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# The Neuroscience Gateway Portal: *facilitating access to high performance computing resources*

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Advances in experimental and computational neuroscience are driving the emergence of modeling projects which impose computational burdens and/or storage requirements that exceed the capabilities of local hardware. That said, few modelers have been able to take advantage of high-performance computational (HPC) resources, largely because of time consuming technical and administrative barriers that differ considerably from one HPC facility to another. These include

- writing a successful request for computer time
- mastering complex administrative policies and batch system details
- optimally installing applications on HPC resources
- managing workflow that involves multiple remote authentication schemes
- handling data transfer, storage, and output retrieval issues

To reduce these barriers, we are developing the Neuroscience Gateway Portal (NSG) <http://www.nsgportal.org/>, which provides neuroscientists a user-friendly Web-based interface for using HPC and other cyberinfrastructure (CI) resources.

## Design and implementation

NSG's design goals are to make it easier for neuroscientists to

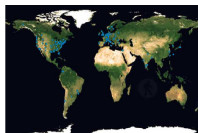
- use HPC time under reasonable usage guidelines and policies
- specify parallel simulation parameters, e.g. number of cores and nodes, estimated job run time etc.
- query job status, and request automatic notification of job completion
- securely access and download output results

## Accomplishments to date

- The NSG offers convenient access to HPC machines on which widely used simulators such as BRIAN, MOOSE, NEST, NEURON, pGENESIS, and PyNN have already been installed and optimally configured.
- Users only need to know how to parallelize their own code and run it on their local hardware.
- They don't even have to apply for CPU time, because each NSG user is given a block of time from NSG's own allocation.

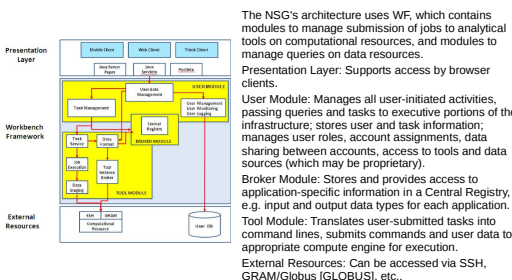
## Milestones

December 2012 Opened to "friendly users"  
March 2013 Initial allocation of 50k CPU hours consumed  
October 2013 Another 250k CPU hours used up  
November 2013 Total CPU usage >350k hours since start.  
~100 users, ~60% "active."



## Technical details

NSG hides CI/HPC-related complexities within the black box of a gateway architecture that is based on and extends the CIPRES Science Gateway framework [CIPRES, Miller 2010]. CIPRES was developed at the San Diego Supercomputer Center (SDSC) for the computational phylogenetics research community. All enhancements and modifications implemented for NSG are contributed back to CIPRES for future use.



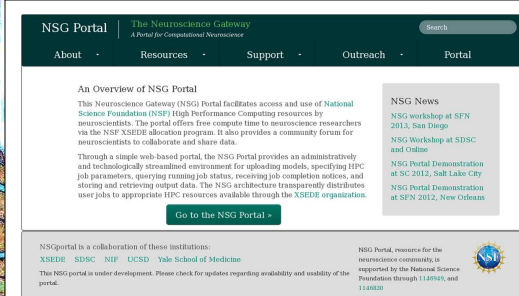
Examples of NSG features that differ from CIPRES:

- Any NSG model may involve multiple files and a complex directory hierarchy.
- Some simulators require compilation of model source code, e.g. NEURON's mod files.
- Results are automatically stored in SDSC's cloud storage.
- User files are automatically deleted based on duration of inactivity.

## Benefits

The Neuroscience Gateway can benefit the broader neuroscience research community in several ways, e.g.:

- Simple interface provides streamlined access to HPC resources, allowing investigators to focus on their research.
- Can be used by investigators with limited local (university-scale) resources to address questions that require access to large scale, advanced systems.
- Can be used by simulator developers to test/debug, benchmark, and scale codes on large scale resources and, when satisfied, make them available to the broader user community.
- Can be used for classes, workshops, and tutorials without requiring instructors to set up simulators on HPC resources or create new accounts for students/participants.



## Work in progress:

- debugging capability
- job bundling, e.g. for parameter exploration and optimization
- programmatic interfaces with model web sites and databases, e.g. ModelDB, neuroConstruct
- sharing of output results, e.g. with NIF
- other enhancements driven by user suggestions and feedback

## Acknowledgements and References

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[WBC] <http://wholebraincatalog.org/>  
[WF] <http://www.ngbw.org/wbframework/>  
[XSEDE] <http://www.xsede.org/>