Cluster Computing

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Overview

- Parallel computing allows us (for certain problems) to split a big job up into many smaller parts and run them in parallel.
- Our laptops or desktops can split a job up into as many threads as are available.
- This is likely a relatively small number like 4, 8, or 12.

Overview

- **Cluster computing** connects many computers (nodes) together on a local network.
- This allows a pooling of resources to increase computing power.
- This allows a user to access hundreds or even *thousands* of cores (if they need them).

MGHPCC

- The Massachusetts Green High Performance Computing Center (MGHPCC) is one of these clusters.
- Each of the participating instiutions has their own distinct cluster. We will be using the UMass cluster.
- In order to connect to this cluster, a user has to be on the UMass campus (or use VPN to the UMass campus.)
- We will need to VPN into the UMass network since we are currently off campus.

Hypothetical cluster computing workflow

- Transfer data/scripts to cluster
- Log in to the cluster
- Submit a job to the "scheduler"
- Transfer data/results from cluster if needed

The process we will use today

Our order of operations...

- Log in to the cluster
- Transfer data/scripts to cluster
- Submit a job to the “scheduler”
- Look at results

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How to pretend you are at UMass using VPN

- Mac: System Preferences > Network > VPN on left
- Windows: Cisco VPN client
  - Server address: vpn2.oit.umass.edu
  - Group name: umass
  - Password: vpn4umass
  - Account name: UMass user ID OR bip[number] (temporary for BIP2014)
  - Password: Enter your password

Accessing the MGHPCC

- Register for the MGHPCC (for UMass): https://www.umassrc.org/hpc/
- A login and password will be (have been?) assigned to you.
- At the moment, this will be different than your UMass user ID or email address. (NetID integration coming soon!)

Accessing the MGHPCC

- Unix or Mac
  - Unix or Mac: Create a secure shell: ssh username@ghpcc06.umassrc.org
- Windows
  - PuTTY: ghpcc06.umassrc.org (you will be prompted for user name and password)
- Enter password when prompted. (First time you login, you will need to change your password, then login again.)
- You are now connected to the cluster!
- Remember: You can only access the MGHPCC if you are on UMass's network (physically on campus or VPN)

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Transferring Data to MGHPCC

- We recommend using Cyberduck, a graphical SFTP client.
- Other options include scp and sftp for Mac/Unix command line users or PSCP/PSFTP for Windows users.
- Let's try to move the BiPSandbox folder to your /home/username folder on the MGHPCC.

The process we will use today

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Software available on the MGHPCC

- Once logged in, you will be placed in your home directory (/home/username).
- Full list of available software: http://wiki.umassrc.org/wiki/index.php/Provided_Software
- There is a wide array of available software options.

Using software on the MGHPCC

- In order to use software on the server, you'll need to load modules that contain the software.
- We are interested in using R here.
- To load R we use the command: `module load R/3.0.1`
- We can also unload R with the command: `module unload R`

Software

- Loading the R module will allow us to run R interactively (by typing R at the prompt) on the MGHPCC servers.
- But you should not do this!

Batch Mode

- Rather than running R code interactively, we can also run R in BATCH mode.
- This first requires you to write an R script that you want to run.
- Then at the command prompt, you can submit the script by typing: `R CMD BATCH [options] scriptName.R`
- But you should not do this either!
- We want to submit batch jobs to the cluster, not to the machine that you login to.

Submitting jobs to the cluster

- In order to submit a job to the cluster we need:
  - A R script that we wish to run
  - A shell script that calls the R script and submits the job to the cluster.
- We will then submit the job to the LSF (Load Sharing Facility) scheduler.
- **Note**: Commands submitted to LSF are just like if they were run from a command prompt.

LSF common commands

- `bsub` - submit a job
- `bkill` - kill a job
- `bjobs` - view status of jobs
- `bpeek` - view output / error files
- `bhist` - job history
- `bqueues` - available queues

Batch Mode

- Once we have a .R file that we want to run we can submit it to the LSF job scheduler.
- What actually gets submited to the LSF scheduler is a shell script that calls the R file (which we'll call example.R).
- We need to create a file that contains all of the code we would have run at the shell prompt.
- Example of a shell script is below. We'll call this shell script example.sh

```
$ module load R/3.0.1
$ R CMD BATCH --vanilla example.R
```

Submiting jobs to the cluster

- The command **bsub** allows us to submit the shell script to the cluster.
- The command below will submit the shell script example.sh to the cluster.

```
$ bsub example.sh
```

Submiting jobs to the cluster: Options

- We can also set many options in our job submission.
- -n: Number of cores requested
- -W: Wall clock time
- -R: Memory per job
- -q: Which queue to submit to

```
$ bsub -n 4 -R "rusage[mem=2048]" -W 0:10 -q long
example.sh
```

Submiting jobs to the cluster: Local

- An example shell script is in `BiPSandbox/module3/submitLocalParallelJob.sh`.
- Here we submit to the short queue.
- Commands to submit from within a .sh file is the same as when submitting from the command line:
  `bsub < submitLocalParallelJob.sh`

Submiting jobs to the cluster: Distributed

- We can also specify options in the shell script that we submit to the LSF scheduler.
- An example shell script is in `BiPSandbox/module3/submitDistrParallelJob.sh`.
- Commands to submit is again:
  `bsub < submitDistrParallelJob.sh`
- "Proper" way to distribute your job is using something like MPI.
- In this example, output is also distributed, less convenient.