Finding a software package on the NYU HPC clusters

The command for seeing what software packages are available is:

```bash
$ module avail
```

The module command selects its subcommand based on the first unique match it finds for the letters typed so far, hence "avail" matches "available". You can in fact shorten it further, to "ava".

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:

```bash
$ 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

```bash
$ 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.