

A Neuroscience Gateway: Software and Implementation

www.nsgportal.org


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Outline

1. Introduction – Right time for Neuroscience Gateway
2. Background – CIPRES Workbench Framework
3. Adaptation – CIPRES to NSG 
4. Summary
5. Acknowledgement

1. Introduction – Right time for Neuroscience Gateway

Growth of Computational Neuroscience

- Growth of computational modeling in neuroscience research

Evidence:

- *New Journals* (Neural Computation, J. of Computational Neuroscience)
 - *Increase in Modeling papers* (J. of Neurophysiology, J. of Neuroscience, Neuron - >1176 publications; ~10% annual growth)
- Trend in research proposals to NSF, NIH in US, and similarly in other countries
- Driven the evolution and refinement of powerful simulation tools
 - NEURON, GENESIS, MOOSE, NEST, PyNN, Brian etc

Research Bottleneck

- Modeling projects start “small” and many stay “small”
- Increase in development of complex models require CI, HPC
- Very few neuroscientists have access to extreme scale HPC
- Widely used simulators (NEURON, GENESIS, MOOSE, NEST, PyNN, Brian) are parallel
- Wider computational neuroscience community needs access!

We want to bring HPC to more neuroscientists

Barriers to Entry

- HPC/CI resources are available from national supercomputer centers

BUT

- Requesting time requires preliminary access to be able to write proposals every year
- Difficulty in understanding HPC machines, complex OS/software
- Need to learn policies, batch system details – different on different HPC systems
- Challenge of managing workflows involving multiple remote authentication systems
- Figuring out data transfer, output result retrieval, storage issues

Our Goals

1. Easy user interface – providing easy model upload, running of codes
2. Complete set of neuronal simulation tools – widely used by computational neuroscientists
3. Ability to easily get to the results, download results

NSG Portal

NSG Portal

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A Portal for Computational Neuroscience

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Missing
results?

Send us the
[job handle](#),
and we may
be able to
help.

More
Information

About Us

Usage
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publications

Latest News

Welcome to NSGportal! Currently NEURON, PGENESIS, NEST, BRIAN, and PyNN codes can be run on Trestles, HPC resource at SDSC. Please login to proceed

First Time Users: Please review our [usage policies](#)

New users who are interested in getting an account should fill out the [form](#) and email it to nsghelp@sdsc.edu

NSGPortal Login

*Username:

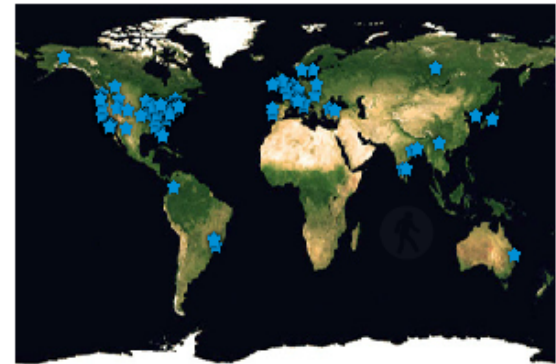
*Password:

Login

Reset

[Forgot Password?](#)

Location of users



2. Background – CIPRES Workbench Framework

Background

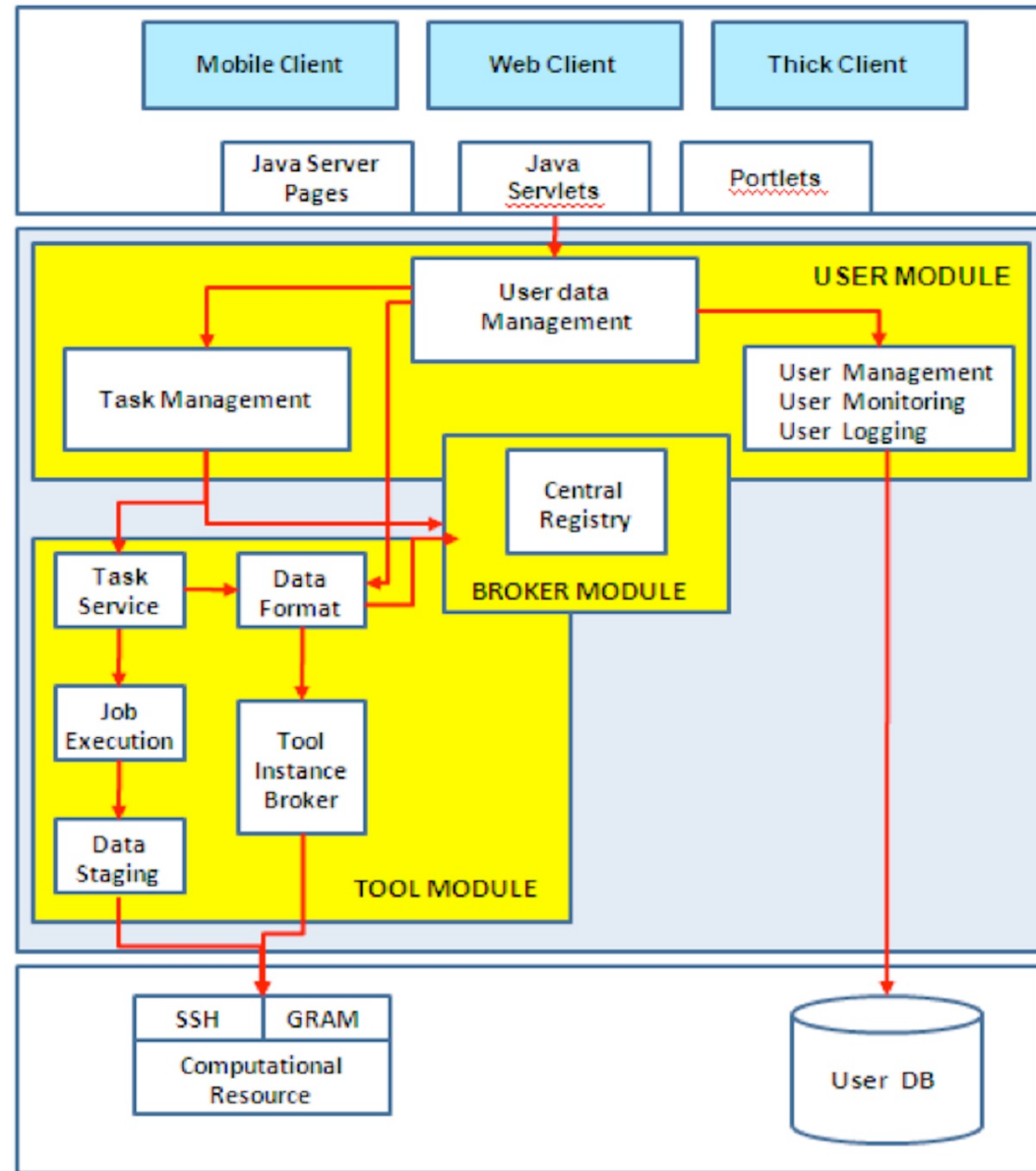
- Why CIPRES (Cyberinfrastructure for Phylogenetic Research) ?
- Well-established, robust, and mature S/W
- Adapted by other gateways
- CIPRES developers and researchers are at SDSC
- Reuse of existing NSF funded software was considered a good practice
 - viewed positively by the NSF

Workbench Framework (from <http://www.ngbw.org/wbframework/>)

Presentation Layer

Workbench Framework

External Resources



• Presentation Layer

- Accesses SDK capabilities
- Provides lightweight web access
- Architecture based on Linux, Apache Tomcat, MySQL and Java Struts2
- Allows data and task management in user-created folders
- Users can create a login protected personal account
- Users can store data, records of their activities for a defined period

• User Module

- Passes user-initiated queries and tasks to executive portions of the infrastructure
 - Done via data and task management modules
- Stores user data and task information in MySQL
- Supports individual user roles, accounts, sharing of data
- Supports selective access to tools, data sources
- Mapping user information happens in this layer
- Allows tracking the individual usage on comp resources

• Broker Module

- Provides access to all application specific information in a Central Registry
- Contains information about all data types for input, output for each application
- Concepts and concept relationships are formed in XML and read by Central Registry
- Tools, data types defined in single location
- Allows adding new tools, data types without impacting any functioning outside of the Registry

• Tool Module

- Translates submitted tasks into command lines; submits command line strings, w/ user input data to compute engines
- Handles data formatting for jobs and job staging
- Tracks which tool can be run on which resources
- Allows adding of computational resources by editing the tool resource config file
- The application can send command line scripts, receive output by any well defined protocol
 - Unix command line, web services, SSH, GRAM, gsissh

3. Adaptation – CIPRES to NSG



Adaptation of CIPRES to NSG - Effort

- Minimal effort as opposed to starting from scratch
- Contributing factor - help provided by SDSC CIPRES experts
- Set up - Tomcat, Apache, database, VM, Cloud storage (courtesy of a separate SDSC grant) - all from SDSC IT department
- Acquired NSF XSEDE startup allocation on Trestles (SDSC), Lonestar (Texas Advanced Computing Center)
- Received XSEDE community account
- Installed NEURON on Trestles
- (Have more codes/tools now – GENESIS, NEST, PyNN, MOOSE, Brian)

Adaptation of CIPRES to NSG – continued

What's different from CIPRES?

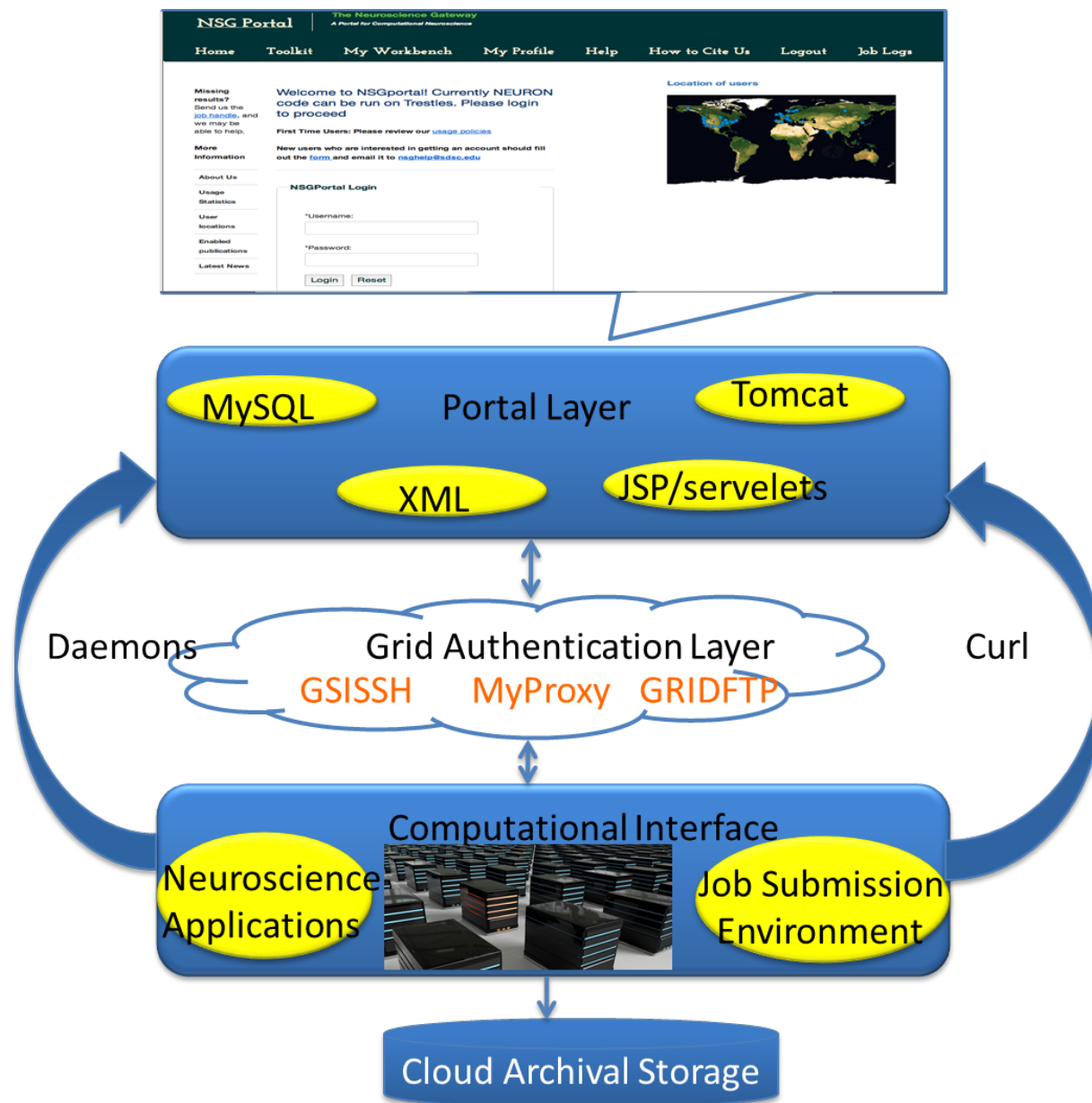
- NSG models have multiple files (e.g. NEURON models)
 - Need to accommodate directory hierarchy containing model code files
 - uuencode/uudecode to support zip file upload to the data handling function
- Requirement to compile input model through NSG
 - mod files for custom mechanisms in C++ are compiled to calculate the biophysical effect (NEURON)
 - Modifications to data staging, job submission
- Define neuronal tools in the XML format
- Automatic storing of output file in SDSC's Cloud storage from HPC resources
- Automatic deletion of user files based on time length of inactivity

Adaptation of CIPRES to NSG – continued

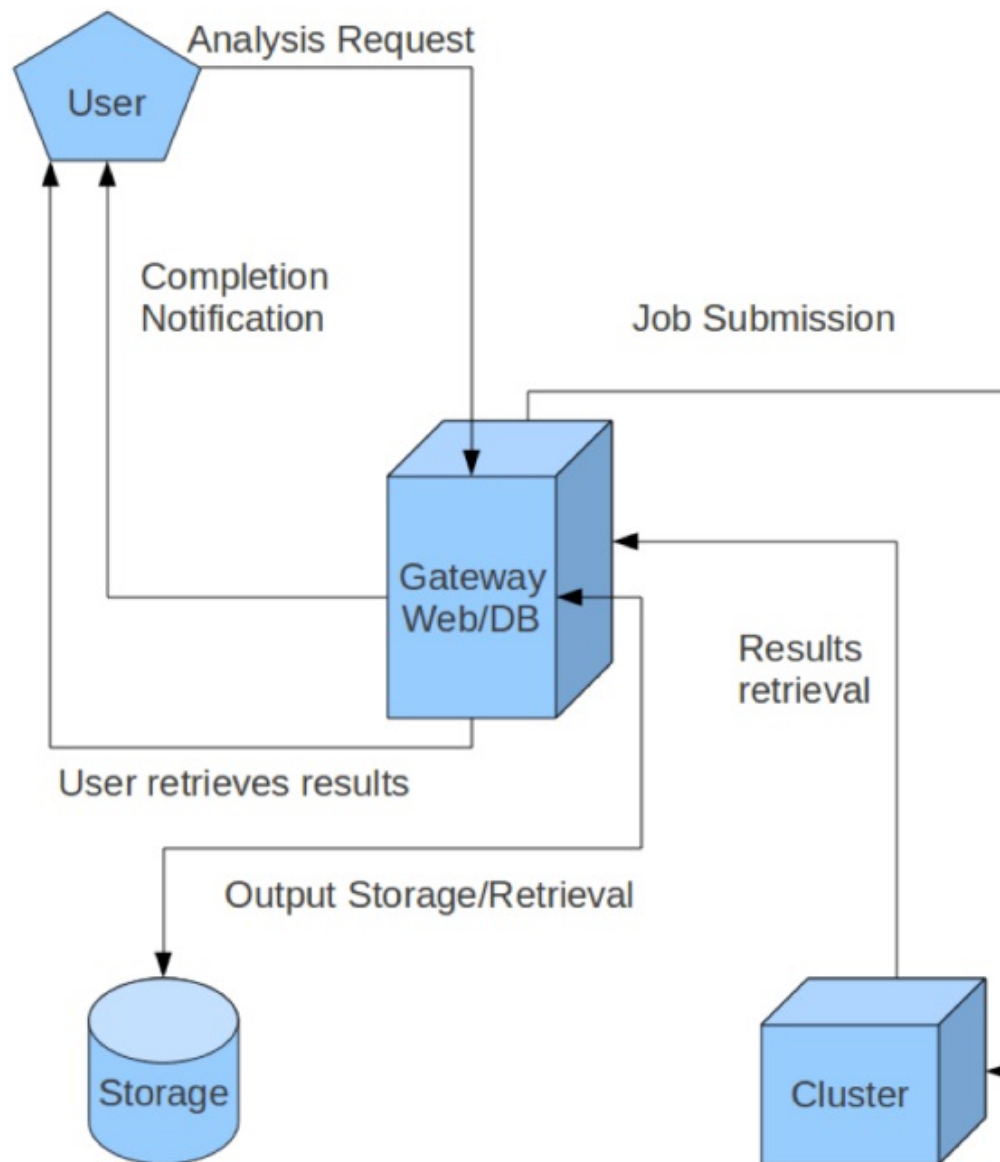
What's different from CIPRES?

- User account creation via user “vetting” process in place
- Why the manual “vetting” process ?
 - As it is possible for user-submitted code to perform actions via HOC, C++ or shell languages (NEURON)
 - For GENESIS the interpreter has access to shell commands
 - To provide user accountability for malicious or incorrect use of HOC/MOD/SHELL languages
- Account creation process is used to verify users
 - Users submit brief contact and technical information
 - We manually “vet” by web searches
 - Then provide account creation instruction

Functional Diagram of NSG Architecture



Users View of NSG



Users View of NSG – continued

Screen after portal log in

NSG Portal

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A Portal for Computational Neuroscience

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Folders

+ tst

+ NEURON 7.2 test

+ test

- MOOSE test run with input1

- Data (2)
- Tasks (5)

User "majumdarnsg" successfully logged in.

Welcome **majumdarnsg** to the NeuroScience Gateway (NSG)



Create New Folder

Current Folder Details:

Label: MOOSE test run with input1


Description: Trying first MOOSE run

Create Subfolder Edit Folder Delete Folder

 Report an Issue  Subscribe to Portal News

NSGportal is a collaboration of these institutions:
[XSEDE](#) [SDSC](#) [NIF](#) [UCSD](#) [Yale School of Medicine](#)
This NSG portal is under development. Please check for updates regarding availability and usability of the portal.

NSG Portal, resource for the neuroscience community, is supported by the National Science Foundation.



Users View of NSG – continued

Can clone task - reproducibility and data validation

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Folders

- test_5_8_13
 - Data (1)
 - Tasks (0)
- NIF-demo
 - Data (1)
 - Tasks (7)
- JonesEtA12009_r31
 - Data (2)
 - Tasks (4)

Tasks

Refresh Tasks

Current CPU Hr Usage: 0 [Explain this?](#)

There are currently 4 tasks in this tab.
(Items 1 - 4 are shown here.)

Show 20 records on each page

<< Page 1 of 1 >>

<input type="checkbox"/>	Select all	Label	Tool	Input	Parameters	Output	Date Created	Action
<input type="checkbox"/>	Clone	test_4_18_13.3	NEURON7.3	View (1)	View (4)	View (2)	4/19/13, 13:35	View Output
<input type="checkbox"/>	Clone	test_4_18_13.2	NEURON7.3	View (1)	View (4)	None	4/19/13, 13:17	View Error
<input type="checkbox"/>	Clone	test_4_18_13.1	NEURON7.3	View (1)	View (4)	View (2)	4/18/13, 20:14	View Output
<input type="checkbox"/>	Clone	test_4_18_13	NEURON7.3	View (1)	View (4)	View (2)	4/18/13, 20:01	View Output

Move selected to JonesEtA12009_r31

GO

Create New Task

Delete Selected

Users View of NSG – continued

- Create new task (job); specify tool, parameters

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Folders

- test IWSG
 - Data (1)
 - Tasks (1)
- tst
- NEURON 7.2 test
- test
- MOOSE test run with input1

Task Summary Select Data Select Tool Set Parameters

You may edit your task using the tabs above.

Current CPU Hr Usage: 0 [Explain this?](#)

* Required

*Description: IWSG test

*Input: 1 Inputs Set

*Tool: Brian [click for more info](#)

Parameters: 4 Parameters Set

[Save Task](#) [Save and Run Task](#) [Discard Task](#)

Saved tasks can be run later from the task list Your task will be saved Clear all user-entered information

XSEDE tasks are limited to 320 hours per job task.

• Input/output Users View of NSG - continued

- Zipped directory
- Single file
- Save folders
- Multiple data sets

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Folders

test IWSG

Data (0)

Tasks (0)

tst

NEURON 7.2 test

test

MOOSE test run with input1

Data (2)

Tasks (5)

Upload File

Label:

Upload your file:

Browse...

For NEURON runs, please create a folder containing your files including subdirectories and upload a zipped version of the main folder.

Save


Cancel

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Users View of NSG – continued

- Select a Tool

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Folders

test IWSG

Data (1)

Tasks (0)

tst

NEURON 7.2 test

test

MOOSE test run with input1

Data (2)

Tasks (5)

Task Summary

Select Data

Select Tool

Set Parameters

Computational Neuroscience Tools

Tools

[Brian](#) (1.4.1) ⓘ - Brian is a simulator for spiking neural networks

[Moose](#) (2.0.0 Kalakand) ⓘ - Multiscale Object-Oriented Simulation Environment

[NEST](#) (2.2.1) ⓘ - Neural Simulation Technology using Python

[NEST](#) (2.2.1) ⓘ - Neural Simulation Technology

[NEURON7.3](#) (7.3) ⓘ - Latest NEURON simulation software package

[NEURON](#) (7.2) ⓘ - NEURON is a simulation environment for modeling individual neurons and networks of neurons.

[PGENESIS](#) (2.3) ⓘ - Parallel Genesis software

[PyNN](#) (0.7.5) ⓘ - Python package for simulator-independent specification of neuronal network models

Users View of NSG – continued

- Advanced users – set parameters

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- NEURON 7.2 test
- test
- MOOSE test run with input1
 - Data (2)
 - Tasks (5)

Task SummarySelect DataSelect ToolSet Parameters

Brian: Brian is a simulator for spiking neural networks
([Romain Brette and Dan Goodman](#))

[Simple Parameters](#) OPEN / CLOSE

[Maximum Hours to Run \(click here for help setting this correctly\) *](#)

[Enter Main Input Python Filename and any arguments\(click here for help setting this correctly\) *](#)











[Enter sub-directory name \(OPTIONAL - click here for help setting this correctly\)](#)

[Enter Number of Nodes \(click here for help setting this correctly\) *](#)

[Enter Number of Cores per Node \(click here for help setting this correctly\) *](#)


Users View of NSG – continued

- Monitor task progress

 **test IWSG**
 Data (1)
 Tasks (1)
 **tst**
 **NEURON 7.2 test**
 **test**
 **MOOSE test run with**
 **input1**
 Data (2)
 Tasks (5)

View Task Details

Refresh Task

Task:	IWSG test
Owner:	majumdarnsg
Group:	majumdarnsg
Date Created:	6/3/13, 03:19
Tool:	Brian
Input:	View (1)
Parameters:	View (4)
Output:	None
Intermediate Results:	 List
Status:	PROCESSING

Task Messages:
Mon Jun 03 03:23:57 PDT 2013 > INITIALIZE : SUCCESS : NGBW-JOB-BRIAN_TG-626E7169BDB44EF5B3B331619DC73A0D : Task 8902 successfully initialized.
Mon Jun 03 03:23:57 PDT 2013 > INPUTCHECK : SUCCESS : NGBW-JOB-BRIAN_TG-626E7169BDB44EF5B3B331619DC73A0D : Input data successfully checked, data valid.
Mon Jun 03 03:23:57 PDT 2013 > COMMANDRENDERING : SUCCESS : NGBW-JOB-BRIAN_TG-626E7169BDB44EF5B3B331619DC73A0D : Command rendered successfully: /home/diag/opt/python2.7_4.6.1/bin/python inputfile
Mon Jun 03 03:23:59 PDT 2013 > INPUTSTAGING : SUCCESS : NGBW-JOB-BRIAN_TG-626E7169BDB44EF5B3B331619DC73A0D : Input files staged successfully to /projects/ps-nsg/home/nsguser/ngbwdev /workspace/NGBW-JOB-BRIAN_TG-626E7169BDB44EF5B3B331619DC73A0D/
Mon Jun 03 03:24:05 PDT 2013 > PROCESSING : SUCCESS : NGBW-JOB-BRIAN TG-

Users View of NSG – continued

Download output

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olders

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 - Tasks (5)



View Task Output

Click on an output file below to review its contents.

Select all	Tool Output	File Name	File Size (Bytes)		
<input type="checkbox"/>	PROCESS_OUTPUT	STDOUT	1225	View	Download
<input type="checkbox"/>		STDERR	10264	View	Download
<input type="checkbox"/>	outputfile	scheduler_stdout.txt	284	View	Download
<input type="checkbox"/>		scheduler_stderr.txt	941	View	Download
<input type="checkbox"/>		output.tar.gz	4701	View	Download

Download Selected

[View Current Task](#) [Return to Task List](#)



Operational Features

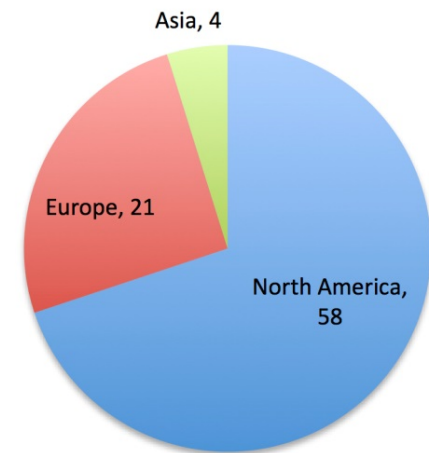
- Two daemons – loadResultsD and recoverResultsD run as nightly cron to retrieve any failed output transfer
- Every job has unique job handle associated with the user – stored in DB
- Nightly cron to gather usage from TGCDB and update DB

Policies

- Any researcher, student from anywhere can use NSG
- Will go through manual “vetting” process – we verify user’s existence
- Current early production state – each user limited to 5000 core hours/year – will increase as we have more users, usage
- If more than 5K/year needed, user’s can use their own allocation via NSG

Early Use

- Opened for friendly users around Dec, 2012
- Received 50,000 hours of core hours on SDSC Trestles and TACC Lonestar machine
- 50K on Trestles was used up by end of Feb
 - We received supplemental 200K on Trestles
 - Another 60K has been used up in the last few weeks
 - Will write yearly XSEDE allocation proposal by the October deadline
- Currently about 80 users – usage picking up slowly
 - We made it more robust, adding hardware
 - Now doing outreach to users
 - XSEDE-wide tutorial in March, 2013
 - SFN demo/outreach in 2012 and in Nov, 2013
 - Summer projects by HS and UG students



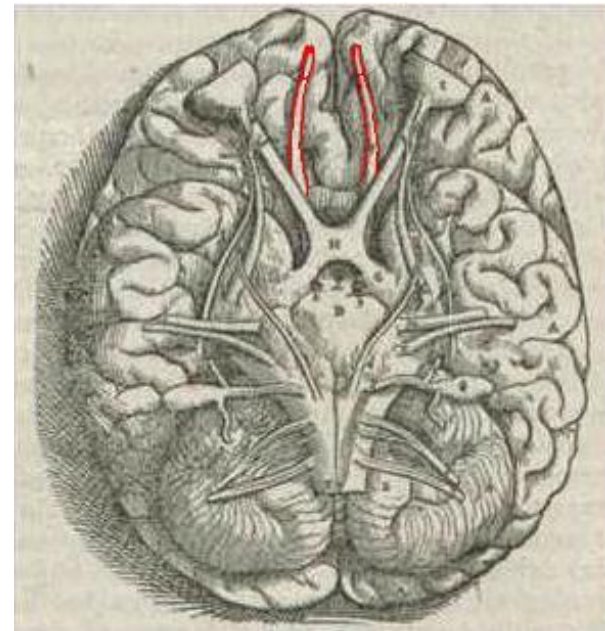
Current Issues – Being Addressed

- Data transfer issue
 - GridFTP occasionally fails during data transfer between VM home directory and HPC resource
 - Alternate implementation – gsissh/scp
- NFS home dir issue on SDSC Trestles machine
 - Automount issue or home dir unavailable due to heavy load
 - Alternate – NSG's own project space as Trestles home dir
 - Use this for input staging, job submission, output staging retrieval

Example Parallel Performance

- Using the NEURON7.3 parallel code
- For 500 mitral cells and 10000 granule cells a large-scale model of the olfactory bulb – small test case run for parallel scaling
- Ran for 40,000 time steps to simulate 1 sec
- <https://senselab.med.yale.edu/modeldb/ShowModel.asp?model=144570>

# of Gordon cores	Time (sec)	Speedup
48	1947	
96	1016	1.91
192	485	4.01
384	249	7.81
768	163	11.94



Future Development

- Computational neuroscience requires
 - Interface with model websites/databases (modelDB, neuroConstruct)
 - Output results sharing (NIF, Wholebrain catalogue)
- Will be implemented using the REST API
- Any enhancement or modification we do for NSG, will be contributed back to CIPRES software for future use

4. Summary

NSG – Enabling Computational Neuroscience

- Providing all the benefits of a science gateway
 - Eliminating technical and administrative barriers to access HPC/CI
- Enable neuroscience education and research for institutions with less resources (and unable to bring up wet labs)
- *Democratize Computational Neuroscience Research and Education*

5. Acknowledgement

- NSF collaborative grant:
DBI 1146949 (PI A. Majumdar, SDSC, Co-PI Martone, NIF, UCSD)
DBI 1146830 (PI T. Carnevale, Yale School of Medicine)
Collaborative Research: ABI Development: Building A Community Resource for Neuroscientists
- Mark Miller, Terri Schwartz, SDSC for CIPRES software (based on which NSG is implemented) and help with implementation
 - XSEDE ECSS support
- SDSC Internal (CID) grant – S. Sivagnanam, K. Yoshimoto
- XSEDE – www.xsede.org
 - Providing HPC resources for the NSG

Thank You



SAN DIEGO SUPERCOMPUTER CENTER

XSEDE13, San Diego, 37
July 22-25, 2013

at the UNIVERSITY OF CALIFORNIA; SAN DIEGO

