Deploying Community Codes

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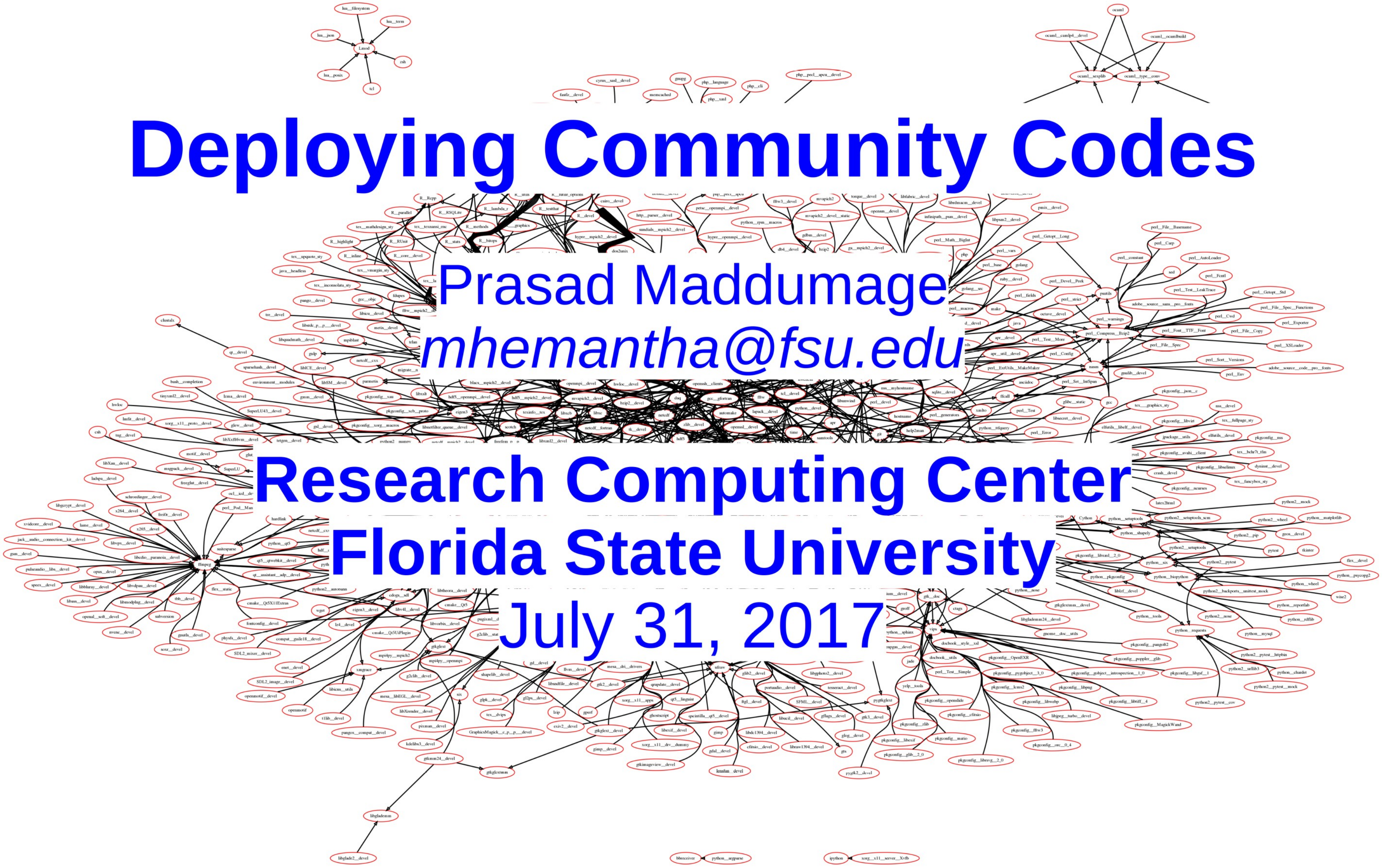


Overview

- What are community packages?
- Who installs what?
- How to compile and install?
  - Dependency hell
- Setup at FSU RCC
  - Where to install?
- Using RPMs vs regular install
  - Getting RPMs
  - How to build an RPM
- Automated package building
  - EasyBuild
  - Spack

What are community packages?

- Libraries
  - Scalapack (linear algebra routines)
  - SuperLU (solving sparse matrices)
- Languages
  - Python (2 and 3)
  - R (several versions per year)
  - Julia (relatively new yet powerful)
- Software packages
  - LAMMPS (molecular dynamics simulation)
  - TopHat (RNA sequencing)

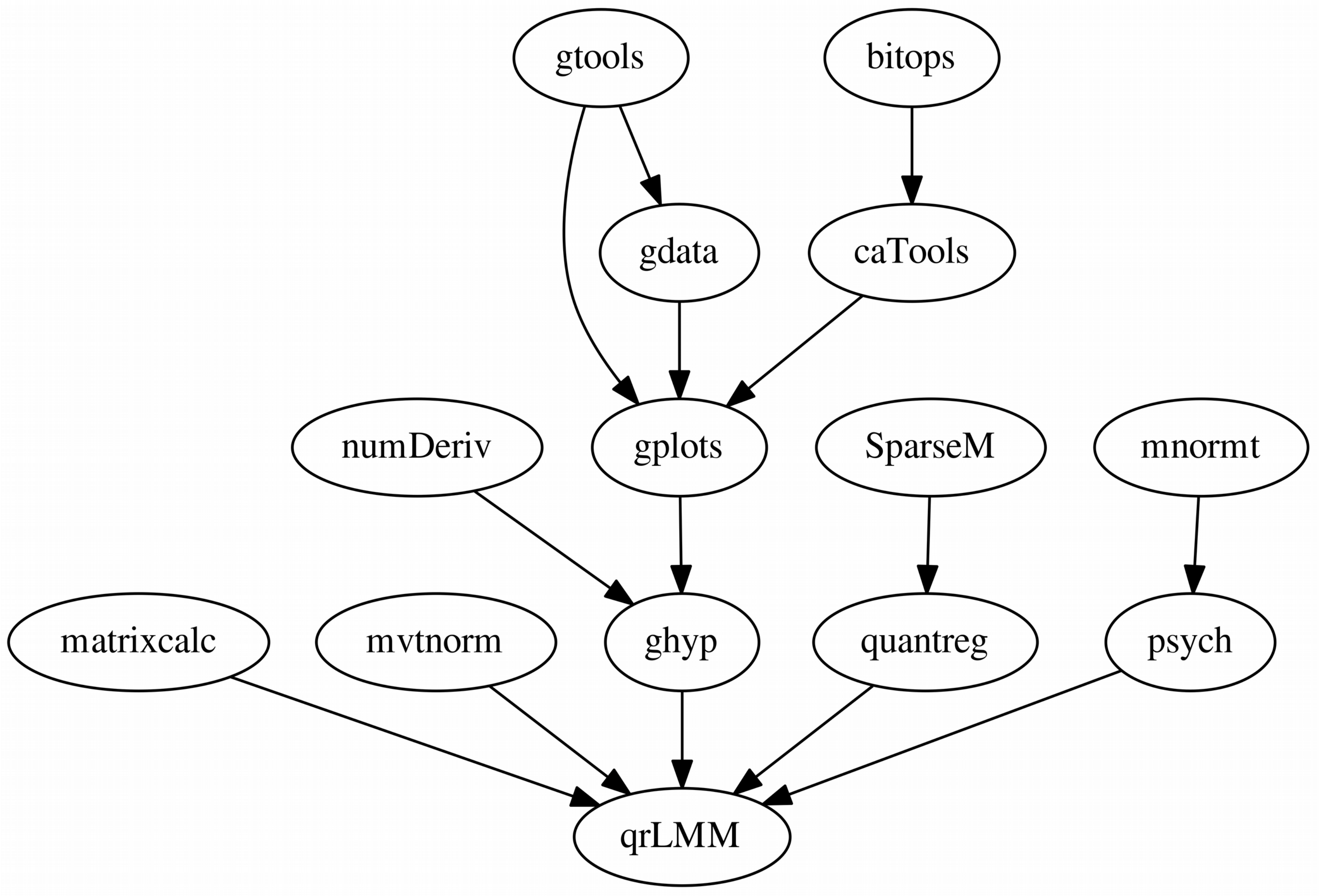
Who Installs What?

- Two policies
  - Administrators install the basics and users install packages on their home directories
    - Cluster maintenance is relatively simple
    - User support could become complicated
  - Support staff install packages system-wide for users
    - Cluster upgrades and maintenance is complicated
    - Eliminates most package install and version related issues

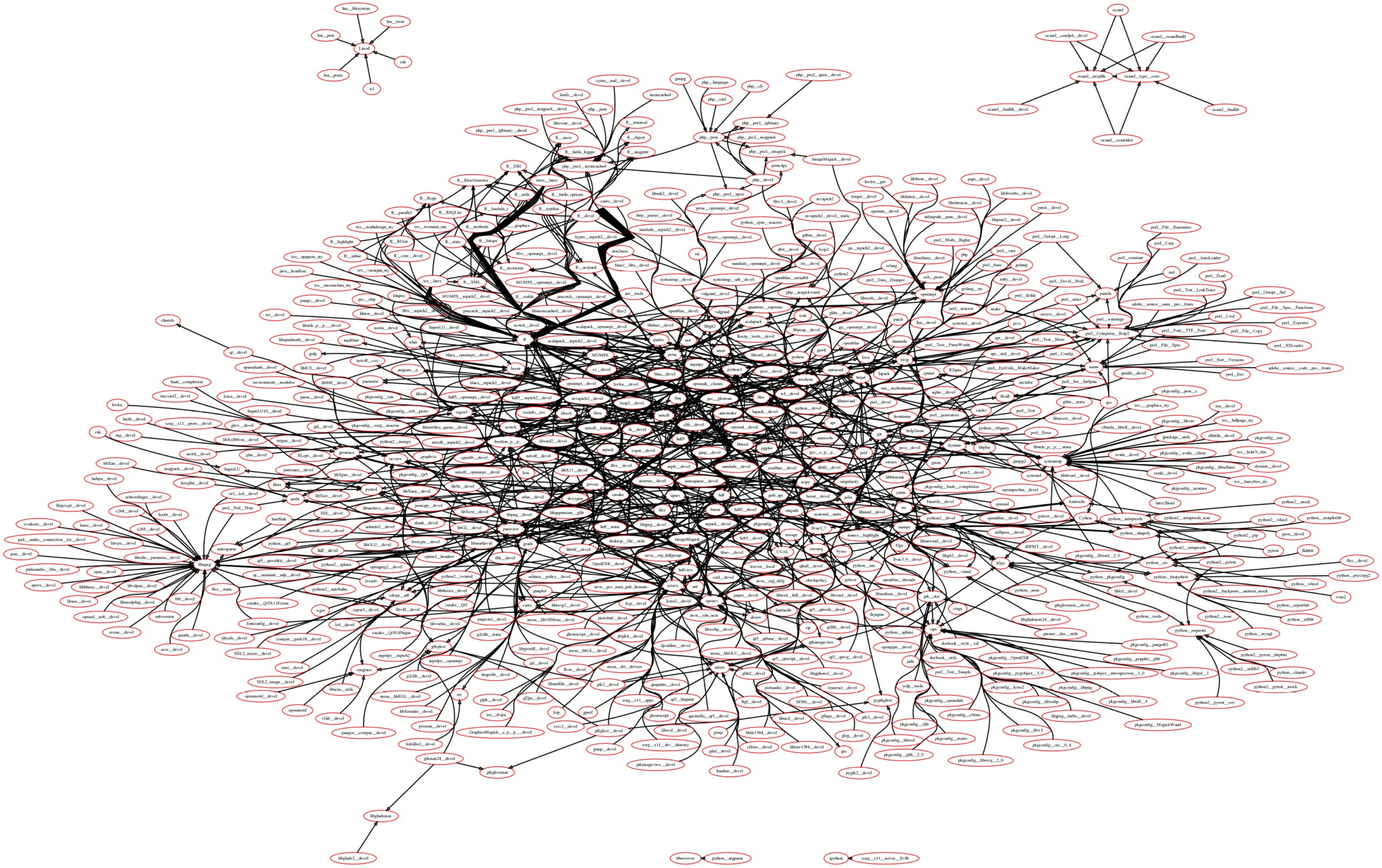
How to compile and install?

- `configure/cmake`, `make`, `make install`
  - Most packages install this way
  - Best if only had to do once
  - `cmake` offers many configuration options
  - May need lot of researching (Google) to find best options
- Binaries from the developer
  - No need to compile
  - Library version incompatibilities (eg: `boost`)
  - Only use if source is not available
- Use RPMs (on RHEL and CentOS)

Dependency hell



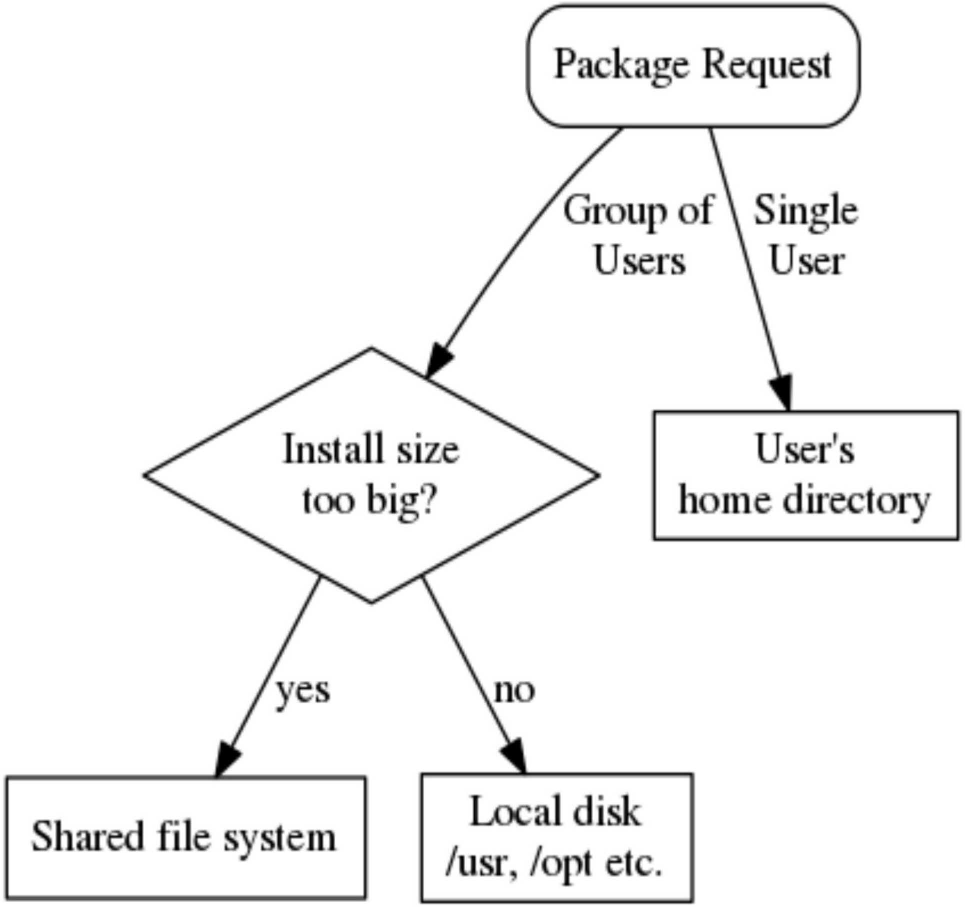
Dependency hell



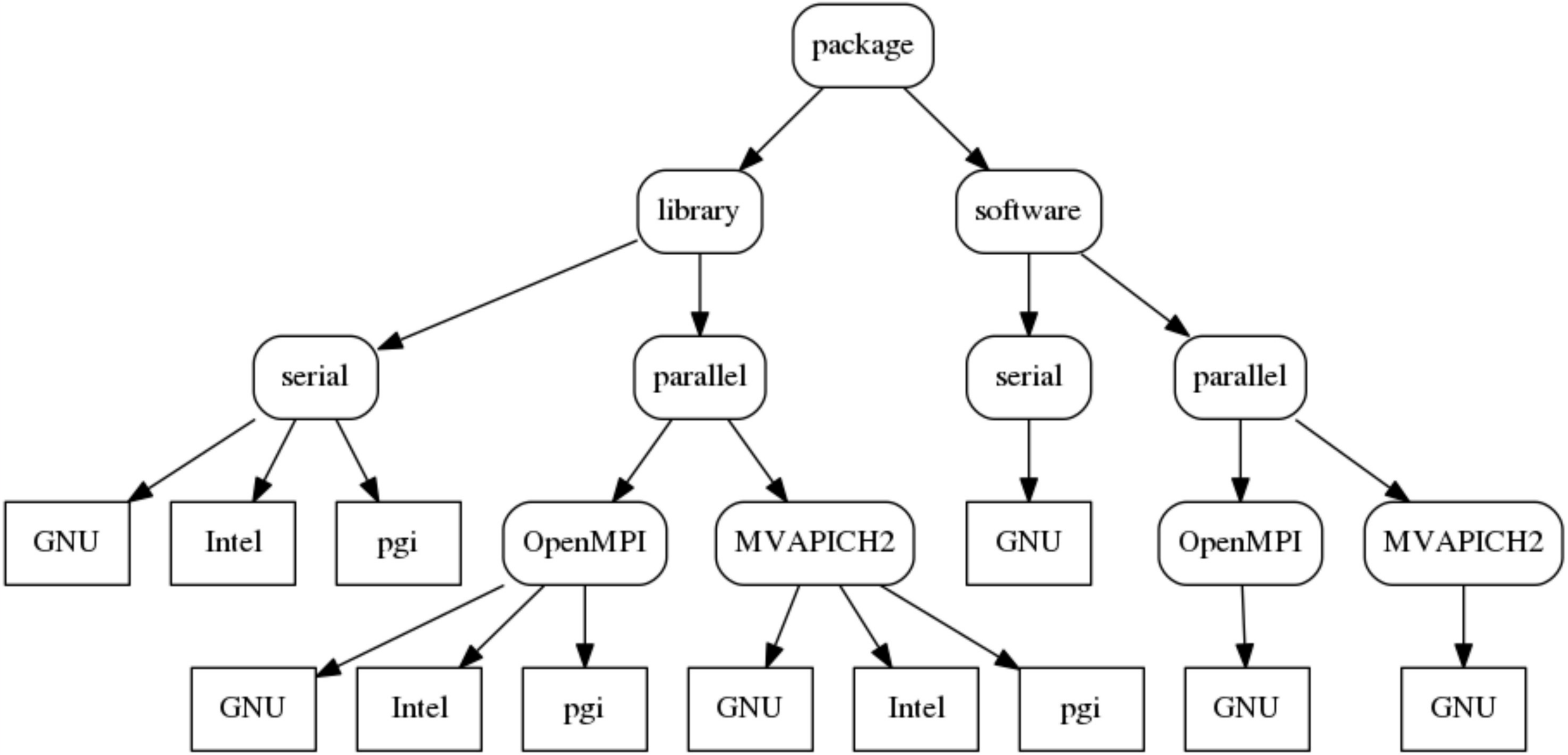
Setup at FSU RCC

- FSU RCC manages 550 custom packages
  - 171 R packages (mostly bioconductor)
  - Only install basic Python packages and Python 3
    - Users can install Python packages in their home directories via `virtualenv (pip` installs dependencies automatically)
- All packages are installed via RPMs
  - Few exceptions for very large packages installed on parallel file system (eg: `orca`)
- Only support the packages we install
  - `WRF` is widely used but managed by users and we respond to support requests

Where to install?



Where to install?



Using RPMs vs regular install

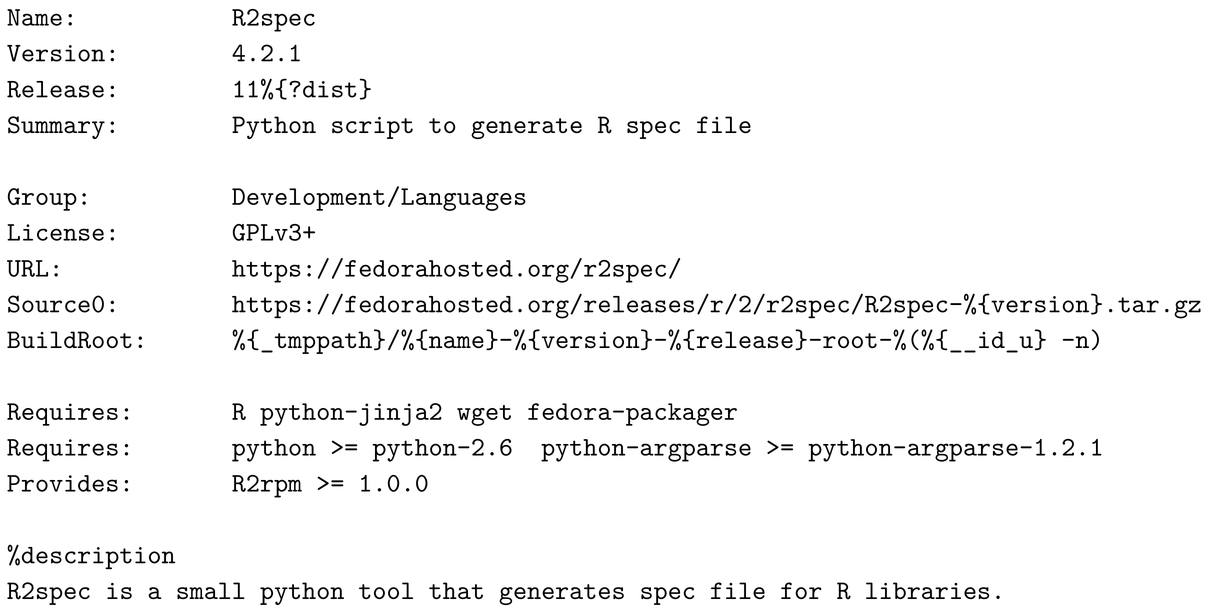
- Pros
  - No need to figure out how to install a package if a pre-built RPM exists
  - Self documenting
  - Easy file lookup (using `yum provides` ...)
  - Easy up/downgrade to different versions (using `yum`)
  - Clean uninstall
- Cons
  - Need local disks on every node
- Best practices
  - Local repo for custom built RPMs
  - Minimal (clean) system for building RPMs

Getting RPMs

- Multiple sources
  - Public repos (EPEL, fedora, rpmfusion, …)
  - Some packages offer RPMs (eg: `LAMMPS`)
  - Customize an existing source RPM
- Create a custom RPM
  - Get the source
  - Find the installation instructions
  - Create a spec file
  - Use `rpmbuild` to create the RPM
  - Resulting source RPM contains the .spec file and all the source files
  - The RPM(s) preserve the install directory structure

How to build an RPM

- Need the package source and `.spec` file



```
Name:           R2spec
Version:        4.2.1
Release:        11%{?dist}
Summary:        Python script to generate R spec file

Group:          Development/Languages
License:        GPLv3+
URL:            https://fedorahosted.org/r2spec/
Source0:        https://fedorahosted.org/releases/r/2/r2spec/R2spec-%{version}.tar.gz
BuildRoot:      %{_tmppath}/%{name}-%{version}-%{release}-root-%(%{__id_u} -n)

Requires:       R python-jinja2 wget fedora-packager
Requires:       python >= python-2.6  python-argparse >= python-argparse-1.2.1
Provides:       R2rpm >= 1.0.0

%description
R2spec is a small python tool that generates spec file for R libraries.
```

How to build an RPM

```
%prep
%setup -q

%build
%{__python} setup.py build
sed -i '1i %%define Rver 3.4.0' r2spec/specfile.tpl
sed -i '2i %%define _prefix            \/opt\/hpc\/R\/R-%{Rver}' r2spec/specfile.tpl
sed -i '3i %%define distnum %%(\/usr\/lib\/rpm\/redhat\/dist.sh --distnum)' r2spec/specfile.tpl
sed -i 's|%%{?dist}.*|%%{?dist}%%{distnum}3|' r2spec/specfile.tpl
sed -i 's|^Name:             R-%%{packname}|Name:             R-%%{Rver}-%%{packname}|' r2spec/specfile.tpl
sed -i '44i module purge;module load R/\%{Rver}' r2spec/specfile.tpl
sed -i '62,70d' r2spec/specfile.tpl
sed -i '62i %%{rlibdir}/%%{packname}/*' r2spec/specfile.tpl

%install
rm -rf %{buildroot}
%{__python} setup.py install --root=%{buildroot}
install r2spec/specfile.tpl %{buildroot}/%{python_sitelib}/r2spec/
chmod -x %{buildroot}/%{python_sitelib}/r2spec/specfile.tpl

%clean
rm -rf %{buildroot}

%files
%defattr(-,root,root,-)
%doc README LICENSE CHANGELOG
%{python_sitelib}/*
%config(noreplace) %{_sysconfdir}/%{name}/repos.cfg
%{_bindir}/%{name}
%{_bindir}/R2rpm
%{_mandir}/man1/%{name}.1.gz
%{_mandir}/man1/R2rpm.1.gz
```

Automated package building

- Dependencies make package building very tedious
- Fedora uses `Koji` RPM build system
  - `https://pagure.io/koji`
  - Used by CERN, Caltech, and, Amazon etc.
  - Very complicated and less flexible
- RPM building process can be scripted in many cases
  - R package RPM creation was completely automated
    - Recursively download all dependencies
    - `R2spec` package was used to create spec files for RPMs
  - General RPM creation at FSU RCC was mostly automated
    - Package source locations had to be manually supplied

EasyBuild

- Automatic build and installation of (scientific) programs
- Flexible and configurable (build recipes)
- Automatic dependency resolution
- Module file generation, logging, archiving
- Good documentation, increasing community acceptance
- Relatively simple to set up and use when using defaults
- Due to its flexibility, more complicated to customize
- Best deployed as a fresh build-out

Spack

- Package management tool designed to support multiple versions and configurations of software
- Designed for large HPC clusters
- Automatic installation of scientific packages through prebuilt recipes
- Strong CLI support
- Different versions of packages can coexist
- Easy to integrate with existing systems
- Module files are auto generated (Tcl and LMOD)

Demo