



Backgrounding and Task Distribution In Batch Jobs

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Overview

- Description of the Problem Environment
- Quick Review of Command Shell Job Control
- WQ Components
- Simple Serial Example
- Multi-Threaded Example
- MPI Example
- Comments on Monitoring and Statistics









The Problem Environment









LSU HPC Environment

- Traditional Moab/Torque (PBS) environment.
- Usage is allocation controlled.
- Large clusters tuned for large-scale parallel processing.
- Small 39 node cluster for serial work.
- Growing interest in bioinformatics causing an explosion in serial job requirements.









BIG File Counts

- Jobs with 10's of thousands of input files and identical processing tasks.
- Most workflow tools not well suited to timelimited batch queuing systems.
- Current approach: background or otherwise manually distribute work in the PBS batch script.
 - Requires intermediate level shell scripting skills
 - Scripting is foreign to non-traditional users.









Desired Solution

- Avoid detailed scripting requirements but allow flexibility and adaptability.
- Minimize customization and do most things automagically.
- Make method batch environment aware, particularly wallclock time constraints.









Command Shell Job Control









Shell Job Control

- Shell job control features manage, background, suspend, foreground.
- Not to be confused with batch jobs!
- Typically used interactively.
- Available for use in any shell script.









Common Commands

- Ctrl-Z . . suspends an interactive process.
- bg %M . . . sends job #M into background.
- fg %N . . . brings job #N into foreground
- cmd & . . . starts cmd in the background.
- kill %L . . kills job #L.
- jobs . . . lists known jobs.

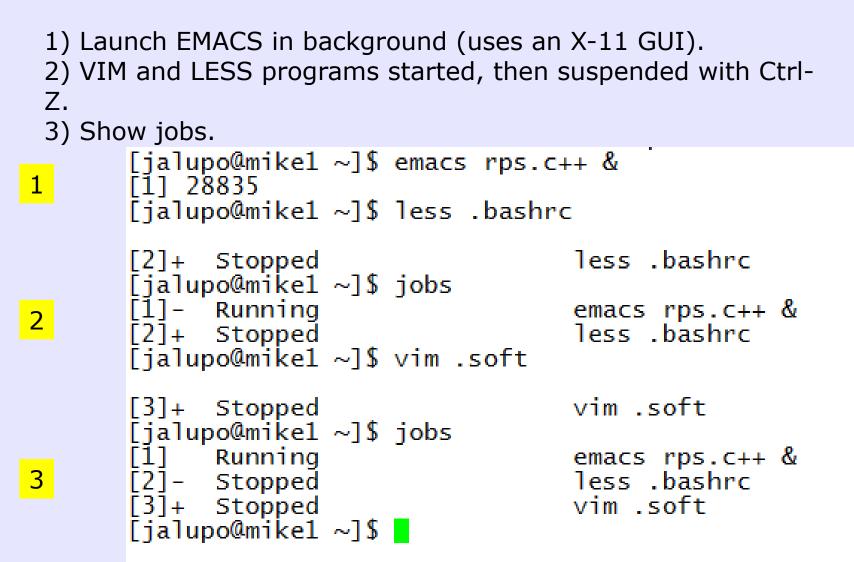








Example











Hands-On Example

```
1) Run: $ vimtutor
2) Suspend with Ctrl-Z.
3) Run: $ ls -l
4) Run: $ jobs
5) Identify which job is vimtutor.
6) Run: $ fg %N
7) Suspend again.
8) Run: $ vim &
9) Run: $ vim &
10) Run: $ kill %N %M
```









Launching Processes With &

Syntax: \$ cmd [-switches] [args] [< stdin] [> stdout] &

- Interactive jobs are suspended.
- Non-interactive jobs start running.
- stdio* streams stay as is unless redirected.
- Parent shell determines how jobs are handled when shell terminates.



* stdin, stdout, stderr

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PBS Script Running 4 Serial Programs

```
#! /bin/bash
#PBS -l nodes=1:ppn=4
#PBS . . . other settings . . .
myprog < infile1 > outfile1 &
myprog < infile2 > outfile2 &
myprog < infile3 > outfile3 &
myprog < infile4 > outfile4 &
wait
```

The **wait** makes sure all 4 tasks have completed, else when the script ends, the job manager will kill all the user's running programs in preparation for the next job.









Running 2 Multi-Threaded Programs

• With 4 cores there is the ability to run 2 2-thread programs - almost as easy as running serial programs.

```
#! /bin/bash
#PBS -l nodes=1:ppn=4
#PBS . . . other
settings . . .
export OMP_NUM_THREADS=2
myprog < infile1 > outfile1 &
```

```
myprog < infile1 > outfile1 &
myprog < infile2 > outfile2 &
```

wait









Multi-Process MPI Programs

On an 8-core node, 2 4-process MPI tasks can be run.

#! /bin/bash
#PBS -l nodes=1:ppn=8
#PBS . . . other settings . . .

NPROCS=4
mpirun -np \$NPROCS -machinefile \$PBS_NODEFILE mprog < infile1 > outfile1 &
mpirun -np \$NPROCS -machinefile \$PBS_NODEFILE mprog < infile2 > outfile2 &

wait









Higher Core Counts

- Multiple multi-threaded or multi-process tasks allows one script to take advantage of all cores in a node.
- 4, 8, 16, 20, and 40 cores per node are available on the various local clusters.
- The types of programs can be mixed, so long as the required number of cores is consistent with what the node provides.
- Scaling up (more cores plus more nodes) will obviously complicate the scripting required.



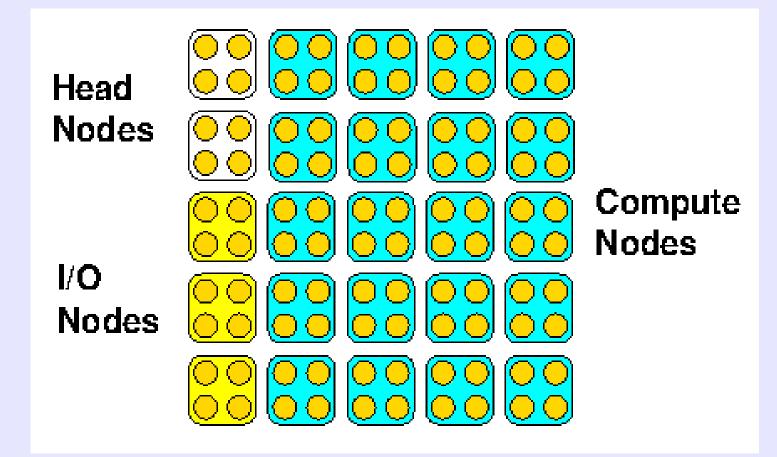




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Use Multiple Nodes?



On typical cluster, the work must be done on the compute nodes. We could submit multiple single node job scripts, but how about using more than one node at a time?









Multi-Node Considerations

- The *mother superior* node is only one with all the job information, like environment variables.
- The programs on other nodes can be started with remote shell commands, like ssh.
- Must account for shared or local file systems.
- Must assure all programs finish before script exits.
- Must be aware of efficiency (load balancing).







8 Serial Programs on 2 4-core Nodes

8 Cores Total	<pre>#! /bin/bash #PBS -l nodes=2:ppn=4 #PBS other settings export WORKDIR=/path/to/work/directory cd \$WORKDIR</pre>
Node 1 Mother Superior 4 Tasks	<pre>myprog < infile1 > outfile1 & myprog < infile2 > outfile2 & myprog < infile3 > outfile3 & myprog < infile4 > outfile4 &</pre>
	<pre># Discover second host name, somehow, then</pre>
Node 2 Compute Node 4 Tasks	<pre>ssh -n \$HOST2 "cd \$WORKDIR; myprog < infile5 > outfile5" & ssh -n \$HOST2 "cd \$WORKDIR; myprog < infile6 > outfile6" & ssh -n \$HOST2 "cd \$WORKDIR; myprog < infile7 > outfile7" & ssh -n \$HOST2 "cd \$WORKDIR; myprog < infile8 > outfile8" &</pre>
	woit

wait



-n suppresses reading from stdin and just starts the program. The path to myprog is assumed known (.bashrc?)







Some Real Scripting Required

- 8 programs on 2 nodes clearly starts to make life complicated.
- Real shell magic needed to figure out host names - maybe a little opaque:

NAMES=(\$(uniq \$PBS_HOSTFILE))
HOST2=NAMES[1]

Assumes host names are assigned starting with the mother superior, and in sorted order. More work if this is not the case!









Automating Multiple Nodes

	# Get the node names
	NODES=(\$(uniq \$PBS_NODEFILE))
	# Get the number of names
	NUMNODES= \$(uniq \$PBS_NODEFILE) wc -l awk '{print \$1-1}')
	# Do commands on first node:
Node 1	cmd stuff &
Mother Superior	start as many as desired (but customize each line!)
4 Tasks	cmd stuff &
	# Loop over all the nodes, starting with the second name:
	for i in \$(seq 1 \$((NUMNODES-1))); do
Node N Compute Node	<pre>ssh -n \${NODES[\$i]} cmd stuff &</pre>
	start as many as desired (but customize each line!)
4 Tasks	<pre>ssh -n \${NODES[\$i]} cmd stuff &</pre>
	done
	wait

Really not fun if you don't like shell scripting, yet it gets worse!









Consider Multi-Threaded / MPI Task Requirements

- Have to pass the thread count.
- Have to construct partial host name lists.
- Involves basic shell programming, and maybe gets involved with fussy quoting rules to get everything passed correctly.
- It doesn't really SCALE!









Solution Requirements

- Isolate the things that change with each task.
- Make user setup as simple as possible.
- Automate most of the magic.
- Try to deal with batch job wall time issues.









Questions?

- Before we move on, any further clarifications of the basic shell scripting concepts needed?
- Any concerns over difference between a shell script and a PBS job script?









WQ and It's Components









What Is WQ?

- A work distribution system (distributor/worker model). WQ roughly stands for "Work Queuing".
- Handles tasks a task is defined as the work necessary to process one input file.
- Multiple workers execute the tasks one worker for each simultaneous task desired all nodes.
- Workers request a task from the *distributor*.
- Workers and the distributor share elapsed time information, estimate remaining time, and won't start a new task if insufficient time remains.







Design Assumptions

- Task viewed as work needed to process one input file.
- The distributor manages a list of input file names, and hands out one at a time.
- A work request includes run time of last task executed.
- A work handout includes longest known task run time.









WQ Components

- wq.py A Python script that implements the distributor and workers (as they say, no user serviceable parts inside!).
- wq.pbs A PBS batch script template with a few user required variable settings and most of the magic cooked in.
- wq.sh A user created script (could be a program) that accepts an input file name as it's only argument.
- wq.list A user created file containing input file names, one per line (suggest using absolute path names).

The names of files can be changed – just keep consistent with the contents of the PBS script – changing name of **wq.py** would require a bit more work than changing any of the other 3.









wq.pbs : PBS Preamble Section

The PBS script is divided into 2 parts: the WQ prologue (which includes the PBS preamble), and the WQ epilog. Only prologue contains items the user should adjust. The PBS preamble portion should look familiar (not all PBS options are shown here):

#! /bin/bash ####################################	
<pre># Begin WQ Prologue section</pre>	
######################################	
<pre>#PBS -A hpc_myalloc_03 #PBS - l nodes 44</pre>	
<pre>#PBS -l nodes=4:ppn=4 #PBS -l walltime=00:30:00</pre>	
#PBS -q workq	
#PBS -N WQ_Test	

The PBS script itself must be set executable, as it will be run by nodes other than the mother superior, if necessary.









wq.pbs : Prologue Section

Have the script run 1 worker per core on each node assigned. # The system to run on has 4 cores per node (i.e. ppn=4):

- #1 WPN=4
 - # Set the working directory:
- #2 WORKDIR=/work/user

Use a file with 82 names listed:

#3 FILES=\${WORKDIR}/82_file_list

Name the task script each worker is expected to run on the file
name provided as it's only argument.

4 TASK=\${WORKDIR}/wq_timing.sh

5 START=1









wq.pbs : Epilogue Section

- Serious magic happens in the Epilogue section so dabble with at your own peril.
- Does some sanity checking of settings.
- Determines if running as mother superior.
- Mother superior preps information exchange process and starts job script on all other compute nodes.
- Mother superior starts dispatcher, and it's workers.
- Compute nodes start required number of workers.
- All workers start the *request execute report* cycle until time runs out or no more tasks to assign.











This name represents an actual shell script, program, or any other type of executable which works on the provided input file name. What it does should be consistent with the settings (i.e. multi-threaded, multi-process, serial) in wq.pbs.

Before launching, it can/should be tested with a single file:

\$./wq.sh filename

If it works manually, it should function correctly when called by a worker.









wq.list

This is nothing more than a file containing input file names, one per line. For a really large number of input files, generate it with the **find** command:

\$ find `pwd` -name '*.dat' -print > wq.list

In many cases, using absolute paths for the file names is best since the script can extract information about the location from the name (hence the use of `pwd` to get the current working directory).

Some examples are in order.









A Serial Example









A Simple **wq.sh**

Let's not try to do much except waste some time and show what can be done with the file name:

```
#! /bin/bash
# First, some basic processing of the input file name.
FILE=$1
DIR=`dirname ${FILE}`
BASE=`basename ${FILE}`
# Now just echo the results.
echo "DIR=${DIR}; BASE=${BASE}"
echo "That's all, folks!"
sleep 2
```

A real-world script can be arbitrarily complex!









An Input File List

Let's look for files with .bf extensions:

\$ find /work/user -name '*.bf' -print > file_list

And assume it produces names like so:

/work/user/chr13/chr13_710.bf
/work/user/chr13/chr13_727.bf
/work/user/chr13/chr13_2847.bf
/work/user/chr13/chr13_711.bf
/work/user/chr13/chr13_696.bf









A Serial **wq.pbs**

We can try to run on 32 cores. If the system has 16 cores per node, we would need to request 2 nodes. The PBS preamble option would look like:

#PBS -l nodes=2:ppn=16

Now we just need to make the 5 PBS prologue variables agree:

WPN=16 WORKDIR=/work/user FILES=\${WORKDIR}/file_list TASK=\${WORKDIR}/wq.sh START=1









Serial Example STDERR

```
Dispatcher:Start:1
mike044_0:Taking:1:0.00:90.00
. . . .
mike045_15:Taking:32:0.00:90.00
Dispatcher:Maxtime:mike044_6:2.03:1393524348.06
. . . .
mike045_0:Taking:81:4.03:85.97
Dispatcher:Shutdown:32
Dispatcher:Last:82
mike045_1:Taking:82:4.03:85.97
```

Dispatcher – event, task number involved, event data Worker ID – action, task number involved, start time, remaining time.









Serial Example STDOUT

Each worker emits a report using 4 groups of lines as so:

```
Task:7:mike044_6:Ran:True:/work/user/wq_timing.sh /work/user/chr13/chr13_720.bf
Timings:7:mike044_6:1393524346.03:1393524348.06:2.03:2.03
Stdout:7:
    DIR=/work/user/chr13; BASE=chr13_720.bf
    That's all, folks!
Stderr:7:
```

- Task task number, worker ID, action, success, task command
- Timings task number, worker ID, start time, end time, elapsed, max.
- Stdout task number, followed by task stdout lines produced, if any.
- Stderr task number, followed by task stderr lines produced, if any.









A Multi-Threaded Example









Adjust For Multi-Threading

- wq.sh set up for multi-threading. We'll use OpenMP for this example.
- wq.pbs adjust so number of threads and number of workers is consistent with number of cores on the nodes.







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Multi-Threaded Example wq.sh

	#! /bin/bash
	# Set a variable as the absolute path to the blastn executable:
Shortcut	BLASTN=/usr/local/packages/bioinformatics/ncbiblast/2.2.28/gcc-4.4.6/bin/blastn
# Threads	export OMP_NUM_THREADS=4
	FILE=\$1 DIR=`dirname \${FILE}` BASE=`basename \${FILE}`
	# Build the rather complex command line.
Keep It Readable	CMD="\${BLASTN} -task blastn -outfmt 7 -max_target_seqs 1" CMD="\${CMD} -num_threads \${OMP_NUM_THREADS}" CMD="\${CMD} -db /project/special/db/img_v400_custom/img_v400_custom_GENOME" CMD="\${CMD} -query \${FILE}" CMD="\${CMD} -out \${DIR}/IMG_genome_blast.\${BASE}"
	<pre># For testing purposes, use "if false". For real runs, use "if true":</pre>
	if true ; then
Production vs Testing	eval "\${CMD}" else echo "\${CMD}" # This just slows things way down for testing. sleep 1
	fi









Multi-Threaded Example **wq.pbs**

Assume the system has 16 cores per node. That means we could run 4 4-thread tasks per node. On 2 nodes we could run 8 tasks at a time, so let's set that up in the PBS preamble:

#PBS -l nodes=2:ppn=16

Now we just need to make the PBS prologue variables agree:

WPN=4 WORKDIR=/work/user FILES=\${WORKDIR}/file_list TASK=\${WORKDIR}/wq.sh START=1









Multi-Threaded Example STDERR

Dispatcher:Start:1 mikel11_0:Taking:1:0.00:252000.00 mikel11_1:Taking:2:0.00:252000.00 mikel11_2:Taking:3:0.00:252000.00 Dispatcher:Maxtime:mikel11_1:64223.42:1393836959.93 mikel11_1:Taking:5:64223.42:187776.58 Dispatcher:Maxtime:mikel11_2:123837.43:1393896573.95 mikel11_2:Skipping:6:123837.44:128162.56 Dispatcher:Timeup:mikel11_2:1393896573.95 Dispatcher:Shutdown:3 Dispatcher:Last:6

Note Task 6 was last handed out, but mike111_2 skipped it because to little time remained to safely start it and finish.









Multi-Threaded Example STDOUT

```
Task:3:mike111_2:Ran:True:/work/jalupo/WQ/BLASTN/wq_blastn.sh
/work/jalupo/WQ/BLASTN/GS049.blast/xai.fna
Timings:3:mike111_2:1393772736.52:1393896573.95:123837.43:123837.43
Stdout:3:
Stderr:3:
```

```
Task:6:mikell1_2:Skipped:False:/work/jalupo/WQ/BLASTN/wq_blastn.sh
/work/jalupo/WQ/BLASTN/GS049.blast/xaa.fna
Timings:6:mikell1_2:-1.00:-1.00:-1.00:123837.44
Stdout:6:
    Insufficient Time
Stderr:6:
    Time left: 128162.56; Max Time: 123837.43; Margin: 1.25
```









An MPI Example





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Adjust For MPI

- wq.sh set up for small number of MPI processes per task.
- wq.pbs adjust so number of processes and number of workers is consistent with number of cores on the nodes.







Build

Host

Lists

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MPI Example wq.sh

```
#! /bin/bash
FILE=$1
DIR=`dirname ${FILE}`
BASE=`basename ${FILE}`
# Assume we want 16 processes per task (i.e. 1 worker per node).
PROCS=16
HOSTNAME=`uname -n`
HOSTLIST=""
for i in `seq 1 ${PROCS}`; do
   HOSTLIST="${HOSTNAME},${HOSTLIST}"
done
HOSTLIST=${HOSTLIST%,*}
CMD="mpirun -host ${HOSTLIST} -np ${PROCS} mb < ${FILE} > ${BASE}.mb.log"
cd $DIR
# Clean out any previous run.
rm -f *.[pt] *.log *.ckp *.ckp~ *.mcmc
# For testing purposes, use "if false". For production, use "if true"
if false ; then
   eval "${CMD}"
else
   echo "${CMD}"
   echo "Faking It On Hosts: ${HOSTLIST}"
   sleep 2
fi
```







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MPI Example wq.pbs

Set number of workers per node:

WPN=1

Set the working directory:

WORKDIR=/work/user

Name of the file containing the list of input files:

FILES=\${WORKDIR}/wq.lst

Name of the task script

TASK=\${WORKDIR}/wq_mb.sh

START=1









MPI Example STDERR

Only the end of the file looks interesting:

```
mike333_0:Taking:513:15336.63:2663.37
mike241_0:Taking:514:15367.58:2632.42
mike331_0:Taking:515:15401.42:2598.58
mike322_0:Skipping:516:15459.29:2540.71
Dispatcher:Timeup:mike322_0:1393617821.63
Dispatcher:Shutdown:31
Dispatcher:Last:516
```

Last task handed out was number 516, but looks like mike322_0 skipped it. The Dispatcher expects to order 31 other workers to stop the next time they request a task.









MPI Example STDOUT

The stdout file really doesn't change much, though the file paths are long.

```
Task:513:mike333_0:Ran:True:/work/user/wq_mb.sh
/work/user/PostPredYeast/YHL004W_DNA/SeqOutfiles/YHL004W_DNA.ne
x.run3_2868000/GTRIG.bayesblock
Timings:513:mike333_0:1393617699.01:1393618496.73:797.72:16134.
34
Stdout:513:
Stderr:513:
```

Task:515:mike331_0:Ran:True:/work/jalupo/WQ/MrBayes/wq_mb.sh /work/jalupo/WQ/MrBayes/PostPredYeast/YHL004W_DNA/SeqOutfiles/Y HL004W_DNA.nex.run3_4180000/GTRIG.bayesblock Timings:515:mike331_0:1393617763.78:1393618516.08:752.30:16153. 72 Stdout:515: Stderr:515:









Load Balancing Issues

- The more uniform the runtimes are across all tasks, the more likely a job will end gracefully.
- Take a look at the concepts.
- Illustrate potential problem.
- Discuss how to analyze a job's efficiency.



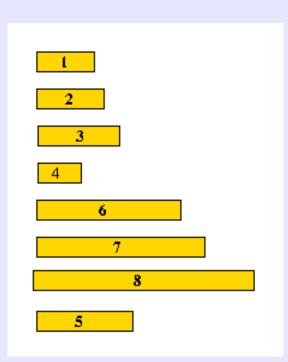






Task Run Times

Imagine a set of 8 tasks, number for identification only, and represented by bars propotional to their run times.







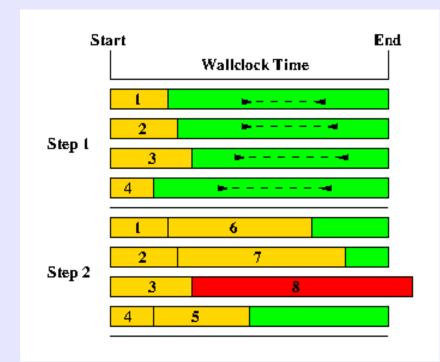


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Insufficient Walltime

PBS walltime sets the maximum wallclock time a job is allowed. Imagine the tasks get assigned in the following order:



Dashed bars show estimated times for next task - they all appear to fit remaining time.

Bad estimate for Task 8!









Sufficient Walltime











Load Balance Implications

- Order by longest running first, if possible.
- Run many tasks so representative times are seen early in the job.
- If range of times not known, there is no good way to make sure jobs complete gracefully.
- Output format allows analysis.









Monitoring and Statistics









Output Format Rational

- The colon-delimited format and seemingly redundant data items was intentional.
- Gawk, Perl, Python, and other scripting languages have easy facilities for parsing lines with character delimited fields.
- A few examples illustrate the idea.









Identifying Failed Tasks

The Task lines in the output file have the following format (fields are numbered):

1 2 3 4 5 6 Task:1414:mike104_0:Ran:True:/yada/script /data/path/filename

That means we just have to find the "Task" lines, check field 5 for True/False, and output the file name (i.e. could use to generate a new input list). Consider using Gawk:







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Timing Jitter

- Use Python to find the timing jitter between the longest and shortest running workers using Timing records. Field 5 is the walltime the task ended, so we just need to find the minimum and maximum end times.
 - 1 2 3 4 5 6 7

Timings:3:mike243_0:1406673580.51:1406673582.52:2.02:2.02

```
#! /bin/env python
import sys
f = open( sys.argv[1], 'r' )
raw = f.readlines()
f.close()
worker = {}
max end = 0.0
min end = 1.0e+37
for l in raw:
   u = l.strip().split(':')
   if u[0] == 'Timings' :
      t = float(u[4])
      if t > 0.0 :
         worker[u[2]] = t
for k, v in worker.iteritems() :
   if v < min end :
      min end = v
   if v > max end :
      max end = v
print( "End times between %.2f and %.2f - %.2f sec spread." %
        ( min end, max_end, max_end - min_end ) )
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```

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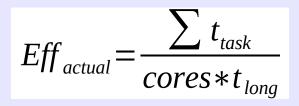


Efficiency

Important because job charges are based total walltime (in hours):

 $SU = cores * t_{long}$

$$Eff_{ave} = \frac{t_{long} + t_{short}}{2 * t_{long}}$$



 Want uniform end times. If one task keeps many nodes idle waiting to end, not good!

> t_{long} = longest worker walltime t_{short} = shortest worker walltime t_{task} = individual task walltime

 Eff_{ave} = average parallel efficiency Eff_{actual} = actual parallel efficiency









Examples

- Consider a job that runs 64 tasks on 64 cores.
- Well balanced, min of 69 hrs, max of 71 hours:
 - 98.6% ave efficiency.
- Highly imbalanced, 63 finish in 1 hour, 1 finishes in 71 hours.
 - 50.7% ave efficiency.
 - 2.9% actual efficiency.









Resources

- Moodle version at:
 - http://moodle.hpc.lsu.edu
 - HPC121 Background and Distribute Tasks
 - Distribution zip archive file provided.
- On SuperMike-II:
 - /work/jalupo/WQ/WQ-20140801r145.zip









Hands-On Test

- 1. Need +Python-2.7.3-gcc-4.4.6 in .soft
- 2. Create a directory.
- 3. unzip /work/jalupo/WQ/WQ-20140801-r145.zip
- 4.cd Examples/Timing
- 5.cp ../../wq.py .
- 6. chmod u+x wq_timing*
- 7. Edit wq_timing.pbs: set PBS output directory, proper allocation, and work directory.
- 8. Generate a proper file list:
 - 1. rm 82_file_list
 - 2. for i in `seq 1 82` ; do echo "`pwd`/file\$i" >> 82_file_list; done
- 9. Submit the PBS file: qsub wq_timing.pbs > jid







Hands-On Test Results

When job completes, the directory will look like this:

\$ ls 82 file list	iid	wq.py	WQ Timing.o228557
wq timing.sh	JIG	wq·ρy	
hostlist.228557 \$	pbs.228557	WQ_Timing.e228557	wq_timing.pbs

jid		Job ID (228557 in this case).
hostlist.228557 .		Job specific host list.
pbs.228557		PBS job script copy.
WQ_Timing.e228557		stderr (note use of job name and jobID).
WQ Timing.o228557		stdout (note use of job name and jobID)









Final Suggestions

- Organize data files in meaningful way.
 - More than 10,000 files per directory will cause performance degradation.
- Use Linux tools to generate file lists.
- Stay aware of job performance.



