SDSC SAN DIEGO SUPERCOMPUTER CENTER



Zero to Neuro

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Abstract

Using supercomputers drastically increases the efficiency of completing a task by using multiple nodes and tasks per node to spread out the work. The Neuroscience Gateway (NSG) is an effective tool for neuroscientists to gain access to supercomputers to run computational neuroscience simulations, eliminating the need to go through the supercomputer's backend to submit their scripts. We compared the steps for using NSG and going through the backend to demonstrate how the simple user interface of NSG makes it efficient and less complicated for neuroscientists around the world to further their research.

Introduction

The research intends to explore the convenience of providing gateways on supercomputers, such as the Neuroscience Gateway. Supercomputers increase the efficiency of research by assigning work to multiple cores, thus distributing the workload and decreasing the work time. The utilization of supercomputers require knowledge of operating Linux, using compiling tools and understanding schedulers and file systems. Gateways like NSG are used to make up for the lack of cyber-infrastructure knowledge for some scientists. The comparison between the NSG interface and Comet back end highlights the ease of use of NSG, which enables any scientist to make full use of the supercomputers regardless of their cyber-infrastructure background. Neuroscientists can also use computer simulated environments to recreate processes in the brain, and can increase complexity and test many variables to predict what might happen in a real life situation.

Methods/Tools

1. Comet

Comet is a dedicated eXtreme Science and Engineering Discovery Environment (XSEDE) cluster designed by Dell and SDSC delivering 2.76 peak petaflops. It features Intel next-gen processors with AVX2, Mellanox FDR InfiniBand interconnects, and Aeon storage.

2. NEURON

NEURON is a simulation environment for modeling individual neurons and networks of neurons. It provides tools for conveniently building, managing, and using models in a way that is numerically sound and computationally efficient. It is particularly well-suited to problems that are closely linked to experimental data, especially those that involve cells with complex anatomical and biophysical properties.

3. Neuroscience Gateway

The Neuroscience Gateway (NSG) project facilitates access and use of National Science Foundation funded High Performance Computing (HPC), High Throughput Computing (HTC) and cloud resources by neuroscientists.

- 4. Jones model
- An example of biophysically realistic neural model.

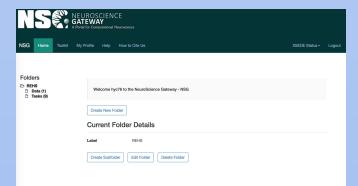
Research and Results

Access through Neuroscience Gateway (NSG) Portal

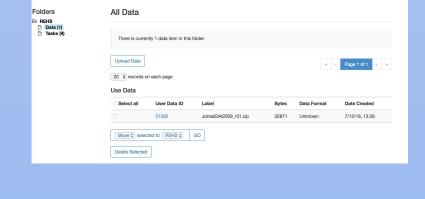
1. Access the NSG (Neuroscience Gateway) Portal [1].



- Click "Register Account" to create an account and fill in all the information 2. needed.
- Once the account is created, click "Access NSG Portal" to access the login 3. page.
- Inside the account, create a folder with a meaningful name. 4.



Inside the folder, go to "data" folder and upload zip files into the folder. (In 5. our project, we uploaded the Jones Model zip file).



Folders De REHS Data (1) Tasks (9)	Tasks	${\cal G}$ Refresh Tasks
	Current CPU Hr Usage: 0 Explain this? There are currently 9 tasks in this tab. (Items 1 - 9 are shown here.)	
	Create New Task	

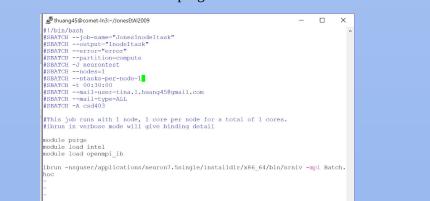
7. Modify number of cores through the parameter list, where the final number of

Access through Comet Backend

- 1. Make a Comet account.
- 2. Go to Model DP [2] and download the zip file.
- Download "WinSCP" to transfer the Jones file to your own Comet directory. 3.
- Log into your Comet account. 4.
- Drag and drop the Jones script from your computer's files into your Comet 5. directory.
- Download "putty" to access your Comet account, or use terminal for Macs. 6.
- Log into Comet [3].
- Log in with your Comet username and password. 8.
- 9. Type "ls" to display all of your files. "JonesEtAl2009" should be listed.

login as: thuang45 Using keyboard-interactive authen Password: Last login: Fri Jul 27 13:33:57 20	tication.		~
Rocks 6.2 (SideWinder) Profile built 16:45 08-Feb-2016			
Kickstarted 17:27 08-Feb-2016			
WELCOME TO			
* * * * * * * * * * * * * * * * * * * *	*****	*****	
[1] Example Scripts: /share/apps/	examples		
[2] Filesystems:			
(a) Lustre scratch filesystem (Preferred: Scalable larg	m : /oasis/scratch/comet/\$USER/temp_proj ge block I/O)	ect	
(b) Compute/GPU node local S: (Meta-data intensive job:	SD storage: /scratch/\$USER/\$SLURM_JOBID s, high IOPs)		
(c) Lustre projects filesyste	em: /oasis/projects/nsf		
(d) /home/\$USER : Only for se *Do not* use for I/O inte	ource files, libraries, binaries. ensive jobs.		
[3] Comet User Guide: http://www.s	sdsc.edu/support/user_guides/comet.html		
Lthuang45Bcomet-in3 -18 1s C. hello, Slum_script error hello, C.17687124.comet-6-53.out hellompi.1790768.comet-16-53.out hellompi.17901504.comet-18-59.out hellompi.17901504.comet-18-59.out hellompi.17901504.comet-18-59.out hellompi.17901504.comet-02-68.out hellompi.17901504.comet-02-68.out	Jones_script mpi_hello mpi_hello.c	****	

- 10. Enter the "JonesEtAl2009" directory by typing "cd JonesEtAl2009/".
- 11. Create or edit a pre existing script and call it "Jones_script". This will be used to submit the Batch.hoc file to run the program.
- 12. Type "vi Jones_script" to edit the script. Type "i" then enter to insert and edit the information.
- 13. Set the job and output name to a meaningful name to keep track of varying nodes and tasks. Change the mail-user to your own email to receive notifications of when the submitted task is finished. Set the number of nodes and ntasks per node both to 1. Add in "module purge", "module load intel", "module load openmpi_ib", and "ibrun ~nsguser/applications/neuron7.5single/installdir/x86_64/bin/nrniv -mpi Batch.hoc" at the end of the program.



14. Hit the "esc" key, then type "ZZ" to exit and save the edited script. 15. Enter "sbatch Jones_script" to submit the job.

We accessed the NEURON + Python Basics page [4] and created a simple neuron with a passive cell membrane using Python code. We inserted an alpha synapse, set up recording variables, then ran the simulation using NEURON's software.

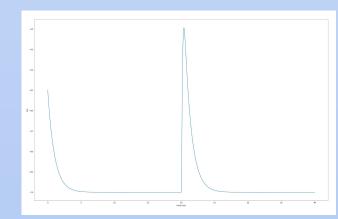


Figure 2 Action potential graph using NEURON of a simple neuron model with a passive cell membrane.

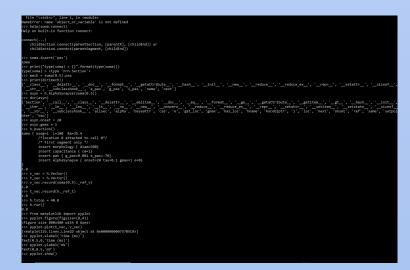


Figure 3 Code written in Python to create a graph of action potential using NEURON.

After familiarizing ourselves with the NEURON software and design, we continued the ball and stick tutorial to create a model of a soma connected to a dendrite. We added biophysical mechanisms, and then stimulated the neuron by sending a current pulse through the distal end of the dendrite. Varying the number of segments on the dendrite resulted in different outputs.

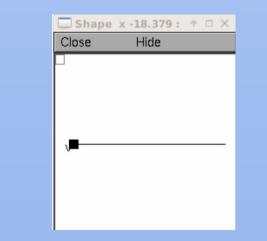
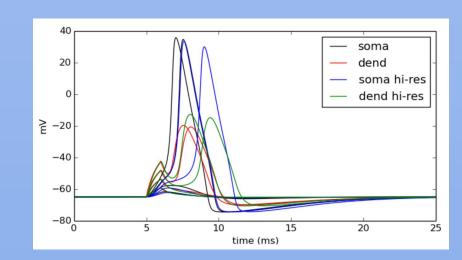
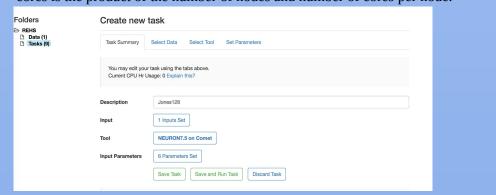


Figure 4 A simple ball and stick model of a neuron with a soma and dendrites.



cores is the product of the number of nodes and number of cores per node.



- "Save and Run Task" to NSG. 8.
- An email would be sent informing the completion of a task. 9.
- Once the job is completed, view the output and download the "STDOUT" file. 10.

L	abel	Tool		Input	Parameters	Date Created	Action
Clone	Jones128	NEURON7	.5 on Comet	View (1)	View (6)	7/26/18, 14:21	View Output
Select all	Tool Outpu		File Name	Eile Siz	e (Bytes)		
	PROCESS		STDOUT	69		Download	
			STDERR	370		Download	
	outputfile		output.tar.gz	545037		Download	

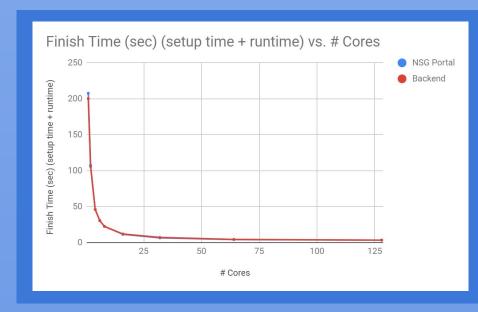
Record the time used to complete the task. 11.

	STDOUT	
numprocs=128 setuptime = 0.37 runtime = 34.71		
0 finishtime = 35.19		

- - 16. There should be a new line that says "Submitted batch job _____" with a string of numbers.
- 17. Check your email to see when the submitted job is completed, then type "ls" to find the output file. It should be listed as the name you've given the output file, for example "1node1task".
- Type "cat _____" with your output file name to see the contents of the output file. 18.
- Record the finish time time as a data point. This time includes the set up time 19. and the run time.

thuang45@comet-In3:~/JonesEtAl2009		-		×
WELCOME 1	0			^
	/// // //			
*****	*******	* * * * * * * * * * * * * * * * * * * *	*****	- 11
[1] Example Scripts: /share/app	s/examples			
[2] Filesystems:				
(a) Lustre scratch filesys(Preferred: Scalable 1		met/\$USER/temp_proje	ct	
(b) Compute/GPU node local (Meta-data intensive j		\$USER/\$SLURM_JOBID		
(c) Lustre projects filesy	stem: /oasis/projects/n	sf		
(d) /home/\$USER : Only for *Do not* use for I/O i		s, binaries.		
<pre>[thuang45@comet-ln3 ~]\$ ls Inodeitask C_hello_Slurm_script error hellompi.17796783.comet-l6-53.out hellompi.1779576.comet-l8-45.comet-l8-45.comet-l8-45.comet-l8-45.comet-l10mpi.17801504.comet-l8-45.comet-l8-45.comet-l10mpi.1780507.comet-l8-45.comet-l8-4</pre>	nut Jones_script nut mpi_hello nut mpi_hello.c nut mpi_hello_Slurm_scr test sEtAl2009/	ip	****	
Inde6task errInd61task Ind68task error Znd632task Jones_script [thuang45@comet=ln3 JonesEtAl20 [thuang45@comet=ln3 JonesEtAl20 scuptime = 1.67 runtime = 198.56 0	09]\$ sbatch Jones_scrip 09]\$ ls mod_files mosInit.hoc MuBurst_10.hoc Mu_output.dat 10.hoc noise2D_V2.hoc .txt out.dat. parlib.hoc readme.txt 09]\$ vi Jones_script	scale_ep_thresh.hoc sj10-cortex.hoc STATES wiring_proc_2Dv2.ho	с	
finishtime = 200.26 [thuang45@comet-1n3 JonesEtA120	0010			

20. Repeat steps 12 through 19 with varying numbers of nodes and tasks per node, making sure to also update the job and output names accordingly to keep track.



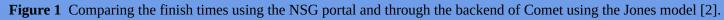


Figure 5 Measuring the action potential along various parts of the neuron. The number of segments was also another factor that modified the output.

Summary

After 2 months of research on NSG and Comet, we have learned that gateways greatly increase the efficiency of executing computational neuroscience tasks. Neuroscientists can easily use simulation environments, such as NEURON, to model brain structures and activities, such as action potentials in neurons. Modeling real life processes in hypothetical environments can push the limits of experiments that can be accomplished in laboratories.

Future Work

We plan to continue our work by exploring how to model more complex functions of the brain using NEURON. Our first step would be to create a model of a network of cells that can run on a parallel machine, then investigate how different neurotransmitters affect synapses.

References

[1] https://www.nsgportal.org/index.html [2] https://senselab.med.yale.edu/ModelDB/ShowModel.cshtml?model=136803 [3] https://www.sdsc.edu/services/hpc/hpc_systems.html#comet [4] https://www.neuron.yale.edu/neuron/static/docs/neuronpython/firststeps.html#what-is-neuron