Neuroscience Gateway - Enabling HPC for Computational Neuroscience

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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, GENESIS, PyNN, MOOSE, and FreeSurfer
• Provided The Virtual Brain (TVB) connectome pipeline through NSG
• Around 150 researchers at 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, NEURON simulation of multiple sclerosis
• NIH sponsored MSI visit & NSG workshop at New Mexico State University, Mar 2015

Example science use case

Investigator: Dr Patrick R Hof (Mount Sinai School 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-Unpaired (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 265 since October 2014 till April 2015.

Resulting Publication:


Latest Publications enabled by NSG

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

Gite NSG as follows


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