Running Simulations on Different Pathways

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Abstract
The purpose of this project was to inform students about the differences between the pathways to run a certain code on a supercomputer. In order to reach our conclusion, our group experimented by using both pathways and observing the differences between the steps taken to get results. Many scientists use the Neuroscience Gateway Portal in order to run simulations; however, there is more to the backend of the portal. Even if both pathways yield the same results, the steps to run the simulation would be much simpler when users use the portal. Following our research, we found the significance of shortcuts making the lives of scientists or researchers easier.

What We Learned
While part of our internship was learning how to use unix in order to run programs on the Comet Supercomputer we also learned a lot about the super computer's uses, and what SDSC does with it. Approximately every four years they submit a proposal to acquire a new Supercomputer. SDSC then helps scientists get accesses to these computers for their research.

Methods
The technology we used in this project is the supercomputers. We used Linux which is an open source operating system to run the simulation for one of the pathways. For another pathway, we used a Neuroscience Gateway Portal to run the simulations.

NSG Portal

1. Download a file for the "jonesmodel" (make sure the file is a zip file because the NSG portal can only read zip file)

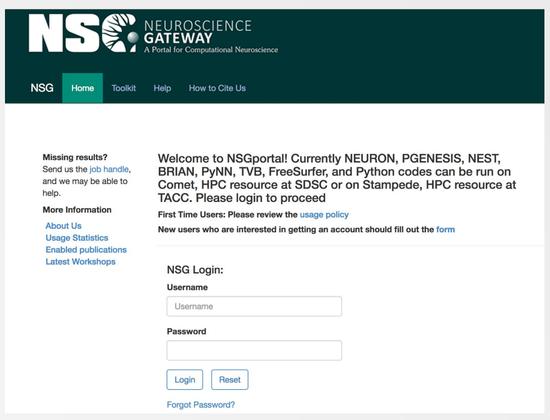
2. Log onto the Neuroscience Gateway Portal

3. Create a New Folder and upload the zip file for the "jonesmodel" in the Data subfolder.

4. Create a "New Task" on the Task subfolder.

5. Name the Task in the Description, choose the "jonesmodel" data for the input, choose the "NEURON7.4 on Comet" for the tool, and choose the number of hours you want to run the program in, type in "Batch.hoc" for the main input file name, the number of nodes to use, and the number of cores you want to use from each node for the parameters.

6. Wait for an email from the NSG portal for completing the job. Download the files in the output.



Comet

1. Log onto Comet from Linux.
(type in "ssh -l <username> comet.sdsc.edu")

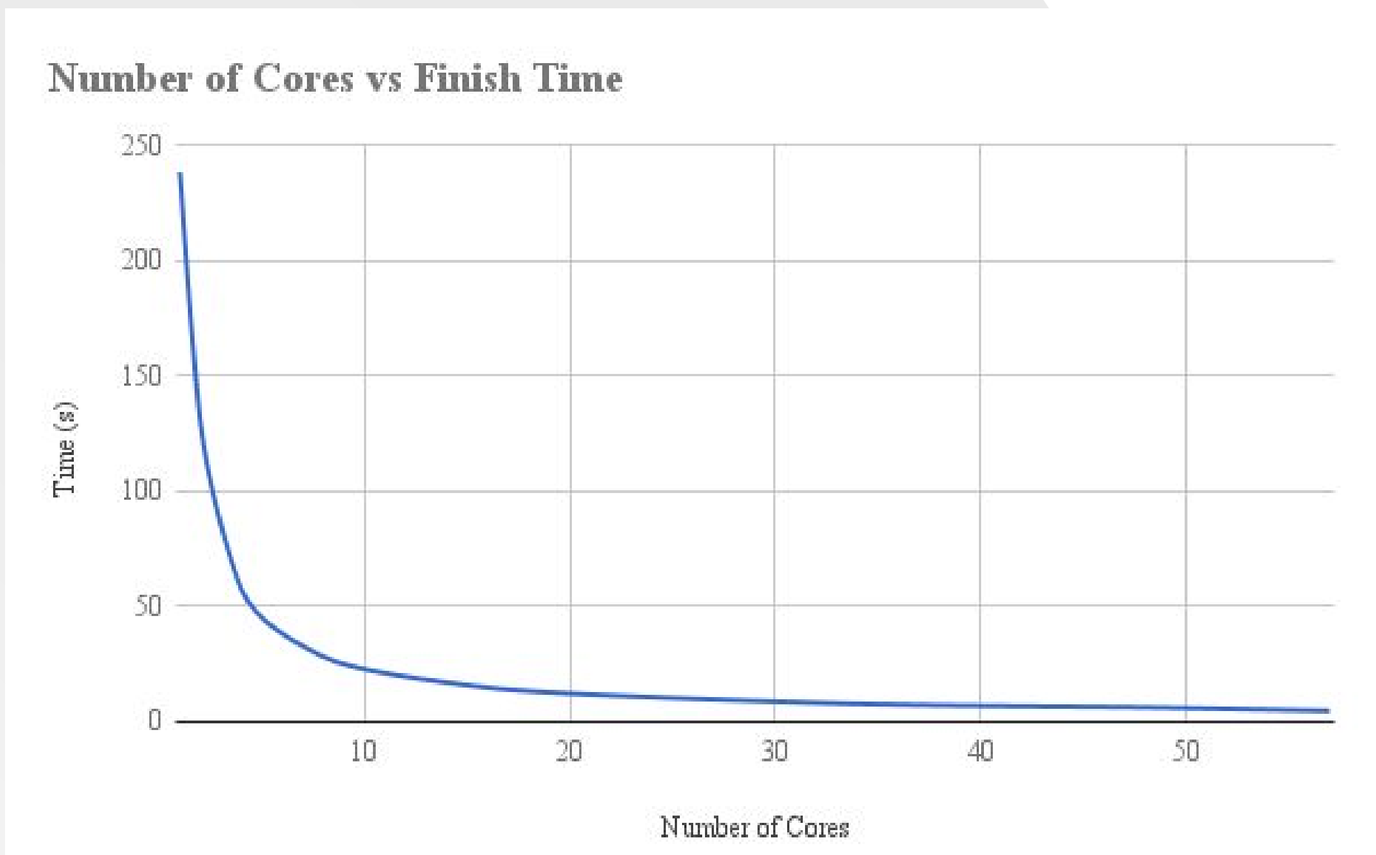
2. Download the Jones model by downloading the zip file onto the comet account.
("scp <filename> <username>@comet.sdsc.edu:~/")

3. create a file in the Jonesmodel directory.
(cd <directory>; touch <newfilename>)

4. Source a nrnenv file: . /projects/ps-nsg/home/nsguser/applications/neuron7.4/nrnenv
Then verify by typing in "which nrnivmodl" and run "nrnivmodl mod_files"

5. Edit the new file by typing in "vi <newfilename>" then type in the code for the simulation.

6. run the code and wait for the code to finish running and view the results.



As the number of cores increase, the time to finish each job decrease. However, if there are too many cores requested, it may take more time to send information between nodes.

Summary
The time to go through the path is shorter and the pathway itself is much simpler with the portal than programming on Linux. In conclusion, using the portal to run simulations is more convenient than actually programming the information into Comet.