Managing Environment with Modules

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Linux Environment Review

- Shell is command-line interface between user and operating system
- The shell's behavior can be customized by setting environment variables

  (eg, `export PATH=$PATH:~/bin`)
- Some commonly used environment variables include
  - `PATH`: list of directories to search for commands
  - `DISPLAY`: screen where graphical output will appear
  - `MANPATH`: directories to search for manual pages
  - `LANG`: current language encoding
  - `LD_LIBRARY_PATH`: directories to search for shared objects (dynamically-loaded libs)
  - `LM_LICENSE_FILE`: files to search for FlexLM software licenses

Setting Environment “By Hand”

- Can set default environment variables at login by putting “export” commands in ~/.bash_profile .
- Different applications might need different environment settings
  - For example, a third-party compiler might have executables and libraries stored in a non-default location
  - To find these, PATH and LD_LIBRARY_PATH would need to be modified
- Different versions of applications may also require different environments
- Modifying your environment by hand each time you want to use an application (or switch versions) is tedious and time-consuming

Environment Modules

- “module” command is an easier way to set the appropriate environment for using a specific application
- The necessary environment variable settings or modifications are defined in a “modulefile”, normally maintained by the system administrator
- However, you can create your own modulefiles
- Modules are “loaded” prior to using the corresponding application

Examples

- Show what modules you currently have loaded
  - `module list`
- Show what modules are available on this computer
  - `module avail`
- Load a module
  - `module load intel-13.0.1`
- Unload a module
  - `module unload fftw/3.3.4`
- Clear all loaded modules
  - `module purge`

Loading Modules Automatically

- Can put module load commands in shell initialization scripts, such as .bash_profile , to set up a default environment every time you log in
- But, depending on which scheduling software a site uses, it may also be necessary to put module commands in the batch script for each job
- In my opinion, it's a good idea to load the modules needed for a job in the job script