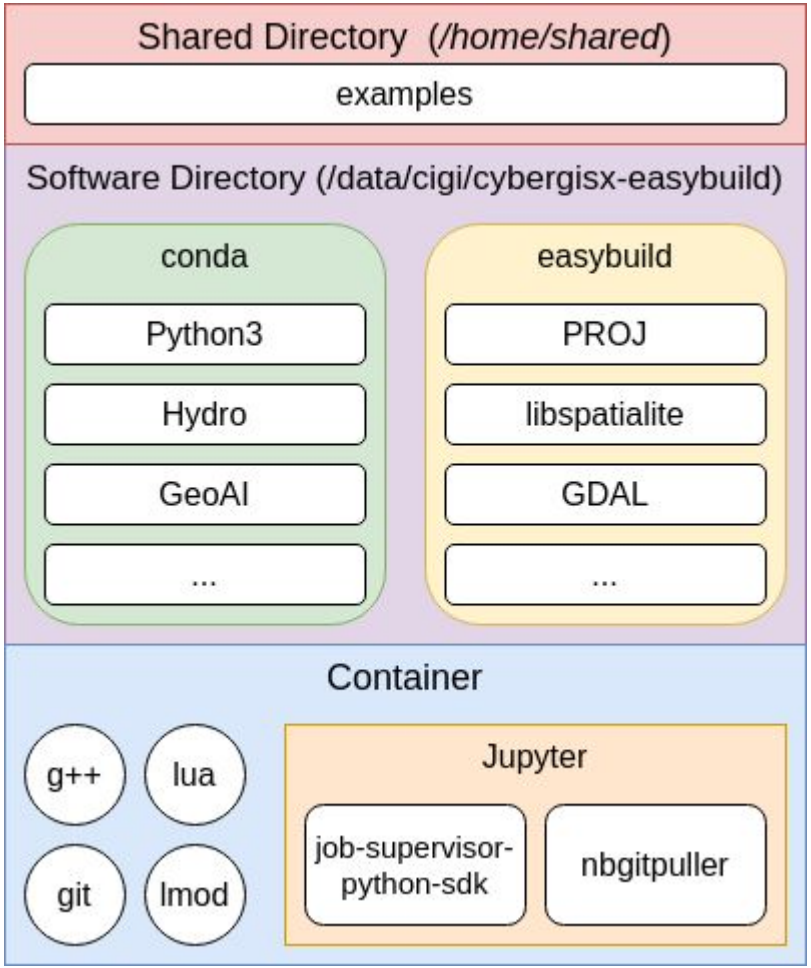
a. software is built at the time it is needed
b. the onus of specifying and managing software installations is passed to notebook developers

https://mybinder.org/

Our New Approach

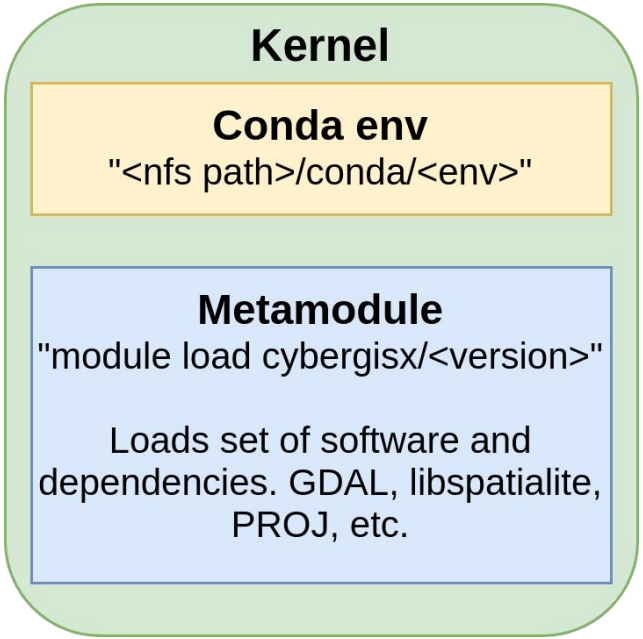
Compute environment software is moved outside of the container. To do this, we utilize:

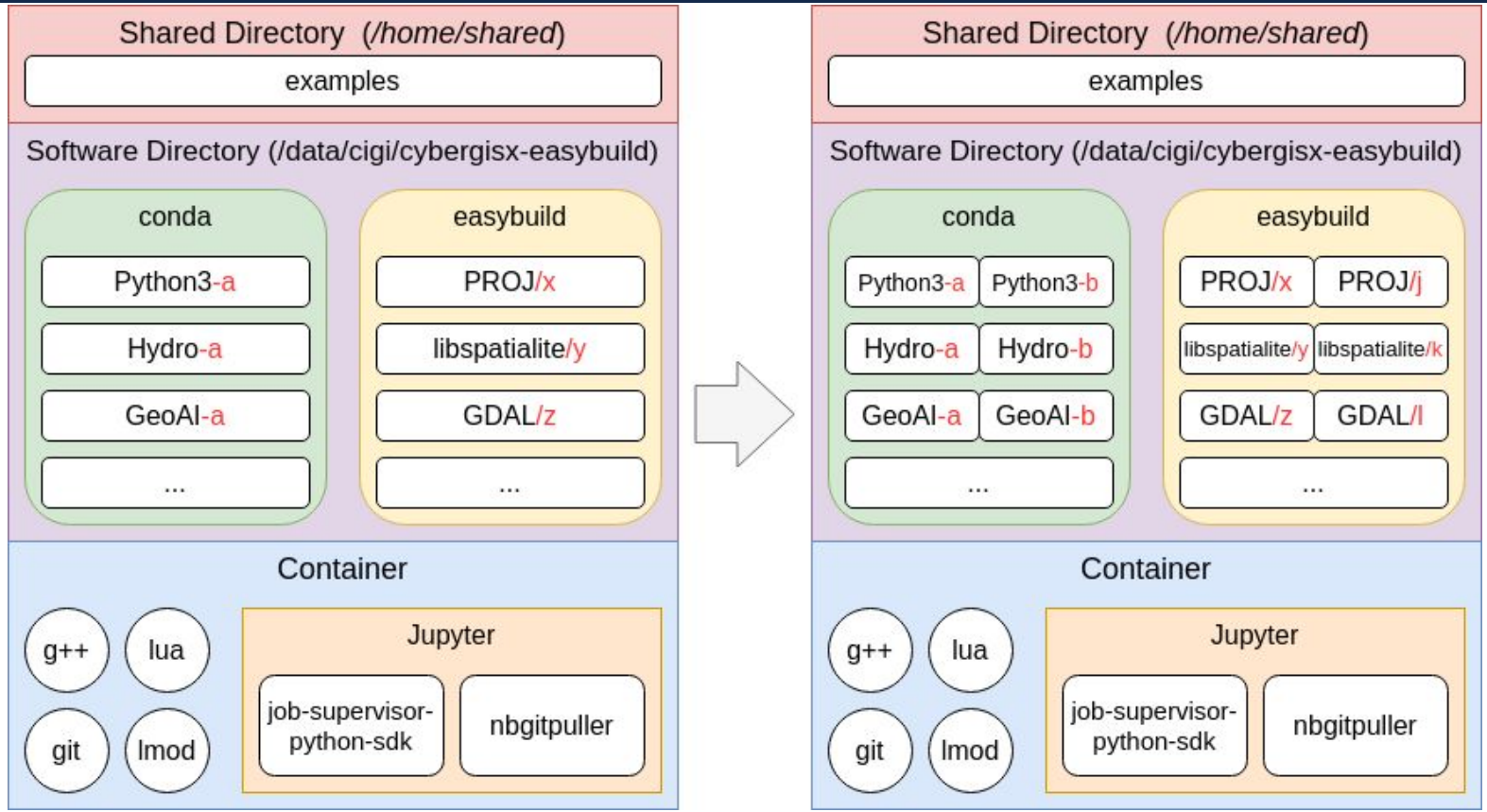
- **Easybuild** - to build software and provide use with modulefiles
- **Lmod** - for users to manage software
- **Conda** - for Python environments



Kernels in the New Approach

The specifications for kernels are given by a JSON file and a script which runs before the kernel is started.





Updating in Our New Approach

User Experience

We have had this approach deployed for over a month on CyberGISX and its sister platform CyberGIS-Jupyter for Water (CJW), with minimal issues.

The average user doesn't know anything changed.

Accessing/managing "old" versions adds a bit of complexity. CyberGISX CLI designed to alleviate this, but more work needs to be done.

Future Work

- User Experience
- Scalability concerns
- Availability outside of the gateway

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Questions?

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