Titan – Getting started

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Outline

- hpc@usit
- Titan fun facts
- Getting started with Titan
- An MPI example

Research Computing Services

hpc@usit.uio.no

- Computational Physics requires High Performance Computing (HPC) resources
- USIT and the Research Computing Services (RCS) provides HPC resources and HPC support
- Resources: `titan.uio.no`
- Support: 14 people, 7 with PhD, one PhD student (me)
- Contact: `hpc@usit.uio.no`

Titan

Hardware

- 546 X2200m2, 7 X4200, Magnum 3456 IB switch
- 174 Dell 1425, + 20 HP DL385 servers
- EVA8K 120 TB storage
- Dual core Intel and AMD ($\sim$ 2500 cores in total)
- Infiniband and ethernet
- From 4GB to 64GB RAM
- Heterogenous cluster!
- To come: quad-core CPUs (april?), petabyte storage?

Software

- Batch system: Sun Grid Engine (SGE)
- Message Passing Interface (MPI):
  - Scampi
  - MPICH2
  - OpenMPI
- Compilers: GCC, Intel, Portland and Pathscale
- Optimized math libraries and scientific applications
- All you need may be found under `/site`
- Available software: `http://www.hpc.uio.no/index.php/Titan_software`

Getting started

Sounds nice. But how do we use it?

Getting started

Batch systems

- A batch system controls the use of the cluster resources
- Submits the job to the right resource
- Monitors the job while executing
- Restarts the job in case of failure
- Takes care of priorities and queues to control execution order of unrelated jobs

Sun Grid Engine

- SGE is the batch system used on Titan
- Jobs are executed either interactively or through job scripts
- Useful commands: `showq`, `qlogin`, `qsub`
- `http://www.hpc.uio.no/index.php/FAQ#QUEUE_SYSTEM`

Modules

- Different compilers, MPI-versions and applications need different sets of user environment variables
- The `modules` package lets you load and remove the different variable sets
- Useful commands:
  - List available modules: `module avail`
  - Load module: `module load <environment>`
  - Unload module: `module unload <environment>`
  - Currently loaded: `module list`
- `http://www.hpc.uio.no/index.php/FAQ#MODULES`

Example

Interactively

```
# login to titan
$ ssh titan.uio.no
# ask for 4 cpus
$ qlogin -P uio -pe mpi 4
# we want to use mpich2
$ module load mpich2
$ mkdir -p fys4410/mpiexample/
$ cd fys4410/mpiexample/
# download program5.cpp from the course pages:
$ wget http://tinyurl.com/39hrah/program5.cpp
# compile the program
$ mpicxx -O3 -o program5.x program5.cpp
# and execute it
$ mpiexec ./program5.x
Result: 3.14159
# finished, so logging out
$ exit
```

The job script

job.sge

```
#!/bin/sh
# 4 cpus with mpi (or other communication)
#$ -pe mpi 4
# 10 mins of walltime
#$ -l s_rt=0:10:0
# project uio
#$ -P uio
# we need 512 MB of memory per process
#$ -l s_vmem=512M
# name of job
#$ -N program5

source /site/bin/jobsetup

# load the module used when we compiled the program
module load mpich2

# start program
/site/bin/mpiexec ./program5.x

#END OF SCRIPT
```

Example

Submitting

```
# login to titan
$ ssh titan.uio.no
# we want to use mpich2
$ module load mpich2
$ cd fys4410/mpiexample/
# compile the program
$ mpicxx -O3 -o program5.x program5.cpp
# and submit it
$ qsub job.sge
$ exit
```

Checking execution

```
# check if job is running:
$ qstat -u jonkni
job-ID  prior   name       user         state submit/start at     queue
                              slots ja-task-ID
-----------------------------------------------------------------------------
 379931 2.50073 rectangle  jonkni       r     01/17/2008 06:02:39 normal@compute
      -13-6.local          4
# results are in rectangle.o379931
$ cat rectangle.o379931
Starting job 379931 on node compute-13-6.local at Thu Jan 17 06:02:39 CET 2008
Creating /work/379931.undefined.d
Result: 3.14159
Terminating job 379931 on compute-13-6.local at Thu Jan 17 06:02:44 CET 2008
Deleting /work/379931.undefined.d
```

Tips and admonitions

Tips

- Titan FAQ: `http://www.hpc.uio.no/index.php/FAQ`
- man-pages, e.g. `man qsub`
- Ask us

Admonitions

- Remember to exit from qlogin-sessions; the resource is reserved for you untill you exit
- Don't run jobs on login-nodes; these are only for compiling and editing files

Good luck!