Neuroscience Gateway - Enabling HPC for Computational Neuroscience

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http://www.nsgportal.org

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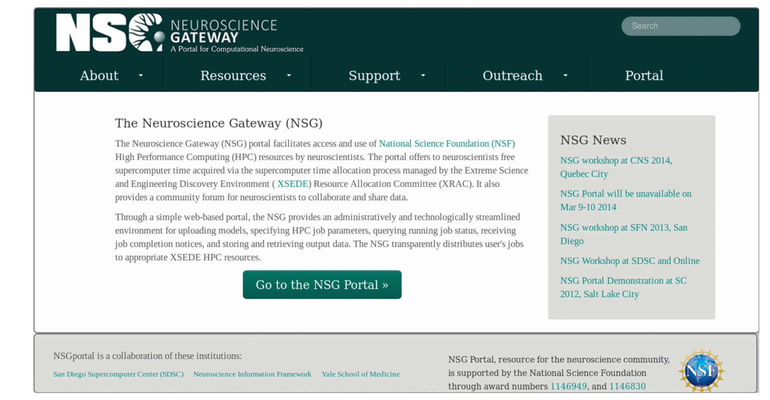


We present the **Neuroscience Gateway (NSG) http://www.nsgportal.org/**, which allows neuroscientists to easily use High Performance Computing (HPC) resources for computationally intensive modeling tasks such as simulating large-scale networks or exploring high-dimensional parameter spaces. Potential HPC users typically face a high entry barrier because of numerous complex side-issues, such as applying for CPU time, installing and configuring simulation software, remote authentication, data transfer and retrieval, batch system management, and administrative policies--all of which may vary from one HPC site to another. The NSG reduces this entry barrier by streamlining administrative procedures and providing a convenient web browser-based interface that hides technical details, so that researchers use XSEDE HPC and other cyberinfrastructure (CI) resources without being distracted from scientific issues relevant to their research.

Key accomplishments to date

- NSG users used in the last two and half years, over **4.5** million SUs on SDSC's Trestles, Comet and TACC's Stampede machines
- Around **270** researchers since early 2013
- Installed and made available widely used computational neuroscience tools such as Brian, NEST, NEURON, pGENESIS, PyNN, MOOSE, and FreeSurfer
- Provided The Virtual Brain (TVB) connectome pipeline through NSG
- Around 150 researchers attended 5 NSG workshops held at Society for Neuroscience (SFN), Computational Neuroscience meeting (CNS) and XSEDE workshops in the past two years

Benefits

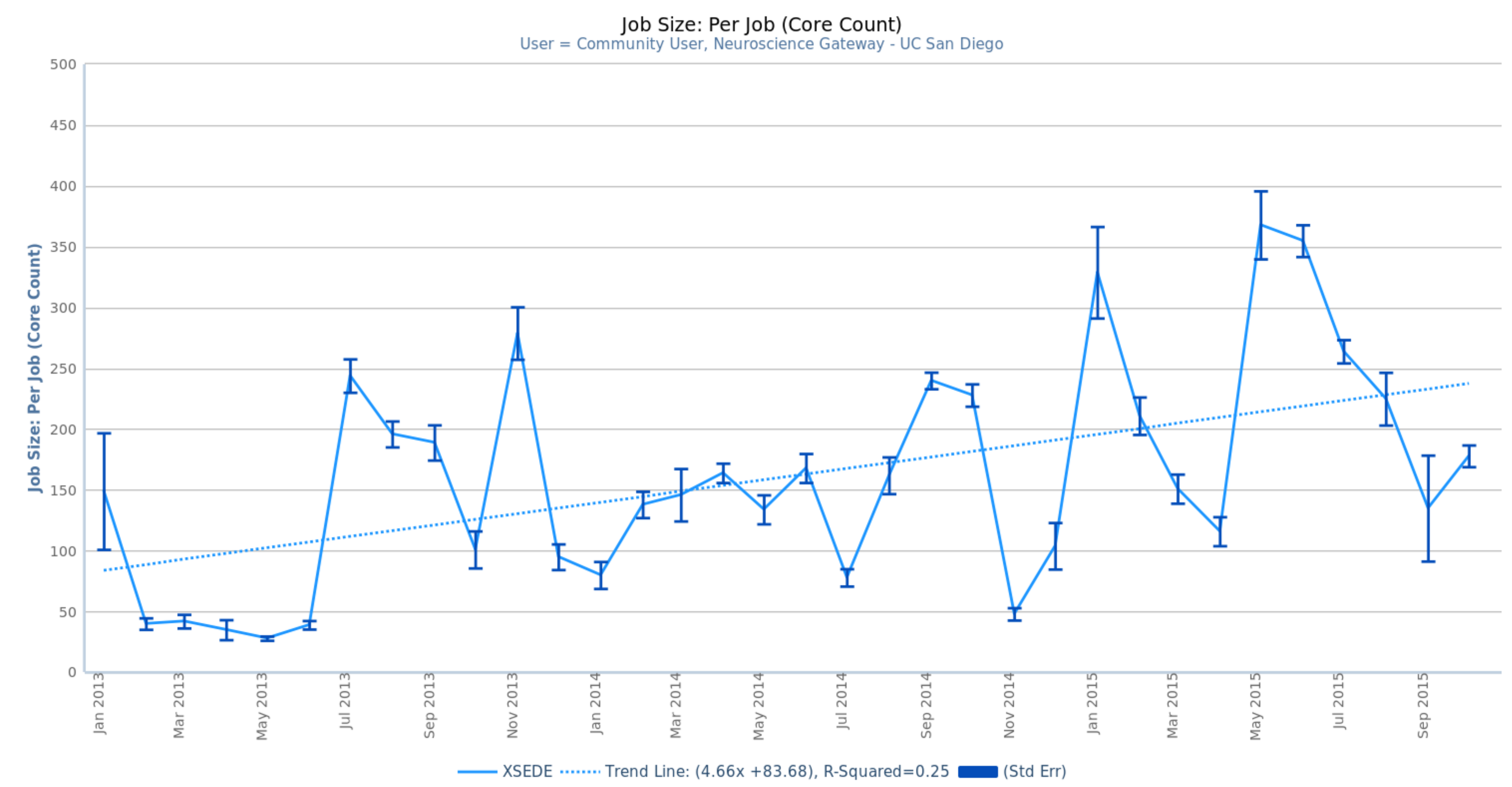
NSG benefits the broader neuroscience research community in several ways, e.g.:

- Researchers can run larger complex neuronal networks and parameter sweep simulations
- Easy to use web interface provides streamlined access to HPC resources, allowing researchers to focus on their research
- Can be used by researchers with limited local (university-level) resources to address questions that require access to large scale, advanced systems
- Can be used by simulator developers to test, benchmark, and scale codes on large scale resources
- Can be used for classes, workshops, and tutorials

Education and Outreach

- REHS students (two in 2013, three in 2014, two in 2015), UCSD undergrad (one in 2013) – web development, running and validation of parallel models, providing input to Neuroscience Information Framework (NIF), developing NEURON simulation of multiple sclerosis
- NIH sponsored MSI visit & NSG workshop at New Mexico State University, Mar 2015

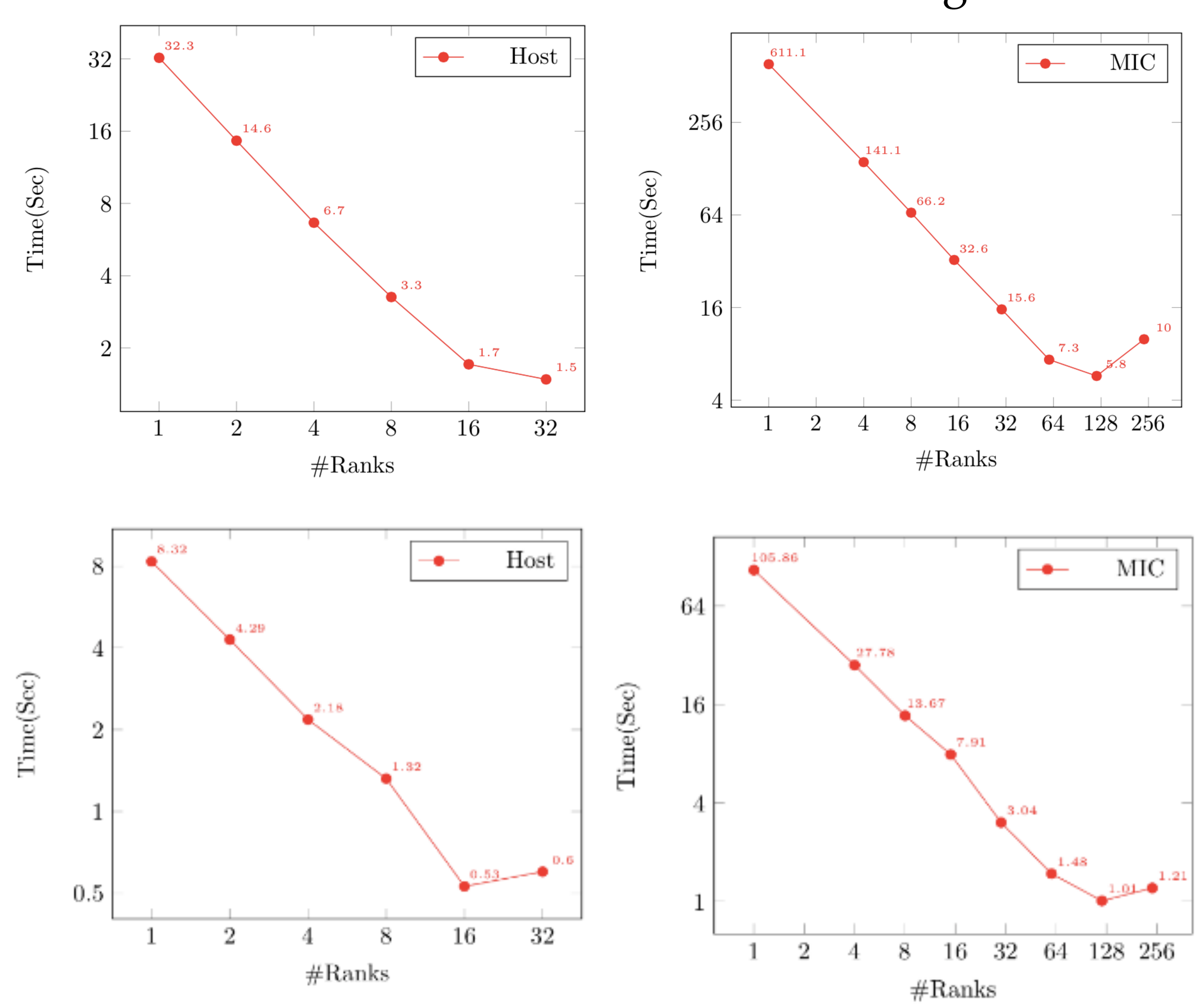
Usage characteristics



Prilminary NEURON performance work on Intel MIC:

Work done on MIC development system at Juelich Supercomputing Center (HOST: Intel XEON 2.6 GHz Dual socket, 8 core/socket, 16GB DRAM ; MIC 61 cores, 1.23 GHz, 16 GB DRAM)

Host only Vs. MIC only
Before and After Load Balancing



- Linear scaling on CPU as well as on MIC
- Two mpi ranks per core benefits on CPU/ MIC
- MIC is 3.8x slower compare to CPU

- Using larger problem NEURON load balance on MIC improves
- MIC is only 1.93 times slower compared to dual socket Xeon
- No performance tuning or optimization yet

Upcoming Feature:

Provide programmatic access through REST services that will allow users of neuroscience community projects (OSB, NIF, ModelDB) to readily access and run simulations on HPC resources. Experienced model developers will be able to run their models directly on HPC from the familiar software environment within their laptop or desktop.

Example science use case

Investigators: Dr Patrick R Hof (Mount Sinai Schoo l of Medicine, New York, NY) , Dr Christina M Weaver (Franklin & Marshall College, Lancaster, PA) with postdoc Tim Rumbell (Mount Sinai School of Medicine, New York, NY).

Science: Investigating the cellular mechanisms underlying cognitive decline with aging in rhesus monkeys, the laboratory species most closely related to humans. It aims to predict cellular mechanisms that account for increased firing rates in layer 3 neocortical pyramidal neurons of aged versus young monkeys recorded in vitro.
This group plans to identify parameters for a total of ten model cells among three groups of rhesus monkeys: Young; Aged-Unimpaired (with cognitive testing scores matched to young monkeys); and Aged Impaired (with cognitive scores significantly impaired relative to young monkeys)
Over 100 jobs were run using NSG on SDSC Trestles machine with an average core size of 256 since October 2014 till April 2015.

Resulting Publication:

1.Compartmental model optimization predicts altered channel densities and kinetics in aged versus young pyramidal neurons of rhesus monkey prefrontal cortex T. RUMBELL, D. DRAGULJIC, J. I. LUEBKE, P. R. HOF, C. M. WEAVER; Society for Neuroscience Annual Meeting, Washington D.C., Nov. 15-19, 2014
2.Rumbell, Timothy, Danel Draguljić, Jennifer Luebke, Patrick Hof, and Christina M. Weaver. "Automatic fitness function selection for compartment model optimization." BMC Neuroscience 15, no. Suppl 1 (2014): O5.

Latest Publications enabled by NSG

1.Lee S, Marchionni I, Bezaire MJ, Danielson N, Lovett-Barron M, Losonczy A, Soltesz I. GABAergic Basket Cells Differentiate Among Hippocampal Pyramidal Cells. Neuron, 1129-1144, June 4, 2014.
2.Ingber L, Pappalepore M, and Stesiak R, "Electroencephalographic fiend influence on calcium momentum waves," J. of Theoretical Biology, Vol 343, pp 138-153, Feb 2014.
3.Forrest MD, Simulation of Alcohol Action upon a Detailed Purkinje Neuron Model and a Simpler Surrogate Model that runs >400 times faster. BMC Neuroscience, 2014.
4.M. Schirner, S. Rothmeier, V. K. Jirsa, A. R. McIntosh, P. Ritter, An Automated Pipeline for Constructing Personalized Virtual Brains from Multimodal Neuroimaging Data, NeuroImage, March 2015; doi:10.1016/j.neuroimage.2015.03.055
5.N.A. Pelot, C.E. Behrend, W.M. Grill. Modeling the Response of Small Myelinated and Unmyelinated Axons to Kilohertz Frequency Signals. 7th International IEEE EMBS Neural Engineering Conference (2015). Montpellier, France.

Cite NSG as follows

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