Neuroscience Gateway: Enabling Easy Path to Supercomputing for Neuroscience Research and Education

Amitava Majumdar[1], Subhashini Sivagnanam[1], Ted Carnevale[2], Kenneth Yoshimoto[1]

[1]UCSD, San Diego, CA; [2]Yale University, New Haven, CT

Neuroscience's Growing Need for High Performance Computing (HPC)

- Increased size and complexity of computational models
- Wider use of optimization and parameter space exploration
- Projects that require generating a large ensemble of simulations, e.g. to examine roles of noise or stochasticity, determine parameter sensitivity, evaluate learning rules
- Expanding use of experimental methods that generate massive amounts of data requiring computationally intensive analysis

Barriers to Using HPC

- Writing peer-reviewed proposals for computer time.
- Understanding HPC machines, policies, complex OS/software.
- Installing and benchmarking complex tools on HPC resources.
- Understanding and managing multiple remote authentication systems.
- Dealing with data transfer, management, and storage issues.

Result: few neuroscientists could access HPC before the Neuroscience Gateway was developed. Projects may have started small by design, but entry barriers forced many to stay small.

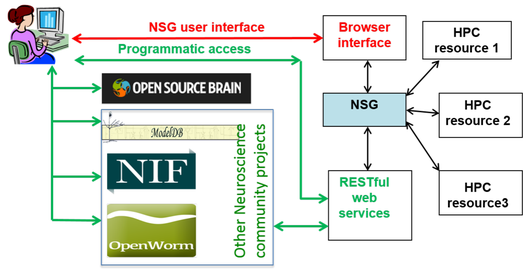
The Neuroscience Gateway (NSG)

The Neuroscience Gateway https://www.nsgportal.org provides simple, secure access to the XSEDE project's HPC resources. NSG's portal and programmatic service, make it easy to use neuroscience-related software and tools.

Partial list of tools currently available at NSG:

Brian	NetPyNE	EEGLAB	FREESURFER
CARLsim	NEURON	MATLAB	FSL
DynaSim	PyNN	Octave	TensorFlow
GENESIS	BluePyOpt	Python	The Virtual Brain
NEST		R	Empirical Pipeline

New tools are added on request.



GUI and Programmatic Access

NSG Portal's simple, easy to use web interface provides

- access to XSEDE HPC resources, HPC software stack.
- access to architectures such as GPUs, KNL.
- support for "bundling" of jobs, i.e. multiple single core executions in parallel (e.g. for embarrassingly parallel tasks, such as parameter sweep studies).
- support for custom workflows, e.g. Virtual Brain pipeline.

A RESTful API (NSG-R) offers most portal functionality

- submit, cancel, and delete jobs
- list and check status of submitted jobs
- list and download results
- list working directory

Example:

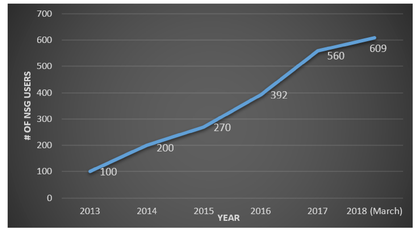
```
curl –u username:$PASSWORD -H cipres-appkey:
$KEY $URL/job/username -F tool=NEURON74_TG -F
input.infile_=@./JonesEtAl2009_r31.zip  -F
vparam.number_nodes_=2
```

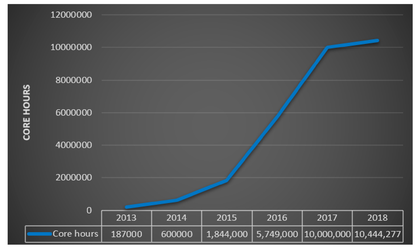
Getting an Account

To use NSG directly through its portal or RESTful interface, you will need your own NSG account. Fill out the form at https://www.nsgportal.org/gest/reg.php. Contact and brief technical information are required for user verification. Accounts are usually set up within 24 hours. Users are added to the NSG email list, which gets occasional news posts.

Several neuroscience community projects, such as OpenSourceBrain and BluePyOpt, take advantage of NSG's RESTful services and have their own "umbrella account." Their users can run jobs on NSG without having to register with NSG. Similarly, users of downloadable software packages that have integrated NSG access, such as SimTracker, don't need individual accounts.

Growth of NSG Usage





Evolution of NSG

We initially implemented NSG to provide streamlined access to HPC resources for neuroscientists dealing with large scale modeling projects. Subsequently we have expanded its domain of utility to meet other HPC needs of the broader neuroscience community, especially cognitive and experimental neuroscientists faced with computationally challenging tasks. Some recent applications include:

Neuroscience software tools/application development and dissemination

- Integration with EEGLAB (Scott Makeig, UCSD)
- Integration with Human Neocortical Neurosolver (HNN) (Stephanie Jones, Brown University)
- Integration of BluePyOpt from HBP (Michele Migliore, CNR, Italy)
- CARLsim--GPU-accelerated SNN simulator (Jeffrey Krichmar, UCI)
- LSNM--Large Scale Neural Simulator (Antonio Ulloa, Neural Bytes LLC)

Education and training

- NEURON summer course
- NIH-funded computational neuroscience training course (Satish Nair, U. Missouri)
- Workshops at SFN, OCNS meetings
- NSF-supported cyberinfrastructure neuroscience training (U. Missouri, UCSD)

Collaborative environment

- for application development and testing
- sharing
- survey of future feature needs

Key Points

- Any student or researcher anywhere can use NSG for free.
- Inactive user files are deleted based on length of inactivity.
- Users may request addition of new software, pipelines.
- If you need a large individual allocation, we will help you write your own XSEDE allocation proposal.
- You may use NSG with your own individual allocation.
- Online documentation and support are available at nsghelp@sdsc.edu

Summary

- NSG catalyzes and democratizes computational neuroscience research for everyone, regardless of local or institutional resources.
- Please cite us if you use NSG (**S. Sivagnanam, A. Majumdar, K. Yoshimoto, V. Astakhov, A. Bandrowski, M.E. Martone, and N.T. Carnevale. Introducing the Neuroscience Gateway, IWSG, vol. 993 of CEUR Workshop Proceedings, CEUR-WS.org, 2013**, or see https://www.nsgportal.org/citation.html)
- Also please notify us nsghelp@sdsc.edu of your presentations and publications so we can include them in reports.

Other Acknowledgments and References

This work was partially supported by these current and past grants:
NSF 1458840 (A.M., S.S., K.Y)
NSF 1458495 (N.T.C.); N.T.C. was also partly supported by NIH/NIDCD DC 009977 PI G. Shepherd and NIH/NINDS NS 011613 PI M. Hines.
Technical support for NEURON via NIH/NINDS NS 011613 and the European Human Brain Project [GrantID101445]
BBSRC #BB/N005236/1, NSF 1730655, NIH 1R01EB023297-01A1, NSF 1339856, NSF 1146949, NSF 1146830.

[BluePyOpt] https://github.com/BlueBrain/BluePyOpt/
[Brian] http://briansimulator.org/
[CARLsim] https://github.com/UCI-CARL/CARLsim3
[DynaSim] https://github.com/DynaSim/DynaSim
[EEGLAB] https://sccn.ucsd.edu/eeglab/index.php
[FREESURFER] http://surfer.nmr.mgh.harvard.edu/
[FSL] https://fsl.fmrib.ox.ac.uk/fsl/fslwiki/FSL
[GENESIS] http://www.genesis-sim.org/GENESIS/
[LSNM] https://github.com/NIDCD/lsnm_in_python
[MATLAB] https://www.mathworks.com/products/matlab.html
[NEST] http://www.nest-initiative.unifreiburg.de/index.php/Software:About_NEST
[NetPyNE] http://neurosimlab.org/netpyne/
[NEURON] http://www.neuron.yale.edu/
[NSG] See Summary above.
[Octave] https://www.gnu.org/software/octave/
[OSB] http://www.opensourcebrain.org
[PyNN] http://neuralensemble.org/PyNN/
[Python] https://www.python.org/
[R] https://www.r-project.org/
[REST] Rodriguez, A. RESTful web services: the basics. IBM developerWorks, 2008, last accessed 10/12/2015. http://www.ibm.com/developerworks/library/ws-restful/index.html
[SimTracker] http://mariannebezaire.com/simtracker/
[TensorFlow] https://www.tensorflow.org/
[VirtualBrain] https://github.com/the-virtual-brain
[XSEDE] http://www.xsede.org/