Parallel and Distributed Computing for Optimization and Statistics

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[1]Special thanks to Sebastien Martin for providing many of the slides!

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- Machine Learning on large datasets
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Or repetitive computations:

- Parameter tuning
- Benchmarking

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- Limited computational power.
- Limited number of cores.
- Limited time available. (You, presumably, have better things to do than sitting and watching your program run.)

Resources

There are several ways to have access to a remote computer or a cluster.

- Another personal computer you own.
- Athena at MIT.
- Resources of your department/lab (Engaging at Sloan).
- Cloud computing as a service (Amazon AWS, Google Cloud Computing...).

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- Remote computing - execute commands on a remote machine
- Parallel computing - execute multiple commands simultaneously
- Distributed computing - parallel computing without shared memory

Why Should I Use This?

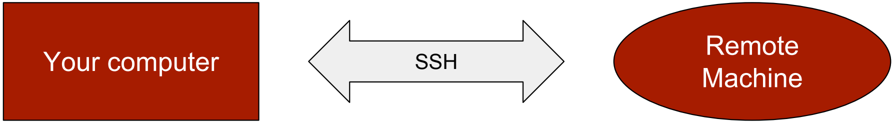
For research:

- Tackle bigger data sets in Stats and Optimization.
- Parallelize your computations.
- Longer computational times: run overnight or for a whole week!
- Can be very simple to use with interactive sessions (RStudio...)

In general:

- Valuable skill, used everywhere in industry.

How does it work: using a remote computer



- We use SSH (see lecture 1) to run commands on a remote machine through our computer.
- We can use the shell to do almost anything on the remote computer: create files, run a program, use Julia...
- It is also possible to use GUI applications like R-Studio or Matlab.
- It works with any computer, including your own machines.

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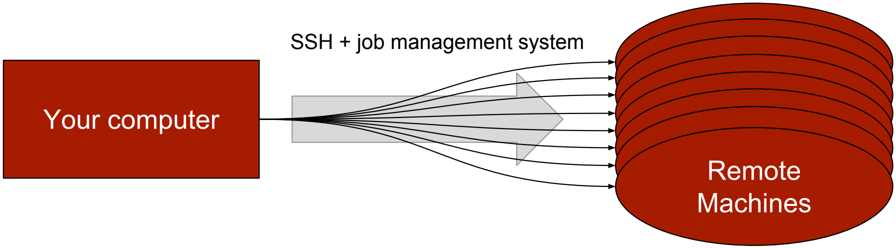

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- Different job management systems exist, we will use the example of Slurm, which the cluster Engaging uses.
- More complex to use, but far more powerful.

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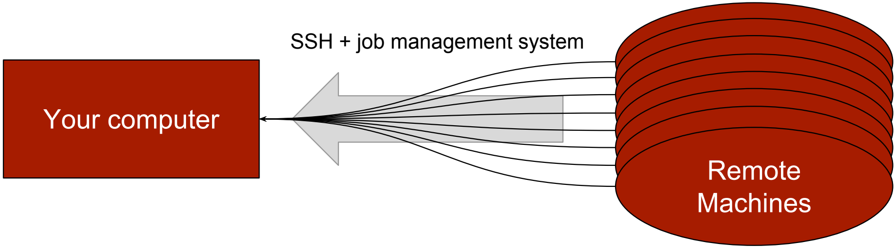

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Engaging

Engaging is a powerful computing cluster for MIT Sloan affiliates, request an account at `stshelp@mit.edu`. It uses the job management system Slurm, that we will use in this presentation.

Connecting to Engaging

Hostname	`eosloan.mit.edu`
Username	MIT Kerberos username
Password	MIT Kerberos password

`wikis.mit.edu/confluence/display/sloanrc/Engaging+Platform`

Athena

Any MIT affiliate can access the Athena distributed computing environment, you can use it to follow if you do not have access to Engaging.

Connecting to Athena

Hostname	`athena.dialup.mit.edu`
Username	MIT Kerberos username
Password	MIT Kerberos password

`http://web.mit.edu/dialup/www/ssh.html`

SSH

As seen in Lecture 1, we can connect to the remote machine through SSH:

```
ssh <user_name>@eosloan.mit.edu
```

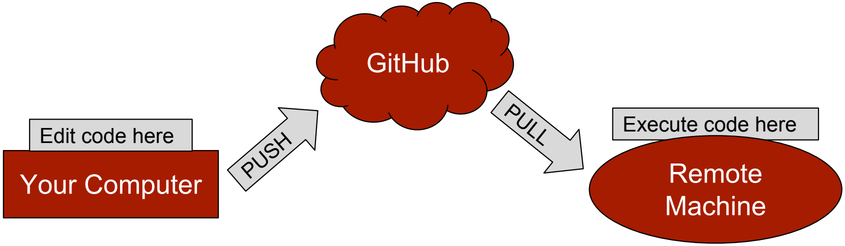
File Transfer

- Downloading from the Internet (useful to install software, or download datasets): wget
- Transferring files between the local and remote machines: Secure Copy scp

```
scp file_name.csv <user_name>@eosloan.mit.edu:
```

Using Git/GitHub to Synchronize Code

If you need to run code on the remote machine, an elegant way is to use git and GitHub:



For Advanced Users

Feel free to read up if you're interested!

- sshfs allows you to access the files of the remote machine as if they were on your own (magic)!
- screen allows you to keep your session active after you disconnect.
- tmux (terminal multiplexer) is like screen with lots of additional functionalities (panes...)

Running Jobs on a Computing Cluster

Important!

Do not run jobs/processes on the login node!

- When we login to Engaging, we are actually logging into a special login node.
- The login nodes are not designed for performing computations, but rather just for submitting jobs to the job management system.
- The actual work will be done by the computing nodes.

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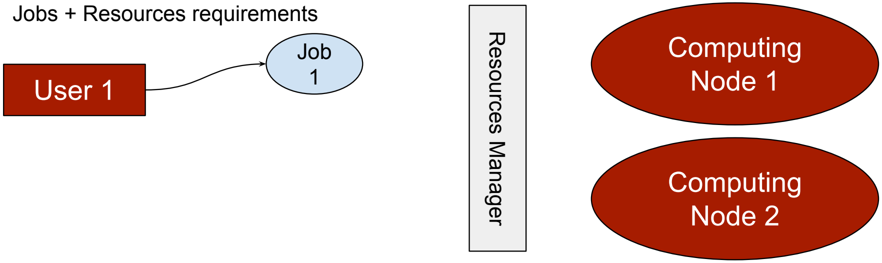

Job
: A program to be executed. (running a R/Julia/Python source file, a bash script, etc..)

Resources
: Resources required to run the job (memory, cpus, time, software requirements...)

The Job/Resource manager allocates the available resources of the computing nodes of the cluster to the different users.

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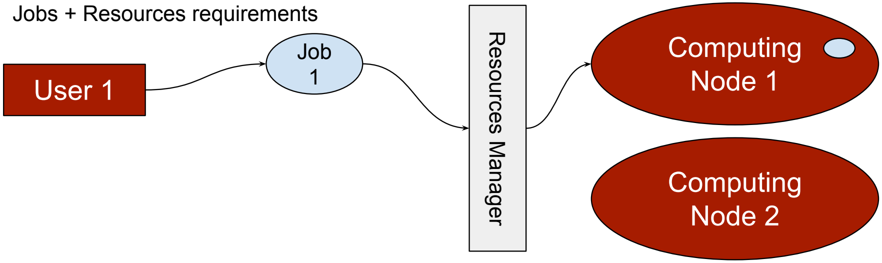

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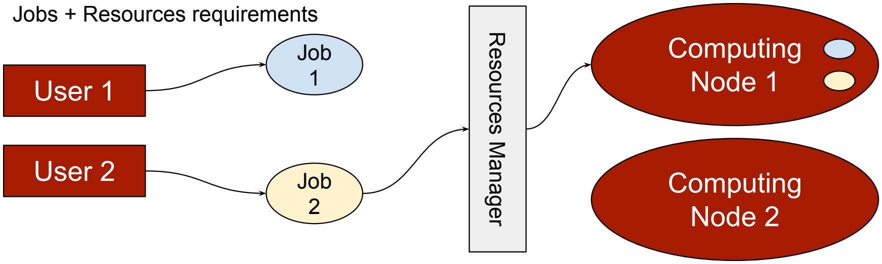

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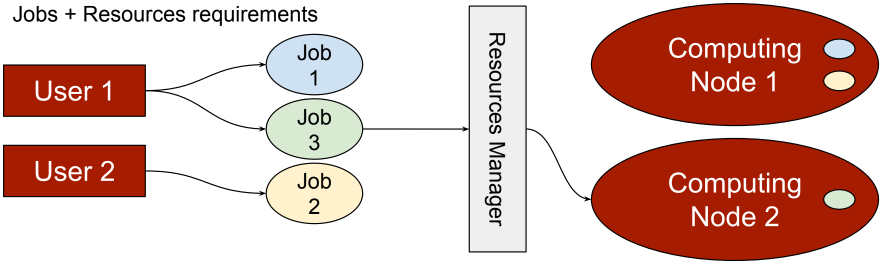

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Module Loading

Many packages are installed on the cluster. To use them, we use the following special commands.

- Show all modules: `module avail`
- Search for modules: `eo-module-find julia`
- Load a module: `module load engaging/julia/0.6.1`

Running an Interactive Job on Engaging - `srun`

To ask SLURM, we use the command `srun`.

- The main resource parameters are:

Memory	`--mem-per-cpu=1G`
CPUs	`--cpus-per-task=1`
Time	`--time=1-12:00` (for 1 day and 12 hours)
Partition	`--partition=sched_mit_sloan_interactive`

- The partition is the name of the cluster you want to use. The two main partitions you should use are `sched_mit_sloan_interactive` and `sched_mit_sloan_batch`.
- When running interactive jobs, we should use the `--pty` flag to start the session in the current window.

Monitoring Jobs

- You can check if your job is running or in the queue: `eo-show-myjobs`
- Cancel a job: `scancel <JOB_ID>`

Running a Batch Job on Engaging - `sbatch`

- A nice way to run jobs is to save them and all their parameters in a special bash file, and use `sbatch` to run them.
- The job can be run using “`sbatch myjobname.sh`”
- The output of your jobs (what would normally appear in the console) will be saved in a `slurm-<yourjob>.out` log file where you ran `sbatch`.

Types of Parallel Computing Jobs

- “Embarassingly parallel”
  - Multiple instances of the same program with different inputs
  - Each instance can run independently, no need for shared memory
  - eg. grid search for hyperparameter tuning
- Parallel computing with shared memory
  - Commands execute simultaneously on separate processors, but work on shared memory
  - Computation cannot (easily) be split across separate nodes because communication between processes is necessary
  - eg. matrix multiplication, parallel SGD
- Advanced topics
  - Distributed computing with a message passing interface (MPI)
  - GPU computing

Other Things to Explore

There are a lot of possibilities with Engaging and other systems! Read the Engaging and SLURM documentation, use Google, etc.. For example:

- Running interactive jobs (ie with a console that you control)
- Running graphical interfaces (RStudio, SAS, Matlab...)
- Receive an email when your job completes
- Use Jupyter Notebooks on the cluster...