BIOTEAM
Enabling Science

Cluster User Training

From Bash to parallel jobs under SGE in one terrifying hour

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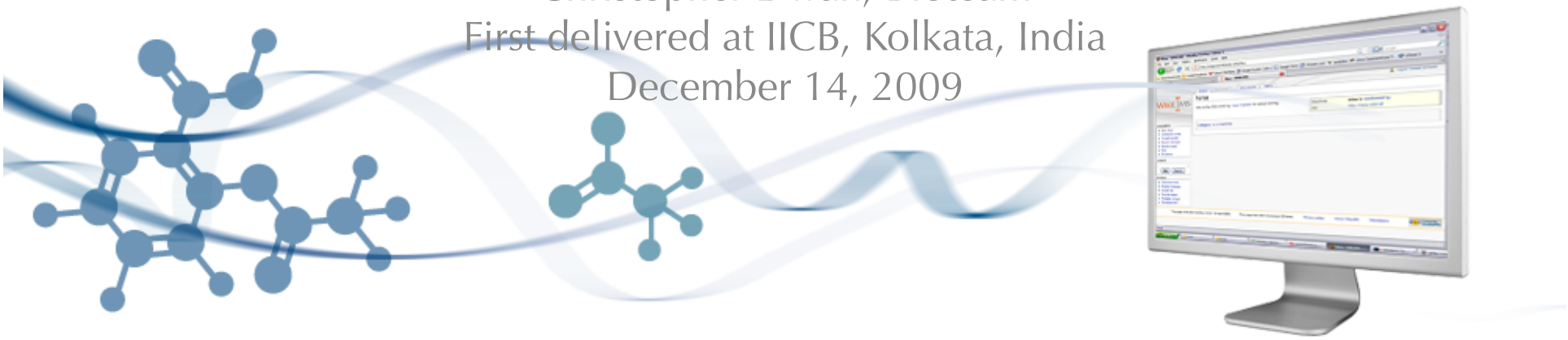


UNIX ESSENTIALS

Unix command line essentials

"**pwd**":	Print current working directory (where am I?)
"**ls**":	File listing
"**ls –l**":	Detailed file listing, including permissions
"**cd**":	Change directory
"**chmod":**	Change file permissions
"**echo**":	Print something to the terminal
"**more**":	Show contents of a text file
"**pico**"	Text editor

"**man**": Documentation on any Unix command:

Basic Unix Exercises: Making directories

What directory am I currently in?

```
Remora:~ cdwan$ pwd
/Users/cdwan/
```

Create a directory named "test_1"

```
Remora:~ cdwan$ mkdir test_1
Remora:~ cdwan$ ls
test_1
```

Change into that directory, and verify that we are there.

```
Remora:~ cdwan$ cd test_1
remora:test_1 cdwan$ pwd
/Users/cdwan/test_1
```

More basic Unix

Return to your home directory:

"**cd**" with no arguments

Exit the session:

"**exit**"

File editing.

"The best script editor" is the subject of an ongoing religious war in technical circles

You should use the tool that does not get in your way.

"**vi**": lightweight, complex, powerful, difficult to use
"**emacs**": heavyweight, complex, powerful, difficult to use
"**pico**": Possibly the simplest editor to use

To edit a file: "**pico filename**"

Hello world in 'bash'

"Bash" is a shell scripting language.

- It is the default scripting language that you have at the terminal.
- I.e: You are already using it.
- We will take this command:

```
remora:test_1 cdwan$ echo "hello world"
hello world
```

And create a wrapper script to do the same thing:

```
remora:test_1 cdwan$ pico hello.sh
remora:test_1 cdwan$ chmod +x hello.sh
remora:test_1 cdwan$ ./hello.sh
hello world
```

Running a set of bash commands

Using pico, create a file named “hello.sh” containing a single line:

```
echo "hello world"
```

Exit pico. Verify the contents of the file:

```
remora:ex_1 cdwan$ more hello.sh
echo "hello world"
```

Then invoke it using the ‘bash’ interpreter:

```
remora:ex_1 cdwan$ bash hello.sh
hello world
```

Hello world script

```
remora:test_1 cdwan$ pico hello.sh

#!/bin/bash

echo "hello world"
```

The "#!" line tells the system to automatically run it using bash

Ctrl-O: Save the file

Ctrl-X: Exit pico

File permissions

Files have properties:

- Read, Write, Execute
- Three different types of user: "owner", "group", "everyone"

To take a script you have written and turn it into an executable program, run "**chmod +x**" on it.

```
remora:test_1 cdwan$ ls -l hello.sh
-rw-r--r--  1 cdwan  staff  32 Dec 14 21:56 hello.sh

remora:test_1 cdwan$ chmod +x hello.sh

remora:test_1 cdwan$ ls -l hello.sh
-rwxr-xr-x  1 cdwan  staff  32 Dec 14 21:56 hello.sh
```

Execute the hello world script

```
remora:test_1 cdwan$ pico hello.sh

remora:test_1 cdwan$ chmod +x hello.sh

remora:test_1 cdwan$ ./hello.sh
hello world
```

SUBMITTING SGE SCRIPTS

Most useful SGE commands

- qsub / qdel
  - Submit jobs & delete jobs
- qstat & qhost
  - Status info for queues, hosts and jobs
- qacct
  - Summary info and reports on completed job
- qrsh
  - Get an interactive shell on a cluster node
  - Quickly run a command on a remote host
- qmon
  - Launch the X11 GUI interface

Interactive Sessions

To generate an interactive session, scheduled on any node:
"qlogin"

```
applecluster:~ cluster$ qlogin

Your job 145 ("QLOGIN") has been submitted
waiting for interactive job to be scheduled ...
Your interactive job 145 has been successfully scheduled.
Establishing /common/node/ssh_wrapper session to host node002.cluster.private ...
The authenticity of host '[node002.cluster.private]:50726 ([192.168.2.2]:50726)'
    can't be established.
RSA key fingerprint is a7:02:43:23:b6:ee:07:a8:0f:2b:6c:25:8a:3c:93:2b.
Are you sure you want to continue connecting (yes/no)? yes
Warning: Permanently added '[node002.cluster.private]:50726,[192.168.2.2]:
    50726' (RSA) to the list of known hosts.
Last login: Thu Dec  3 09:55:42 2009 from portal2net.cluster.private

node002:~ cluster$

all.q@node002.cluster.private  BIP   1/8       0.00     darwin-x86
    145 0.55500 QLOGIN     cluster      r     12/15/2009 09:15:08
```

Requesting the whole node

```
qlogin -pe threaded 8
```

```
all.q@node014.cluster.private  BIP   8/8        0.00     darwin-x86
    146 0.55500 QLOGIN     cluster       r     12/15/2009 09:34:58     8
```

We request a parallel environent called “threaded” (note, this PE does not exist by default in SGE – we create it in iNquiry)

We request 8 slots within that environment

Now, no other jobs will be scheduled to your node while that login is in place.

Most basic job example

```
qsub –b y /bin/hostname
```

You will see two new files in your home directory:

```
hostname.oYYY
hostname.eYYY
```

YYY is the job id provided by the queuing system.

These are the standard output and standard error files from running /bin/hostname on one of the nodes.

Argument **"-b y"** indicates that this is a a compiled binary. SGE will not try to parse the input, but merely run it.

Creating the sleeper script

```
#!/bin/bash

echo "hello world"
sleep 60
hostname
```

Then run like this:

```
remora:test_1 cdwan$ cp hello.sh sleeper.sh
remora:test_1 cdwan$ pico sleeper.sh
remora:test_1 cdwan$ ./sleeper.sh
hello world
remora.local
```

Submitting the sleeper script

```
genesis2:example bioteam$ qsub -cwd -S /bin/bash sleeper.sh
Your job 217 ("sleeper.sh") has been submitted

genesis2:example bioteam$ qstat
job-ID  prior   name       user         state submit/start at
   queue                          slots ja-task-ID
-----------------------------------------------------------------
   ------
    217 0.55500 sleeper.sh bioteam      r     12/14/2009 12:00:46
   all.q@node004.cluster.private      1
```

Adding arguments directly into the script

```
#!/bin/bash
#$ -S /bin/bash
#$ -cwd

echo "hello world"
sleep 60
hostname
```

Any comment that starts with "#$" is interpreted as an argument to qsub.

In case of conflict, the command line wins.

More SGE commands

- "**qstat –f**": Show all queues, even the empty ones
- "**qstat –u** *": Show jobs from all users
- "**qstat –f –u** *": Both all queues and uses

- "**qdel job_id**": Delete a particular job
- "**qdel –u cdwan**": Delete all jobs run by user cdwan

Giving your job a name

```
#!/bin/bash
#$ -S /bin/bash
#$ -cwd
#$ -N sleeper

echo ”Hello world”
sleep 60
hostname
```

```
genesis2:demo bioteam$ qsub sleeper.sh
Your job 222 ("sleeper") has been submitted
```

Resource Requirements

```
genesis2:demo bioteam$ qsub -l arch=solaris sleeper.sh
Your job 225 ("sleeper") has been submitted


genesis2:demo bioteam$ qstat
job-ID  prior   name       user         state
-----------------------------------------------
    225 0.00000 sleeper    bioteam      qw
```

We specify a resource requirement that cannot be met (there are no solaris machines in the cluster)

Qstat –j 225 tells the story:

(-l arch=solaris) cannot run at host "node008.cluster.private" because it offers only hl:arch=darwin-ppc

Environment variables from SGE

SGE sets several variables in the script for you.

- JOB_ID numerical ID of the job

```
#!/bin/bash
#$ -S /bin/bash
#$ -cwd
#$ -N sleeper

echo "My job id is " $JOB_ID
sleep 60
```

```
genesis2:demo bioteam$ more sleeper.o221
My job id is  221
```

Job dependencies

```
genesis2:demo bioteam$ qsub -N "primary" sleeper.sh

genesis2:demo bioteam$ qsub -hold_jid primary -N
   "secondary" sleeper.sh
Your job 224 ("secondary") has been submitted


genesis2:demo bioteam$ qstat
job-ID  prior   name       user         state
---------------------------------------------
    223 0.55500 primary    bioteam      r
    224 0.00000 secondary  bioteam      hqw
```

Redirecting output

```
#!/bin/bash
#$ -S /bin/bash
#$ -cwd
#$ -o task.out
#$ -e task.err

echo "Job ID is " $JOB_ID
```

Task arrays

```
#!/bin/bash
#$ -S /bin/bash
#$ -cwd
#$ -N task_array
#$ -o task.out
#$ -e task.err

echo "Job ID is " $JOB_ID " Task is " $SGE_TASK_ID
```

Task arrays

```
genesis2:example_2 bioteam$ qsub -t 1-10  task.sh
Your job-array 228.1-10:1 ("task_array") has been
   submitted

genesis2:example_2 bioteam$ more task.out
Job ID is  228  Task ID is  10
Job ID is  228  Task ID is  1
Job ID is  228  Task ID is  3
Job ID is  228  Task ID is  4
```

- ...

Perl instead of bash

My “hello world” script, using Perl instead of Bash:

```
remora:~ cdwan$ more hello_world.pl
#!/usr/bin/perl
#! –S /usr/bin/perl

sleep(60);
print "Hello world\n";
```

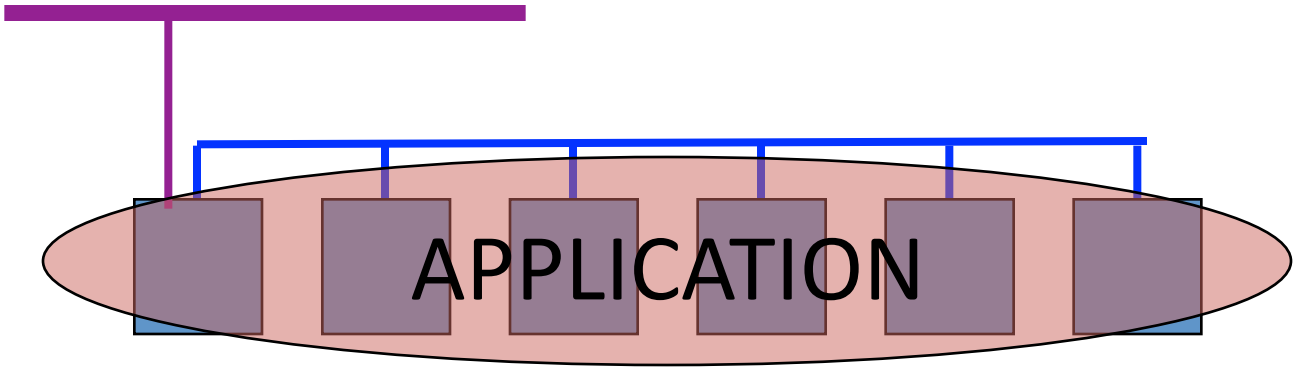
Submitted to the queuing system:

```
qsub hello_world.pl
```

PERFORMANCE TUNING / PARALLELIZATION

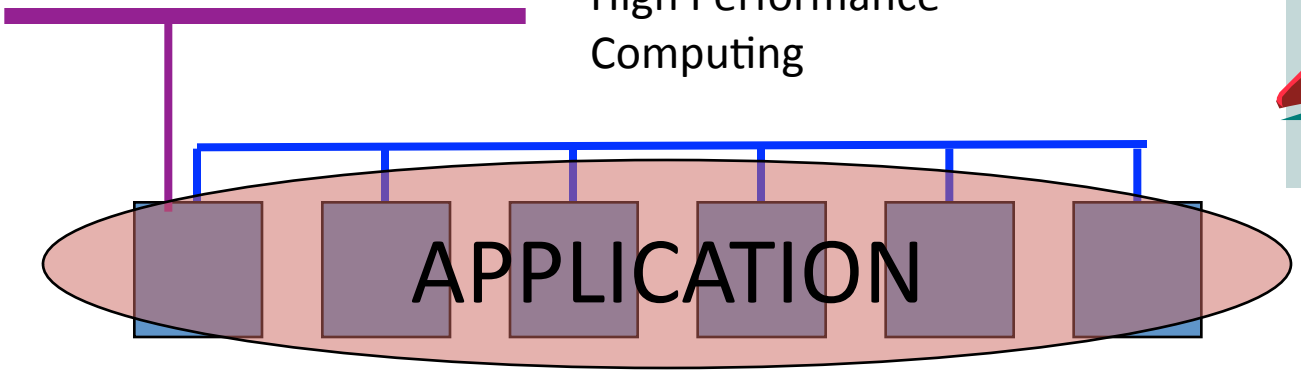
Parallel Jobs

- A parallel job runs simultaneously across multiple servers
  - Biggest SGE job I've heard of: Single application running across 63,000 CPU cores: TACC "Ranger" Cluster in Texas
  - Distinction with 'batches' of processes that include many tasks to be done in any order

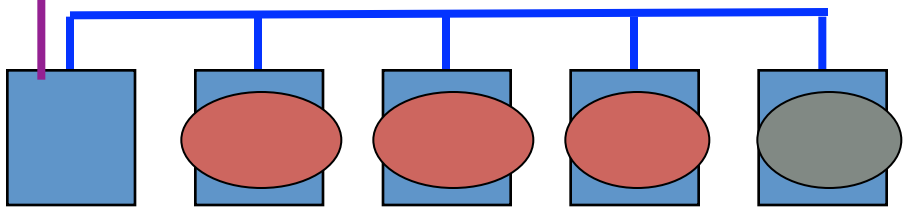


Parallel computing 101

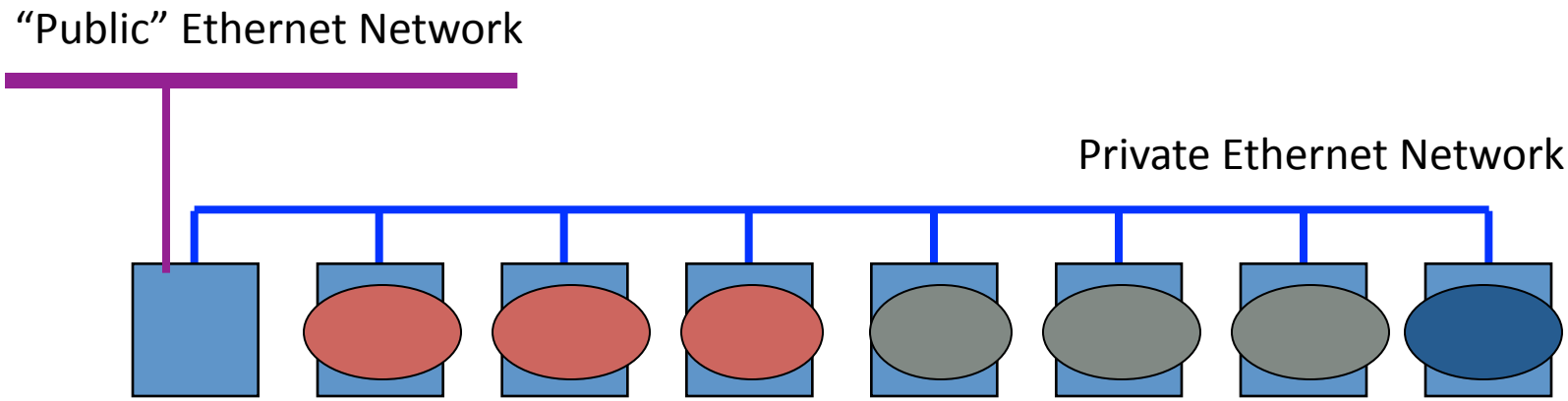
High Performance Computing



High Throughput Computing (farm)



Batch Jobs



- Independent applications running at the same time
- Many jobs (batch)
- Maximum efficiency, simple to write

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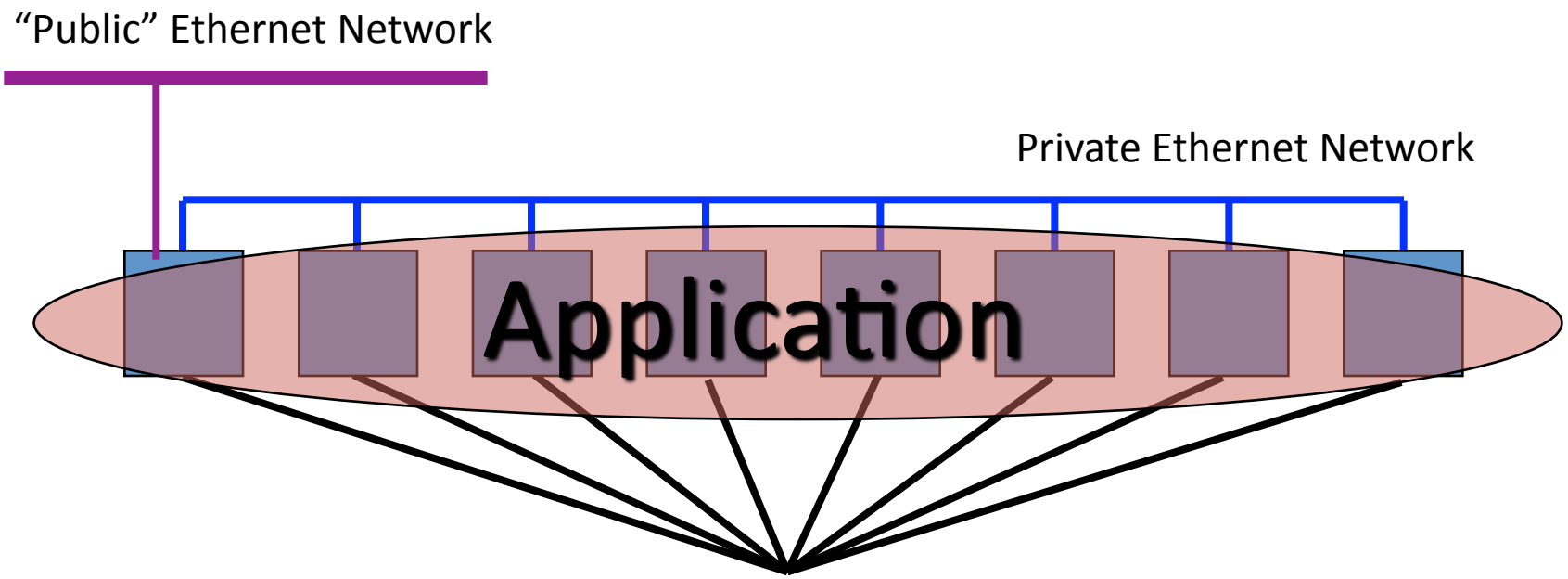
Tightly Coupled / Parallel



One parallel application running over the entire cluster

- One job, where response time is important.
- Overall efficiency is lower
- Scalability is hard

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Amdahl's Law

Maximum expected speedup for parallelizing any task

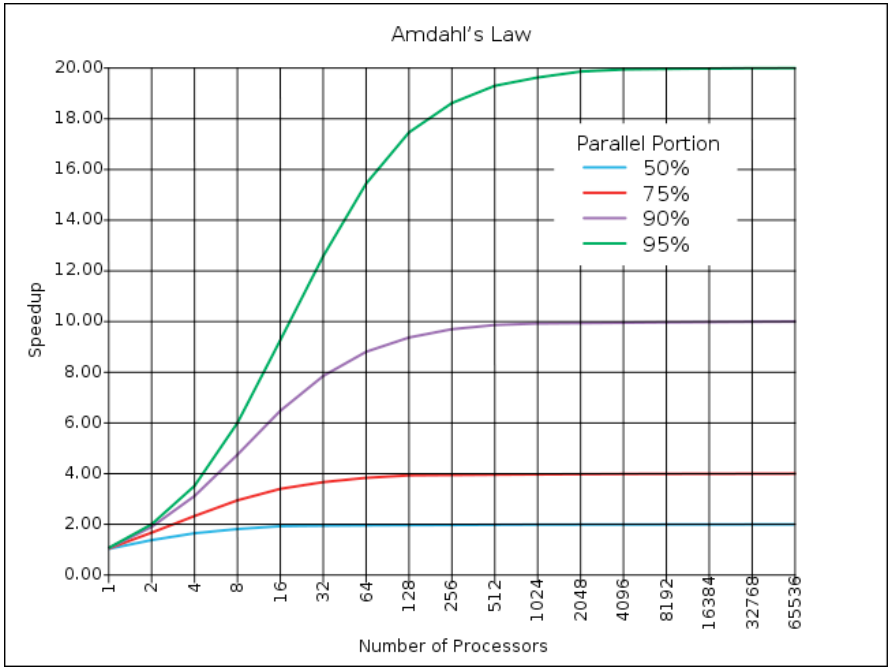
- Serial portion (non parallelizable)
- Parallel portion (can be parallelized)

Additionally:

- Cost associated with using more machines (startup, teardown)
- At least, scheduling. Possibly some other factors like communication
- Communication scales with number of processes

Important to note:

Re-stating the problem can radically alter the serial / parallel ratio



Network Latency

- **Latency**:
  - Time to initiate communication
- **Throughput**:
  - Data rate once communication is established

- **Gigabit Ethernet:**
  - Latencies: ~100ms
  - Throughputs up to 80% of wire speed (800Mb/sec)
  - $10 / network port

- **Myranet / Infiniband:**
  - Latencies: ~3ms
  - Throughput: 80% of wire speed
  - $800 / network port

RUNNING PARALLEL TASKS

Parallel Jobs

Many different software implementations are used to support parallel tasks:

- MPICH
- LAM-MPI
- OpenMPI
- PVM
- LINDA

No magic involved

- Requires work
- Your application must support parallel methods

Submitting a standalone MPI job

Build the code with a particular version of MPI:

```
genesis2:examples bioteam$ pwd
/common/mpich/ch_p4/examples

genesis2:examples root# which mpicc
/common/mpich/ch_p4/bin/mpicc

genesis2:examples root# mpicc cpi.c

genesis2:examples root# mpicc -o cpi cpi.o
```

Run without any MPI framework:

```
genesis2:examples root# ./cpi
Process 0 on genesis2.mit.edu
pi is approximately 3.1416009869231254, Error is
   0.0000083333333323
wall clock time = 0.000214
```

Submitting a standalone MPI job (no SGE)

MPI needs to know which hosts to use: We create a hosts file which simply lists the machine

```
genesis2:~ bioteam$ more hosts_file
node001
node002
Node003
node004
```

Then start the job using 'mpirun'

```
genesis2:~ bioteam$ mpirun -machinefile hosts_file \
          -np 4 /common/mpich/ch_p4/examples/cpi
Process 0 on genesis2.mit.edu
Process 2 on node002.cluster.private
Process 3 on node003.cluster.private
Process 1 on node001.cluster.private
pi is approximately 3.1416009869231249, Error is 0.0000083333333318
wall clock time = 0.002106
```

Critical Notes

In order to have MPICH jobs work reliably, you need to compile and run them with the same version of MPICH.

/common/mpich

/common/mpich2

/common/mpich2-64

All user account issues must be in order for this to work.

- Password free ssh in particular

If the application does not work from the command line, SGE will not help.

Loose Integration with SGE

Loose Integration

- Grid Engine used for:
  - Picking when the job runs
  - Picking where the job runs
  - Generating the custom machine file
- Grid Engine does not:
  - Launch or control the parallel job itself
  - Track resource consumption or child processes

Advantages of loose integration

- Easy to set up
- Can trivially support almost any parallel application technology

Disadvantages of loose integration

- Grid Engine can't track resource consumption
- Grid Engine must "trust" the parallel app to honor the custom hostfile
- Grid Engine can not kill runaway jobs

Tight integration with SGE

Tight Integration

- Grid Engine handles all aspects of parallel job operation from start to finish
- Includes spawning and controlling all parallel processes

Tight integration advantages:

- Grid Engine remains in control
- Resource usage accurately tracked
- Standard commands like "`qdel`" will work
  - Child tasks will not be forgotten about or left untouched

Tight Integration disadvantages:

- Can be really hard to implement
- Makes job debugging and troubleshooting harder
- May be application specific

Running an mpich job with loose SGE integration

Step one: Job must work without SGE.

- Until you can demonstrate a running job using a host file and manual start up, there is no point to involving SGE

Step two: Create a wrapper script to allow SGE to define the list of hosts and the number of tasks

Step three: Submit that wrapper script into a 'parallel environment'

- Parallel environment manages all the host list details for you.

MPICH Wrapper for CPI

A trivial MPICH wrapper for Grid Engine:

```
#!/bin/bash

## ---- EMBEDDED SGE ARGUMENTS ----
#$ -N MPI_Job
#$ -pe mpich 4
#$ -cwd
#$ -S /bin/bash
## -------------------------------------
MPIRUN=/common/mpich/ch_p4/bin/mpirun
PROGRAM=/common/mpich/ch_p4/examples/cpi
export RSHCOMMAND=/usr/bin/ssh

echo "I got $NSLOTS slots to run on!"
$MPIRUN -np $NSLOTS -machinefile $TMPDIR/machines $PROGRAM
```

Job Execution

Submit just like any other SGE job:

```
[genesis2:~] bioteam% qsub submit_cpi
Your job 234 ("MPI_Job") has been submitted
```

Output files generated:

```
[genesis2:~] bioteam% ls -l *234
-rw-r--r--  1 bioteam  admin  185 Dec 15 20:55 MPI_Job.e234
-rw-r--r--  1 bioteam  admin  120 Dec 15 20:55 MPI_Job.o234
-rw-r--r--  1 bioteam  admin   52 Dec 15 20:55 MPI_Job.pe234
-rw-r--r--  1 bioteam  admin  104 Dec 15 20:55 MPI_Job.po234
```

Output

```
[genesis2:~] bioteam% more MPI_Job.o234
I got 5 slots to run on!
pi is approximately 3.1416009869231245, Error is
   0.0000083333333314
wall clock time = 0.001697

[genesis2:~] bioteam% more MPI_Job.e234
Process 0 on node006.cluster.private
Process 1 on node006.cluster.private
Process 4 on node004.cluster.private
Process 2 on node013.cluster.private
Process 3 on node013.cluster.private
```

Parallel Environment Usage

- "qsub -pe mpich 4 ./my-mpich-job.sh"
- "qsub -pe mpich 4-10 ./my-mpich-job.sh"
- "qsub -pe lam-loose 3 ./my-lam-job.sh"

Behind the Scenes: Parallel Environment Config

```
genesis2:~ bioteam$ qconf -sp mpich
pe_name            mpich
slots              512
user_lists         NONE
xuser_lists        NONE
start_proc_args    /common/sge/mpi/startmpi.sh $pe_hostfile
stop_proc_args     /common/sge/mpi/stopmpi.sh
allocation_rule    $fill_up
control_slaves     FALSE
job_is_first_task  TRUE
urgency_slots      min
```

Behind the scenes: MPICH

The "`startmpi.sh`" script is run before job launches and creates custom machine file

The user job script gets date required by '`mpirun`' from environment variables:

`$NODES, $TEMPDIR/machines`, etc.

The "`stopmpi.sh`" script is just a placeholder

Does not really do anything (no need yet)

Behind the scenes: LAM-MPI

- Just like MPICH
- But 2 additions:
  - The “lamstart.sh” script launches LAMBOOT
  - The “lamstop.sh” script executes LAMHALT at job termination
- In an example configuration, lamboot is started this way:
  - `lamboot -v -ssi boot rsh -ssi rsh_agent "ssh -x -q" $TMPDIR/machines`

Behind the scenes: LAM-MPI

- A trivial LAM-MPI wrapper for Grid Engine:

```
#!/bin/sh

MPIRUN="/common/lam/bin/mpirun"

## ---- EMBEDDED SGE ARGUMENTS ----
#$ -N MPI_Job
#$ -pe lammpi 3-5
#$ -cwd
## --------------------------------------
echo "I have $NSLOTS slots to run on!"
$MPIRUN C ./mpi-program
```

OpenMPI

In absence of specific requirements, a great choice

Works well over Gigabit Ethernet

Trivial to achieve tight SGE integration

Recent personal experience:

- Out of the box: 'cpi.c' on 1024 CPUs
- Out of the box: heavyweight genome analysis pipeline on 650 Nehalem cores

Behind the scenes: OpenMPI

OpenMPI 1.2.x natively supports automatic tight SGE integration

- Build from source with "--enable-sge"
- `mpirun -np $NSLOTS /path-to-my-parallel-app`

OpenMPI PE config:

```
pe_name            openmpi
slots              4
user_lists         NONE
xuser_lists        NONE
start_proc_args    /bin/true
stop_proc_args     /bin/true
allocation_rule    $round_robin
control_slaves     TRUE
job_is_first_task  FALSE
urgency_slots      min
```

OpenMPI Job Script

```
#!/bin/sh

## ---- EMBEDDED SGE ARGUMENTS ----
#$ -N MPI_Job
#$ -pe openmpi 3-5
#$ -cwd
## --------------------------------------

echo "I got $NSLOTS slots to run on!"
mpirun -np $NSLOTS ./my-mpi-program
```

Application profiling

- **Most basic: System Monitoring**
  - 'top'
  - Ganglia
- **Apple 'shark' tools**
- **Deep understanding of code.**

Tuning parallel jobs

- **Round Robin:**
  - Jobs are distributed to as many nodes as possible
  - Good for tasks where memory may be the bottleneck

- **Fill up:**
  - Jobs are packed onto as few nodes as possible
  - Good for jobs where interprocess communications may be the bottleneck

- **Single chassis**
  - “threaded” environment from earlier sessions
  - For multi-threaded programs (BLAST)

Thank you