

Programming Environment

John Urbanic

Parallel Computing Scientist
Pittsburgh Supercomputing Center

Lightning Overview

Just the basics.

- Docs and other answers
- Modules
- Compilers
- Debugging
 - DDT
 - idev
 - perf tools (later)
- Scripting & Not the usual HPC
 - Python
 - R
 - Scala (hadoop/Spark later)
 - Matlab (later)
 - Java

For deeper questions...

Docs and Other Answers

- Docs
 - <http://psc.edu/index.php/bridges/user-guide/programming-environment>
 - Rapidly evolving. Your feedback welcome.
- Real People
 - <http://psc.edu/index.php/home/contact-us#consulting>
 - Mail / Phone. Backed by expertise. Not a black hole.

Modules

The sane way to deal with a flexible environment. We are adding rapidly.

- module avail
- module load
- module help

```
[urbanic@br005 ~]$ module avail
----- /opt/modulefiles -----
-----
Abinit/7.10.5
blasr/1.3.1
blast/2.2.31
blat/v35
boost/1.60.0
bowtie/1.1.2
bowtie2/2.2.7
cuda/7.5(default)
detonate/1.10
diamond/0.7.11
discovardenovo/52488
falcon/0.4.1
fastqc/0.11.3
fraggenescan/1.20
gamess/V2014
gaussian/09.E.01
gcc/5.3.0(default)
hmmer/3.1b2
icc/16.0.2(default)
idba-ud/1.1.1
java/jdk8u73(default)
java7/jdk7u80
jpeg/9b
matlab/R2016a
maven/3.3.9
maxbin/2.1.1
megan/5.11.3
modulefiles/blast/2.2.31
modulefiles/R/3.2.3-mkl
modulefiles/ray/2.3.1
modulefiles/rsem/1.2.21
modulefiles/samtools/0.1.19
modulefiles/signalp/4.1c
modulefiles/slurm/15.08.8
modulefiles/sra-toolkit/2.5.7
modulefiles/tiff/4.0.6
modulefiles/tmhmm/2.0c
modulefiles/trinity/2.0.6
modulefiles/trinity/2.1.1
modulefiles/trinotate/2.0.2
modulefiles/trinotate_db/2.0
modulefiles/velvet/1.2.10-maxk63-big
modulefiles/velvet/1.2.10-maxk63-categ14-big
modulefiles/zlib/1.2.8
namd/2.11
netcdf/3.6.2-gcc
netcdf/3.6.2-icc(default)
nwchem/6.6
pbjelly/15.8.24
perl/5.18.4-threads
petsc/3.6.1
petsc/3.6.1-intel(default)
phylosift/1.0.1
picard/2.1.1
png/1.6.21
psc_path/1.0
```

Compilers

Traditional HPC:

- PGI
- GNU
- Intel (*much more to come*)

- C
- C++
- Fortran

- MPI
 - *OpenMPI*
 - *Intel*
 - *MVAPICH2*

- OpenMP
- CUDA / OpenACC(PGI)
- *PGAS?*

No Matrix
Necessary!

Scripting & non-HPC

First class citizens here.

- Python
- R
- Matlab (*more to come*)
- Java

Debugging & Profiling

Worth accessing the platform just for friendly environment and licensed tools during development.

- idev
 - Simple interactive access
- Performance Profiling
 - Intel (much more to come)
- DDT
 - X windows
 - Client!
 - Great, intuitive GUI



Example from our MPI course... View Array

The screenshot displays the Allinea DDT - Allinea Forge 6.0.2 interface. The main window shows the Fortran source file `laplace_mpi.f90` with the following code:

```
34 integer, parameter :: left=100, right=101
35
36 !usual mpi variables
37 integer :: mype, npes, ierr
38 integer :: status(MPI_STATUS_SIZE)
39
40 double precision, parameter :: max_temp_error=0.01
41
42 integer :: i, j, max_iterations, iteration=1
43 double precision :: dt, dt_global=100.0
44 real :: start_time, stop_time
45
46 double precision, dimension(0:rows+1,0:columns+1) :: temperature, temperature_last
47
48 !usual mpi startup routines
49 call MPI_Init(ierr)
50 call MPI_Comm_size(MPI_COMM_WORLD, npes, ierr)
51 call MPI_Comm_rank(MPI_COMM_WORLD, mype, ierr)
```

The `Locals` panel on the right shows the current state of variables:

Variable Name	Value
columns	250
rows	1000
temperature	
temperature_last	

The `Input/Output` panel at the bottom left shows the program's output:

```
Maximum iterations [100-4000]?
100
----- Iteration number: 100 -----
( 995, 995): 69.93 ( 996, 996): 72.67 ( 997, 9
Max error at iteration 100 was 0.35
Total time was 0.257431000 seconds.
```

The `Evaluate` panel at the bottom right is empty, and the status bar at the bottom right indicates "Ready Connected to: gomez@bridges.psc.edu".

Visualize...

