

Seamless Integration of Neuroscience Models and Tools with High Performance Computing

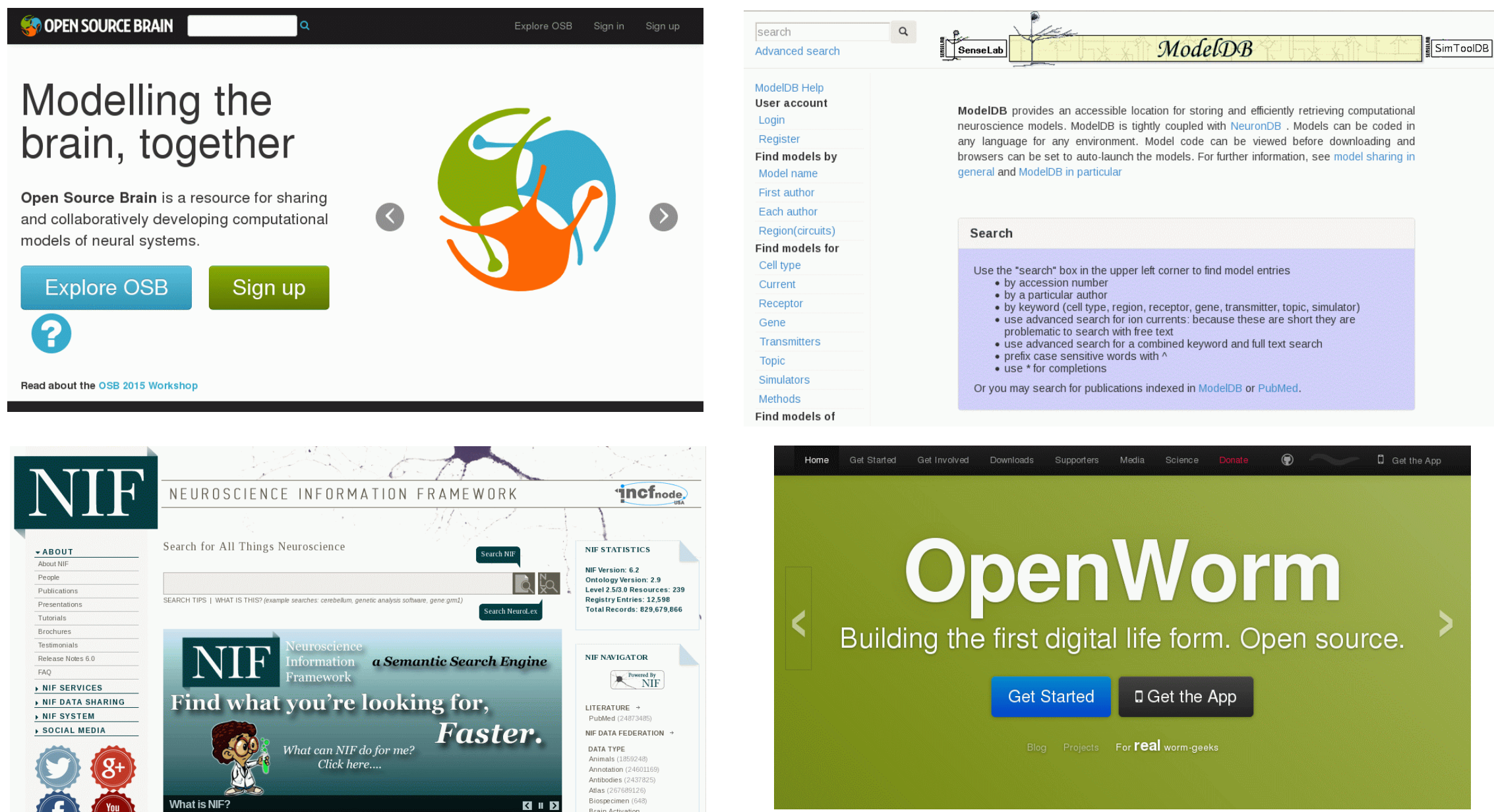
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Introduction and background

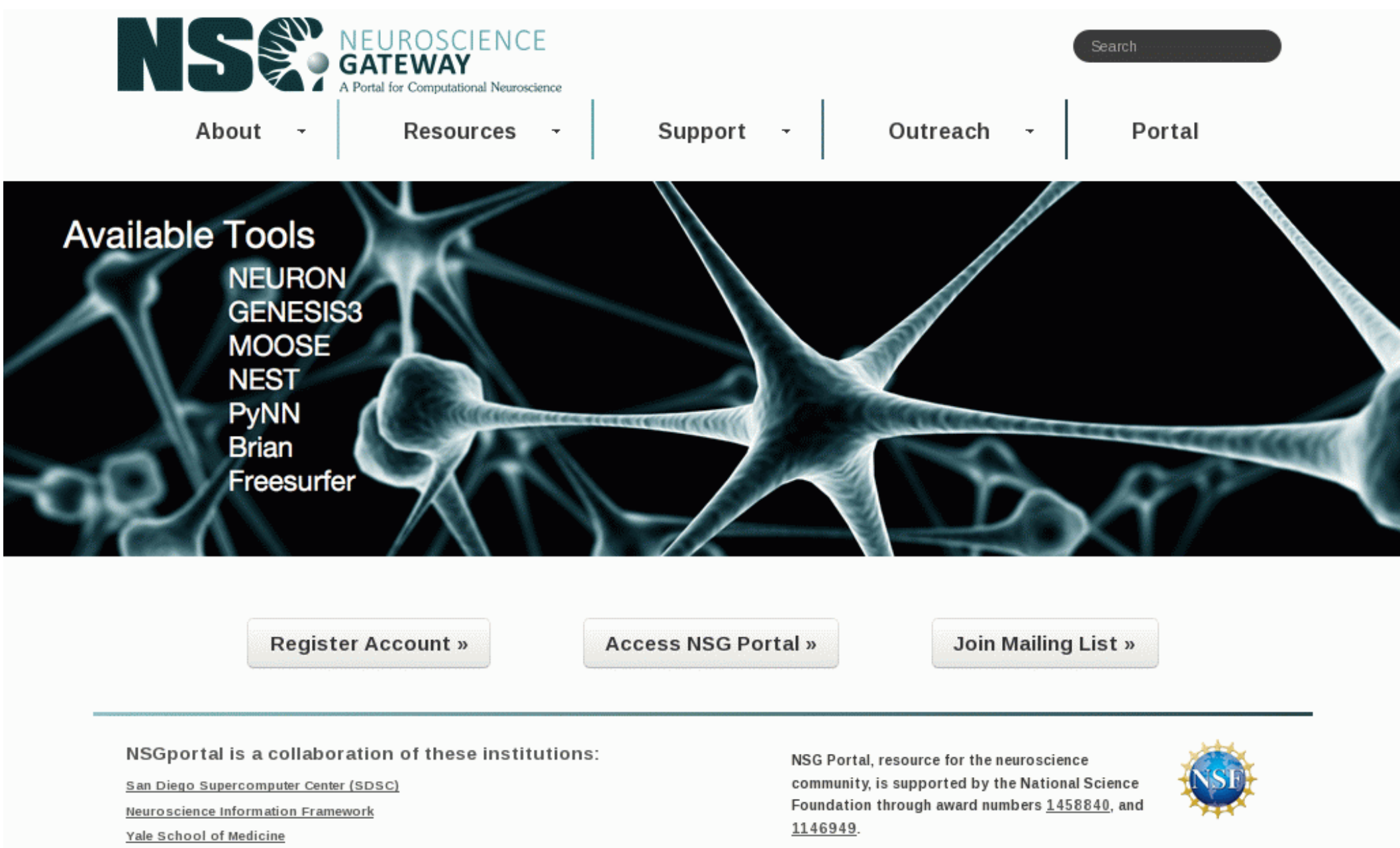
A central challenge in neuroscience is to understand how brain function emerges from interactions of a large number of biological processes at multiple physical and temporal scales. Computational modeling is an essential tool for developing this understanding. This has led to the development of powerful, open source simulators that run efficiently on parallel hardware (e.g. Brian, GENESIS, MOOSE, NEST, NEURON) and creation of neuroscience community projects (NCPs) that facilitate modeling by promoting data and model source code sharing, and enabling collaborative model development, such as Open Source Brain (OSB), ModelDB, Neuroscience Information Framework (NIF), and OpenWorm.



However, experimental and theoretical advances are increasingly driving the formulation of models and simulation protocols that exceed the capabilities of the computational resources available to most neuroscientists. This trend has been intensified by recent research initiatives, such as the BRAIN Initiative in the US and the Human Brain Project in Europe. The result is a critical need for access to HPC by computational neuroscientists and their colleagues in the broader neuroscience community.

NSG: facilitating access to HPC resources

This motivated us to begin development of the Neuroscience Gateway Portal (NSG, <http://www.nsgportal.org/>) in late 2012 with NSF support. NSG's mission is to facilitate access and use by neuroscientists of HPC resources located at NSF-funded national supercomputer centers. To the best of our knowledge, NSG is the first and only science gateway designed to address the HPC needs of neuroscientists.



NSG eliminates many technical and administrative barriers to the use of HPC in computational neuroscience by:

- providing a single access point for widely used simulators and data analysis tools
- reducing or eliminating administrative bottlenecks by adopting streamlined policies, so that tasks like registering and getting time allocations are quick and easy
- offering a simple browser-based user interface for uploading models or data, performing simulations or analyses, and downloading results

Investigators are rapidly adopting NSG to deal with the growing computational challenges of neuroscience research. As of 9/2015 NSG has >270 users, to whom >4.4 M CPU hours have been allocated. Many are already presenting results at scientific meetings and in refereed publications (see **Publications Enabled by NSG**).

But as much as NSG has helped, there are still opportunities to make HPC resources more widely and readily useful. For example, users of OSB, ModelDB etc. become quite accustomed to the environment and workflow of those tools, but in order to use NSG in its present form they must leave their familiar working environments to log into NSG, upload their model source code, set NSG's job submission parameters, submit NSG jobs, and retrieve output results to their local hardware for further analysis. These manual steps constitute a bottleneck and a diversion of effort from potentially more productive activities.

NSG-R: automating access to HPC resources

We recently began a new multidisciplinary, multi-institutional and multinational collaborative project to eliminate these steps by creating an application programmer interface called NSG-R that exposes NSG's services through Representational State Transfer (REST). This will enable on-demand, automated communication between NSG and neuroscience resources such as OSB, and even directly between NSG and neural simulators running on neuroscientists' own laptop and desktop computers.

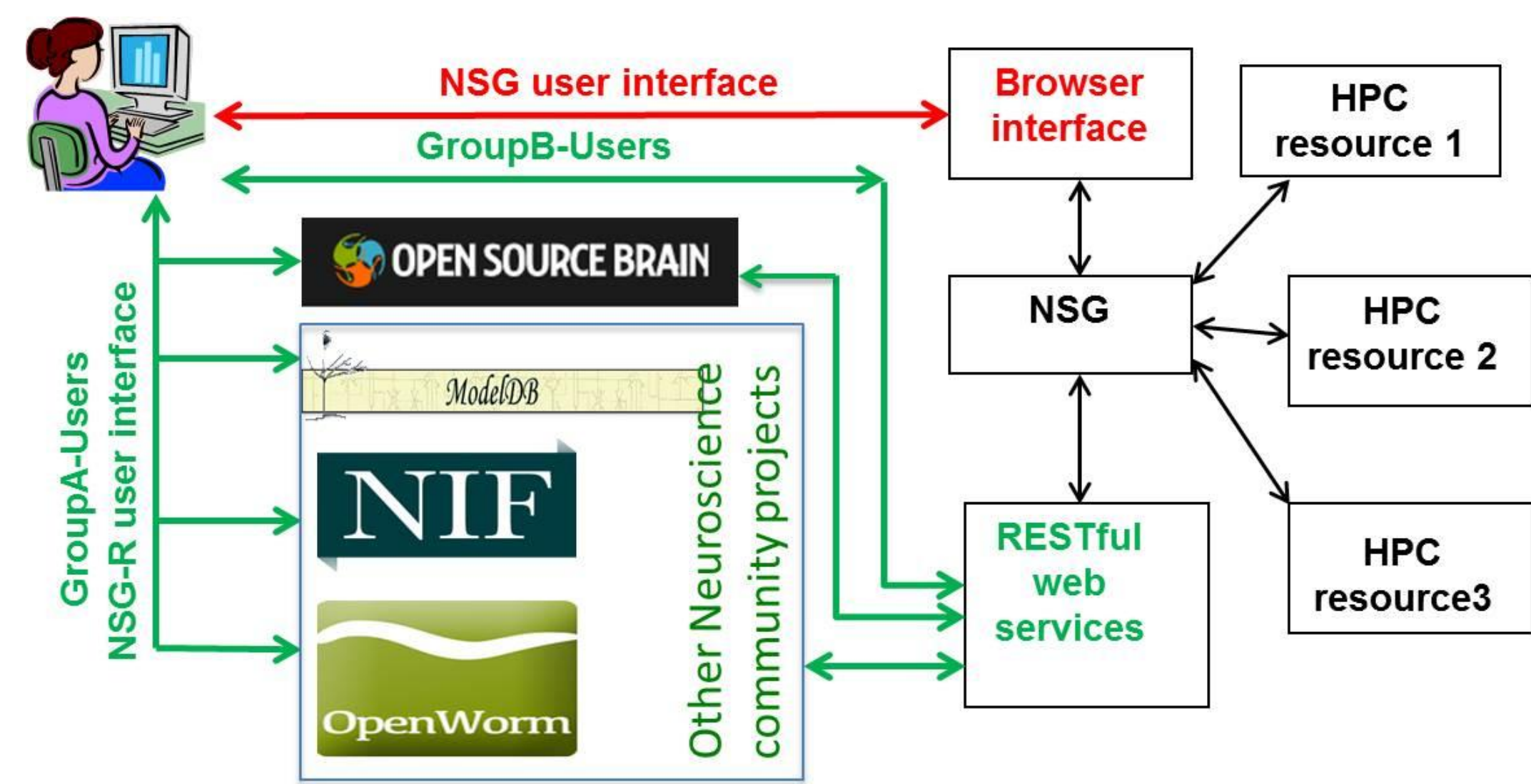


Figure 1. Concept of NSG and NSG-R Web Services.

The US-based members of this collaboration are located at the San Diego Supercomputer Center at UCSD (Majumdar, Sivagnanam, Yoshimoto) and Yale University Medical School (Carnevale) and are collaborators in the project that created NSG.

The UK-based members are at University College London (Silver, Gleeson) and have developed OSB with support from the Wellcome Trust [GrantID101445]. OSB supports the reuse and improvements to the model that happen after initial scientific publication. It supports conversion to open, standardized formats and encourages updates or bug fixes to published model code. It also supports models which are still in development, e.g. the models being created in the OpenWorm project.

This will be a synergistic effort between the US and UK teams, who have complementary expertise in computational neuroscience, cyberinfrastructure/HPC, software engineering, and neuronal simulations. Its first goal is to develop a production quality implementation of the NSG-R web services by interfacing OSB to NSG. This interface will initially be tested by using it to develop and apply a model optimization pipeline that goes from experimental data to working model (in NeuroML on OSB) in the context of a set of cell and network models of interest to the UK team.

Further testing will involve OSB users as early implementation users of NSG-R-enabled seamless, automated access to HPC resources. The experience of integrating NSG-R with OSB will help ensure that it is well tested and robust before it is opened up to the developers of other NCPs and neural simulators, and will guide us in making this process as easy as possible. It will also ensure that NSG-R meets the needs of community developers, and provides a valuable service for end users from within their preferred software environments and workflows. After successful implementation with OSB, we will collaborate with the developers of other NCPs such as ModelDB, NIF, OpenWorm, to help them incorporate NSG-R into their own web interface software.

By enabling seamless access to HPC resources through NSG, NSG-R will

- mutually enhance the utility of NSG, NCPs like OSB, and widely used neural simulators such as Brian, GENESIS, MOOSE, NEST, and NEURON
- improve research productivity and enable greater use of large scale computational modeling by scientists and students
- expand opportunities for educational and career advancement in neuroscience and engineering
- remove barriers that traditionally have limited access to HPC, leveling the playing field for all students and researchers regardless of their institutional affiliation

Publications enabled by NSG

T. Rumbell, D. Draguljić, J.I. Luebke, P.R. Hof, C.M. Weaver. Compartmental model optimization predicts altered channel densities and kinetics in aged versus young pyramidal neurons of rhesus monkey prefrontal cortex. Abstract 372.22, Society for Neuroscience Annual Meeting, Washington D.C., Nov. 15-19, 2014.

T. Rumbell, D. Draguljić, J. Luebke, P. Hof, C.M. Weaver. Automatic fitness function selection for compartment model optimization. BMC Neuroscience 15, Suppl 1: O5, 2014.

S. Lee, I. Marchionni, M.J. Bezaire, N. Danielson, M. Lovett-Barron, A. Losonczy, I. Soltesz. GABAergic basket cells differentiate among hippocampal pyramidal cells. Neuron 82:1129-1144, 2014.

L. Ingber, M. Pappalepore, R. Stesiak. Electroencephalographic field influence on calcium momentum waves. Journal of Theoretical Biology 343:138-153, 2014.

M.D. Forrest. Simulation of alcohol action upon a detailed Purkinje neuron model and a simpler surrogate model that runs >400 times faster. BMC Neuroscience 16:27, 2015.

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. Montpellier, France, 2015.

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 117:343-357, 2015.

A.H. Seidenstein, R.A. McDougal, M.L. Hines, A. Fesharaki, W.W. Lytton. Parallelizing large networks using NEURON-Python. Poster. Computational Neuroscience Annual Meeting, Prague, July 18-23, 2015.

C. Mitelut, S.L. Gratiy, D. Denman, J.H. Siegle, S. Durand, K. Godfrey, C. Lee, R.C. Reid, M. Hawrylycz, C. Koch, N.V. Swindale, C. Anastassiou. Standardizing spike sorting: an in vitro, in silico and in vivo study to develop quantitative metrics for sorting extracellularly recorded spiking activity. Abstract 598.10, Society for Neuroscience Annual Meeting, Chicago, IL, October, 2015.

S.A. Neymotin, B.A. Suter, M. Migliore, S. Dura-Bernal, G.M.G. Shepherd, W.W. Lytton. Optimizing computer models of layer 5 motor cortex pyramidal neurons using somatic whole cell recordings. Abstract 421.02, Society for Neuroscience Annual Meeting, Chicago, IL, October, 2015.

A. Seidenstein, S.A. Neymotin, A. Fesharaki, M.L. Hines, R.A. McDougal, A.S. Bulanova, W.W. Lytton. Neuronal network bump attractors augmented by calcium up-regulation of Ih in multiscale computer model of prefrontal cortex. Abstract 92.05, Society for Neuroscience Annual Meeting, Chicago, IL, October, 2015.

Publications about NSG

S. Sivagnanam, A. Majumdar, P. Kumbhar, M. Hines, K. Yoshimoto, T. Carnevale. Neuroscience Gateway--Enabling HPC for Computational Neuroscience. Poster. Supercomputing 2015, Austin, TX, November, 2015.

T. Carnevale, A. Majumdar, S. Sivagnanam, K. Yoshimoto, P. Gleeson, R.A. Silver. Seamless integration of neuroscience models and tools with high performance computing. Abstract 450.13, Society for Neuroscience Annual Meeting, Chicago, IL, October 17 - 21, 2015.

M. Miller, T. Schwartz, P. Hoover, K. Yoshimoto, S. Sivagnanam, A. Majumdar. The CIPRES workbench: a flexible framework for creating science gateways. Proceedings XSEDE15, St. Louis, MO, July 26-30, 2015.

B. Lytton, M. Hines. NEURON and the Neuroscience Gateway Portal. HPC Workshop, Computational Neuroscience Annual Meeting, Prague, July 18-23, 2015.

T. Carnevale, A. Majumdar, S. Sivagnanam, K. Yoshimoto, V. Astakhov, A. Bandrowski, M. Martone. High performance computing in neuroscience via the Neuroscience Gateway Portal. Abstract 187.01, Society for Neuroscience Annual Meeting, Washington D.C., November 15 - 19, 2014.

T. Carnevale, A. Majumdar, S. Sivagnanam, K. Yoshimoto, V. Astakhov, A. Bandrowski, M. Martone. The Neuroscience Gateway Portal--high performance computing made easy. Poster, Computational Neuroscience Annual Meeting, Quebec City, Canada, July 26-31, 2014.

S. Sivagnanam, A. Majumdar, K. Yoshimoto, V. Astakhov, A. Bandrowski, M. Martone, N.T. Carnevale. Early experiences in developing and managing the neuroscience gateway. Journal of Concurrency and Computation: Practice and Experience, May 2014, UR: <http://dx.doi.org/10.1002/cpe.3283>.

N.T. Carnevale, A. Majumdar, S. Sivagnanam, K. Yoshimoto, V. Astakhov, A. Bandrowski, M. Martone. The Neuroscience Gateway Portal--facilitating access to high performance computing resources. Poster, Society for Neuroscience Annual Meeting, San Diego, November 9-13, 2013.

S. Sivagnanam, K. Yoshimoto, A. Majumdar, N. T. Carnevale, V. Astakhov, M. Martone, A. Bandrowski. A Neuroscience Gateway: software and implementation. Proceedings XSEDE13 Gateway to Discovery, San Diego, CA, July 22-25, 2013.

S. Sivagnanam, A. Majumdar, K. Yoshimoto, V. Astakhov, A. Bandrowski, M. E. Martone, and N.T. Carnevale. Introducing the Neuroscience Gateway, IWSG, volume 993 of CEUR Workshop Proceedings, CEUR-WS.org, 2013

N.T. Carnevale, S. Sivagnanam, K. K. Yoshimoto, V. Astakhov, A. E. Bandrowski, M. E. Martone, A. Majumdar. A Neuroscience Gateway for high performance computing. Poster, Society for Neuroscience Annual Meeting, New Orleans, October 13-17, 2012.

Acknowledgments and References

NSF-BBSRC collaborative grant
USA NSF 1458840 (A.M., S.S., K.Y.)
USA NSF 1458495 (N.T.C.)
UK BBSRC BB/N005236/1 (A.S., P.G.)

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] Grant ID 101445; The Open Source Brain repository: enabling the collaborative development of open and accessible models for neuroscience

[ModelDB] <http://senselab.med.yale.edu/modeldb/>

[MOOSE] <http://moose.sourceforge.net/>

[NEST] http://www.nest-initiative.unifreiburg.de/index.php/Software>About_NEST

[NEURON] <http://www.neuron.yale.edu/>

[NIF] <http://neuinfo.org/>

[NSG] See Publications about NSG.

[OSB] <http://www.opensourcebrain.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>

[XSEDE] <http://www.xsede.org/>

