A Neuroscience Gateway: Software and Implementation

www.nsgportal.org

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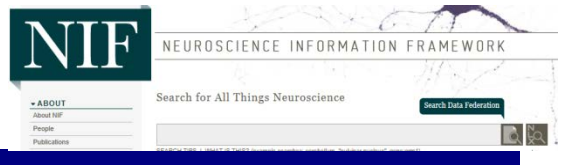


Outline

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 | The Neuroscience Gateway
A Portal for Computational Neuroscience

Home | Toolkit | My Workbench | My Profile | Help | How to Cite Us | Logout | Job Logs

Missing results? Send us the job handle, and we may be able to help.

More Information

- About Us
- Usage Statistics
- User locations
- Enabled 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

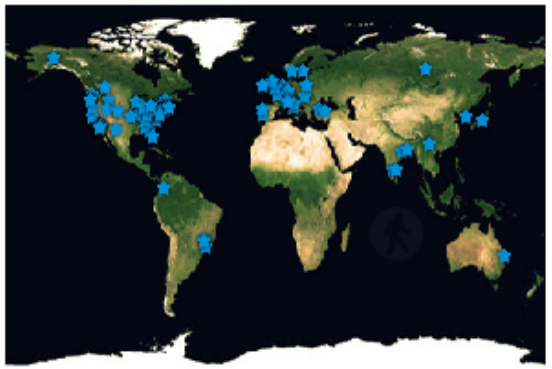
*Username:

*Password:

Login Reset

Forgot Password?

Location of users



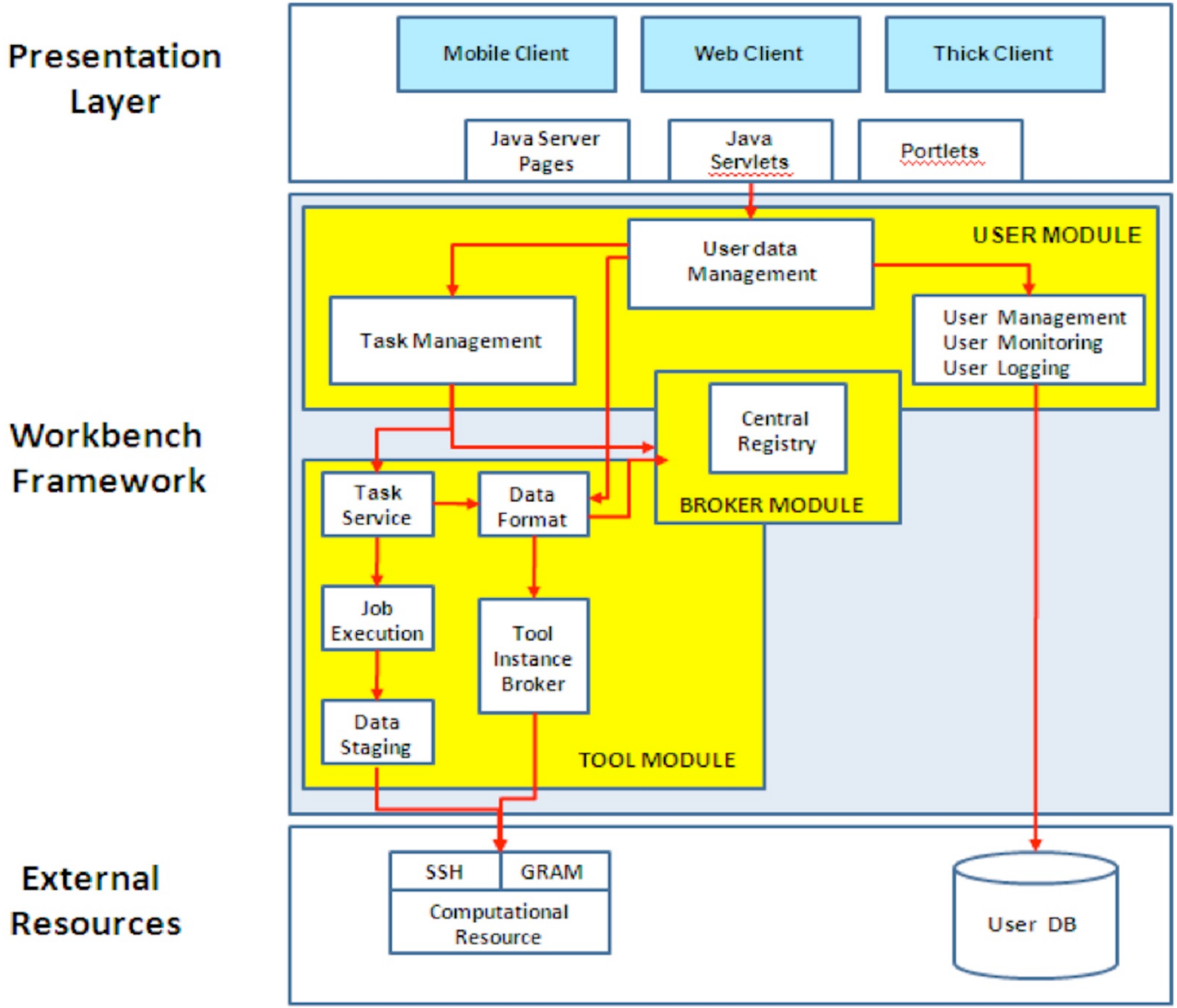
2. Background – CIPRES Workbench Framework

Background

- Why CIPRES (Cyberinfrastructure for Phylognetic 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
- 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

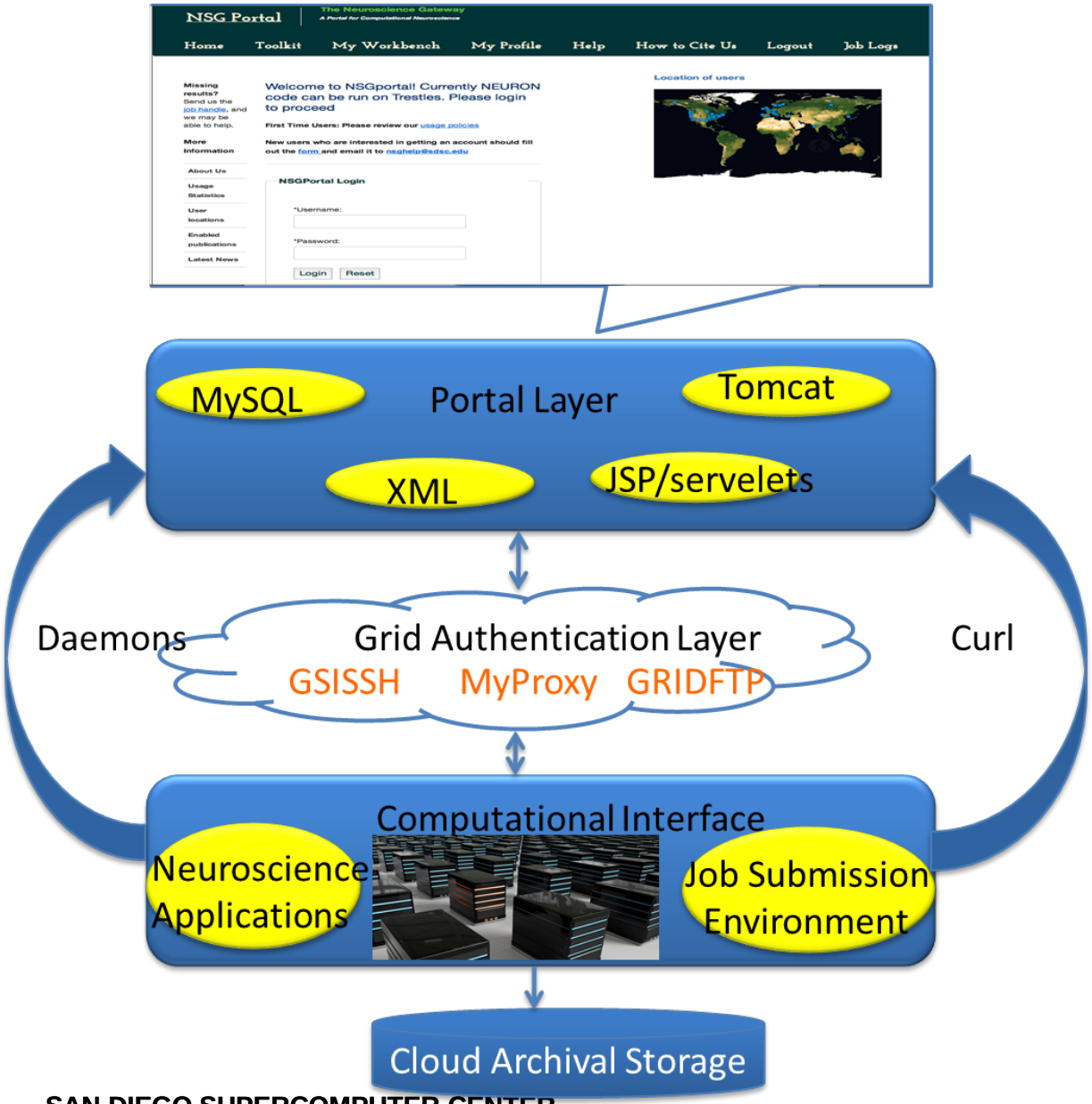
What's different from CIPRES?

- User account creation via user "vetting" process in place

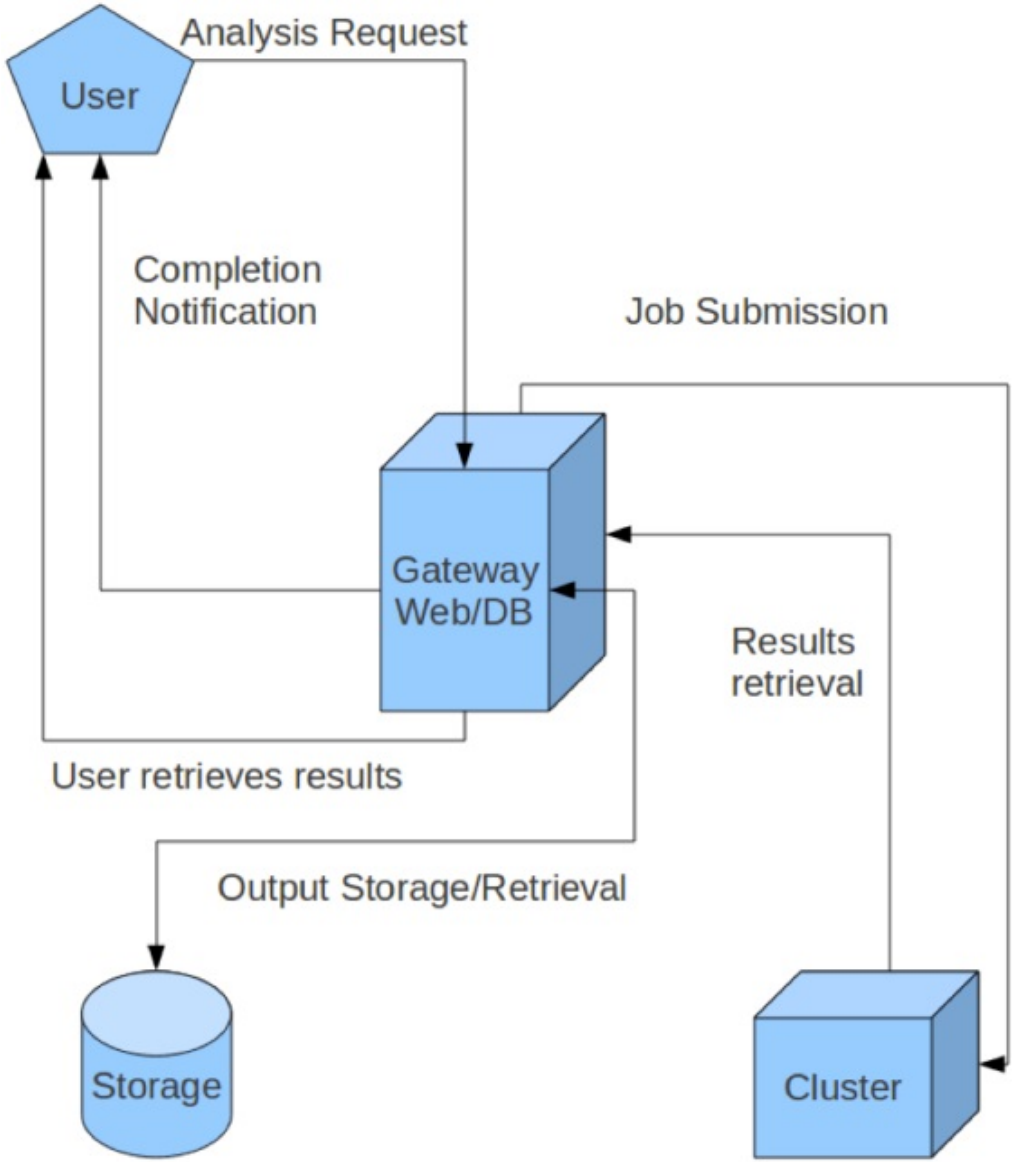
- Why the manual "vetting" process ?
  - As it is possible for user-submitted code to perform actions via HOC, C++ or shell languages (NEURON)
  - For GENESIS the interpreter has access to shell commands
  - To provide user accountability for malicious or incorrect use of HOC/MOD/SHELL languages

- 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

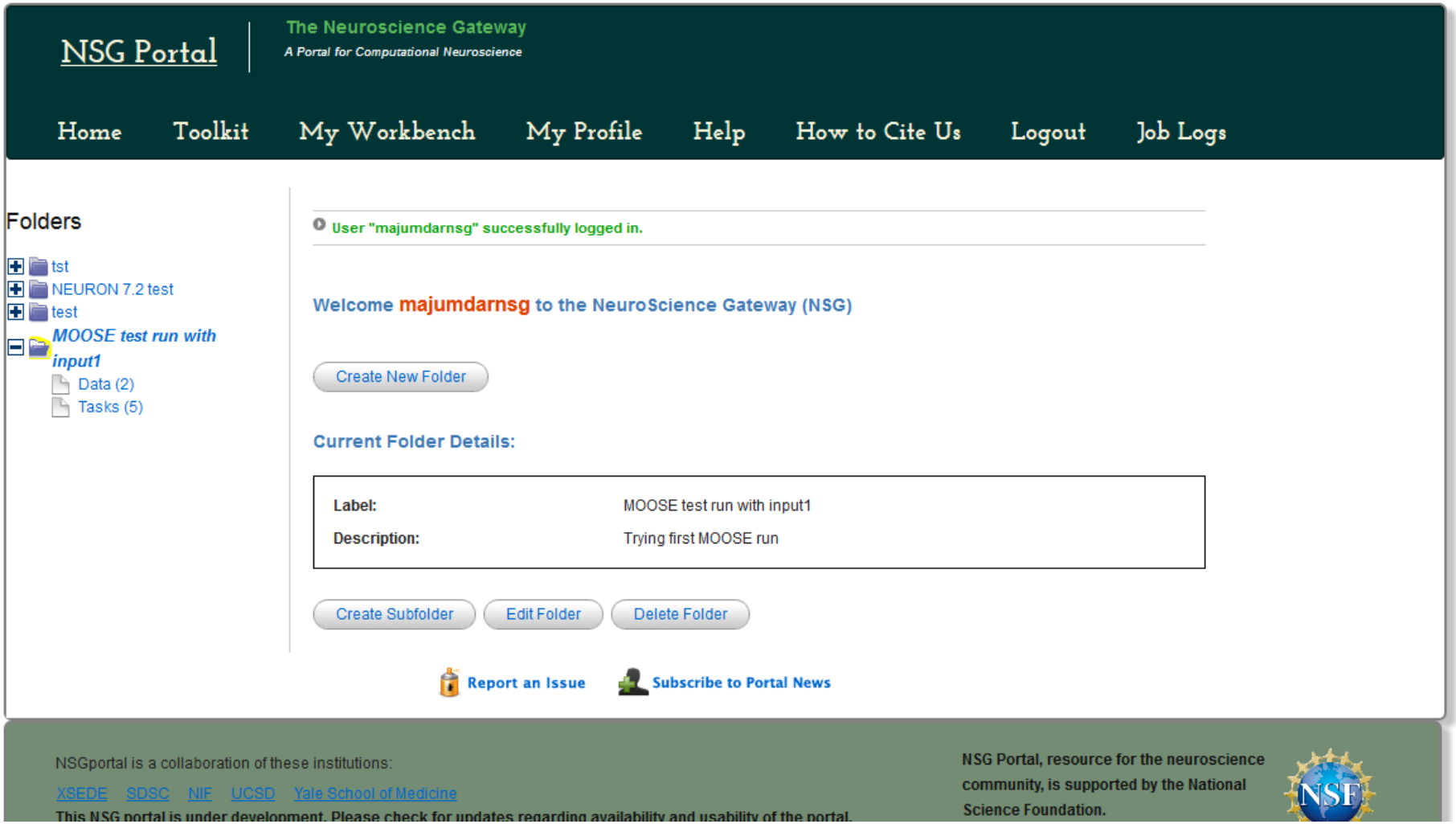


Users View of NSG



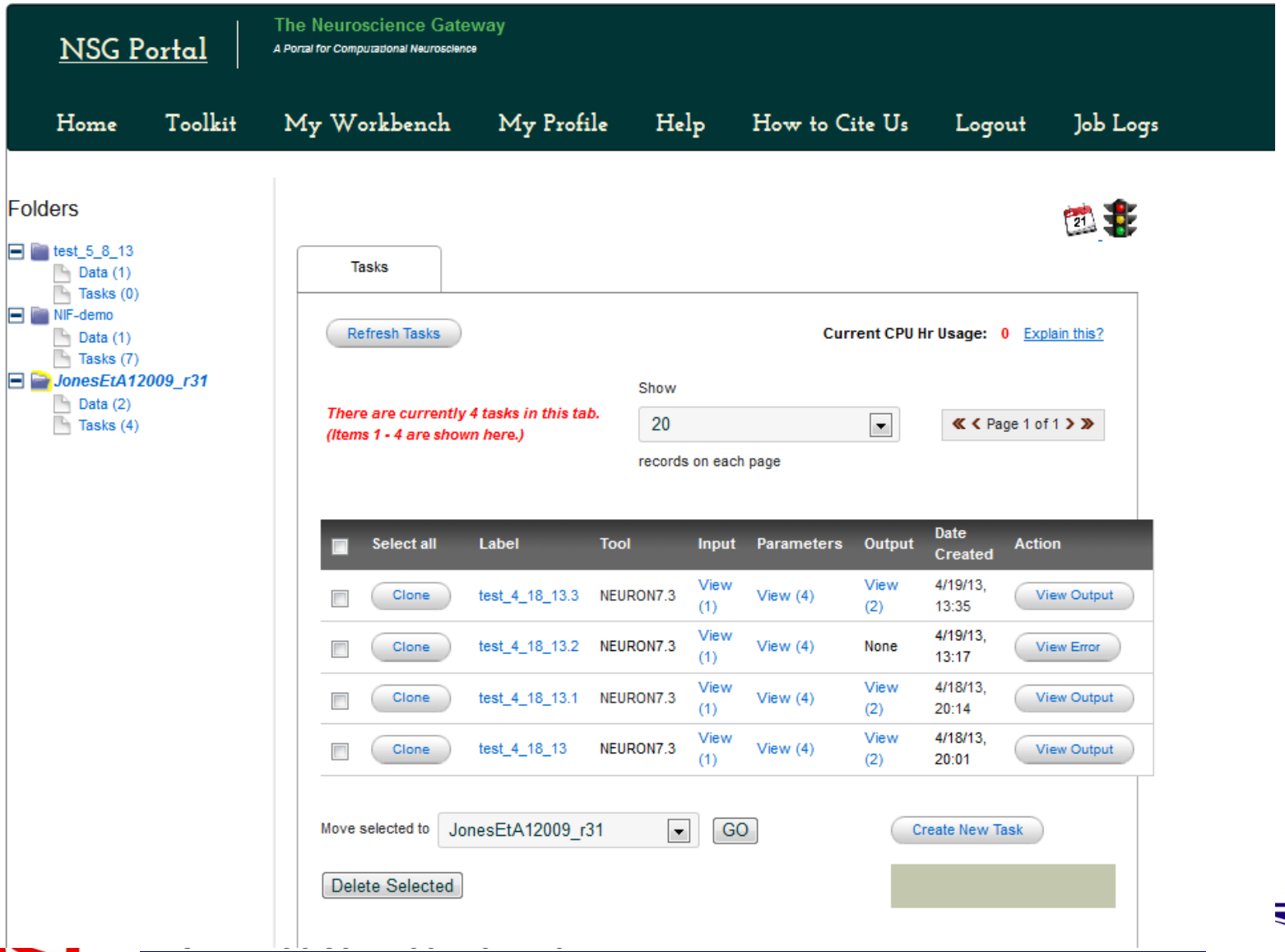
Users View of NSG – continued

Screen after portal log in



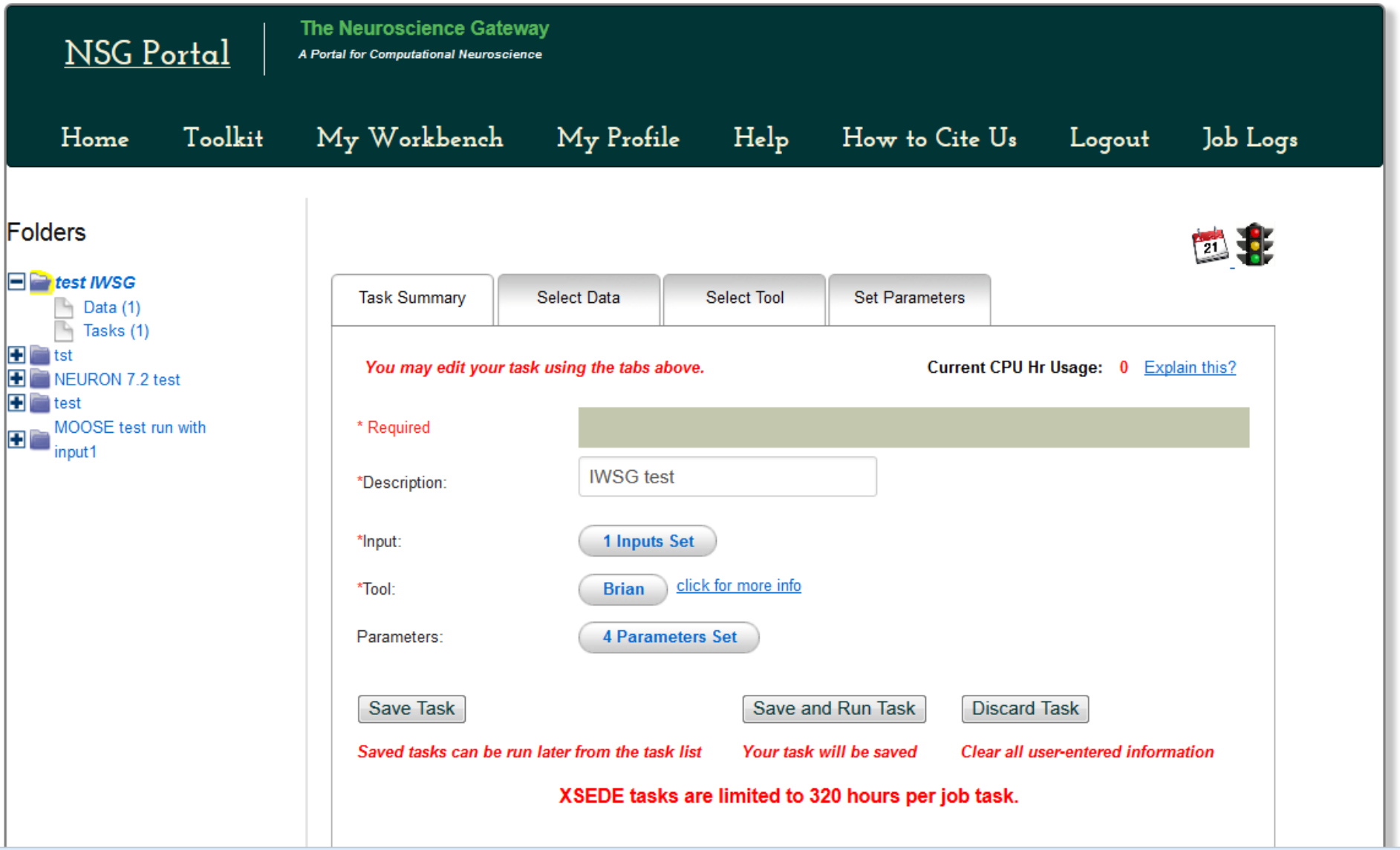
Users View of NSG – continued

Can clone task - reproducibility and data validation



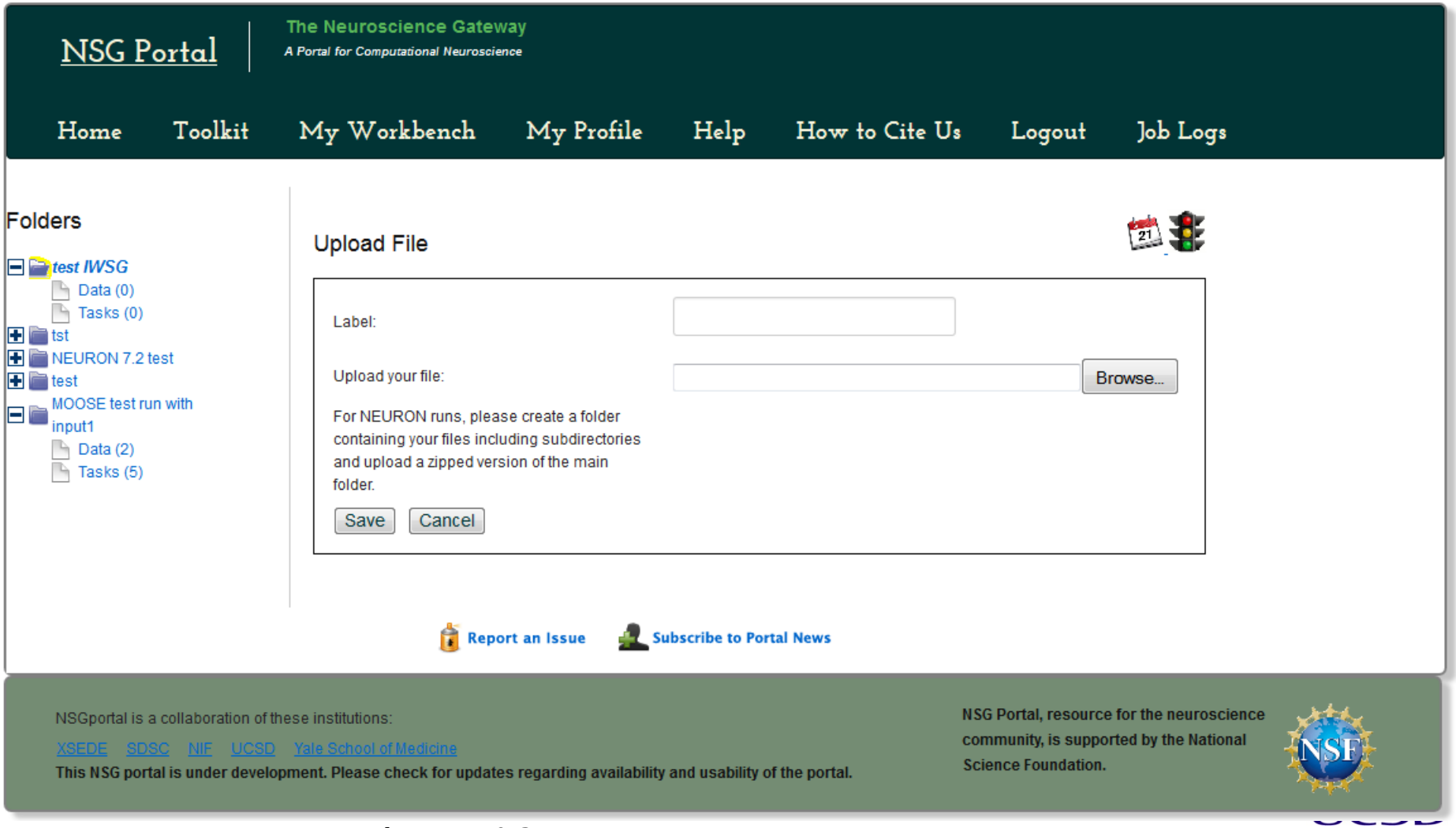
Users View of NSG – continued

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



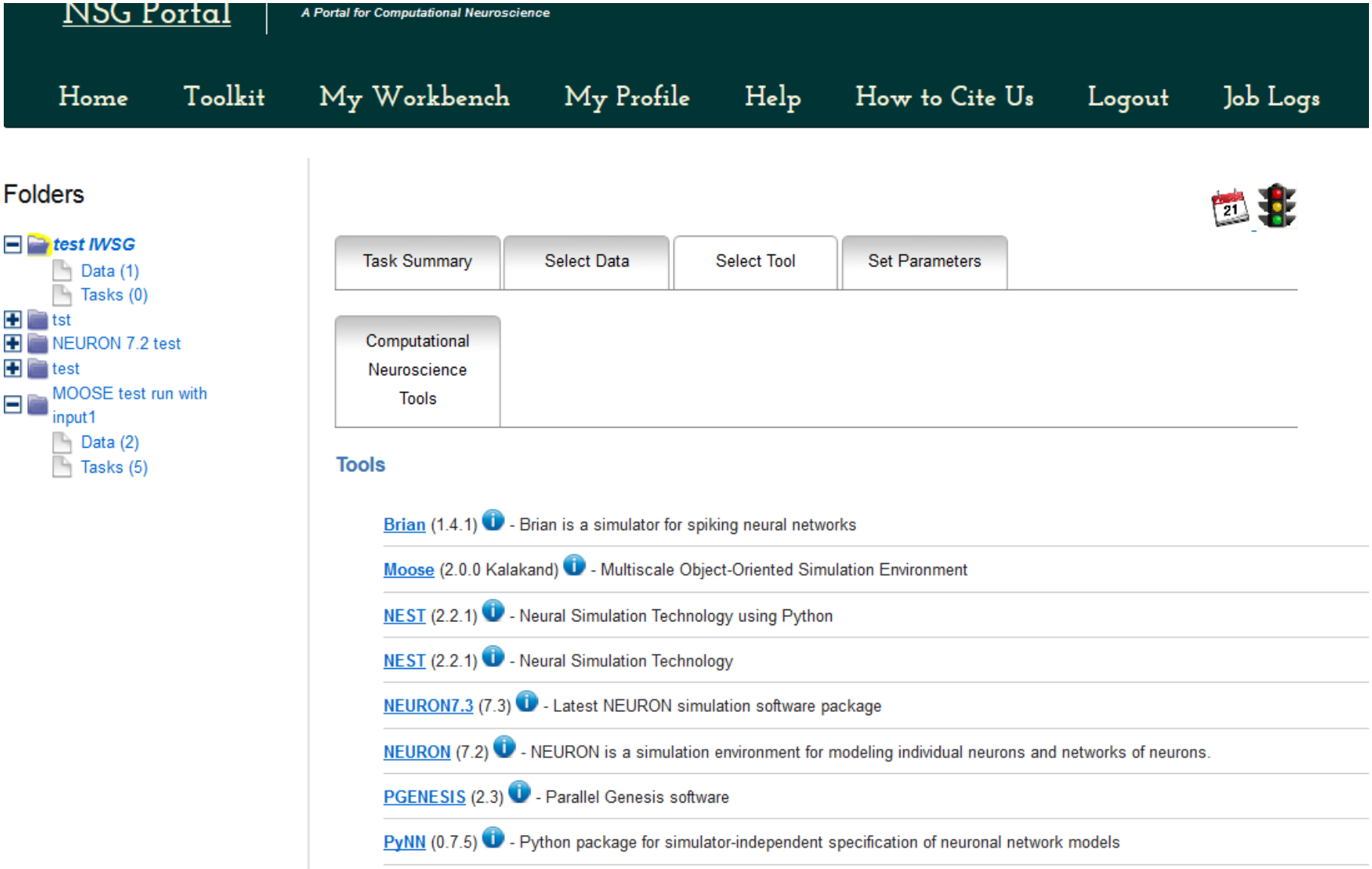
Users View of NSG - continued

- Input/output
  - Zipped directory
  - Single file
  - Save folders
  - Multiple data sets



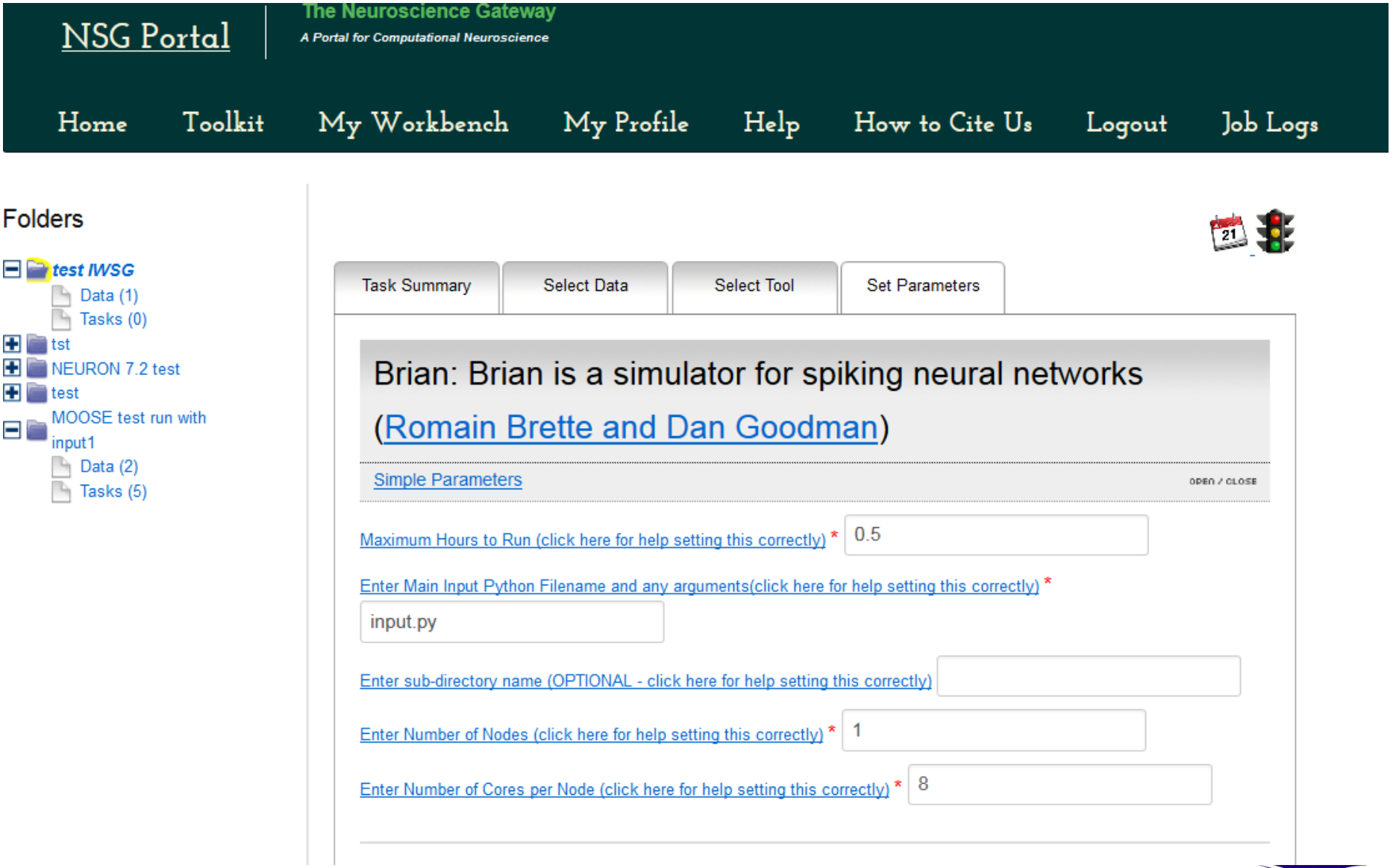
Users View of NSG – continued

- Select a Tool



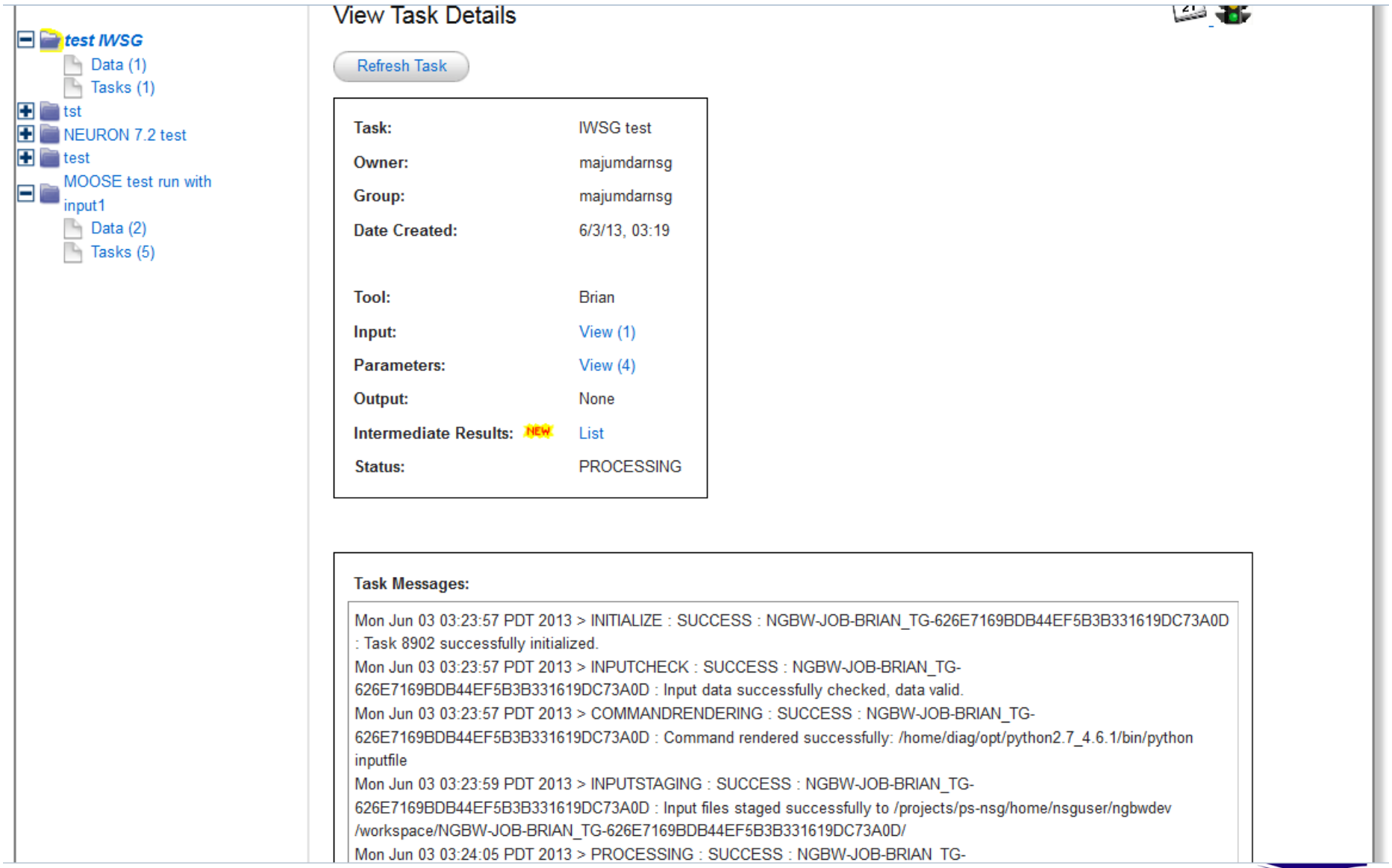
Users View of NSG – continued

- Advanced users – set parameters



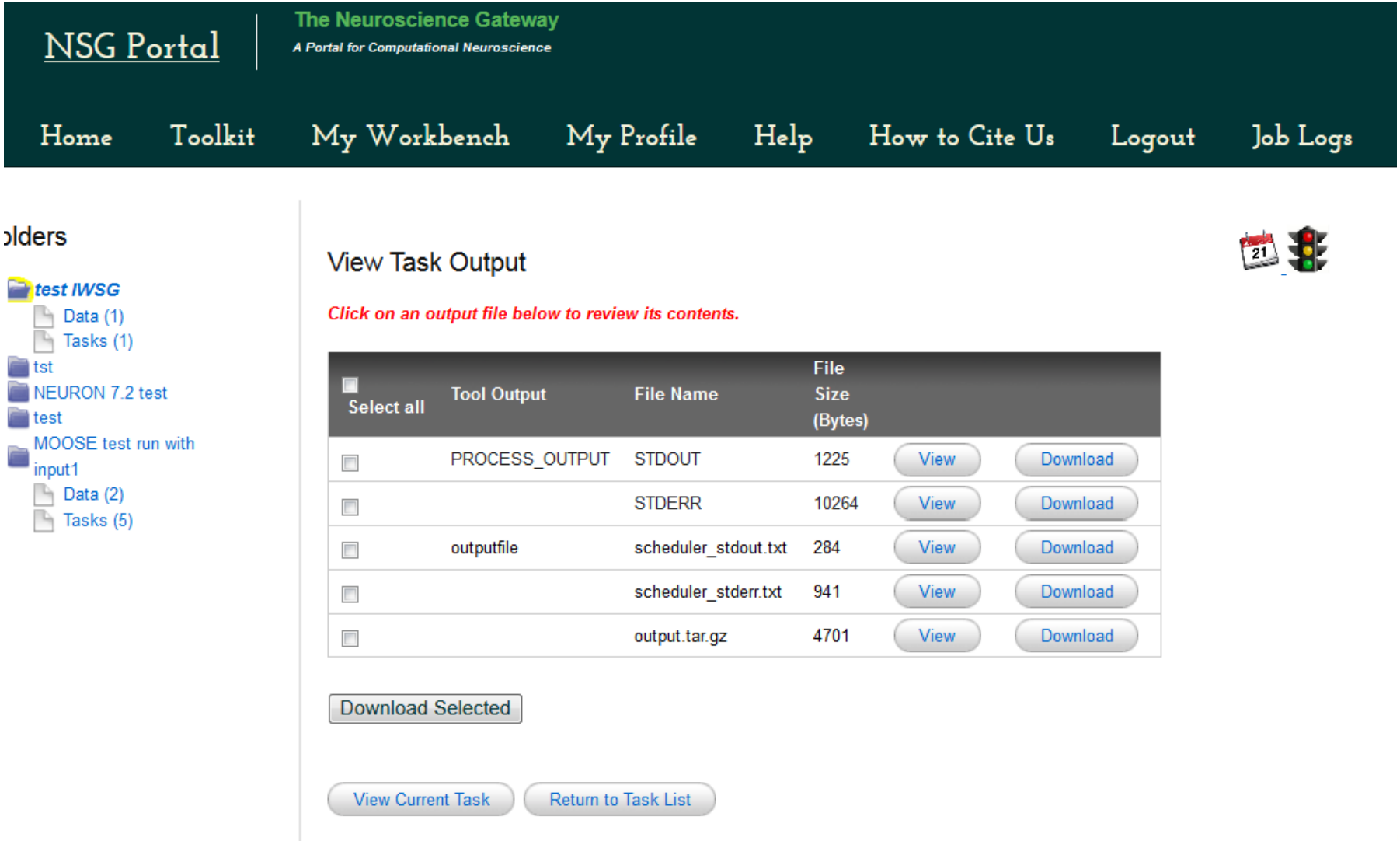
Users View of NSG – continued

- Monitor task progress



Users View of NSG – continued

Download output



Operational Features

- Two daemons – loadResultsD and recoverResultsD run as nightly cron to retrieve any failed output transfer

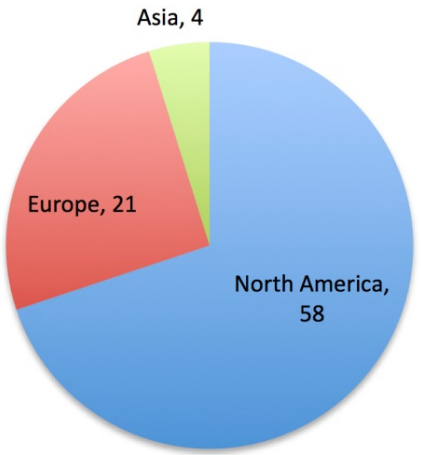
- Every job has unique job handle associated with the user – stored in DB
- Nightly cron to gather usage from TGCDB and update DB

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 hardwar
  - 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

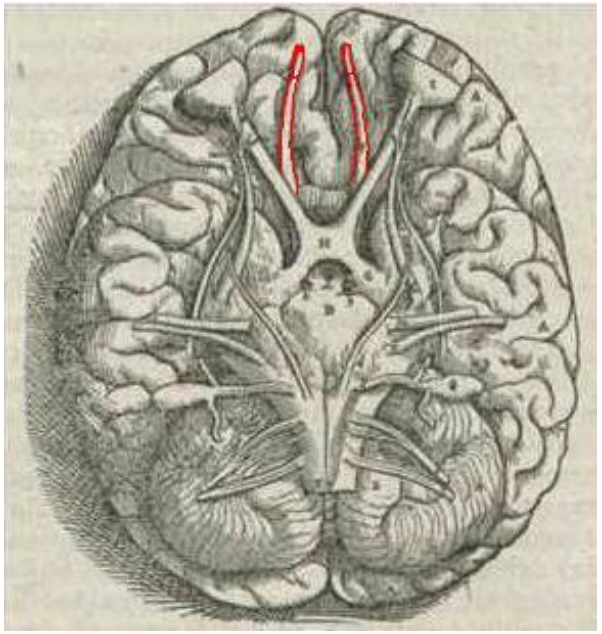
- Data transfer issue
  - GridFTP occasionally fails during data transfer between VM home directory and HPC resource
  - Alternate implementation – gsissh/scp

- 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