Neuroscience Gateway – Enabling HPC for Computational Neuroscience

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ABSTRACT

In this poster, we describe the Neuroscience Gateway that enables HPC access for the computational neuroscience community since 2013. 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. This has also resulted in critical need for access to HPC by computational neuroscientists. 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. We also report on performance of the NEURON application on HPC machines.

Categories and Subject Descriptors

J.3 [**Life and Medical Sciences**]: Biology and Genetics

General Terms

Design, Management

Keywords

Computational Neuroscience, HPC, science gateways

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]. Through a simple web-based portal, 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. NSG CORE SOFTWARE

NSG is based on highly successful gateway software [4], which is used by many other science gateways such as CIPRES [4] enabling phylogenetics on HPC resources. The software has various modules that integrate various protocols for data transfer to HPC resource, job submission to HPC resources and daemons for job monitoring and usage.

3. 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 [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 average core size of NSG jobs submitted by users since 2014 and shows that NSG is allowing computational neuroscientists to run parallel models on HPC resources. Around 250 researchers have signed up in the last two and half years to use NSG. NSG users used in the last two and half years over three million SUs on SDSCs Trestles, Comet and TACC's Stampede machines.

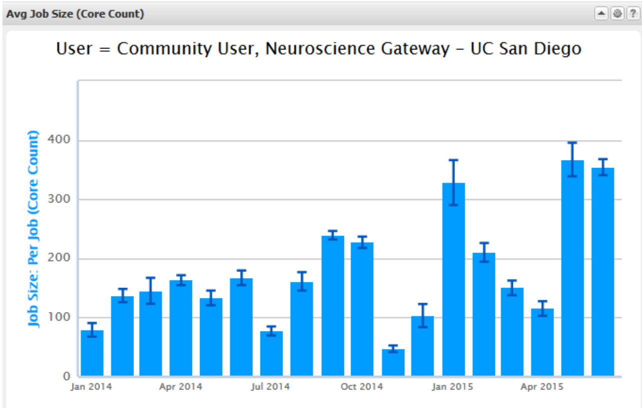

Figure 1. Average NSG job size since 2014.

4. NEURON PERFORMANCE ON HPC

The parallel NEURON code was ported to MIC based Intel HPC machines. For a 100 cell neuronal model [6], running on MICs only, there was significant load imbalance among MPI tasks on MIC cores as 100 cells were too small to distribute work equally among 60 MIC cores. This is shown in figure 2, which shows longer MPI_Allgather wait time among MPI tasks.

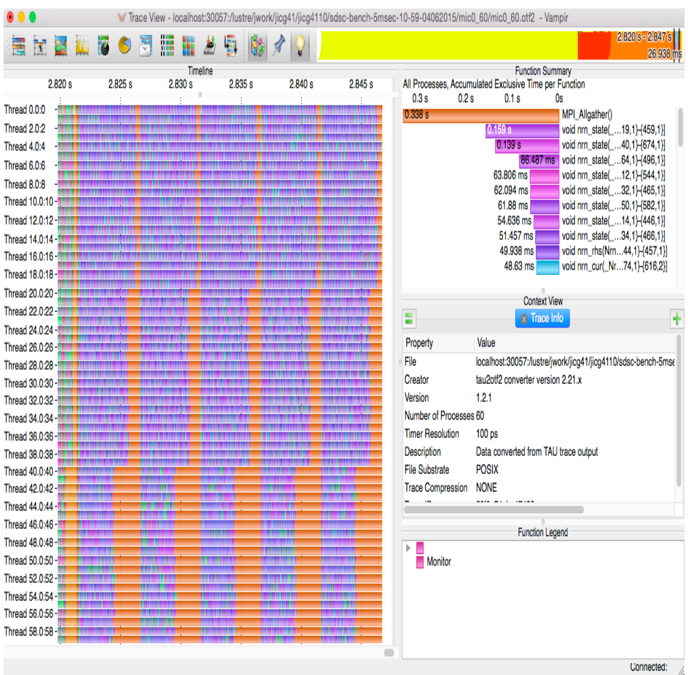

Figure 2. Profiling result of 100 cells test case using NEURON.

For this test case 60 MIC cores took 3.81 times more time than 16 SandyBridge cores.

We also looked at running the model across host (dual socket 16 core SandyBridge) and MIC cores and as expected that showed timing on MIC cores longer than on SandyBridge cores for the 100 cell test case as shown in figure 3 below. This is also attributed to load imbalance.

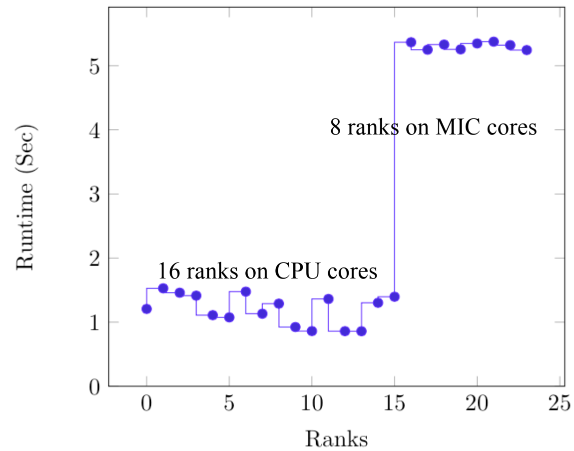

Figure 3. Timing of run across host and MIC cores.

To improve the load balance the problem size was increased to include 480 cells which is multiple of 60 i.e. the number of MIC cores used for the benchmark.

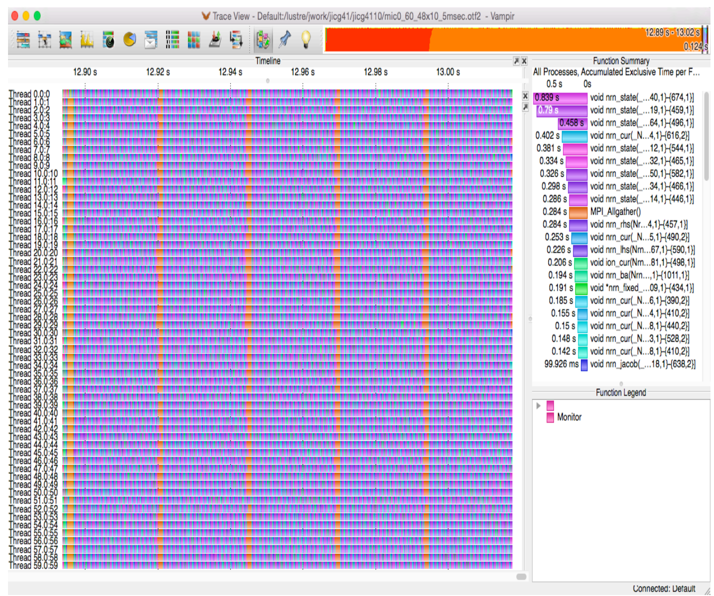

Figure 4. Profiling result of 480 cells test case using NEURON.

The profiling result from figure 4 shows that as the load was increased to 480 cells the MPI tasks on MIC cores had equal distribution of load and all the MPI_Allgather spend very little time on wait. As a result for this 480 cell case, the 60 MIC cores are only about 1.9 times slower than the 16 SandyBridge cores. These timing results are shown in figure 5 and 6.

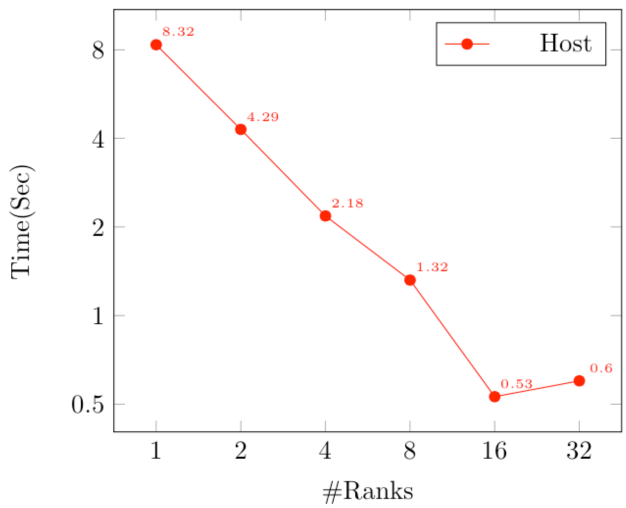

Figure 5. Timing of 100 cells test case on host using NEURON.

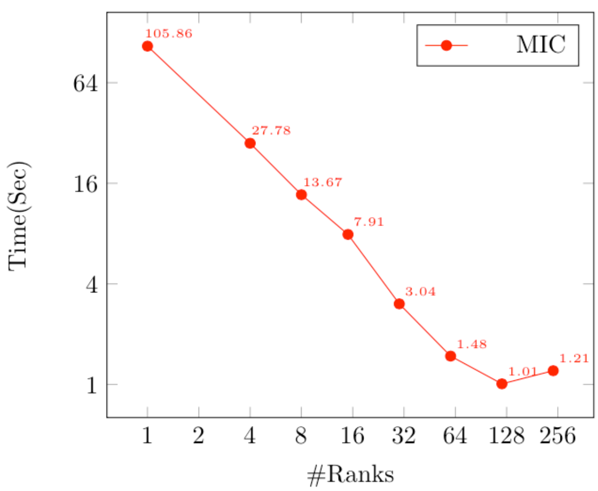

Figure 6. Timing of 480 cells case on MIC using NEURON.

5. WORKSHOPS

Various workshops were conducted to educate users on using NSG. Around 150 researchers attended 5 NSG workshops held at Society for Neuroscience (SFN), Computational Neuroscience meeting and XSEDE workshops in the past two years. In addition, we also held workshops at New Mexico State University a MSI institution.

6. FUTURE WORK

REST service based implementation will allow be done and will allow users of neuroscience community projects (OSB [5], NIF [6], ModelDB) and individual users to readily access and run simulations on HPC resources, and retrieve results.

7. ACKNOWLEDGMENTS

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8. REFERENCES

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