Neuroscience Gateway – Understanding the scaling behavior of NEURON application

Subhashini Sivagnanam
San Diego Supercomputer Center
9500 Gilman Drive
La Jolla, CA 92093
1+858 822 3662
sivagnan@sdsc.edu

Amit Majumdar
San Diego Supercomputer Center
9500 Gilman Drive
La Jolla, CA 92093
1+858 534 8356
majumdar@sdsc.edu

Pramod Kumbhar
Ecole Polytechnique Fédérale de Lausanne
Route Cantonale, 1015 Lausanne
Switzerland
pramod.kumbhar@epfl.ch

Michael Hines
Yale University
333 Cedar Street
New Haven, CT 06520
michael.hines@yale.edu

Kenneth Yoshimoto
San Diego Supercomputer Center
9500 Gilman Drive
La Jolla, CA 92093
1+858 822 0859
kenneth@sdsc.edu

Ted Carnevale
Yale University
333 Cedar Street
New Haven, CT 06520
1+203 737 4232
ted.carnevale@yale.edu

ABSTRACT

In this poster, we describe the Neuroscience Gateway that enables HPC access for the computational neuroscience community since 2013. We will also discuss the scaling performance on various HPC architectures for NEURON application. A central challenge in neuroscience is to understand how brain function emerges from interactions of a large number of biological processes at multiple physical and temporal scales. Computational modeling is an essential tool for developing this understanding. Driven by a rapidly expanding body of empirical observations, models and simulation protocols are becoming increasingly complex. This has stimulated development of powerful, open source computational neuroscience simulators, which run efficiently on HPC systems. NEURON is one such simulator that is widely used by computational neuroscientist. The Neuroscience gateway hides the complexities of using HPC systems directly and allows researchers to seamlessly access computational neuroscience codes that are made available on various HPC resources.

Keywords

Computational Neuroscience, HPC, science gateways, NEURON

1. INTRODUCTION

The Neuroscience Gateway (NSG) [1, 2] facilitates access and use of NSF's HPC resources by neuroscientists. It has been in production since early 2013 and offers to neuroscientists free supercomputer time acquired via the allocation process managed by XSEDE [3]. The NSG can be accessed through a simple web-based portal or programmatically using RESTful services (NSG-R). The NSG provides an administratively and technologically streamlined environment for uploading neuronal models, specifying HPC job parameters, querying running job status, receiving job completion notices, and storing and retrieving output data. The NSG transparently distributes user's jobs to appropriate XSEDE HPC resources.

2. HPC INTERACTION AND USAGE

The computational neuroscience software such as NEURON, PGENESIS, BRIAN, FreeSurfer, PyNN, NEST were benchmarked on HPC resources. Scaling studies were done on neuronal models from Modeldb [4, 5], a repository of published neuronal models, to understand performance and optimal setting for the software. The job submission scripts on various HPC systems are implemented providing support for parameter sweep study simulations. Workflow simulations utilizing various neuronal codes were implemented supporting job dependency. Figure 1 shows the maximum core count job per month submitted by users since 2013 and shows that NSG is allowing computational neuroscientists to scale up their parallel models on HPC resources. Around 350 researchers have signed up since 2013. NSG users used over five million SUs on SDSCs Trestles, Comet and TACC's Stampede machines. The NSG-R makes it possible for users of neuroscience community gateway projects such as Open Source Brain [6] to seamlessly use HPC resources without leaving their familiar work environment. The users of such projects are not required to register with NSG avoiding multiple authentication process. The programmatic access also makes it easier for developers to integrate the HPC access in their code by utilizing the available python or java libraries.

3. NEURON PERFORMANCE ON HPC

NEURON [7] is used by thousands of researchers world-wide for building computational models of neurons and networks of neurons. It has the advantage of allowing models to include anatomical and biophysical properties that are necessary for mechanistic modeling of biological neurons and neural circuits. NEURON has already been used to simulate 10s of millions of neurons on ~100s of thousands of cores. We studied the scaling performance of NEURON code on various HPC resources such as FX10 Kobe supercomputer, KNL, GPUs etc.

Previously we presented performance of Jones model [8] on Intel Knights Corner co-processor. Currently we are running the same model on Intel Knights Landing (KNL) and on Fujitsu SPARC64 IXfx processor on Pi resource (FX10) at Kobe University. The performance scaling on these resources will be presented in the final poster.

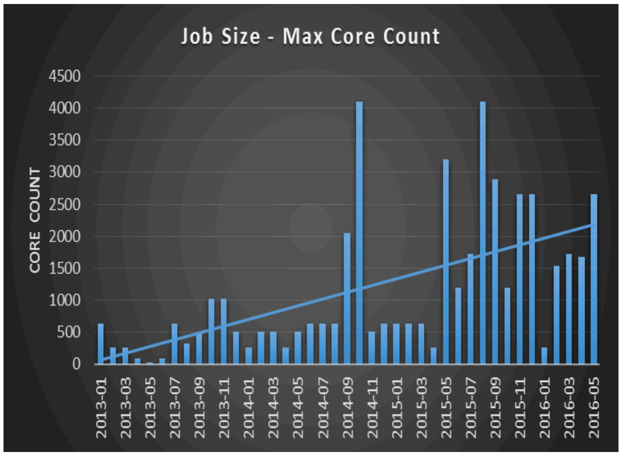

Figure 1. Max core count jobs since 2013.

4. WORKSHOPS

Various workshops were conducted to educate users on using NSG. Around 200 researchers attended multiple NSG workshops held at Society for Neuroscience (SFN), Computational Neuroscience meeting and XSEDE workshops. In addition, we also held workshops at New Mexico State University a MSI institution.

5. FUTURE WORK

Vigorous development efforts are still needed to prepare NEURON code for exascale level machines to be able to simulate ~100 billion neurons; the same consideration holds for other simulators as well. This scaling will require thorough understanding of performance characteristics of NEURON and development of performance models for NEURON. It can be done by carrying out detailed profiling and tracing analysis to understand processor and memory level performance characteristics, communication patterns and characteristics, and I/O behavior. At the same time implementations of NEURON should be further explored on both GPU and Intel Phi accelerators/co-processors. All of these need to be tied back to the algorithms utilized. Some of these algorithms will need to be reframed in order to produce new code that can be optimized and implemented for improved performance at these extremely large scales.

6. ACKNOWLEDGMENTS

We would like to acknowledge the NSF awards DBI 1458840, 1458495, 1146949.

7. REFERENCES

[1] www.nsgportal.org

[2] Sivagnanam, S., Majumdar, A., Yoshimoto, K., Astakhov, V., Bandrowski, A., Martone, M.E., and Carnevale, N. T., 2013. Introducing the Neuroscience Gateway, IWSG, vol. 993 of CEUR Workshop Proceedings.

[3] https://www.xsede.org

[4] https://senselab.med.yale.edu/ModelDB/

[5] https://senselab.med.yale.edu/ModelDB/ShowModel.cshtml?model=136803

[6] http://www.opensourebrain.org

[7] http://www.neuron.yale.edu

[8] http://sc15.supercomputing.org/sites/all/themes/SC15images/tech_poster/tech_poster_pages/post314.html