User Environment on Super Mike II

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User Services
HPC @ LSU

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Outline

- User environment
  - System access and file systems
  - Software stack
  - Compiling programs on Super Mike II – GPU-accelerated code and Open MPI
  - Job management
- Applications benchmark results

SuperMikeII

- Ranked 250 in Nov 2012 Top 500 list
- 440 nodes, dual 8-core Intel Sandy Bridge Xeon processors @ 2.6GHz, including
  - 382 nodes with 32 GB RAM
  - 50 GPU nodes with 64 GB RAM and dual NVIDIA Tesla M2090 GPUs
  - 8 nodes with 256 GB RAM, capable of aggregation into a single virtual symmetric multiprocessing (vSMP) using ScaleMP
- 146 CPU TFLOPS and 66 GPU TFLOPS (double-precision)
- 364 TB of storage space
- Mellanox Infiniband network

Accessing the Clusters

- Host name: ***mike.hpc.lsu.edu***
- Use ssh to connect
  - Unix-alike and Mac: "`ssh <host name>`" in a terminal window
  - Windows: use **Putty** or other ssh clients
- The default log in shell is bash
  - Supported: bash, tcsh, csh, ksh and sh

Connection with X11 Forwarding

- Some software packages have GUI, which requires X11 forwarding to be established with the ssh connection
- Unix/Linux users
  - Use the "-X" option of ssh
- Mac users
  - Use the "X11" application
- Windows users
  - Install X server for Windows (e.g. Xming)
  - Enable X11 forwarding in the ssh client

File Systems

	Distributed	Throughput	File life time	Best used for
Home	Yes	Low	Unlimited	Code in development, compiled executable
Work/Scratch	Yes	High	30 or 60 days	Job input/output
Local scratch	No		Job duration	Temporary files

- Tips
  - Never let you job write output to your home directory
  - Do not write temporary files to /tmp
    - Write to the local scratch or work space
  - The work space is not for long-term storage
    - Files are purged periodically
  - Use "`rmpurge`" to delete large amount of files

Disk Quota

Cluster	Home		Work		Local scratch
	Access point	Quota	Access Point	Quota	Access point
SuperMikeII	/home/$USER	5 GB	/work/$USER	None	/var/scratch

- No quota is enforced on the /work space on Super Mike II (146TB total)
  - Again, it is subject to a purge every 30 to 60 days
- The work directory is created within an hour after the first login
- Command to check current disk usage: `showquota`

Storage Allocation on /project

- One can apply for extra disk space on the /project volume (218TB total on Super Mike II) if
  - your research requires some files to remain on the cluster for a fairly long period of time; **and**
  - their size exceeds the quota of the /home
- The unit is 100 GB
- Storage allocations are good for 6 months, but can be extended based on the merit of the request
- Examples of valid requests
  - I am doing a 6-month data mining project on a large data set
  - The package I am running requires 10 GB of disk space to install
- Examples of invalid requests
  - I do not have time to transfer the data from my scratch space to my local storage and I need a temporary staging area

File Transfer

- From/to a Windows machine
  - Use a client that supports the scp protocol (e.g. WinSCP, Filezilla)
- From/to a Unix/Linux/Mac machine (including between the clusters)
  - `scp` command
    - Syntax: `scp <options> <source> <destination>`
  - `rsync` command
    - Syntax: `rsync <options> <source> <destination>`

Software Stack

- Similar to other LSU HPC Linux clusters
  - Installed under `/usr/local/packages`
- Compiler
  - Default: Intel 13.0.0
  - Also available: Intel 12.1.4, PGI-12.8, PGI-11.5, GCC-4.7.2, GCC 4.4.6
- MPI
  - Default: OpenMPI 1.6.2
  - Also available: Mvapich2 1.8.1, Mvapich2 1.9a2

Software Stack Cont'd

- Script language
  - Python 2.7.3
  - Perl 5.10.1
  - Ruby 1.9.3
- Application software
  - NAMD, Matlab, Mathematica, DDT…
- A complete list available at http://www.hpc.lsu.edu/docs/guides/index.php#Supermike2
  - Or use the `softenv` command to find out
- User requested software will be installed in the user's home space
  - Unless requested by multiple users, in which case it will be installed under /usr/local/packages

Using SOFTENV

- Environment variables
  - PATH: where to look for executables
  - LD_LIBRARY_PATH: where to look for shared libraries
  - Other custom environment variables needed by various software
- **SOFTENV** is a software that helps users set up environment variables properly to use software packages
  - Much more convenient than setting environment variables in .bashrc or .cshrc

Listing All Packages

- Command "softenv" lists all packages that are managed by SOFTENV

```
[lyan1@mike1 ~]$ softenv
SoftEnv version 1.6.2

…

These are the keywords explicitly available:

    +ImageMagick-6.7.9-gcc-4.4.6   @types: library @name: ImageMagick @version:
                                     6.7.9 @build: ImageMagick-6.7.9-gcc-4.4.6
                                     @internal: @external:
                                     http://www.imagemagick.org @about: A
                                     software suite to create, edit, and compose
                                     bitmap images.
    +Intel-12.1.4                  @types: Compiler @name: Intel compiler suite
                                     @version: 12.1.4 @build: Binary
                                     installation @internal: @external:
                                     http://software.intel.com/en-
```

Searching A Specific Package

- Use “-k” option with “softenv”

```
[lyan1@mike1 ~]$ softenv -k fftw
…


These are the keywords explicitly available:

    +fftw-3.3.2-Intel-13.0.0       @types: library @name: fftw @version: 3.3.2
                                     @build: Intel-13.0.0 @internal: @external:
                                     www.fftw.org @about: A fast, free C FFT
                                     library; includes real-complex,
                                     multidimensional, and parallel transforms.
    +fftw-3.3.3-Intel-13.0.0       @types: library @name: fftw @version: 3.3.3
                                     @build: Intel-13.0.0 @internal: @external:
                                     www.fftw.org @about: A fast, free C FFT
                                     library; includes real-complex,
                                     multidimensional, and parallel transforms.
```

Setting up Environment via Softenv – permanent change

- Set up the environment variables to use a certain software package
  - First add the key to $HOME/.soft
  - Then execute resoft at the command line
  - The environment will be the same next time you log in

```
[lyan1@mike1 ~]$ cat .soft
#
# This is the .soft file.
+portland-12.8
@default
[lyan1@mike1 ~]$ resoft
[lyan1@mike1 ~]$ which pgf90
/usr/local/compilers/pgi/linux86-
64/12.8/bin/pgf90
```


Setting up Environment via Softenv – one time change

- Set up the environment variables to use a certain software package **in the current login session only**
  - Add a package: soft add <key>
  - Remove a package: soft delete <key>

```
[lyan1@mike1 ~]$ which gcc
/usr/bin/gcc
[lyan1@mike1 ~]$ gcc --version
gcc (GCC) 4.4.6 20110731 (Red Hat 4.4.6-3)
[lyan1@mike1 ~]$ soft add +gcc-4.7.2
[lyan1@mike1 ~]$ which gcc
/usr/local/compilers/GNU/gcc-4.7.2/bin/gcc
[lyan1@mike1 ~]$ gcc --version
gcc (GCC) 4.7.2
```

Querying a Softenv key

- Command "soft-dbq" shows which variables are set by a SOFTENV key

```
[lyan1@mike1 ~]$ soft-dbq +portland-12.8

Name: +portland-12.8
Description: @types: Compiler @name: The Portland Group Compilers @version: 12.8 @about:
Portland Group's high-performance compilers and tools.
-----------------------------------------
On the Linux architecture,
the following will be done to the environment:

  The following environment changes will be made:
    CUDA_NIC_INTEROP = 1
    LD_INCLUDE_PATH = ${LD_INCLUDE_PATH}:/usr/local/compilers/pgi/linux86-64/12.8/include
    LD_LIBRARY_PATH = ${LD_LIBRARY_PATH}:/usr/local/compilers/pgi/linux86-
64/12.8/libso:/usr/local/compilers/pgi/linux86-64/12.8/lib
    MANPATH = ${MANPATH}:/usr/local/compilers/pgi/linux86-64/12.8/man
    PATH = ${PATH}:/usr/local/compilers/pgi/linux86-64/12.8/bin
    PGI = /usr/local/compilers/pgi
```

Compilers

Language	Vendor			
	Intel	PGI	GNU	NVIDIA
Fortran	ifort	pgf77, pgf90	gfortran	
C	icc	pgcc	gcc	
C++	icpc	pgCC	g++	
CUDA				nvcc

- Usage: <compiler> <options> <your_code>
  - Example: `icc -O3 -o myexec mycode.c`

Compiling CUDA Programs

- Add the softenv keys for CUDA and NVIDIA driver
  - Currently `+cuda-4.2.9` and `+nvidiadriver-default`
- Use the `nvcc` command to compile

```
[lyan1@mike401 asyncAPI]$ nvcc -I../../common/inc/ asyncAPI.cu
[lyan1@mike401 asyncAPI]$ ./a.out
[./a.out] - Starting...
GPU Device 0: "Tesla M2090" with compute capability 2.0

CUDA device [Tesla M2090]
time spent executing by the GPU: 22.31
time spent by CPU in CUDA calls: 0.04
CPU executed 132214 iterations while waiting for GPU to finish
```

Compiling CUDA Fortran Programs

- CUDA Fortran
  - Fortran interface to CUDA
  - PGI v12.8 is the only compiler that supports it on Super Mike II

```
[lyan1@mike405 cudaFortran]$ which pgf90
/usr/local/compilers/pgi/linux86-64/12.8/bin/pgf90
[lyan1@mike405 cudaFortran]$ pgf90 matmul.CUF
[lyan1@mike405 cudaFortran]$ ./a.out
  arrays sized            512  by          1024  by           512
 calling mmul
 Kernel time excluding data xfer:    2665.000      microseconds
 Megaflops excluding data xfer:      100726.3
 Total time including data xfer:     219162.0      microseconds
 Megaflops including data xfer:      1224.827
  C(1,1) =    3.5791874E+11
  C(2,2) =    3.5739933E+11
  No errors found
```

Compiling OpenACC Programs

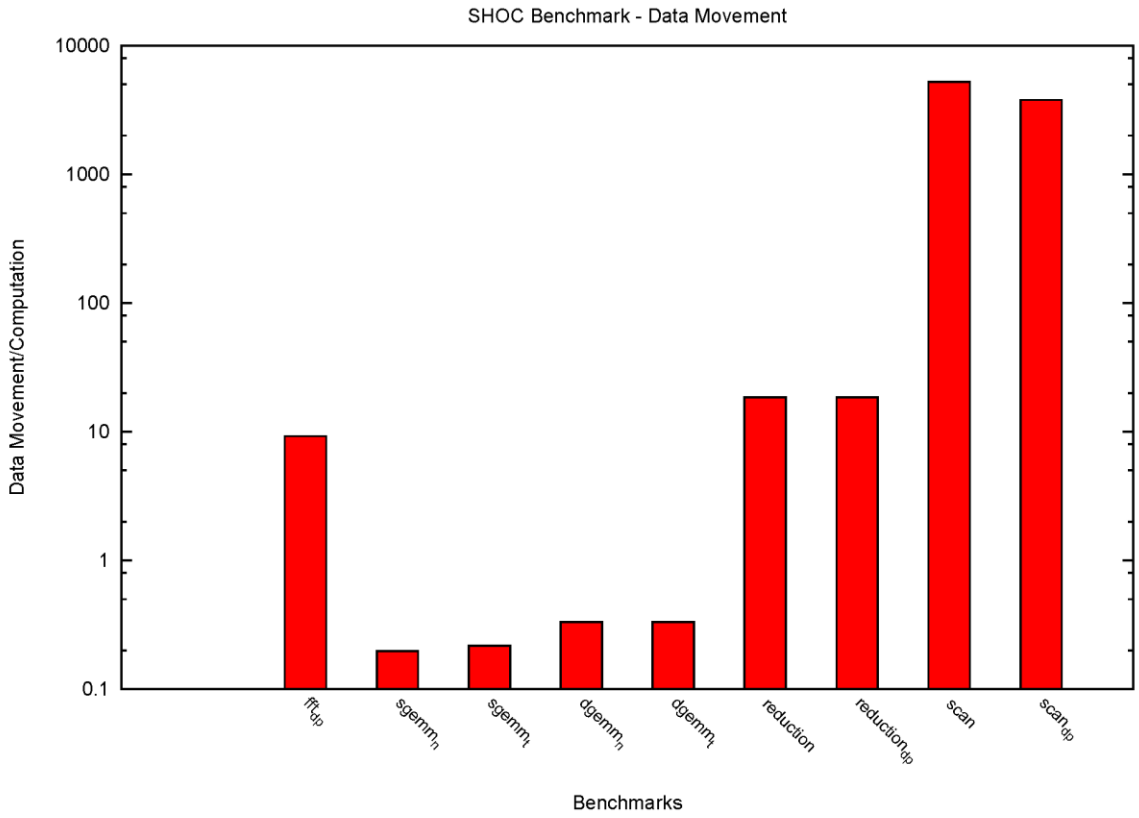
- OpenACC
  - Directive-based programming for code running on accelerators with syntax similar to OpenMP
  - Available in Fortran, C and C++
- Supported via PGI 12.8

```
[lyan1@mike401 openacc]$ pgf90 vecadd.f90 -ta=nvidia -Minfo
vector_add:
     11, Generating copyout(c(1:10))
         Generating copyin(a(1:10))
         Generating copyin(b(1:10))
         Generating compute capability 1.0 binary
         Generating compute capability 2.0 binary
     12, Loop is parallelizable
         Accelerator kernel generated
         12, !$acc loop gang, vector(32) ! blockidx%x threadidx%x
             CC 1.0 : 7 registers; 52 shared, 12 constant, 0 local memory bytes
             CC 2.0 : 14 registers; 0 shared, 68 constant, 0 local memory bytes
```

SHOC Benchmark

- **S**calable **H**eter**O**geneous **C**omputing Benchmark Suite
  - Multiple benchmarks in both CUDA and OpenCL
  - Supports multiple devices per node
  - Inter-node parallel benchmarks with MPI
  - Both performance tests and stability tests

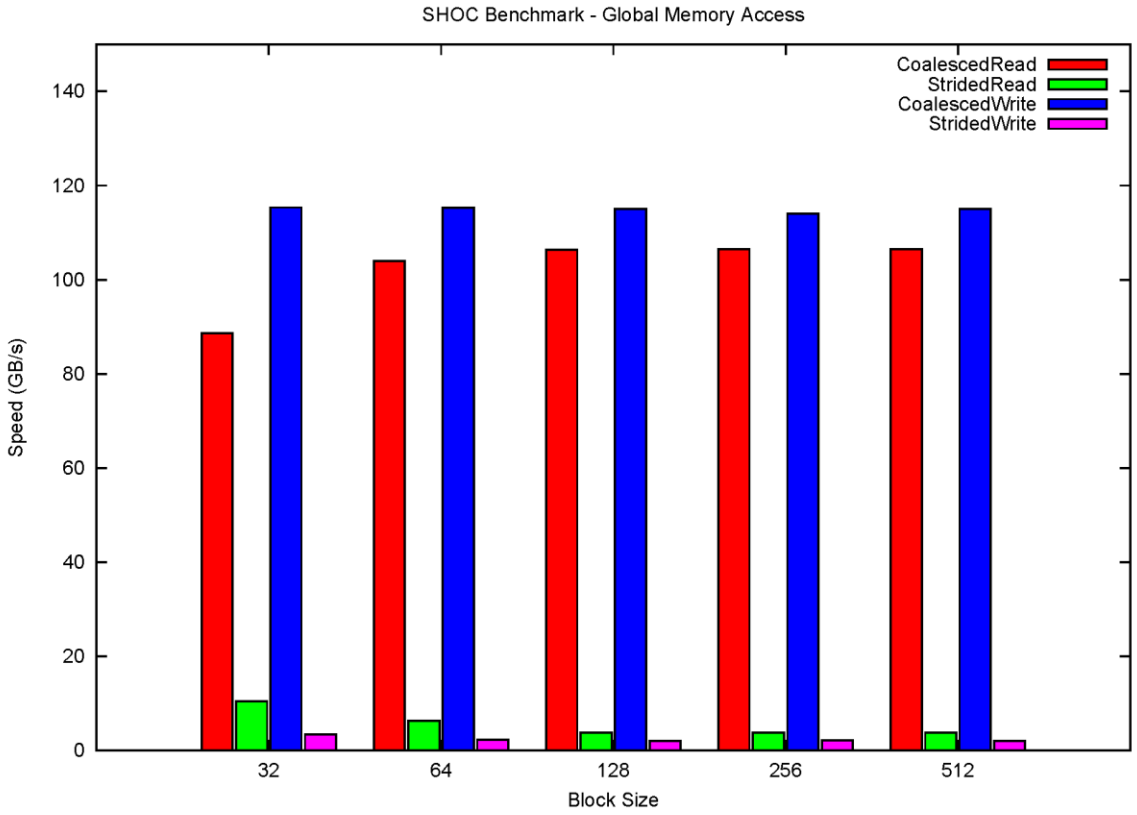
SHOC – Data Movement over PCIe



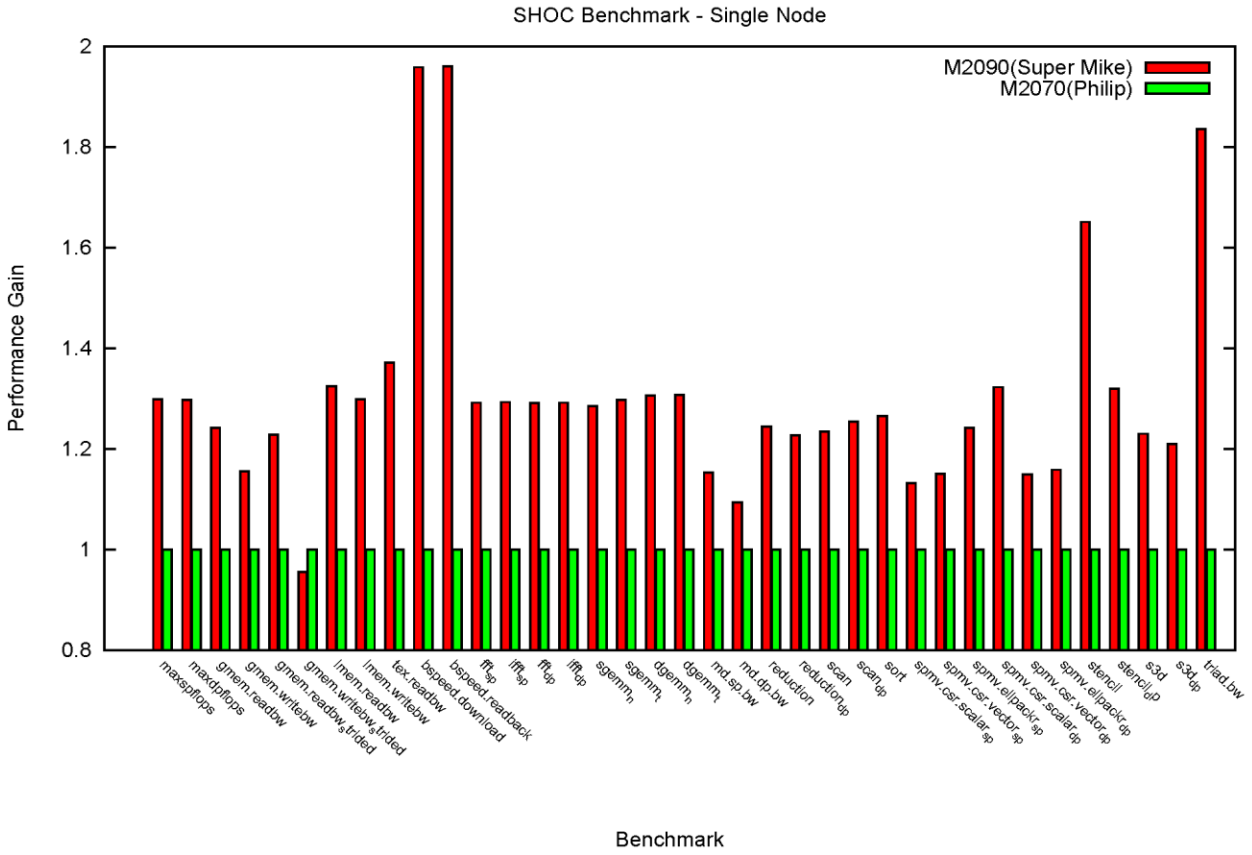
Very slow!

SHOC 1.1.4, Serial (single node) benchmarks, Size 4

SHOC – Coalesced vs Strided Memory Access

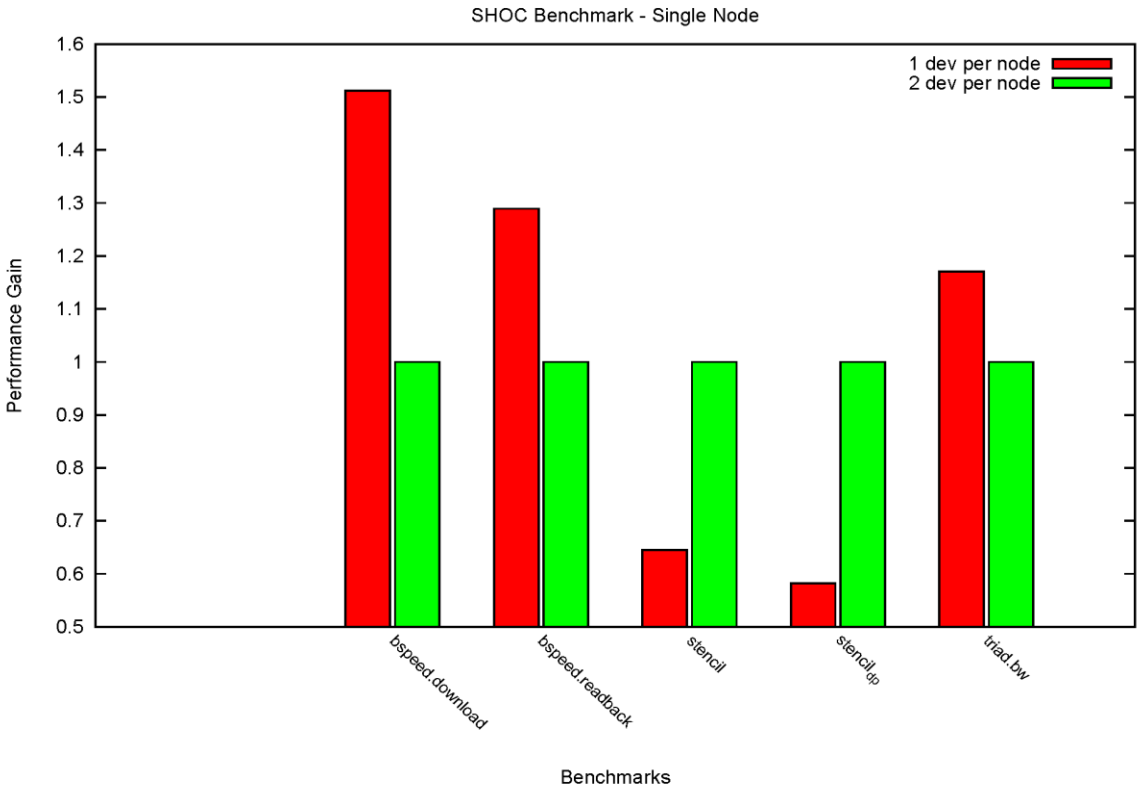


SHOC - Tesla M2090 vs M2070



SHOC 1.1.4, Serial (single node) benchmarks, Size 4

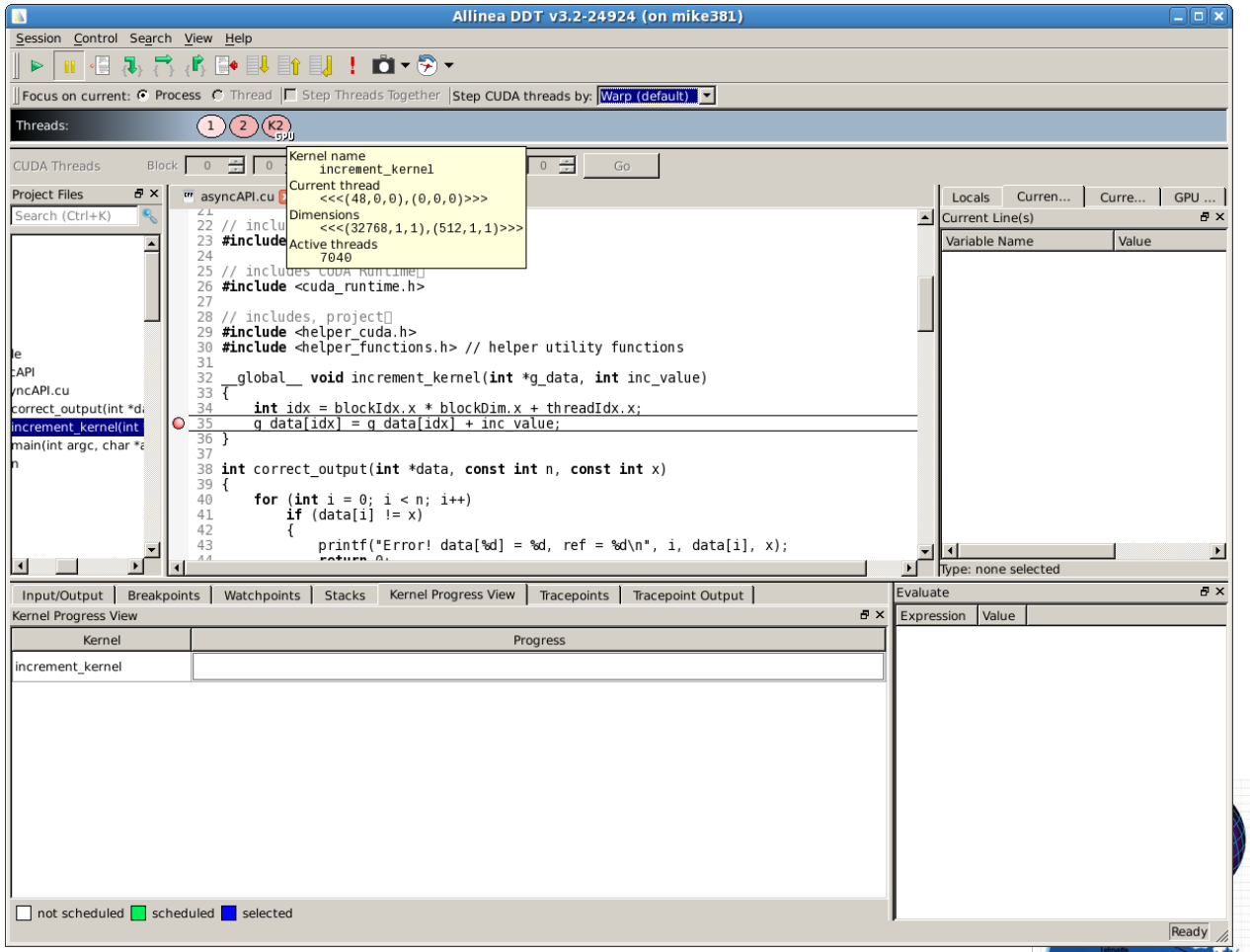
SHOC – Single vs Multiple Devices



SHOC 1.1.4, Parallel (MPI) benchmarks, Size 4

Debugging GPU Programs

- NVIDIA cuda-gdb
  - Command line debugger that comes with CUDA toolkit
  - CUDA only
- DDT
  - Parallel debugger that supports CUDA
    - Step through CUDA kernel
    - Examine data in GPU memory



MPI Compilers (1)

Language	Compiler command
Fortran	mpif77, mpif90
C	mpicc
C++	mpiCC

- Usage: similar to what we have seen
  - Example: `mpif90 -O2 -o myexec mycode.f90`
- On Super Mike II
  - The default MPI is OpenMPI 1.6.2
    - Keys:

```
+openmpi-1.6.2-Intel-13.0.0
+openmpi-1.6.2-gcc-4.4.6
+openmpi-1.6.2-gcc-4.7.2
+openmpi-1.6.2-pgi-12.8
```


MPI Compilers (2)

- The MPI compilers are **wrappers**
  - They still use the compilers we've seen on the previous slide
    - Intel, PGI or GNU
  - They take care of everything we need to build MPI codes
    - Head files, libraries etc.
  - What they actually do can be reveal by the `--show` option
- It's extremely important that you compile and run your code with the same version of MPI
  - Use the default version (+openmpi-1.6.2-Intel-13.0.0) if possible

OpenMPI - mpirun

- Use `mpirun` or `mpiexec` (identical for OpenMPI) to run
- Options
  - `-np`: number of processes
  - `-hostfile` (or `-machinefile`): name of the host file
  - `--mca <parameter> <value>`: specify run-time environment
    - Back-end network, resource manager support etc.
    - Ex: "`--mca btl ^tcp`" prevents tcp from being used for point-to-point communication

OpenMPI – mpirun (cont'd)

- Options (cont'd)
  - `--bind-to-core`: bind processes to specific cores (default is not to)
    - Performance consideration mainly for MPI-OpenMP hybrid programs
    - `--byslot`: assign processes round-robin by slot (default)
    - `--bysocket`: assign processes round-robin by socket
    - `--bynode`: assign processes round-robin by node

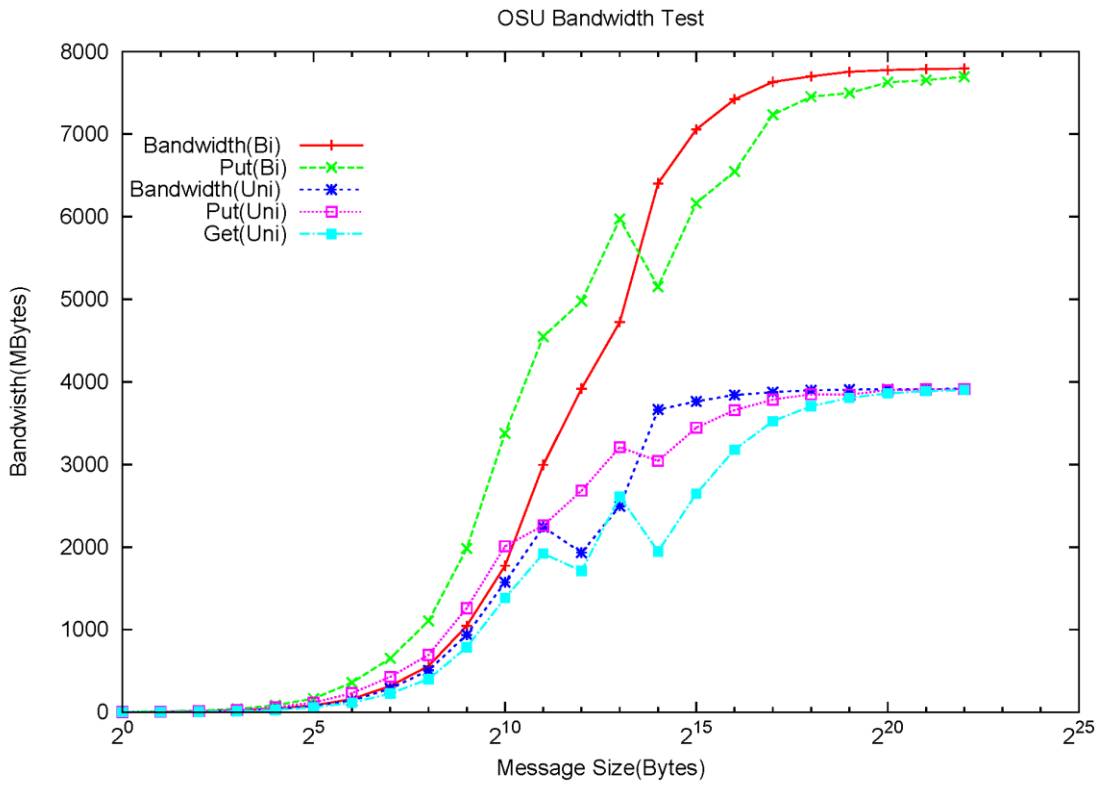
OpenMPI Commands

- Useful commands other than mpirun
  - `ompi_info`: tells everything about the OpenMPI installation
    - Ex: `ompi_info -param btl all`
  - `ompi-top`: Diagnostic to provide process info similar to the popular "top" program
  - `ompi-ps`: Displays information about the active jobs and processes in Open MPI

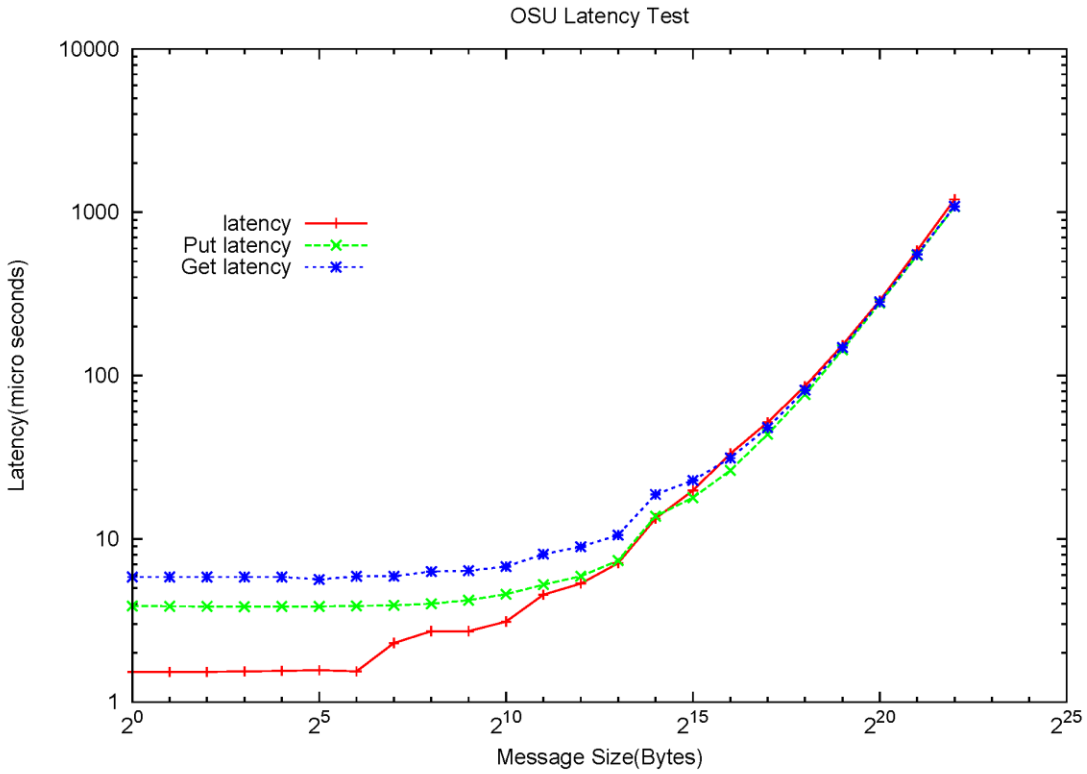
OpenMPI Configuration

- Determined by (in the given order)
  - mpirun command line
  - Environment variables
  - File
    - `$HOME/.openmpi/mca-params.conf`
    - `<OpenMPI installation path>/etc/openmpi-mca-params.conf`
  - Default
- Defined by `openmpi-mca-params.conf` on Super Mike II
  - FCA is turned off by default
    - Because of firmware issues, but
    - Consider to turn it on to reduce latency when you have many collective MPI calls with large message size (`--mca coll coll_fca_enable 1`)
  - MPI_LEAVE_PINNED is turned off by default
    - May hang multi-threaded MPI programs, but
    - Consider to turn it on to sustain high bandwidth when you have lots of large MPI messages (`--mca mpi_leave_pinned 1`)

OSU MPI Benchmarks – Bandwidth



OSU MPI Benchmark – Latency



Batch Queuing System

- A software that manages resources (CPU time, memory etc.) and schedules job execution
  - Super Mike II: Torque (PBS)/Moab
- The batch queuing system determines
  - The order jobs are executed
  - On which node(s) jobs are executed

Job Queues

- There are more than one job queue
- The main purpose is group similar jobs to maximize utilization
- Each job queue differs in
  - Number of available nodes
  - Max run time
  - Max running jobs per user
  - Node characteristics
  - …

Job Queues on Super Mike II

Machine	Queue	Max Runtime	# of nodes	Max running jobs per user	Max nodes per job	Use
SuperMikeII	workq	3 days	346	48	128	Unpreemptable
	checkpt		262		200	Preemptable
	bigmem	2 days	8		2	Big memory
	gpu	1 day	50		32	Job using GPU
	single	3 days	2	8	1	Serial jobs
	Mwfa	Only open to certain users				
	Lasigma					
	Priority					
	Admin					

Job Types

- Interactive job
  - Set up an interactive environment on compute nodes for users
    - Advantage: can run programs interactively
    - Disadvantage: must be present when the job starts
  - Purpose: testing and debugging
    - Do not run on the head node!!!
    - Try not to run interactive jobs with large core count, which is a waste of resources)
- Batch job
  - Executed without user intervention using a job script
    - Advantage: the system takes care of everything
    - Disadvantage: can only execute one sequence of commands which cannot changed after submission
  - Purpose: production run

Basic Commands

- Queue querying
  - Check how busy the cluster is
- Job submission
  - Submit a job to run
- Job monitoring
  - Check job status (estimated start time, remaining run time etc.)
- Job manipulation
  - Cancel/hold jobs

Queue Querying

- Command: qfree
  - Show the number of free, busy and queued nodes

```
[lyan1@mike1 ~]$ qfree
PBS total nodes: 453,  free: 118,  busy: 315,  down: 20,  use: 69%
PBS workq nodes: 168,  free: 30,  busy: 31,  queued: 0
PBS checkpt nodes: 252,  free: 30,  busy: 17,  queued: 248
```

Submitting Jobs

- Interactive job
  - `qsub -I -V -l walltime=<hh:mm:ss>,nodes=<# of nodes>:ppn=16 -A <your allocation> -q <queue name>`
  - Add `-X` to enable X11 forwarding
  - Limited to a maximum of 12 hours on Super Mike II
- Batch job
  - `qsub <job script>`
- On Super Mike II `ppn` must be **16** except for serial jobs

PBS Job Script – Parallel Jobs

```
#!/bin/bash
#PBS -l nodes=4:ppn=16          Number of nodes and processor
#PBS -l walltime=24:00:00       Maximum wall time
#PBS -N myjob                   Job name
#PBS -o <file name>             File name for standard output
#PBS -e <file name>             File name for standard error
#PBS -q checkpt                 Queue name
#PBS -A <hpc_allocation>        Allocation name
#PBS -m e                       Send mail when job ends
#PBS -M <email address>         Send mail to this address

<shell commands>
mpirun  -machinefile $PBS_NODEFILE -np 16 <path_to_executable> <options>
<shell commands>
```

Running GPU-enabled Applications

- One needs to specify
  - How many devices per node
  - How many CPU cores per device
- Varies from one application to another
  - Ex: NAMD will automatically use all devices on the node(s) if built with CUDA
    - The user needs to determine how many CPU cores to use by
      - Creating an appropriate host file (with mpirun) or
      - Using the "`+p<n>`" and "`+ppn<n>`" option (with charmrun)
    - The user can indicate which device(s) to use with the "`+devices`" option (whith charmrun)

Example: Running NAMD on GPU

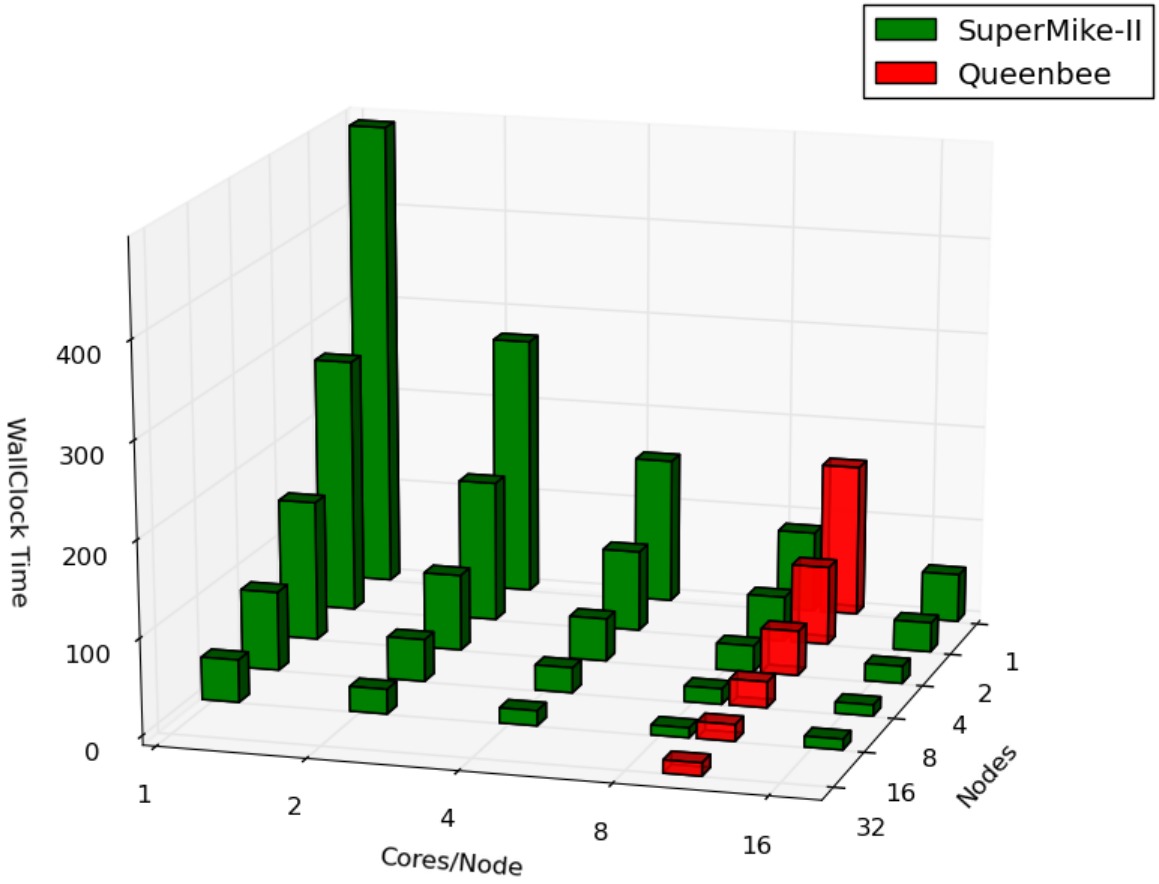
- Running NAMD on 16 nodes with 2 devices per node and 1 CPU process for device:
  - With mpirun

```
mpirun –np 32 –hostfile $newhostfile <path to namd
executable> apoa1.namd
```

  - With charmrun

```
charmrun +p32 ++nodelist <path to host file> <path to
namd excutable> apoa1.namd ++ppn 2 +idlepoll
++remote-shell ssh
```

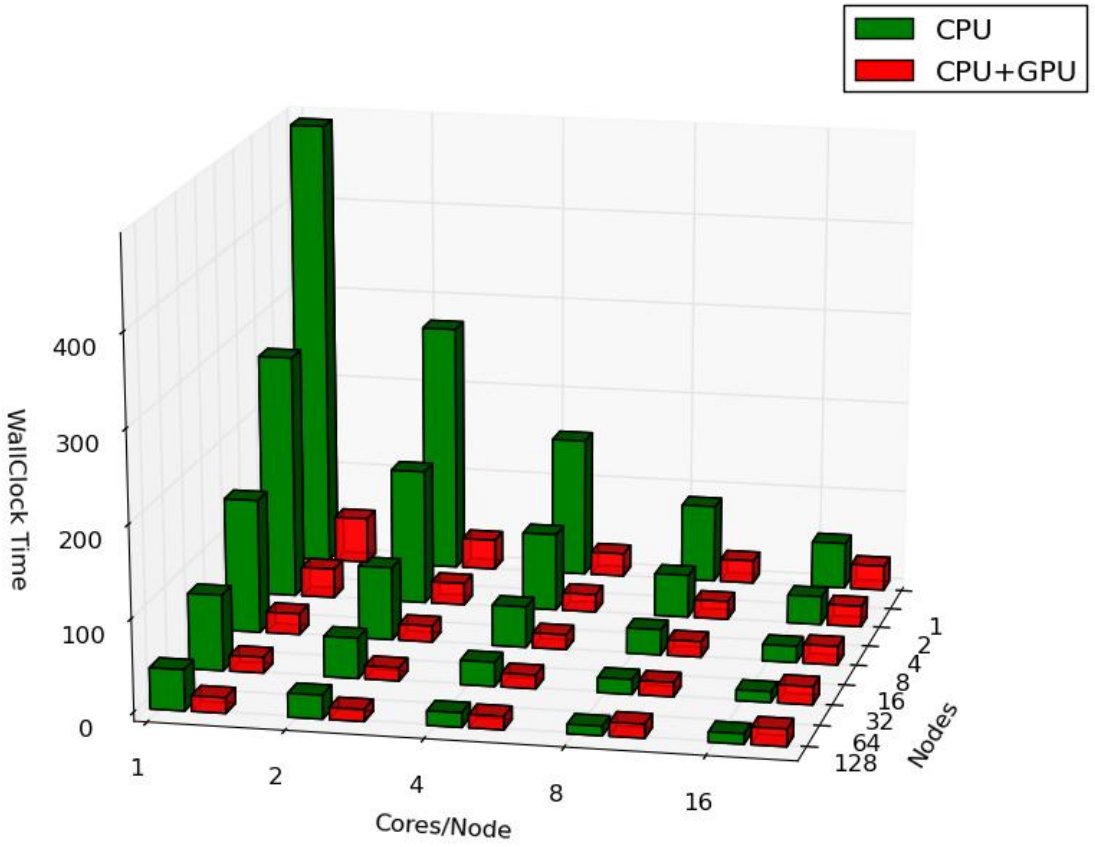
NAMD Benchmark – CPU Only



NAMD 2.9, Apoa1 benchmark

http://www.ks.uiuc.edu/Research/namd/performance.html

NAMD Benchmark – With GPU



NAMD 2.9, Apoa1 benchmark

http://www.ks.uiuc.edu/Research/namd/performance.html

Job Monitoring

- Command: `showstart <job_id>`
  - Check when a job is estimated to start
- Things that can change the estimated start time
  - Higher priority jobs are submitted
  - Running jobs terminate earlier than the system expects
  - The system has trouble starting your job

Job Monitoring cont'd

- Command: `qstat <options> <job_id>`
  - Show information on job status
  - All jobs are displayed if `<job_id>` is omitted
  - Show jobs submitted by a specific user: `qstat -u <username>`
  - Display in the alternative format: `qstat -a <job_id>`
- Command: `qshow <job_id>`
  - Show information on a running job
    - On which node(s) the job is running
    - CPU load
    - Memory usage

Job Manipulation

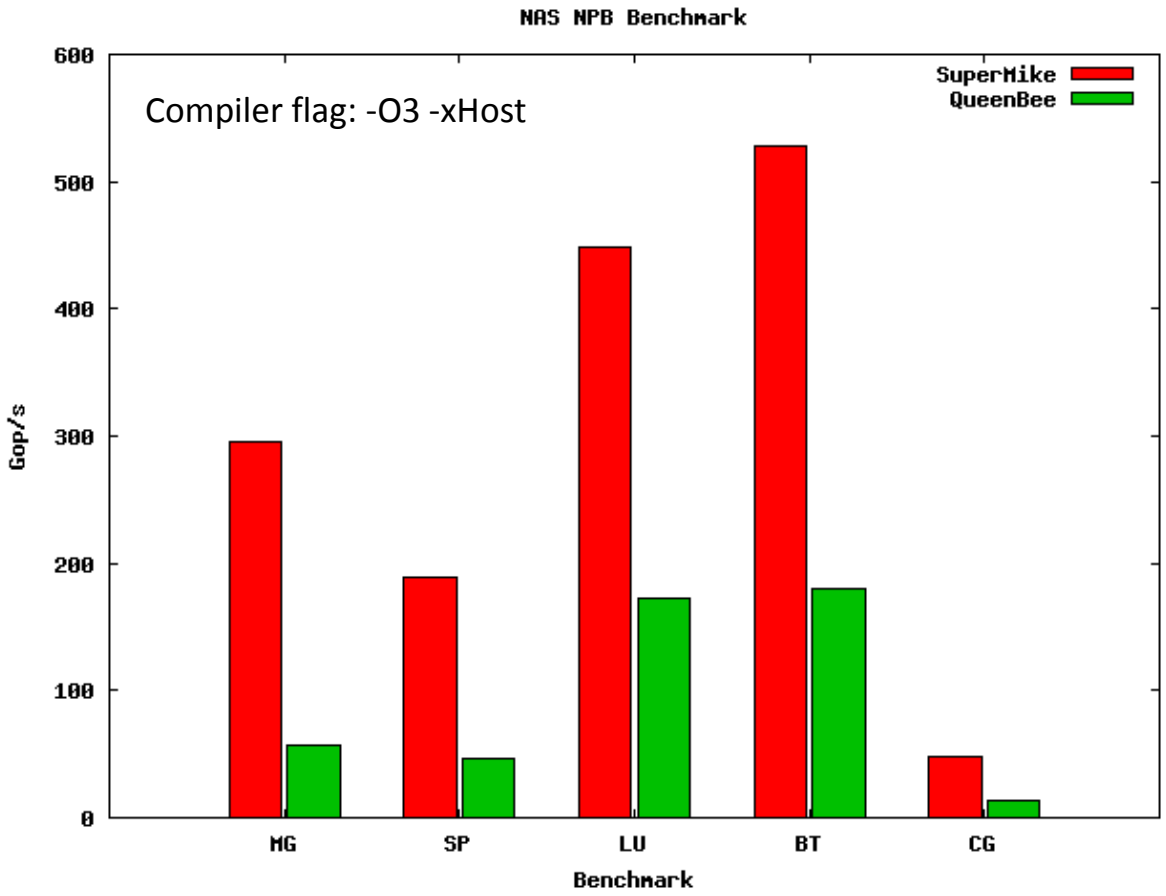
- Command: `qdel <job_id>`
  - Cancel a running or queued job
  - May take some time depending on the size of the job
- Command: `qhold <job_id>`
  - Put a queued job on hold
- Command: `qrls <job_id>`
  - Resume a held job

Benchmark Results on Super Mike II

NAS Parallel Benchmarks

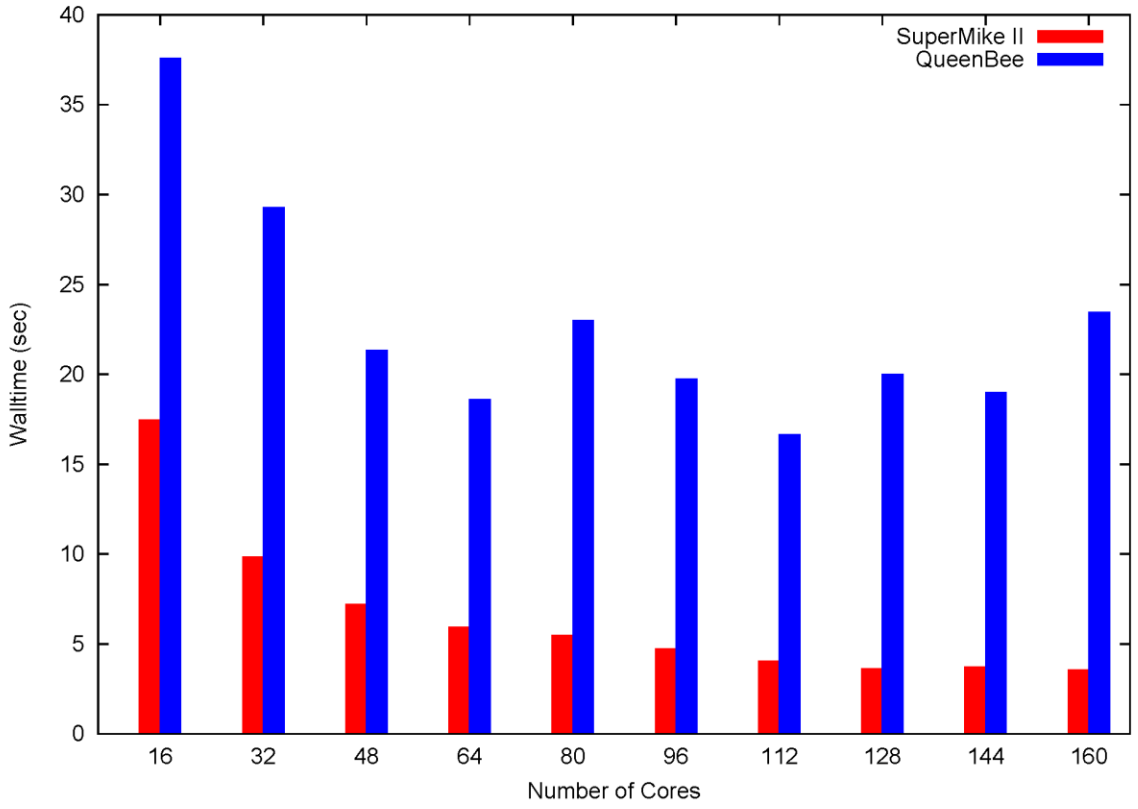
- Developed by NASA Advanced Supercomputing (NAS)
- Derived from CFD applications
  - MG: Multi-grid method for a 3D Poisson problem
  - CG: Conjugate-gradient solver for an unstructured sparse linear system
  - BT: Block tri-diagonal solver
  - SP: Scalar penta-diagonal solver
  - LU: Lower-upper Gauss-Seidel solver

NAS Parallel Benchmarks

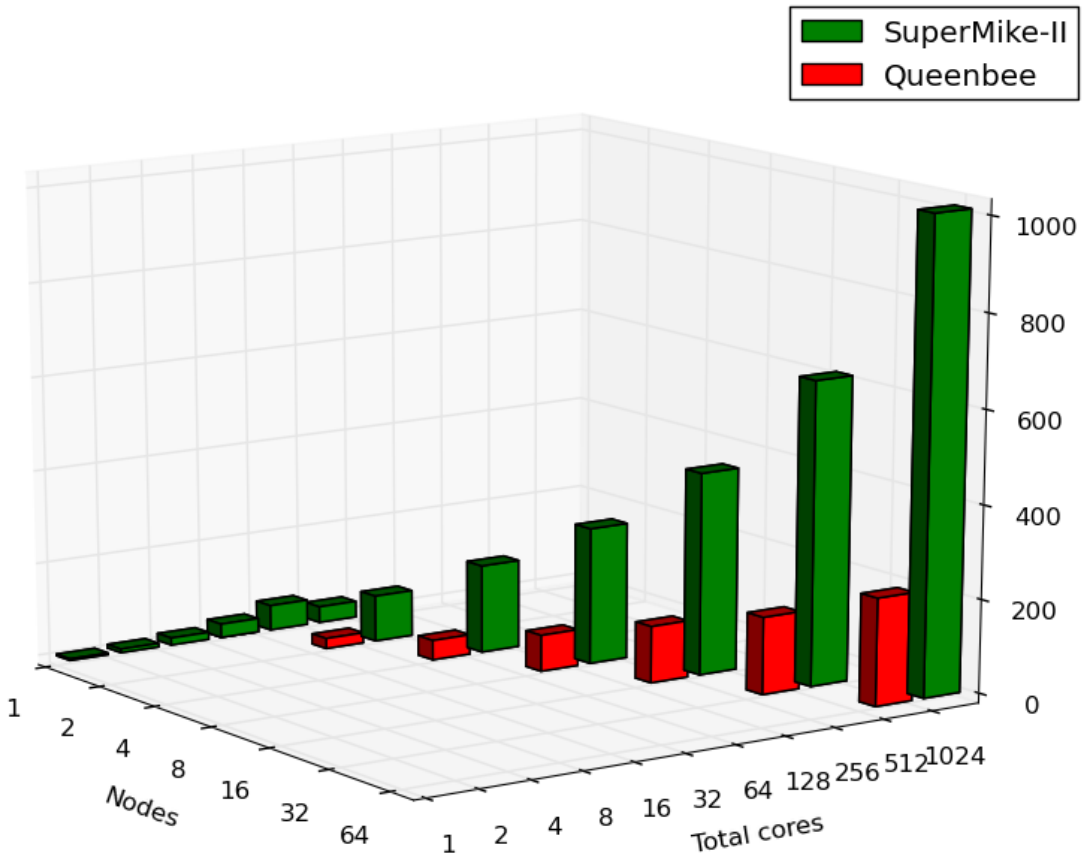


NPB-3.2, problem size D, pure MPI, 256 processes

LAMMPS Benchmark – CPU Only



GROMACS Benchmark



GROMACS 4.5.4, d.dppc benchmark

Questions?


Shreveport
Monroe
Ruston
Alexandria
LONI
Lake Charles
Baton Rouge
Lafayette
New Orleans