Supercomputing on Stampede: Introduction

Using the Stampede-2 supercomputer

- **General machine information**
  - You should have already set up your XSEDE account.
  - Do web search for "*stampede2 user guide"*, which should take you here: *https://portal.tacc.utexas.edu/user-guides/stampede2*
  - TACC is the Texas Advanced Computing Center at Univ. Texas-Austin.
- **Connecting**
  - from a browser, via XSEDE: login to XSEDE, click on your name (top right), then under *My Xsede*, choose *Accounts*, then select *Login* link.
  - from a Linux PC, a Mac running Terminal or Iterm2, or PC/Cygwin:
    ssh -Y yourlogin@stampede2.tacc.utexas.edu
  - from a windows PC:
    use XShell (recommended), Putty or other secure-shell software.
  - for *much more* information, see the class Stampede access page.
- **Setting up your Stampede class account**
  - My home directory on Stampede is: *~tg457444*
  - My ATMS 502/CSE 566 directory is: *~tg457444/502*
  - **Login shell:** To find out what your command interpreter (shell) is on Stampede, type "ps" to list running processes. If the response includes *csh* or *tcsh,* then your login shell is c-shell. Otherwise, your shell is bash.
  - If your shell is c-shell:
    - **To Append** my *login-settings.txt* file to your *.cshrc* file with:
      cat ~tg457444/502/login-settings.txt >> ~/.cshrc
    - **To Replace** your .cshrc file with mine, if your account is **new**:
      cp ~tg457444/502/cshrc-copy ~/.cshrc
  - If your login shell is bash:
    - **To Append** my *login-settings.txt* file to your *.cshrc* file with:
      cat ~tg457444/502/bash-settings.txt >> ~/.bashrc
  - **Now logout** (typing "exit" is a fast way) and log back in.
    - You will never need to type the above settings again.
  - **Did it work**?
    - The following command should *then* work without errors:
      which ncargf90 (if you get *command not found*, see me).

- **Compiling**
  - If you are most familiar with MATLAB, you are used to using an *interpreter* rather than a *compiler*. A *compiler* converts your entire code into a running program; compiled programs run more quickly.
  - Our Fortran compiler is called "ncargf90"; C compiler is called "ncargcc"
    - These are really the Intel Fortran (ifort) and C (icc), with parts of the *NCAR Graphics Package* added on.
- **To compile your program**
  - ncargf90 your_program.f90 -o programname *(Fortran90)*
  - ncargcc your_program.c -o programname *(C)*
- **To debug your program**
  - Compile instead with:
    ncargf90 -g -check all -traceback program.f90 -o programname *(Fortran)*
    ncargcc -g -debug extended program.c -o programname *(C)*
  - More extensive checks:
    ncargf90 -g -traceback -check all -ftrapuv -zero program.f90 -o program
    ncargcc -g -debug extended -traceback -check=uninit -Wuninitialized -Wcheck program.c -o programname
  - For Fortran, these options check for array subscript (bounds) errors, and will stop with an error message listing the line where the error occurred. "ftrapuv" stops if you use a variable whose value was not previously set.
  - Intel C does not have a similar subscript check option.
  - Stampede has the gnu debugger (gdb) and Intel debugger (idb) available. Often, the most useful debugging tool is *still*: many print statements. More on Intel compiler debugging options is available here.
- **To use the NCAR Graphics package**
  - Programs run using the NCAR Graphics package produce a graphics file known as *metacode*. This file is, by default, named ***gmeta***. It can be viewed on a PC, if you have X-windows running, by typing "*idt gmeta*" or "ctrans -d X11 gmeta"
  - I have set up several scripts that help you convert your output metacode (gmeta) file to CGM, GIF, or Postscript. To run them, try:
    ~tg457444/502/Tools/metagif
    ~tg457444/502/Tools/metacgm
    ~tg457444/502/Tools/metaps
- **To lock your account main directory** so it is not viewable by others, type:
  chmod go-rwx ~ *(don't forget the tilde at the end)*