

Instructor Guide

Most supercomputers/cluster computers will have at least three popular environments for development of parallel applications such as:

- a. Vendor specific environment such as Dell on Cedar and Cray on Blue Waters
- b. PGI development environment
- a. GNU development environment

These programming environments will have compilers and libraries optimized for specific architecture or type of applications. There are also three main methods for developing parallel applications such as: multi-threaded, multi-process, and accelerators/GPGPUs. Though sometimes we can combine at least two methods for developing hybrid applications. Therefore, in this module instructors should focus on:

- a. Compiling and running different parallel applications/algorithms under different development environments.
- b. The module should focus on loading the right compiler, libraries, and environment for compiling applications
- c. Compiler flags for different methods of parallelism
- d. Running applications under different environments and on different CPUs
- e. Running applications in an interactive mode vs. submitting to scheduler with batch scripts.

Common pitfalls for students and instructors

Before compiling any of the example codes, make sure:

- a. To load the appropriate modules and software packages
- b. For compiling OpenACC make sure to load the PGI compiler. Once you load the PGI compiler it will make the openmpi/3.1.2 module inactive, and reloading OpenMPI kept through errors. The workaround is to swap the standard environment modules:

```
$ module swap intel/2018.3 intel/2016.4  
$ module swap intel/2016.4 intel/2018.3
```
- c. Make sure to request the correct nodes, and for an appropriate number of hours. Check the Wiki page for which nodes could be used for interactive jobs, and which nodes are frequently available.