Ranger User Guide

Development Section

Programming Models

There are two distinct memory models for computing: distributed-memory and shared-memory. In the former, the message passing interface (MPI) is employed in programs to communicate between processors that use their own memory address space. In the latter, open multiprocessing (OMP) programming techniques are employed for multiple threads (light weight processes) to access memory in a common address space.

For distributed memory systems, single-program multiple-data (SPMD) and multiple-program multiple-data (MPMD) programming paradigms are used. In the SPMD paradigm, each processor loads the same program image and executes and operates on data in its own address space (different data). This is illustrated in Figure 4. It is the usual mechanism for MPI code: a single executable (a.out in the figure) is available on each node (through a globally accessible file system such as $WORK or $HOME), and launched on each node (through the batch MPI launch command, "ibrun a.out").

In the MPMD paradigm, each processor loads up and executes a different program image and operates on different data sets, as illustrated in Figure 4. This paradigm is often used by researchers who are investigating the parameter space (parameter sweeps) of certain models, and need to launch 10s or 100s of single processor executions on different data. (This is a special case of MPMD in which the same executable is used, and there is NO MPI communication.) The executables are launched through the same mechanism as SPMD jobs, but a Unix script is used to assign input parameters for the execution command (through the batch MPI launcher, "ibrun script_command"). Details of the batch mechanism for parameter sweeps are described in the Running Programs section.

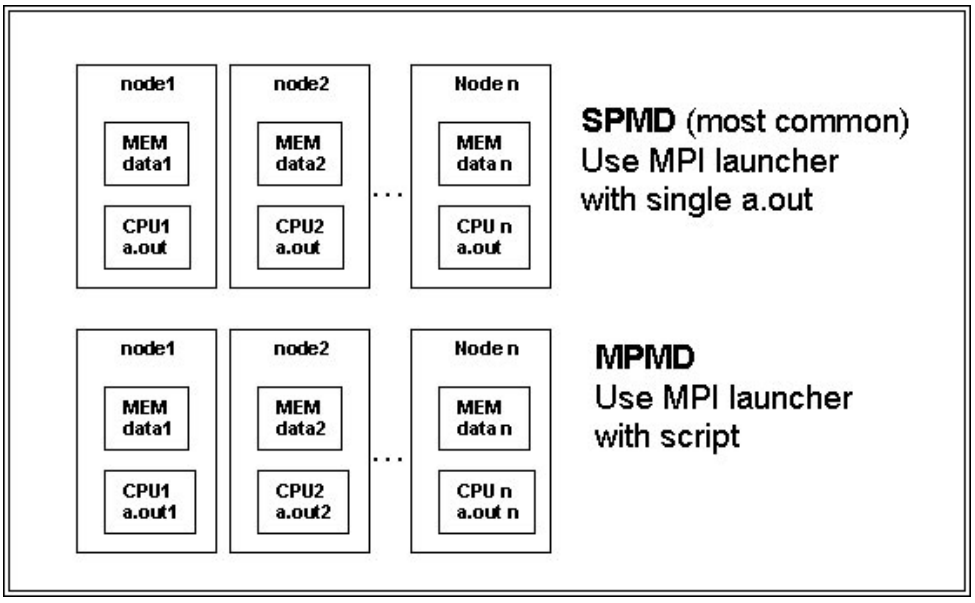


Figure 4. Distributed Memory Paradigm: Single/Multiple-Program Multiple-Data.

The shared-memory programming model is used on Symmetric Multi- Processor (SMP) nodes, like the TACC Champion Power5 System (8 CPUs, 16GB memory per node) or the TACC Ranger Cluster (16 cores, 32GB memory per node).

The programming paradigm for this memory model is called Parallel Vector Processing (PVP) or Shared-Memory Parallel Programming (SMPP). The latter name is derived from the fact that vectorizable loops are often employed as the primary structure for parallelization. The main point of SMPP computing is that all of the processors in the same node share data in a single memory subsystem, as shown in Figure 5. There is no need for explicit messaging between processors as with with MPI coding.

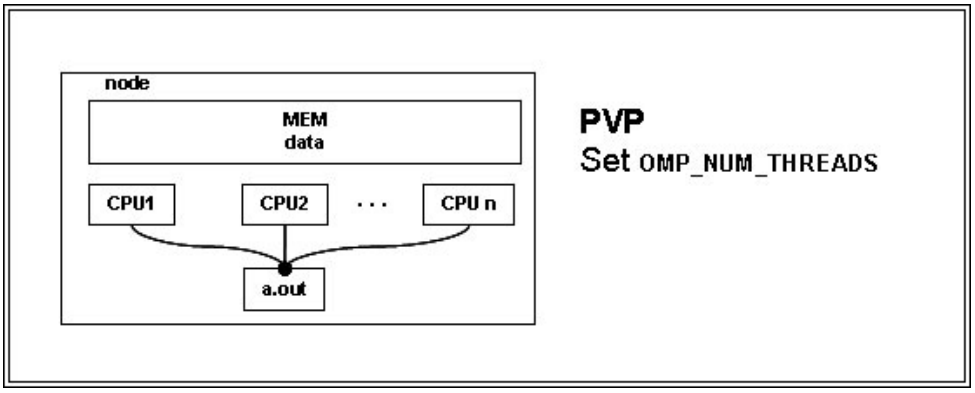


Figure 5. Shared-Memory Parallel Processing.

In the SMPP paradigm either compiler directives (as pragmas in C, and special comments in FORTRAN) or explicit threading calls (e.g. with Pthreads) is employed. The majority of science codes now use OpenMP directives that are understood by most vendor compilers, as well as the GNU compilers.

In cluster systems that have SMP nodes and a high speed interconnect between them, programmers often treat all CPUs within the cluster as having their own local memory. On a node an MPI executable is launched on each CPU and runs within a separate address space. In this way, all CPUs appear as a set of distributed memory machines, even though each node has CPUs that share a single memory subsystem.

In clusters with SMPs, hybrid programming is sometimes employed to take advantage of higher performance at the node-level for certain algorithms that use SMPP (OMP) parallel coding techniques. In hybrid programming, OMP code is executed on the node as a single process with multiple threads (or an OMP library routine is called), while MPI programming is used at the cluster-level for exchanging data between the distributed memories of the nodes.

For further information on OpenMP, MPI and on programming models/paradigms, please see the manuals and packages sections of this document.

Compilation

Compiler Usage Guidelines

The AMD *Compiler Usage Guidelines* document provides the "best-known" peak switches for various compilers tailored to their Opteron products. Developers and installers should read Chapter 5 of this document before experimenting with PGI and Intel compiler options.

See Chapter 5 of the AMD Compiler Usage Guidelines.

The Intel 10.1 Compiler Suite

The Intel 10.1 compilers are NOT the default compilers. You must use the module commands to load the Intel compiler environment (see above). (The 9.1 compilers are available for special porting needs.) The **gcc** 3.4.6 compiler and module are also available. We recommend using the Intel (or the PGI) suite whenever possible. The 10.1 suite is installed with the 64-bit standard libraries and will compile programs as 64-bit applications (as the default compiler mode).

Web accessible Intel manuals are available: Intel 10.1 C++ Compiler Documentation and Intel 10.1 Fortran Compiler Documentation.

The PGI 7.1 Compiler Suite

The PGI 7.1 compilers are loaded as the default compilers at login with the **pgi** module. We are recommending the use of the PGI suite whenever possible (at this time). The 7.1 suite is installed with the 64-bit standard libraries and will compile

programs as 64-bit applications (as the default compiler mode).

A PDF version of the PGI User's Guide is available.

Initially the Ranger programming environment will support several compilers: Intel, PGI, gcc and SUN. The first section explains how to use modules to set up the compiler environment. The next section presents the compiler invocation for serial and MPI executions, and follows with a section on options. All compiler commands can be used for just compiling with the -c option (create just the ".o" object files) or compiling and linking (to create executables).

By default, the pgi compiler environment is set up at login. To use a different compiler you must use module commands to first unload the MPI environment (mvapich2), swap the compiler environment, and then reload the MPI environment. Execute the **module avail** to determine the modulefile names for all the available compilers; they have the syntax ***compiler/version***. The commands are listed below. Place these commands in your .login (C shells) or .profile (Bourne shells) file to automatically set an alternate default compiler in your environment at login.

module unload mvapich2

module swap pgi intel

module load mvapich2

Compiling Serial Programs

The compiler invocation commands for the supported vendor compiler systems are tabulated below.

Compiling Serial Programs

Vendor	Compiler	Program	TypeSuffix
intel	icc	C	.c
intel	icc	C++	.C, .cc, .cpp, .cxx
intel	ifort	F90	.f, .for, .ftn, .f90, .fpp
pgi	pgcc	C	.c
pgi	pgcpp	C++	.C, .cc
pgi	pgf95	F77/90/95	.f, .F, .FOR, .f90, .f95, .hpf
gnu	gcc	C	.c
sun	sun_cc	C	.c
sun	sun_CC	C++	.C, .cc, .cpp, .cxx
sun	sunf90	F77/90	.f, .F, .FOR, .f90, .hpf
sun	sunf95	F95	.f, .F, .FOR, .f90, .f95, .hpf

Note : pgf90 is an alias for pgf95.

Appropriate program-name suffixes are required for each compiler. By default, the executable name is **a.out**. It may be renamed with the **-o** option. To compile without the link step, use the **-c** option. The following examples illustrate renaming an executable and the use of two important compiler optimization options:

intel **icc/ifort -o flamec.exe -O2 -xW prog.c/cc/f90**

pgi **pgcc/pgcpp/pgf95 -o flamef.exe -fast -tp barcelona-64 prog.c/cc/f90**

gnu **gcc -o flamef.exe -mtune=barcelona -march=barcelona prog.c**

sun **sun_cc/sun_CC/sunf90 -o flamef.exe -xarch=sse2 prog.c/cc/f90**

A list of all compiler options, their syntax, and a terse explanation, is given when the compiler command is executed with the **-help** option. Also, man pages are available. To see the help or and man information, execute one of:

compiler* -help / man *compiler with ***compiler* = ifort, pgf90/95** or **sunf90** or
gcc --help / man gcc

sun_cc -help / man sun_cc / sunf90 -help / man sunf90

--> Some of the more important options are listed below.

Compiling Parallel Programs with MPI

The *"mpicmds"* commands support the compilation and execution of parallel MPI programs for specific interconnects and compilers. At login, MPI MVAPICH (**mvapich2**) and Intel 10.1 compiler (**intel**) modules are loaded to produce the default environment which provide the location to the corresponding *mpicmds*. Compiler scripts (*wrappers*) compile MPI code and automatically link startup and message passing libraries into the executable. Note that the compiler and MVAPICH library are selected according to the modules that have been loaded. The following table lists the compiler wrappers for each language:

Compiling Parallel Programs with MPI

Compiler	Program	TypeSuffix
mpicc	c	.c
mpiCC	C++	.cc, .C, .cpp, .cxx
mpif90	F77/F90	.f, .for, .ftn, .f90, .f95, .fpp

Appropriate program-name suffixes are required for each wrapper. By default, the executable name is **a.out**. It may be renamed with the **-o** option. To compile without the link step, use the **-c** option. The following examples illustrate renaming an executable and the use of two important compiler optimization options:

intel **mpicc/mpif90 -o prog.exe -O2 -xW prog.cc/f90**

pgi **mpicc/mpif90 -o prog.exe -fast -tp barcelona-64 prog.f90**

Include linker options such as library paths and library names after the program module names, as explained in the Loading Libraries section below. The Running Code section explains how to execute MPI executables in batch scripts and "interactive batch" runs on compute nodes.

We recommend that you use either the Intel or the PGI compiler for optimal code performance. TACC does not support the use of the gcc compiler for production codes on the Ranger system. For those rare cases when gcc is required, for either a module or the main program, you can specify the gcc compiler with the -cc mpcc option. (Since gcc- and Intel-compiled code are binary compatible, you should compile all other modules that don't require gcc with the Intel compiler.) When gcc is used to compile the main program, an additional Intel library is required. The examples below show how to invoke the gcc compiler in combination with the Intel compiler for the two cases:

```
mpicc -O2 -xW -c -cc=gcc suba.c
mpicc -O2 -xW mymain.c suba.o

mpicc -O2 -xW -c suba.c
mpicc -O2 -xW -cc=gcc -L$ICC_LIB -lirc mymain.c suba.o
```

Compiling OpenMP Programs

Since each of the blades (nodes) of the Ranger cluster is an AMD Opteron quad-processor quad-core system, applications can use the shared memory programming paradigm "on node". With a total number of 16 cores per node, we encourage the use of a shared-memory model on the node.

The OpenMP compiler options are listed below for those who do need SMP support on the nodes. For hybrid programming, use the mpi-compiler commands, and include the openmp options.

Intel : mpicc/mpif90 -O2 -xW **-openmp**
pgi : mpicc/mpif90 -fast -tp barcelona-64 **-mp**

Basic Optimization for Serial and Parallel Programming using OpenMP and MPI

The MPI compiler wrappers use the same compilers that are invoked for serial code compilation. So, any of the compiler flags used with the **icc** command can also be used with **mpicc**; likewise for **ifort** and **mpif90**; and **iCC** and **mpiCC**. Below are some of the common serial compiler options with descriptions.

Intel Compiler

Compiler Options	Description
-03	performs some compile time and memory intensive optimizations in addition to those executed with -O2, but may not improve performance for all programs.
-ipo	Interprocedural optimizations
-vec_report[0|...|5]	control amount of vectorizer diagnostic information:
-xW	includes specialized code for SSE and SSE2 instructions (recommended).
-xO	includes specialized code for SSE, SSE2 and SSE3 instructions. Use, if code benefits from SSE3 instructions.
-fast	-ipo, -O2, -static DO NOT USE -- static load not allowed.
-g -fp	debugging information produced, disable using EBP as general purpose register
-openmp	enable the parallelizer to generate multi-threaded code based on the OpenMP directives
-openmp_report[0|1|2]	control the OpenMP parallelizer diagnostic level.
-help	lists options

Developers often experiment with the following options: *-pad, -align, -ip, -no-rec-div and -no-rec-sqrt*. In some codes performance may decrease. Please see the Intel compiler manual (below) for a full description of each option.
Use the -help option with the *mpicmds* commands for additional information:

mpicc -help
mpif90 -help
mpirun -help {use the listed options with the **ibrun** cmd}

pgi Compiler

Compiler Options	Description
-03	performs some compile time and memory intensive optimizations in addition to those executed with -O2, but may not improve performance for all programs.
-Mipa=fast, inline	Interprocedural optimizations There is a loader problem with this option.
-tp barcelona-64	includes specialized code for the barcelona chip.
-fast	-O2 -Munroll=c:1 -Mnoframe -Mlre -Mautoinline -Mvect=sse -Mscalarsse -Mcache_align -Mflushz
-g, -gopt	debugging information produced
-mp	enable the parallelizer to generate multi-threaded code based on the OpenMP directives
-Minfo=mp,ipa	Information about OpenMP, interprocedural optimization
-help	lists options
-help -fast	lists options for -fast

For detail on the MPI standard go to the URL: www.mcs.anl.gov/mpi.

Loading Libraries

Some of the more useful load flags/options are listed below. For a more comprehensive list, consult the *ld* man page.

- Use the *-l* loader option to link in a library at load time: e.g.

  compiler* prog.f90 -l*name

  This links in either the shared library *libname.so* (default) or the static library *libname.a*, provided that the correct path can be found in *ldd*'s library search path or the LD_LIBRARY_PATH environment variable paths.

- To explicitly include a library directory, use the -L option, e.g.

  compiler* prog.f -L/mydirectory/lib -l*name

  In the above example, the user's *libname.a* library is not in the default search path, so the "*-L*" option is specified to point to the *libname.a* directory.

  Many of the modules for applications and libraries, such as the **mkl** library module provide environment variables for compiling and linking commands. Execute **module help *module_name*** for a description, listing and use cases for the assigned environment variables. The following example illustrates their use for the **mkl** library:

  **mpicc -Wl,-rpath,$TACC_MKL_LIB -I$TACC_MKL_INC mkl_test.c **
  -L$TACC_MKL_LIB -lmkl_em64t

  Here, the module supplied variables TACC_MKL_LIB and TACC_MKL_INC contain the MKL library and header library directory paths, respectively. The loader option **-Wl** specifies that the $TACC_MKL_LIB directory should be included in the binary executable. This allows the run-time dynamic loader to determine the location of shared libraries directly from the executable instead of the LD_LIBRARY path or the LDD dynamic cache of bindings between shared libraries and directory paths. (This avoids having to set the LD_LIBRARY path ("manually" or through a module command) before running the executables.

Running Code

Runtime Environment

Bindings to the most recent shared libraries are configured in the file /etc/ld.so.conf (and cached in the /etc/ld.so.cache file). Cat /etc/ld.so.conf to see the TACC configured directories, or execute

/sbin/ldconfig -p

to see a list of directories and candidate libraries. Use the -Wl,rpath loader option or the LD_LIBARY_PATH to override the default runtime bindings.

The Intel compiler and MKL math libraries are located in the /opt/intel directory (installation date TBD), and application libraries are located in /usr/local/apps ($APPS). The GOTO libraries are located in /opt/apps/gotoblas/gotoblas-1.02 (installation date TBD). Use the

module help *libname*

command to display instructions and examples on loading libraries.

The SGE Batch System

Batch facilities like LoadLeveler, NQS, LSF, OpenPBS or SGE differ in their user interface as well as implementation of the batch environment. Common to all, however, is the availability of tools and commands to perform the most important operations in batch processing: job submission, job monitoring, and job control (hold, delete, resource request modification). In Section I basic batch operations and their options are described. Section II discusses the SGE batch environment, and Section III provides the queue structure on SGE. In the references at the end of this section there are links to SGE manuals. New users should visit the SGE wiki and read the first chapter of the "Introduction to the N1 Grid Engine 6 Software" document. To help users who are migrating from other systems, a comparison of the IBM LoadLeveler, OpenPBS, LSF and SGE batch options and commands is presented in a separate document.

Section I: Three Operations of Batch Processing: submission, monitoring, and control

Step 1: Job submission

SGE provides the qsub command for submitting batch jobs: Use the SGE qsub command to submit a batch job with the following syntax:

qsub ***job_script***

where ***job_script*** is the name of a file with unix commands. This "job script" file can contain both shell commands and special commented statements that include **qsub** options and resource specifications. Details on how to build a script follow.

Table 1. List of the Most Common **qsub** Options

Option	Argument	Function
-q	**queue_name**	Submits to queue designated by **queue_name**
-pe	**pe_name min_proc[-max_proc]**	Executes job via the Parallel Environment designated by **pe_name** with **min_proc-max_proc** number of processes
-N	**job_name**	Names the job **job_name**
-S	**shell** (absolute path)	Use shell as shell for the batch session
-M	**emailaddress**	Specify user's email address
-m	**{b|e|a|s|n}**	Specify when user notifications are to be sent
-V		Use current environment setting in batch job
-cwd		Use current directory as the job's working directory
-o	**output_file**	Direct job output to **output_file**
-e	**error_file**	Direct job error to **error_file**
-A	**account_name**	Charges run to **account_name**. Used only for multi-project logins. Account names and reports are displayed at login.
-l	***resource=value***	Specify resource limits (see qsub man page)

Options can be passed to **qsub** on the command line or, specified in the job script file. The latter approach is preferable. It is easier to store commonly used **qsub** commands in a script file that will be reused several times rather than retyping the **qsub** commands at every batch request. In addition, it is easier to maintain a consistent batch environment across runs if the same options are stored in a reusable job script.

Batch scripts contain two types of statements: special comments and shell commands. Special comment lines begin with **#$** and are followed with **qsub** options. The SGE *shell_start_mode* has been set to unix_behavior which means that the Unix shell commands are interpreted by the shell specified on the first line after **#!** sentinel; otherwise the Bourne shell (/bin/sh) is used. The file job below requests an MPI job with 32 cores and 1.5 hours of run time:

```
#!/bin/bash
                    #Use Bash Shell
#$ -V
                    # Inherit the submission environment
#$ -cwd
                    # Start job in  submission directory
#$ -N myMPI
```

```
                    # Job Name
#$ -j y
                    # combine stderr & stdout into stdout
#$ -o $JOB_NAME.o$JOB_ID
                    # Name of the output file (eg. myMPI.oJobID)
#$ -pe 16way 32
                    # Requests 16 cores/node, 32 cores total
#$ -q normal
                    # Queue name
#$ -l h_rt=01:30:00
                    # Run time (hh:mm:ss) - 1.5 hours
## -M myEmailAddress
                    # Email notification address (UNCOMMENT)
## -m be
                    # Email at Begin/End of job  (UNCOMMENT)
set -x
                    #{echo cmds, use "set echo" in csh}
ibrun ./a.out
                    # Run the MPI executable named "a.out"
```

If you don't want stderr and stdout directed to the same file, remove don't include a -j option line, and insert a -e option (stderr) to name the file that is to receive stderr output.

MPI Environment for Scalable Code

The MVAPICH-1 and MVAPICH-2(default) MPI packages provide runtime environments that can be tuned for scalable code. For packages with short messages, there is a "FAST_PATH" option that can reduce communication costs, as well as a mechanism to "Share Receive Queues". Also, there is a "Hot-Spot Congestion Avoidance" option for quelling communication patterns that produce hot spots in the switch. See Chapter 9, "Scalable features for Large Scale Clusters and Performance Tuning" and Chapter 10, "MVAPICH2 Parameters" of the MVAPICH2 User Guide for more information. The User Guides are available in PDF format at:

MVAPICH User Guides

Understanding the SGE Parallel Environment

Each Ranger node (of 16 cores) can only be assigned to one user; hence, a complete node is dedicated to a user's job and accrues wall-clock time for 16 cores whether they are used or not. The SGE parallel environment option "-pe" sets the number of MPI Tasks per Node (TpN), and the Number of Nodes (NoN). The syntax is:

#$ -pe <TpN > way <NoN x 16 >
e.g.
#$ -pe 16way 64 {16 MPI tasks per node, 4 nodes (= a total of 64 assigned cores/16)}

where:
TpN is the Task per Node, and
NoN is the Number of Nodes requested.

Note, regardless of the value of TpN, the second argument is always **16** times the number of nodes that you are requesting.

Using a multiple of 16 cores per node

For "pure" MPI applications, the most cost-efficient choices are: 16 tasks per node (16way) and a total number of tasks that is a multiple of 16. This will ensure that each core on all the nodes is assigned one task. In this case use:

$# -pe 16way <NoN x 16>

Using fewer than 16 cores per node

When you want to use less that 16 MPI tasks per node, the choice of tasks per node is limited to the set of numbers {1, 2, 4, 8, 12, and 15}. When the number of tasks you need is equal to "Number of Tasks per Node x Number of Nodes", then use the following prescription:

$# -pe <TpN>way <NoN x 16>

where
TpN is a number in the set {1, 2, 4, 8, 12, 15}

If the total number of tasks that you need is less than "Number of Tasks per Node x Number of Nodes", then set the MY_NSLOTS environment variable to the total number of tasks. In a job script, use the following -pe option and environment variable statement:

$# -pe <TpN>way <NoN x 16>
...
setenv MY_NSLOTS <Total Number of Tasks>   { C-type shells }
or
export MY_NSLOTS=<Total Number of Tasks>   { Bourne-type shells }

e.g.
$# -pe 8way 64   {use 8 Tasks per Node, 4 Nodes requested}
...
setenv MY_NSLOTS 31 {31 tasks are launched}

where
TpN is a number in the set {1, 2, 4, 8, 12, 15}

Program Environment for Hybrid Programs

For hybrid jobs, specify the MPI Tasks per Node through the first -pe option (1/2/4/8/15/16way) and the Number of Nodes in the second -pe argument (as the number of assigned cores = Number of Nodes x 16). Then, use the OMP_NUM_THREADS environment variable to set the number of threads per task. (Make sure that "Tasks per Node x number of Nodes" is less than or equal to the number assigned cores, the second argument of the -pe option.) The hybrid job script below illustrates the use of these parameters to run a hybrid job. It requests 4 tasks per node, 4 threads per task, and a total of 32 cores (2 nodes x 16 cores).

```
#!/bin/bash
#                 {use bash shell}
...

#$ -pe 4way 32
#                 {4 cores/node, 32 cores total}
...


set -x            #{echo cmds, use "set echo" in csh}

setenv OMP_NUM_THREADS 4
                  #{4 threads/task}
ibrun ./hybrid.exe
```

The job output and error are sent to **out.o*<job_id>*** and **err.o*<job_id>***, respectively. SGE provides several environment variables for the #$ options lines that are evaluated at submission time. The above **$JOB_ID** string is substituted with the job id. The job name (set with **-N**) is assigned to the environment variable **JOB_NAME**. The memory limit per task on a node is automatically adjusted to the maximum memory available to a user application (for serial and parallel codes).

Step 2: Batch query

After job submission, users can monitor the status of their jobs with the **qstat** command. Table 2 lists the **qstat** options:

Table 2. List of **qstat**s Options

Option	Result
-t	Show additonal information about subtasks
-r	Show resource requirements of jobs
-ext	Displays extended information about jobs

-j <jobid>	Displays information for specified job
-qs {a|c|d|o|s|u|A|C|D|E|S}	Show jobs in the specified state(s)
-f	Shows "full" list of queue/job details

The **qstat** command output includes a listing of jobs and the following fields for each job:

Table 3. Some of the fields in **qstat**s command output

Field	Description
JOBID	job id assigned to the job
USER	user who owns the job
STATE	current job status, includes (but not limited to)
w	waiting
s	suspended
r	running
j	on hold
E	errored
d	deleted

For convenience, TACC has created an additional job monitoring utility which summarizes all jobs in the batch system in a manner similar to the "showq" utility from PBS. Execute

showq

to summarize all running, idle, and pending jobs, along with any advanced reservations scheduled within the next week. Note that **showq -u** will show jobs associated with your userid only (issue **showq --help** to obtain more information on available options). An example output from showq is shown below:

```
ACTIVE JOBS--------------------


JOBID  JOBNAME   USERNAME    STATE  PROC  REMAINING       STARTTIME
14694   equillda    user1  Running    16   18:54:07  Tue Feb 3 17:32:41
14701          V    user2  Running    16    7:02:41  Tue Feb 3 17:41:15
14707          V    user3  Running    16   19:11:02  Tue Feb 3 17:49:36
14708      jet08    user4  Running    32    0:38:36  Tue Feb 3 18:17:10
14713        rti    user5  Running    64    3:58:25  Tue Feb 3 20:36:59
14714        cyl    user6  Running   128   23:16:36  Tue Feb 3 21:55:10


6 Active jobs     272 of 556 Processors Active (48.92%)


IDLE JOBS----------------------
JOBID  JOBNAME   USERNAME    STATE  PROC    WCLIMIT       QUEUETIME
14716     bigjob    user7     Idle   512    0:15:00  Tue Feb 3 22:18:57
14719   smalljob    user7     Idle   256    0:15:00  Tue Feb 3 22:35:31


 2 Idle jobs    BLOCKED JOBS-------------------


JOBID  JOBNAME   USERNAME    STATE  PROC    WCLIMIT       QUEUETIME
14717      hello    user7     Held    16    0:15:00  Tue Feb 3 22:19:07
14718      hello    user7     Held    32    0:15:00  Tue Feb 3 22:19:15


4 Blocked jobs    Total Jobs: 12    Active Jobs: 6     Idle Jobs: 2     Blocked Jobs: 4


ADVANCED RESERVATIONS----------
RESV ID   PROC                    RESERVATION WINDOW
karl#79    556    Tue Mar 23 09:00:00 2004 - Tue Mar 23 17:30:00 2004
```

Step 3: Job control

Control of job behavior takes many forms:

a. **Job modification while in the pending/run state**
Users can reset the qsub options of a pending job with the **qalter** command, using the following syntax:

qalter options <job id>

where **options** refers only to the following **qsub** resource options (also described in Table 1):

-l h_rt=<value>	per-job wall clock time
-o	output file
-e	error file

b. Job deletion
The **qdel** command is used to remove pending and running jobs from the queue. The following table explains the different **qdel** invocations:

qdel <jobid>	Removes pending or running job.
qdel -f <jobid>	Force immediate dequeuing of running job.

** Immediately report the job number to TACC staff through the portal consulting system or the TeraGrid HelpDesk (help@teragrid.org).
(This may leave hung processes that can interfere with the next job.)

c. Job suspension/resumption
The **qhold** command allow users to prevent jobs from running. The syntax is **qhold <job id>**

qhold may be used to stop serial or parallel jobs and can be invoked by a user or a person with SGE sys admin privileges. A user cannot resume a job that was suspended by a sys admin nor can he a job owned by another user.

Jobs that have been placed on hold by **qhold** can be resumed by using the **qalter -hU** command.

Section II: SGE Batch Environment

In addition to the environment variables inherited by the job from the interactive login environment, SGE sets additional variables in every batch session. The following table lists some of the important SGE variables:

Table 4. SGE Batch Environment Variables

Environment Variable	Contains
JOB_ID	batch job id
TASK_ID	task id of an array job subtask
JOB_NAME	name user assigned to the job

Section III: Ranger Queue Structure

Below is a table of queue names and the characteristics (wall-clock and processor limits and default values; priority charge factor; and purpose) for the Ranger queues. The systest and support queues are for TACC system and HPC group testing and consulting support, respectively.

Table 5. LSF Batch Environment Queues

Queue Name	Max Runtime (default)	Max Procs	SU Charge Rate	Purpose
normal	6 hrs	2048 (more soon)		Normal Priority
high	6 hrs	2048 (more soon)		High priority
systest	--	--	--	TACC Staff only, debugging & benchmarking

Please note that the TACC usage policy does not allow users to run interactive (serial) executables (running *a.out*) on the login nodes of the HPC systems. All such executions must be submitted directly to an appropriate queue of the system's batch utility. On the Ranger system, use an SGE job script to submit the job to the serial queue (#$ -q serial).

Process Affinity and Memory Policy

Controlling Process Affinity and Memory Locality

While many applications will run efficiently using 16 MPI tasks on each node (to occupy all cores), certain applications will run optimally with fewer than 16 cores per node and/or a specified arrangement for memory allocations. The basic underlying API (application program interface) utilities for binding processes (MPI Tasks) and threads (OpenMP/Pthreads threads) are sched_get/staffinity , get/set_memopolicy, and membind C utilities . Threads and processes are identical with respect to scheduling affinity and memory policies. In HPC batch systems an MPI task is synonymous with a process, and these two terms will be used interchangeably in this section. The number of tasks, or processes, launched on a node is determined by the "wayness" (the Programming Environment specified after the -pe option (e.g. "#$ -pe 16way 128"). Tasks are easily controlled without any instrumentation. The same level of external control is not available with threads because multiple threads are forked (or spawned) at run time from a single process, and a concise mapping of the threads to cores can only be controlled within the program.

When a task is launched it can be bound to a socket or a specific core; likewise, its memory allocation can be bound to any socket. On the command line, assignment of tasks to sockets (and cores) and memory to socket memories can be made through the **numactl** wrapper command that takes an executable as an argument. The basic syntax for launching MPI executables under "NUMA" control within a batch script is:

ibrun numactl <options> a.out	{options apply to all a.out's}
ibrun numa	{numactl cmd for each a.out is specified within a numa script}

In the first command ibrun executes "**numactl <options> a.out**" for all tasks (a.out's) using the same options. In the second command ibrun launches an executable unix script (here named numa) which tailors the numactl for launching each MPI executable (a.out), as described below.

In order to use numactl it is necessary to understand the node configuration and the mapping between the logical Core IDs, also called CPUIDs (shown in the top and used by numactl), the socket IDs and their physical location. The figure below shows the basic layout of the memory, sockets and cores of a Ranger node.

Ranger Sockets

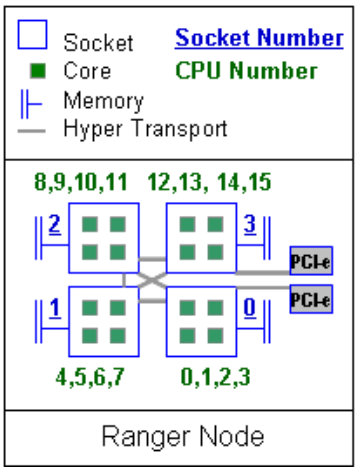


Figure: Node Diagram.

Both memory bandwidth-limited and cache-friendly applications are consequently affected by "numa" instructions to orchestrate a run on this architecture. The following figure shows two extremes cases of core scalability on a node. The upper curve shows the performance of a cache-friendly dgemm matrix-matrix multiply from the GotoBLAS library. It scales to 15.2 for a 16 cores. The lower bound shows the scaling for the Streams benchmark which is limited by the memory bandwidth to each socket. Efficiently parallelized codes should exhibit scaling between these curves.

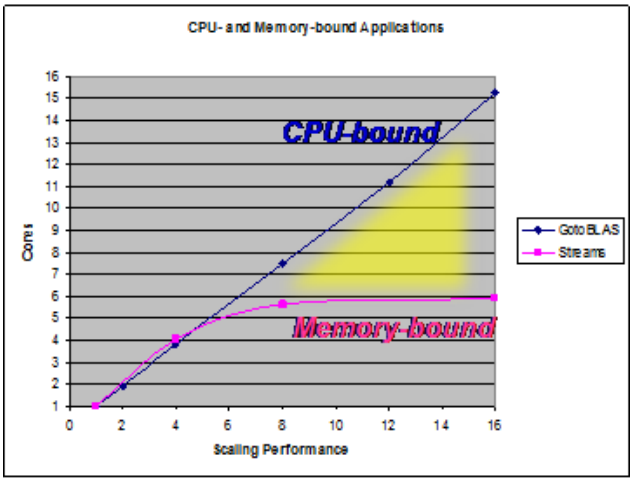


Figure: Application scaling boundaries for CPU-limited and Memory bandwidth-limited Applications.

Additional details are given in the man page and numactl help option:

man numactl
numactl --help

Numactl Command and Options

The table below lists important options for assigning processes and memory allocation to sockets, and assigning processes to specific cores.

	cmd	option	arguments	description
Socket Affinity	numactl	-N	{0,1,2,3}	Only execute process on cores of this (these) socket(s).
Memory Policy	numactl	-l	{no argument}	Allocate on current socket.
Memory Policy	numactl	-i	{0,1,2,3}	Allocate round robin (interleave) on these sockets.

Memory Policy	numactl	--preferred=	{0,1,2,3} select only one	Allocate on this socket; fallback to any other if full .
Memory Policy	numactl	-m	{0,1,2,3}	Only allocate on this (these) socket(s).
Core Affinity	numactl	-C	{0,1,2,3, 4,5,6,7, 8,9,10,11, 12,13,14,15}	Only execute process on this (these) Core(s).

There are three levels of numa control that can be used when submitting batch jobs. These are:

1.) Global (usually with 16 tasks/threads);
2.) Socket level (usually with 4,8, and 12 tasks/threads); and
3.) Core level (usually with an odd number of tasks/treads)

Launch and numactl commands will be illustrated for each. The control of numactl can be directed either at a global level on the ibrun command line (usually for memory allocation only), or within a script (we use the name "numa" for this script) to specify the socket (-N) or core (-C) to run on. (Note, the numactl man pages refers to sockets as "nodes". In HPC systems a node is a blade, and we will only use "node" when we refer to a blade).

The default memory policy is local allocation of memory; that is, any allocation occurs on the socket where the process is executing. The default processor assignment is random for MPI (and should not be of concern for 16way MPI and 1way pure OMP runs). The syntax and script templates for the three levels of control are present below.

Numa Control in Batch Scripts

- GLOBAL CONTROL:
  Global control will affect every launched executable. This is often only used to control the layout of memory for SMP execution of 16 threads on a node. (16-task MPI code should use the default, local, memory allocation policy.) TACC has implemented a script, tacc_affinity, for automatically distributing 4-, 8-, and 12way executions evenly across sockets and assigning memory allocation locally to the socket (-m memory policy).

ibrun	./a.out	{-pe 16way 16 ; local by default; use for MPI}
ibrun numactl -i all	./a.out	{-pe 1way 16 ; interleaved; possibly use for OMP}
ibrun tacc_affinity	./a.out	{-pe 4/8/12way ... ; assigns MPI tasks round robin to sockets, local memory allocation }

- SOCKET CONTROL:
  Often socket level affinity is used with hybrid applications (such as 4 tasks and 4 threads/task on a node), and when the memory per process must be 8/6, two or four times the default (~2GB/task). In this scenario, it is important to distribute 3, 2 or 1 tasks per socket. Likewise, for hybrid programs that need to launch a single task per socket and control 4 threads on the socket, socket level control is needed. A numa script (here, identified as numa.csh and numa.sh for C-shell and Bourne shell control) is created for execution by ibrun. The numa script is executed once for each task on the node. This script captures the assigned rank (PMI_RANK) from ibrun and is used to assign a socket to the task. From a list of the nodes, ranks are assigned sequentially in block sizes determined by the "wayness" of the Program Environment. The wayness is set in the PE variable. So, for example, a 32 core, 4way job (#$ -pe 4way 32) will have ranks {0,1,2,3} assigned to the first node, {4,5,6,7} assigned to the next node, etc. The ibrun command and numa script template are shown for executing 4 tasks, one on each socket (see above diagram for socket numbers). The exported environment variables turn of all affinities of the MPI mvapich interfaces. Both memory allocation and tasks are assigned to 4 different sockets in each node (8 nodes total).

job script

```
...
#! -pe 4way 32
...
```

job script

```
...
#! -pe 4way 32
...
```

export OMP_NUM_THREADS=4
ibrun numa.sh

numa.sh

```
#!/bin/bash
            #Unset all MPI
Affinities
            export
MV2_USE_AFFINITY=0
            export
MV2_ENABLE_AFFINITY=0
            export
VIADEV_USE_AFFINITY=0
            export
VIADEV_ENABLE_AFFINITY=0


            #TasksPerNode
TPN=`echo $PE | sed 's/way//'`
            [ ! $TPN ] && echo TPN NOT defined!

            [ ! $TPN ] && exit 1

            #Get which ever MPI's rank is set


            [ "x$PMI_RANK" != "x" ]
              && RANK=$PMI_RANK


            [ "x$MPI_RANK" != "x" ]
              && RANK=$MPI_RANK

[ "x$OMPI_MCA_ns_nds_vpid" != "x" ] \
            &&
RANK=$OMPI_MCA_ns_nds_vpid
            socket=$(( $RANK % $TPN  ))

            numactl -C $socket -i all ./a.out
```

setenv OMP_NUM_THREADS 4
ibrun numa.csh

numa.csh

```
#!/bin/tcsh
          #Unset all MPI
Affinities
          setenv
MV2_USE_AFFINITY 0
          setenv
MV2_ENABLE_AFFINITY 0
          setenv
VIADEV_USE_AFFINITY 0
          setenv
VIADEV_ENABLE_AFFINITY 0


#TasksPerNode
          set TPN=`echo $PE | sed 's/way//'`


          if(! ${%TPN}) echo TPN NOT defined!

          if(! ${%TPN}) exit 0

#Get which ever MPI's rank is set


if( ${?PMI_RANK} ) eval set RANK=\$PMI_RANK

if( ${?MPI_RANK} ) eval set RANK=\$MPI_RANK

if( ${?OMPI_MCA_ns_nds_vpid} ) \

eval set RANK=\$OMPI_MCA_ns_nds_vpid

@ socket = $RANK % $TPN

numactl -C $socket -i all ./a.out
```

- CORE CONTROL:
  Precise control of mapping tasks onto the cores can be controlled by the numactl -C option, and there may be no simple arithmetic algorithm (such as using the modulo function above), to map the rank to the set of core IDs. In this scenario it is necessary to create an array of the core or node numbers, and use the rank (modulo the wayness) as an index to acquire the binding core or socket from the array. The numa scripts below shows how to use an array for the mapping. In this case the Program Environment is 14way and the set of modulo ranks {0,1,2,3,4,5,6,7,8,9,10,11,12,13,14} are mapped onto the cores {1,2,3,4,5,6,7,8,9,10,11,12,13,14} or sockets {0,0,0,1,1,1,1,2,2,2,2,3,3,3}. This is quite elaborate and may never be used, but the mechanism illustrated in the template is quite general and provides complete control over mapping. The template below illustrates processes being mapped onto cores, while the memory allocations are mapped onto sockets. NOTE: When the number of cores is not a multiple of 16 (e.g. 28 in this case), then the user must set the environment variable MY_NSLOTS to the number of cores within the job script, as shown below, AND the second argument in the -pe option (32 below), but be equal to the value of MY_NSLOTS rounded up the the nearest multiple of 16.

job script

```
...
#$ -pe 14way 32
...
export MY_NSLOTS=28
...
ibrun numa.sh
```

job script

```
...
#$ -pe 14way 32
...
setenv MY_NSLOTS 28
...
ibrun numa.csh
```

numa.sh

```
 #!/bin/bash
                  #Unset all MPI
Affinities
            export
MV2_USE_AFFINITY=0
            export
MV2_ENABLE_AFFINITY=0
            export
VIADEV_USE_AFFINITY=0
            export
VIADEV_ENABLE_AFFINITY=0


#TasksPerNode


TPN=`echo $PE | sed 's/way//'`
            [ ! $TPN ] && echo
TPN NOT defined!
            [ ! $TPN ] && exit 1

#Get which ever MPI's rank is set
            [ "x$PMI_RANK" != "x" ]
              && RANK=$PMI_RANK

            [ "x$MPI_RANK" != "x" ]
               && RANK=$MPI_RANK

            [ "x$OMPI_MCA_ns_nds_vpid"
               != "x" ] \

&& RANK=$OMPI_MCA_ns_nds_vpid

if [ $TPN = 14 ]; then

task2socket=( 0 0 0 1 1 1 1 2 2  2  2
  3  3  3 )

task2core=(   1 2 3 4 5 6 7 8 9 10 11
  12 13 14)  fi

nodetask=$(( $RANK % $TPN  ))

node=$(( $RANK / $TPN  + 1))    #

sh: 1st element is 0

socket=${task2socket[$nodetask]}

core=${task2core[$nodetask]}

numactl -C $core -m $socket ./a.out
```

numa.csh

```
#!/bin/tcsh
           #Unset all MPI
Affinities
           setenv
MV2_USE_AFFINITY 0
           setenv

MV2_ENABLE_AFFINITY
           setenv
VIADEV_USE_AFFINITY 0
           setenv
VIADEV_ENABLE_AFFINITY 0


#TasksPerNode
           set TPN=`echo $PE | sed 's/way//'`


           if(! ${%TPN}) echo TPN NOT defined!


           if(! ${%TPN}) exit 0
#Get which ever MPI's rank is set


if( ${?PMI_RANK} ) eval set RANK=\$PMI_RANK


if( ${?MPI_RANK} ) eval set RANK=\$MPI_RANK


if( ${?OMPI_MCA_ns_nds_vpid} ) \


eval set RANK=\$OMPI_MCA_ns_nds_vpid


if($TPN == 14) then


set task2socket=( 0 0 0 1 1 1 1 2 2 2  2  3
  3   3 )


set task2core=(   1 2 3 4 5 6 7 8 9 10 11 12
  13 14 )


endif


@ nodetask = $RANK % $TPN  #rank module
  tasks/node


@     node = $RANK / $TPN  + 1  #node number


#        Csh: 1st element is 1, add 1


@ nodetask++


set socket  = $task2socket[$nodetask]


set   core  =   $task2core[$nodetask]


numactl -C $core -m $socket ./a.out
```

- CHECKING NUMA SCRIPTS:

To help you test the logic of numa scripts the qchecknuma is provided to list the numactl commands as they will be executed on the nodes. The command syntax is:

qchecknuma <job_script>

This utility scans the job script for the wayness, number of cores (on the #! -pe line) and uses the first argument of the ibrun as the numa script. It then prints a numactl command, as found in the numa script, for the first 128 tasks, in rank order. Details for printing more ranks and other information are explained by invoking the qchecknuma --help command.

Tools

Program Timers & Performance Tools

Measuring the performance of a program should be an integral part of code development. It provides benchmarks to gauge the effectiveness of performance modifications and can be used to evaluate the scalability of the whole package and/or specific routines. There are quite a few tools for measuring performance, ranging from simple timers to hardware counters. Reporting methods vary too, from simple ASCII text to X-Window graphs of time series.

The most accurate way to evaluate changes in overall performance is to measure the wall-clock (real) time when an executable is running in a dedicated environment. On Symmetric Multi-Processor (SMP) machines, where resources are shared (e.g., the TACC IBM Power4 P690 nodes), user time plus sys time is a reasonable metric; but the values will not be as consistent as when running without any other user processes on the system. The user and sys times are the amount of time a user's application executes the code's instructions and the amount of time the kernel spends executing system calls on behalf of the user, respectively.

Package Timers

The time command is available on most Unix systems. In some shells there is a built-in time command, but it doesn't have the functionality of the command found in **/usr/bin**. Therefore you might have to use the full pathname to access the time command in **/usr/bin**. To measure a program's time, run the executable with time using the syntax "**/usr/bin/time -p <args>**" (**-p** specifies traditional "precision" output, units in seconds):

```
/usr/bin/time -p ./a.out          {Time for a.out execution}
real 1.54                         {Output (in seconds)}
user 0.5
sys 0
/usr/bin/time -p ibrun -np 4 ./a.out {Time for rank 0 task}
```

The MPI example above only gives the timing information for the **rank 0** task on the master node (the node that executes the job script); however, the real time is applicable to all tasks since MPI tasks terminate together. The user and sys times may vary markedly from task to task if they do not perform the same amount of computational work (are not load balanced).

Code Section Timers

"Section" timing is another popular mechanism for obtaining timing information. The performance of individual routines or blocks of code can be measured with section timers by inserting the timer calls before and after the regions of interest. Several of the more common timers and their characteristics are listed below in Table 1.

Table 1. Code Section Timers

Routine	Type	Resolution (usec)	OS/Compiler
times	user/sys	1000	Linux/AIX/IRIX/UNICOS
getrusage	wall/user/sys	1000	Linux/AIX/IRIX

gettimeofday	wall clock	1	Linux/AIX/IRIX/UNICOS
rdtsc	wall clock	0.1	Linux
read_real_time	wall clock	0.001	AIX
system_clock	wall clock	system dependent	Fortran 90 Intrinsic
MPI_Wtime	wall clock	system dependent	MPI Library (C & Fortran)

For general purpose or course-grain timings, precision is not important; therefore, the millisecond and MPI/Fortran timers should be sufficient. These timers are available on many systems; and hence, can also be used when portability is important. For benchmarking loops, it is best to use the most accurate timer (and time as many loop iterations as possible to obtain a time duration of at least an order of magnitude larger than the timer resolution). The **times**, **getrussage**, **gettimeofday**, **rdtsc**, and **read_real_time** timers have been packaged into a group of C wrapper routines (also callable from Fortran). The routines are function calls that return double (precision) floating point numbers with units in seconds. All of these TACC wrapper timers (**x_timer**) can be accesses in the same way:

```
external   x_timer                 double x_timer(void);
     real*8  :: x_timer                 ...
real*8  :: sec0, sec1, tseconds    double sec0, sec1, tseconds;
...                                ...
sec0     = x_timer()               sec0     = x_timer();
...Fortran Code                    ...C Codes
sec1     = x_timer()               sec1     = x_timer();
tseconds = sec1-sec0               tseconds = sec1-sec0
```

The wrappers and a makefile are available with a test example from TACC for instrumenting codes.

Standard Profilers

The **gprof** profiling tool provides a convenient mechanism to obtain timing information for an entire program or package. **Gprof** reports a basic profile of how much time is spent in each subroutine and can direct developers to where optimization might be beneficial to the most time-consuming routines, the "hotspots". As with all profiling tools, the code must be instrumented to collect the timing data and then executed to create a raw-date report file. Finally, the data file must be read and translated into an ASCII report or a graphic display. The instrumentation is accomplished by simply recompiling the code using the **-qp** (Intel compiler) option. The compilation, execution, and profiler commands for **gprof** are shown below for a Fortran program:

Profiling Serial Executables

ifort -qp prog.f90	{Instruments code}
a.out	{Produces gmon.out trace file}
gprof	{Reads gmon.out (default args: a.out gmon.out) (report sent to STDOUT)}

Profiling Parallel Executables

mpif90 -qp prog.f90	{Instruments code}
setenv GMON_OUT_PREFIX gout.*	{Forces each tasks to produce a gout.<pid>}
ibrun -np <#> a.out	{Produces gmon.out trace file}
gprof -s gout.*	{Combines gout files into gmon.sum}
gprof a.out gmon.sum	{Reads executable (a.out) & gmon.sum (report sent to STDOUT)}

Detailed documentation is available at www.gnu.org. A documented example of a **gprof** flat profile and call graph output is available to help you interpret **gprof** output.

Timing Tools

Most of the advanced timing tools access hardware counters and can provide performance characteristics about floating point/integer operations, as well as memory access, cache misses/hits, and instruction counts. Some tools can provide statistics for an entire executable with little or no instrumentation, while others requires source code modification.

Debugging with DDT

DDT is a symbolic, parallel debugger that allows graphical debugging of MPI applications. Support for OpenMP is forthcoming but is not available at the current DDT version.

To run on Ranger, please follow the steps below:

1. Logon to login1. DDT is installed *only* on this frontend. Also, make sure that X11 forwarding is enabled when you ssh. This can be done by passing the -X option, if X11 forwarding is not enabled in your ssh client by default.

```
your-desktop$ ssh -X login1.tacc.utexas.edu
```

2. Load the ddt module file:

```
login1$ module load ddt
```

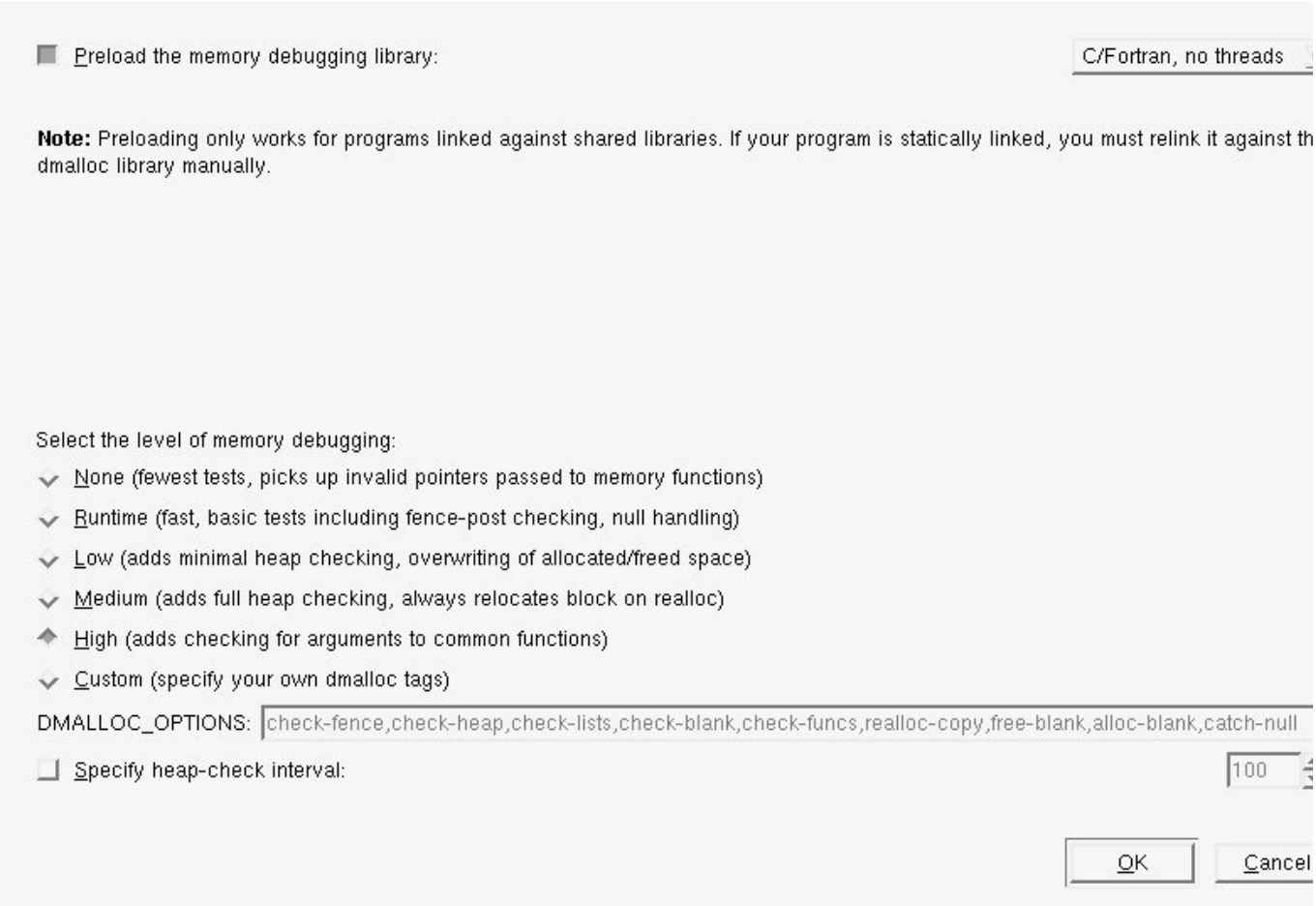
3. Create a .ddt directory in your $HOME area, and copy $DDTROOT/templates/config.ddt:

```
login1$ cd          login1$ mkdir .ddt          login1$ cp $DDTROOT/templates/config.ddt ~/.ddt
```

4. Start the DDT debugger:

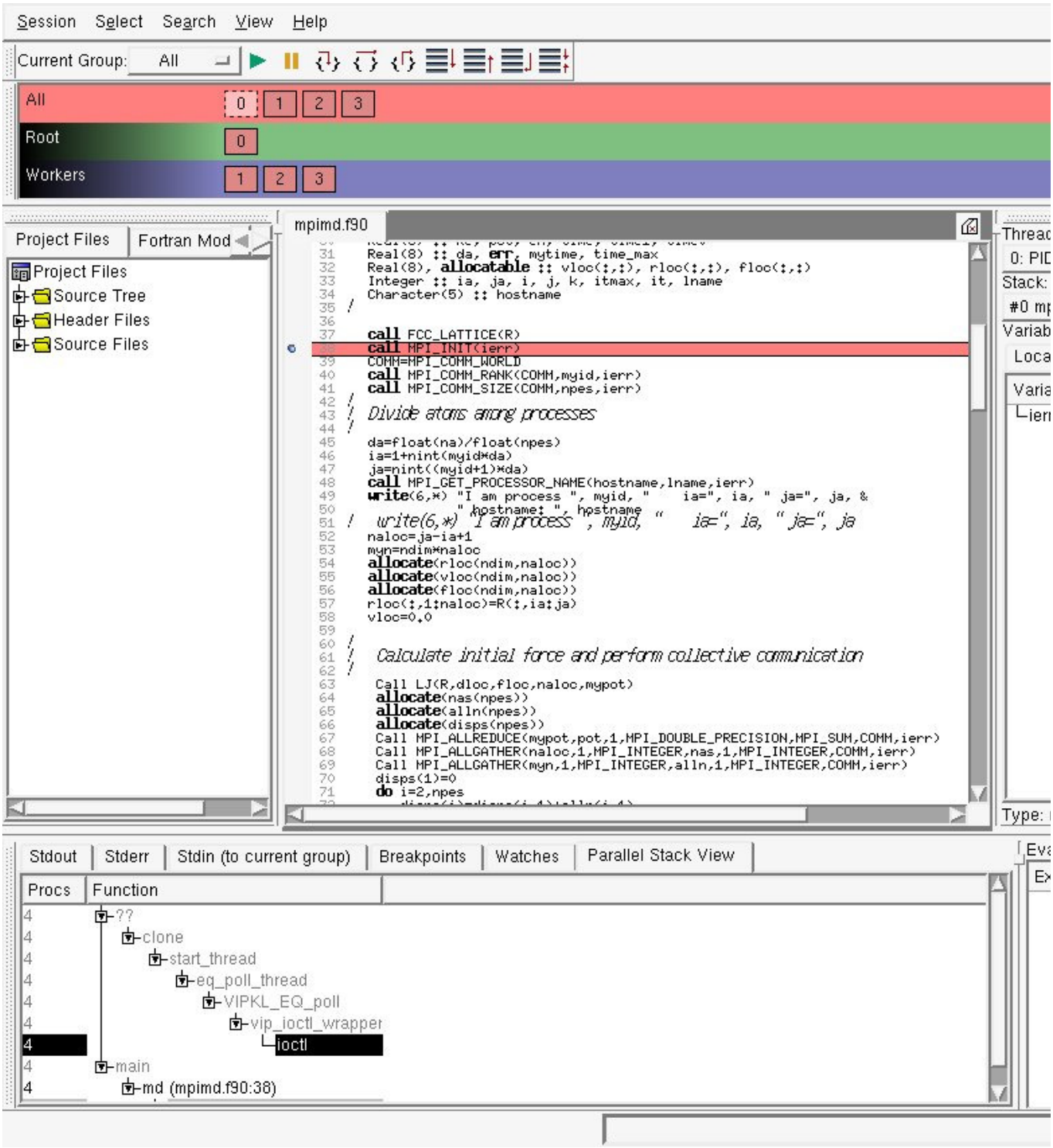
```
login1$ ddt
```

Session control window for DDT. This where you specify the executable path, command-line arguments and processor count.



Different levels of memory debugging can be enabled. Since memory debugging is implemented using DMALLOC, you can customize using DMALLOC-supported options.

5. DDT will thereafter submit a job to the development queue which will request the specified number of processors for 30 minutes. The DDT session will not start until the required resources are available for the debugging job. When the job starts running, you should see the following window appear:



For more information on how to perform parallel debugging using DDT, please consult the DDT user guide.