Finding a software package on the NYU HPC clusters

The command for seeing what software packages are available is:

$ module avail

This will produce a long list of software packages. At NYU, the naming convention for modules is `package/build_configuration/version`
or, for packages provided in binary form, `package/version`.

For example, on Prince we have several installations of the open-source software "fftw", including:

- `fftw/intel/3.3.4` - fftw version 3.3.4, built with the Intel compiler suite
- `fftw/mvapich2/intel/2.1.5` - fftw version 2.1.5, built for MPI with MVAPICH2 and the Intel compiler suite
- `fftw/mvapich2/intel/3.3.4` - fftw version 3.3.4, built for MPI with MVAPICH2 and the Intel compiler suite
- `fftw/openmpi/intel/2.1.5` - fftw version 2.1.5, built for MPI with OpenMPI and the Intel compiler suite

Matlab on the other hand is a commercial package and comes as a binary, not source code, so the only version changes between modules:

- `matlab/2014a`

If you know what the package you need is called, or even what its name starts with, you can see a smaller list of packages by appending all or part of the package name to `module avail`, for example:

$ module avail fftw

```
-------------------------------------------------- /share/apps/modules/modulefiles
--------------------------------------------------
fftw/intel/3.3.4  fftw/mvapich2/intel/2.1.5  fftw/mvapich2/intel/3.3.4  fftw/openmpi/intel/2.1.5
```

will list only the available configurations and versions of `fftw`, while

$ module avail f

will list all packages whose name begins with "f".

Why keep old versions of software?

There are two good reasons to keep old versions even though newer releases are installed:

- **Compatibility**: other software packages may require a specific version of this package, or may not work in conjunction with the newer package.
- **Reproducibility**: the specific version and build configuration of a software package can lead to minor differences in the results of simulations using it. In order to exactly replicate an experiment, the same version of software should be used.