Rotman Research Node (RRN)

Jay / TDMDAL

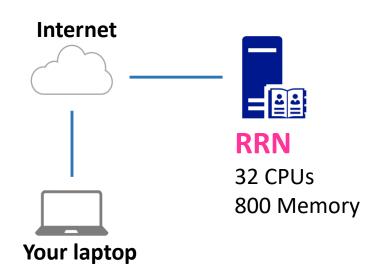
Plan for Today

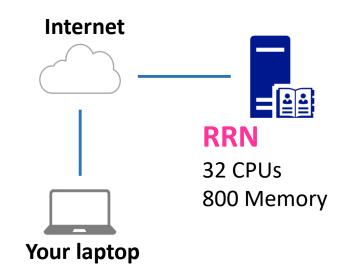
- Agenda
 - What is RRN?
 - When will you choose to use it?
 - How to use it depending on your use cases (demo)?

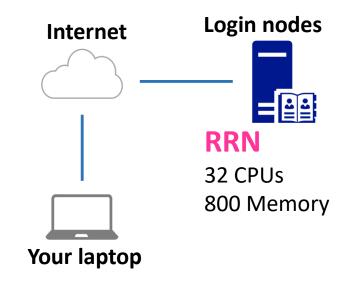
- We will focus on big pictures so
 - You get a good general understanding of the system
 - You know where to look for the details and what details
 - user manuals, Internet, TDMDAL support, etc.

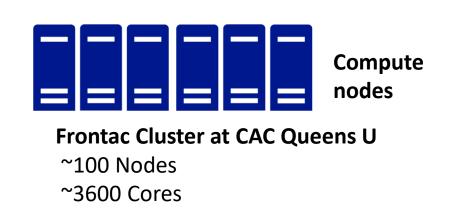
What is RNN (1)

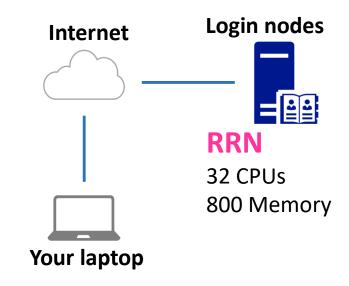
- A shared research server
 - Hardware: 32 Xeon CPUs; 800G Memory
 - Storage: Home directories; 50T shared project directory
 - Software: Linux OS; Python, R, Matlab, Stata, Julia, C, C++, Fortran, etc.
 - Dedicated to Rotman researchers
 - Hosted at Centre for Advanced Computing (CAC) at Queens U
- A gateway to a pool of computing resources
 - Zoom out (next slides)

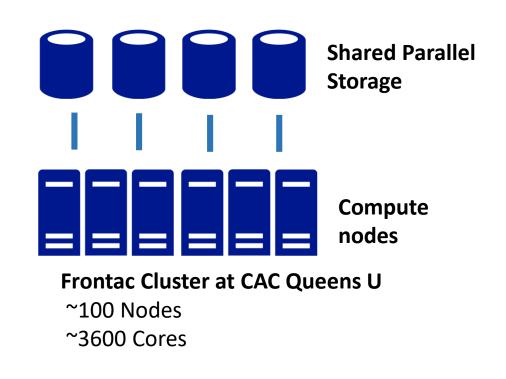


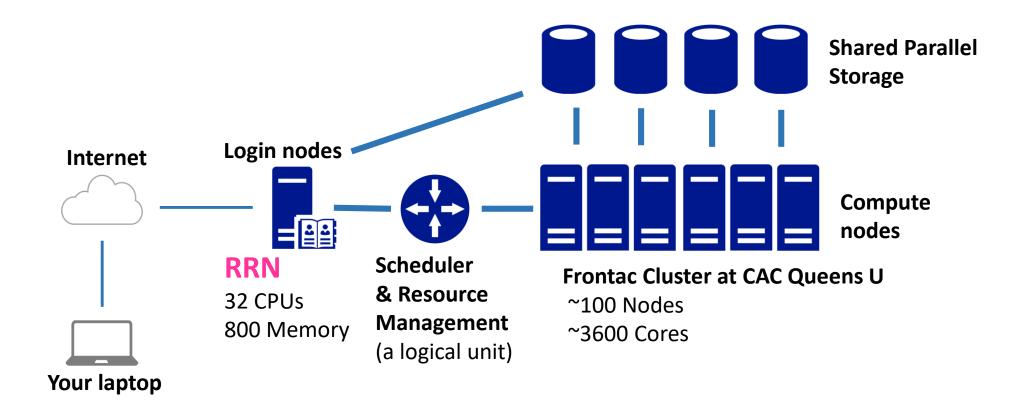


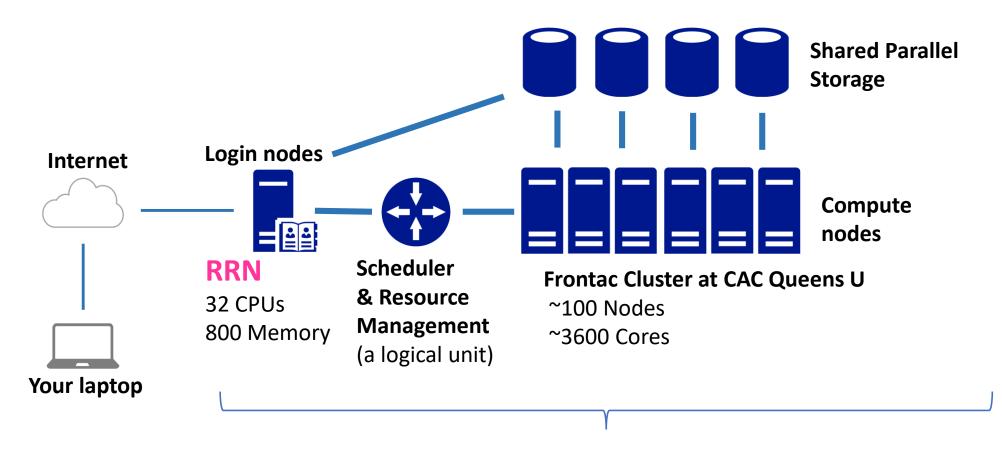












High Performance Computing System (HPC)

Why using RRN

- My code takes too long to run
 - it need more CPUs (i.e. computing intensive work)
 - it need more memory (i.e. memory intensive work)
- I want to use XYZ (ex. Matlab), but the license cost is too high

- I want a stable environment for a long running code
 - ex. collecting data through web scraping

Questions to ask before considering RRN

- One big misunderstanding
 - my (unmodified) code will run faster on the server (NO in most cases)
- I need more CPUs
 - have I optimized my code (vectorization; better algorithm)?
 - have I tried parallel computing on my desktop?
 - modern desktop has 2-4 CPUs (4-8 with hyperthreading)
 - no license cost if you use open source language (R, Python, Julia, etc.)
- I need more memory
 - do I really need to load all those data
 - have I optimized my code (delete big variables/objects after use; better algorithm)

How to Use RRN — User Manuals

- Our RRN <u>User Manual</u>
 - Focus on RRN
 - Good for getting started

- CAC <u>User manual</u>
 - Including HPC usage (Compute Nodes)
 - For users with highly compute-intensive jobs

How to Use RRN – Account & Logon

• Email tdmdal@rotman.utoronto.ca for an account

- SSH (Secure Shell) client
 - Windows (ex. <u>Mobaxterm</u>)
 - Mac (terminal + <u>Xquartz</u>)

ssh -X yourUserName@rrlogin.cac.queensu.ca

Folder Structure & Disk Quota

Folder	Path	Quota	Usage
Home	/global/home/yourUserName/	3T	Main storage
Project	<pre>/global/project/rotman_research/you rUserName/</pre>	50T shared	Additional storage
Scratch	/global/scratch/yourUserName/	5T	Temporary storage

Note: 1) Only you have access to those 3 folders

- 2) Your project folder shares the 50T quota with other Rotman project folders
- 3) project and scratch folders can also be accessed via two shortcuts in the home folder:

rotman_research and scratch

How to Use RRN — Transfer Files

- a SFTP client (transfer files between local PC and RRN)
 - Windows (ex. WinSCP, Cyberduck, FileZilla)
 - Mac (Cyberduck, FileZilla)
- Other methods available too
 - scp, rsync, etc.
 - globus
 - •

Using Software – Module System

A software Environment Module system

module avail

module load <module_name>

module list

	Interactive Mode	Batch Mode
RRN (1 node)		
Compute Nodes (Many nodes)		

	Interactive Mode	Batch Mode
 RRN (1 node) CPU: 32 cores Memory: 800G; quite large Shared (among Rotman researchers) Easy to use: Code runs as soon as you ask it to run 		
Compute Nodes (Many nodes)		

	Interactive Mode	Batch Mode
 RRN (1 node) CPU: 32 cores Memory: 800G; quite large Shared (among Rotman researchers) Easy to use: Code runs as soon as you ask it to run 		
 Compute Nodes (Many nodes) CPU: 24- up to 128-core node Memory: mostly 256G nodes; a few large ones (512G, 1T & 2T) Exclusive use once allocated to you Slightly harder to use Need to write a script to talk to the schedular/resource manager Need to wait in a queue to compete for resources 		

	Interactive Mode	Batch Mode
 RRN (1 node) CPU: 32 cores Memory: 800G; quite large Shared (among Rotman researchers) Easy to use: Code runs as soon as you ask it to run 	Debug code Run small jobs • < 6 cores • < 0.5 hrs.	
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Ex.1 Matlab - RNN Interactive Mode

Load matlab module

module load matlab/R2018b

Run matlab with GUI

matlab

Run matlab without GUI

matlab -nodesktop -nosplash -nodisplay

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 RRN (1 node) CPU: 32 cores Memory: 800G; quite large Shared (among Rotman researchers) Easy to use: Code runs as soon as you ask it to run 	Debug code Run small jobs • < 6 cores • < 0.5 hrs.	Run intermediate compute & memory intensive jobs • ~12 cores • 1-2 hrs. or
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Ex.2 Matlab - RNN Batch Mode

Load matlab module

module load matlab/R2018b

- Run in foreground
 - prompt taken; need to wait for result; not recommend

```
matlab -nodesktop -nosplash -nodisplay <matlab_test.m
&>matlab_test.log
```

Run in background and no hang up after logout (recommend)

```
nohup matlab -nodesktop -nosplash -nodisplay
<matlab_test.m &>matlab_test.log &
```

	Interactive Mode	Batch Mode
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Ex.3 Matlab – Interactive Compute Node

Allocate an interactive node

Load matlab module

- Run matlab in interactive mode with or without GUI
- Run matlab in batch mode. However, don't exit the interactive node!

	Interactive Mode	Batch Mode
 RRN (1 node) CPU: 32 cores Memory: 800G; quite large Shared (among Rotman researchers) Easy to use: Code runs as soon as you ask it to run 	Debug code Run small jobs • < 6 cores • < 0.5 hrs.	Run intermediate compute & memory intensive jobs • ~12 cores • 1-2 hrs. or
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Write a job submission script (an example, job.sh)

```
use bash shell to
                  #!/bin/bash
execute this script
                  #SBATCH --job-name=MATLAB_test
                  #SBATCH --partition=standard
                  #SBATCH --mail-type=ALL
                  #SBATCH --mail-user=jay.cao@rotman.utoronto.ca
request resources
                  #SBATCH --output=STD.out
(Slurm command)
                  #SBATCH --error=STD.err
                  #SBATCH -c 4
                  #SBATCH --time=30:00
                  #SBATCH --mem=5000
                  module load matlab/R2018b
  load matlab &
                  matlab -nodesktop -nosplash -nodisplay <matlab_test.m</pre>
  run my code
```

```
#!/bin/bash
#SBATCH --job-name=MATLAB test # set job name
#SBATCH --partition=standard
                                # set job partition (group of nodes)
#SBATCH --mail-type=ALL
                                # email me when job start, stop, etc.
#SBATCH --mail-user=jay.cao@rotman.utoronto.ca
#SBATCH --output=STD.out # save standard output to STD.out
                                # save std. error output to STD.out
#SBATCH --error=STD.err
                                # ask for 4 CPUs
#SBATCH -c 4
#SBATCH --time=30:00
                                # set wall time to be 30mins
#SBATCH --mem=5000
                                # ask for 5G memory
module load matlab/R2018b
matlab -nodesktop -nosplash -nodisplay <matlab test.m</pre>
```

```
#!/bin/bash
#SBATCH --job-name=MATLAB test # set job name
#SBATCH --partition=standard
                                # set job partition (group of nodes)
#SBATCH --mail-type=ALL
                                # email me when job start, stop, etc.
#SBATCH --mail-user=jay.cao@rotman.utoronto.ca # set my email address
#SBATCH --output=STD.out
                        # save standard output to STD.out
                                # save std. error output to STD.out
#SBATCH --error=STD.err
                                # ask for 4 CPUs
#SBATCH -c 4
#SBATCH --time=30:00
                                # set wall time to be 30mins
#SBATCH --mem=5000
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module load matlab/R2018b
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#SBATCH --output=STD.out
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                                # save std. error output to STD.out
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                                # set wall time to be 30mins
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                                # ask for 5G memory
module load matlab/R2018b
matlab -nodesktop -nosplash -nodisplay <matlab test.m</pre>
```

- run job script to submit your code to a compute node
 - currently CAC doesn't enable inter-node jobs

• Show status of jobs

Cancel jobs

Extra Stuff

Persist Your Sessions: tmux & x2go

- What does it mean
 - after you log out the system, you can still log in back to where you left off
- Why is it useful
 - long running code on RRN in foreground
- Tools to achieve it
 - persist a non-GUI session: tmux (recommended; demo) or screen
 - persist a GUI session: x2go (recommended; demo), VNC or xpra

tmux: minimum to get started

```
launch: tmux
split current pane vertically: ctrl-b %
split current pane horizontally: ctrl-b "
moving between panes: ctrl-b \uparrow, \downarrow, \rightarrow, \leftarrow
close a pane (close the last pane to exit tmux): exit
detach from a session: ctrl-b d
re-attach to a session (assuming you only have 1 session): tmux attach
```

more on getting started with tmux: https://www.hamvocke.com/blog/a-quick-and-easy-guide-to-tmux/

Processes: ps, top, htop, kill, pkill

check all the process you are running

ps -u yourUserName

- display system info (CPU & memory usage, process, etc)
 top or htop (type q to exit)
- terminate a process

kill processID

terminate all processes you have (this will log you out too)

pkill -u yourUserName