Using the CITRIS Cluster and the NERSC Seaborg System

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Outline

CITRIS Cluster
  - Hardware
  - Storage
  - Running Jobs
  - Tools
  - Reporting Problems

Measuring Performance

NERSC Seaborg
  - Hardware
  - Storage
  - Running Jobs
  - Tools
  - Reporting Problems

x86 Millennium Cluster
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x86 Millennium Cluster
CITRIS Cluster – Itanium 2

- 64 Dual Itanium 2 nodes (61 compute, 3 frontend).
- 900 MHz Slow Nodes (22) – McKinley
- 1.3 GHz Fast Nodes (42) – Madison
- 32 KB L1, 256 KB L2, and 1.5 / 3.0 MB L3 Cache
- 4 GB memory per node.
- Nodes c16-c32 are on fast Myrinet network
  \( \approx 800 \text{ MB/s} - 1 \text{ GB/s} \).
Itanium 2 (1.3 GHz)

- Two FMA (fused multiply-add) units, peak of 5.2 GFlop/s.
- Also has vector instructions (two single-precision entries).
- 128 integer (64-bit) and floating-point (82-bit) registers.
- Caches: 32 KB, 256 KB, 3 MB
- Line sizes: 64 b, 128 b, 128 b.
- Cache bandwidth: 32 GB/s.
- Memory bandwidth: 6.2 GB/s.
- Details in *Intel Itanium 2 Processor Reference Manual for Software Development and Optimization*
Storage

- **Home directory – NFS, slow.**
  Semi-permanent space. Use for keeping long term files.

- **Shared workspace /work.**
  - Shared by all the nodes.
  - `mkdir /work/username`
  - 30-day deletion policy.
  - Not backed up, meant for staging runs.

- **Local scratch space /scratch**
  - Fast, but each node has its own /scratch.
  - High-speed RAID0 storage.
  - 10-day deletion policy.
  - Not backed up, for use with program checkpointing.
Shared Interactive Use

▶ 45 nodes (both 900 MHz and 1.3 GHz) for shared use.
▶ Frontend login nodes
  \{lemon, lime\}.millennium.berkeley.edu
▶ Shared use: immediately starts, but speed depends on the load.
▶ Don’t run heavy jobs on login nodes.
▶ Use gexec to run jobs.
  ▶ Set environment variable GEXEC_SVRS.
    \texttt{export GEXEC_SVRS="c1 c2 c3 c4"}
  ▶ Specify number of processors to gexec
    \texttt{gexec -n 4 /path/to/my/program}
  ▶ Can use screen program to detach from terminal session to reattach later.
▶ Use gstat to show the load on each node.
Batch System

- 16 nodes (all 1.3 GHz).
- Frontend login node: grapefruit.millennium.berkeley.edu
- Queue system:
  - gets exclusive use of nodes requested, but must wait in queue.
  - Jobs requesting many nodes may spend long time in the queue.
- PBS (Portable Batch System)
  - Installed in /usr/pbs/bin, man pages in /usr/pbs/man.
  - Use qsub myscript to submit jobs.
    Still need gexec or mpirun in the script.
  - Use qstat for queue status.
  - Use qdel to cancel a submitted job.
- When a node is allocated, you get both processors.
Example Script

```bash
#!/bin/sh
#PBS -l nodes=7:ppn=2
#PBS -l mem=400mb
#PBS -l walltime=1:00:00
gexec -n 0 /path/to/my/program
```

- Lines starting with `#PBS` are PBS directives.
  - Requests 7 nodes, 2 processors each (total of 14 processors).
  - Will use maximum of 400 MB of memory.
  - Will run at most 1 hour.
  - Always specify these to guard against program bugs.
  - Many other directives described in *PBS Pro Users Guide*.

- Submit with `qsub myscript`.

- After execution, output (stdout and stderr) saved in files `myscript.o<job_id>` and `myscript.e<job_id>`
Tools on CITRIS

- Located in /usr/mill, /usr/mill/pkg.
  - Add /usr/mill/bin to your $PATH.
  - Add /usr/mill/lib to your $LD_LIBRARY_PATH.
  - Add /usr/mill/man to your $MANPATH.

- Compilers
  - GNU gcc version 3.3.5 in /usr/bin.
  - Intel C++/Fortran 90 compiler icc and ifort (version 8.1) in /usr/mill/bin.

- Debuggers: gdb, ddd, idb (Intel).


- PAPI: /usr/mill/lib.
Reporting Problems

▶ Mail support@millennium.berkeley.edu.
▶ Visit 505 Soda Hall if above doesn’t solve the problem (also inform me as well).
▶ Semi-Frequent issues
  ▶ Home directory gone: file server problem.
  ▶ gexec hangs. meanwhile try other nodes in GEXEC_SVRS.
  ▶ Installed program doesn’t work. Inform support@millennium, and/or install them yourself.
  ▶ Batch system doesn’t work. Inform support@millennium, perhaps visit 505 Soda.
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x86 Millennium Cluster
Things that Affect Performance

- Parallel use of functional units:
  - Floating point vs. integer operations.
  - Multiple functional units
  - Fused multiply-accumulate units.
- Cache effects: cache hit / miss numbers.
- Paging effects: TLB miss numbers.
- Algorithm (e.g., basic matrix multiply vs. Strassen)
Timing and Counting

- Modern systems generally have good timing routines.
  - High resolution (micro- or nano-seconds).
  - Overhead much higher than resolution.
    ⇒ Need enough work to measure time spent.
  - Wall clock (real time): actual time elapsed.
  - Processor time: CPU time spent by that process.

- Most processors have hardware counters for various events.
  - Cache / TLB misses, Floating point operations, etc.
  - Number of events that can be counted may be limited.
Timing Routines

- `clock()` (res 1 ms, overhead 0.4 µs)
  - Measures time used by the process
  - Resolution OS/Hardware dependent
  - `CLOCKS_PER_SEC` does not indicate resolution.

- `gettimeofday()` (res 1 µs, overhead 0.4 µs).
  - Wall clock
  - Usually in microsecond resolution.

- `clock_gettime()` (res 1 µs, overhead 0.4 µs).
  - `CLOCK_REALTIME` measures wall clock.
  - `CLOCK_PROCESS_CPUTIME_ID` measures process time.
  - May require linking with `-lrt`.

- MPI: `MPI_Wtime()`

- PAPI: `PAPI_get_real_cyc()`, `PAPI_get_real_usec()`
Profilers and Counters

- `gprof` - general profilers, gives a general idea of where the bottleneck is.
- `perfctr` - Linux x86
- `hpm` - IBM Power series
- `PAPI` - common API for many platforms (including CITRIS and Seaborg).
  - Various events: number of cycles, cache misses, flops, etc.
  - Note: not all events on all platforms.
  - Different incompatible versions
    (3.0 on Seaborg, 2.3.x on CITRIS).
#include <stdio.h>
#include <unistd.h>
#include <papi.h>

int main() {
    long_long tm1, tm2;
    PAPI_library_init(PAPI_VER_CURRENT);
    tm1 = PAPI_get_real_cyc();
    sleep(1);
    tm2 = PAPI_get_real_cyc();
    printf("%lld\n", tm2 - tm1);
    return 0;
}
Using PAPI

% gcc -o papi -O2 -Wall  
  -I/usr/mill/pkg/papi/include/papi-2.3.4  
papi.c -L/usr/mill/lib -lpapi  
% ./papi  
1300064584  
%

- Gives $1.3 \times 10^9$ cycles,  
  which is what we expect on 1.3 GHz system.
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NERSC Seaborg

- 416 (380 compute) 16-way SMP nodes (peak of 10 TFlop/s).
- Total of 6656 (6080 compute) 375 MHz IBM Power 3+ processors.
- Total of 7.3 TB memory.
- 44 TB of disk space in GPFS.
- Additional storage in HPSS: 8.8 PB, 50 TB disk cache, 3.2 GB/s theoretical bandwidth.
- Two high speed network card per node.
- Rest of nodes for GPFS, login, network, spare.
IBM Power 3+

- Clock speed: 375 MHz.
- Two FMA units: peak performance of 1.5 Gflop/s.
- Caches: L1 inst. 32 KB, L1 data 64 KB, L2 8 MB (6.4 GB/s).
- L1 line size: 128 b.
- Memory per node: 16-64 GB (4 have 64 GB; 64 have 32 GB; 312 have 16 GB).
- Memory bandwidth: 1.6 GB/s (1.3 GB/s daxpy).
Seaborg Storage

- **Home directory ($HOME)**
  - 15 GB (GPFS), available from every node.
  - Not backed up.

- **Scratch space ($SCRATCH)**
  - 33 TB (GPFS), shared by everyone, user quota of 250 GB.
  - Available from every node.
  - Nominal 7-day deletion policy, but files may be deleted anytime after the job finishes.
  - Not backed up.

- User quota can be checked by `myquota`.

- Do not use `/tmp` or `/var/tmp`.
Interactive Jobs

- Login nodes: seaborg.nersc.gov
- Debug on login nodes and special debug nodes.
- Interactive jobs limited to 8 nodes, 30 minutes.
Batch System

- LoadLeveler queue system
  - Batch jobs use commented shell script (as in CITRIS).
  - `llqs` – lists full queue.
  - `llqs -u username` – lists your jobs.
  - `llsubmit myscript` – submit a job in myscript.
  - `llcancel <job_id>` – cancel a job in queue.

- More information at
Example Script

```bash
#@ job_name = myjob
#@ account_no = mp309
#@ output = myjob.out
#@ error = myjob.err
#@ job_type = parallel
#@ notification = complete
#@ network.MPI = csss,not_shared,us
#@ node_usage = not_shared
#@ class = regular
#@ tasks_per_node = 16
#@ node = 1
#@ wall_clock_limit = 01:00:00
#@ queue
./my_program
```

Class Repository

- Supercomputer time is a limited resource!
- Class repository: mp309.
- Class allocation: 20,000 processor-hours.
- Each person has been allocated $\approx 6\%$ of this.
- Please conserve allocated processor time by
  - Debug thoroughly before submitting large job.
  - Using as many of the 16 processors in each node. (If you use a node, you will be charged for all 16 processors on it.)
  - Setting memory and time limits to your jobs.
  - Use CITRIS cluster.

- If you run out of your allocation:
  - Use your project partners’ allocation.
  - Contact me, I’ll see what I can do.
Tools on Seaborg

- **Modules**
  - See all modules: module avail.
  - To use a particular module: module use <modulename>.
  - IBM C compiler: module xlc.

- **Compilers**
  - gcc/g++/g77 3.4.1, 3.3, 3.2.1.
  - IBM compilers xlc (C), xlC (C++), xlf (F77), xlf90 (F90).

- **Debuggers**: gdb, totalview, ddd, dbx.

- **GNU Tools**: module use gnu.
Using PAPI on Seaborg

% module load papi
% xlc -o papi papi.c $PAPI
% ./papi
375064125

► PAPI version 3.0 on Seaborg (2.3.2 on CITRIS).
Reporting Problems

- Check status
  - http://www.nersc.gov/nusers/status/
  - http://www.nersc.gov/nusers/status/motd.php

- Contacts
  - Seaborg Docs:
    http://www.nersc.gov/nusers/resources/SP/
  - Help page: http://www.nersc.gov/nusers/help/

- Password issues
  - Log into sadmin.nersc.gov to set/change password.
  - Wait an hour after password changes.
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- Pentium IIIs, some dual, some quad.
- Mix of 500, 550, 700 MHz nodes.
- 512 KB, 1 MB L2 caches.
- Use for testing / fun.
- Login nodes \{napa, sonoma\}.millennium.berkeley.edu.
- Use gexec with nodes mm1, mm2, etc.