

Student Opportunities with the TeraGrid



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TeraGrid

- **“TeraGrid is an open scientific discovery infrastructure combining leadership class resources at eleven partner sites to create an integrated, persistent computational resource.”**
- **Began in 2001, ORNL in 2003**
- **Funded by the National Science Foundation**
- **Community account**



TeraGrid Facilities



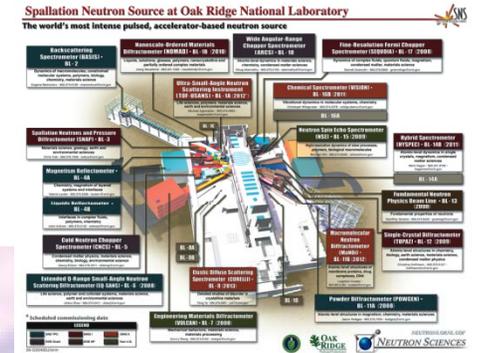
- San Diego Supercomputer Center
- National Center for Atmospheric Research
- Texas Advanced Computing Center*
- National Center for Supercomputing Applications*
- Louisiana Optical Network Initiative
- University of Chicago/ Argonne National Laboratory
- Purdue University
- Pittsburgh Supercomputing Center
- Indiana University
- Oak Ridge National Laboratory*
- National Institute for Computational Sciences

*sites available for the fitting service

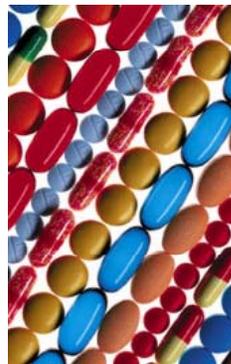
Spallation Neutron Source

➤ Built for material research

- Accelerator-based neutron source
- \$1.4 billion project
- Most intense pulsed beams in world
- Need tools for analysis to make data useful



Spallation Neutron Source (aerial view)



Spallation Neutron Source Portal

The screenshot displays the SNS Portal web application in Internet Explorer. The browser address bar shows <https://neutronsr.us/portal/>. The application interface includes a menu bar with options like File, Visualization, SearchOps, Applications, Job Monitoring, Tools, Sample Activation, Simulation, and Help. Below the menu, there are tabs for Data Browser, Dashboard, and Search.

The main workspace is divided into three sections:

- Workspace:** A file browser showing a directory structure with folders named 'vel-200809151121-5058' through 'vel-200810031525-20298', and a sub-directory 'vel-2008101017-13900' containing 'in', 'out', and 'mcstas.nxs' files.
- McStas Simulation [simulator]:** A control panel for the simulation. It includes a 'Submit' button and a 'Close' button. Below the buttons, there are 'Resource Declarations' for 'Number of Neutron Rays' with fields for 'Base Value' (1.0), 'Exponent' (6.0), and 'Energy Range Min' (2.0).
- 2-D View:** A plot titled '/entry/bank1/data (data 'Backscattering Spectrometer Upper Detector Bank') [-,.,{0-299}]'. The plot shows intensity versus 'Pixel_ID (Pixel IDe) (metre)' on the y-axis (ranging from -0.06 to 0.06) and 'LPSD_Tube_ID (LPSD Tube ID) (metre)' on the x-axis (ranging from -0.3 to 0.3). A color scale on the right indicates intensity values from 0E0 to 1E-1.

The Windows taskbar at the bottom shows the system clock at 8:56 AM and several open applications, including Internet Explorer and a file explorer window.

To be successful, a student should ...

➤ **Work well with a team**

- Instrument scientists
- Portal developers
- TeraGrid developers

➤ **Learn new concepts independently**

- Examples
- Documentation
- Web help pages

Student projects for 2007 and 2008



- **Develop a GUI for fitting service**
 - Analyze data at SNS
 - Allow scientists to fit data without having to know anything about the code or parallel computing

- **Run on TeraGrid from SNS portal**
 - Add to simulation tab in portal
 - Use community account

Fitting_Service [driver]

Fitting Service for Neutron Science Experiments.

[Support URL: https://flathead.ornl.gov/trac/InstrumentSoftware](https://flathead.ornl.gov/trac/InstrumentSoftware)

Please Verify or Enter All Required Parameters,
Then Press the 'Submit' Button to Perform the Simulation Operation.

(* = Required Fields)

Number of CPUs *:

Input Filename *:

Number of Data Points *:

Number of X-Values Per Data Point *:

Model *: (Select Instrument)

Fitting Code *: (Select Code)

Output Filename *:

Fitting_Service X

Job Parameters

Model Parameters

Code Parameters

Number of Fitting Parameters *: 3

chisqr: Undefined

Name: Amplitude

Value: 2

Max: 10

Min: 1

vary

This is the maximum value for the above parameter.

Name: Center

Value: 2

Max: 10

Min: 1

vary

Name: Std. Dev.

Value: 2

Max: 10

Min: 1

vary

Fitting_Service X

Job Parameters

Model Parameters

Code Parameters

IV(1): 12

IV(covprt): 1

IV(covreq): 1

IV(dtype): 1

IV(mxfcals): 200

IV(mxiter): 150

IV(outlev): 1

IV(parprt): 1

IV(prunit): 6

IV(solprt): 1

IV(statpr): 1

IV(x0prt): 1

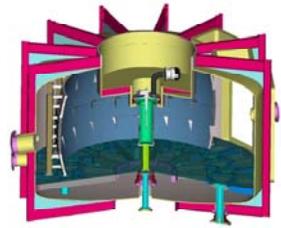
IV(inits): 0

V(tuner1): 0.1

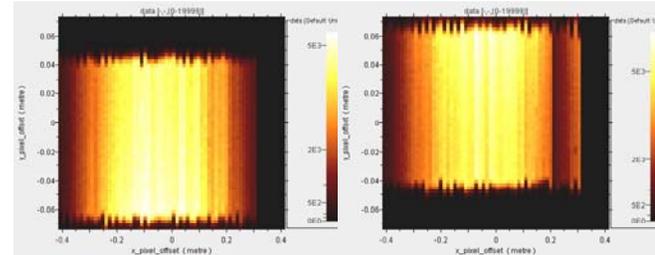
V(afctol): 1e-20

Gives the maximum number of iterations allowed. Also indirectly limits number of gradient evaluations. If number does not suffice, NL2SOL returns with IV(1) = 10.

Sequence



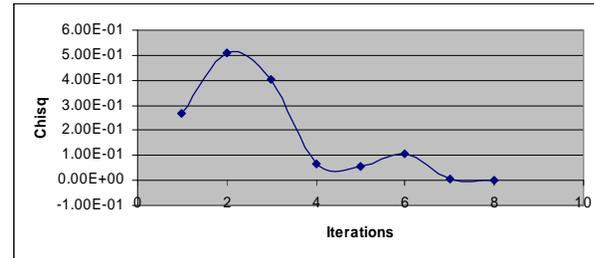
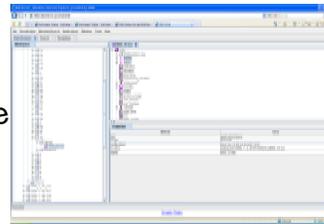
Data to portal



Visualize from portal



Choose a service



Configuration File

```
# Base: 1. Instrument name (char)
Gaussian
# Wdir: 2. Working directory (char)
/users/chemall/LaTeX/FitDirve_BB
# DataF: Data file name (char)
gaussData.dat
# DataS: Data array size (int), X dimensions (int), (reserved for late P90 usage:
dynamically defined array)
1000 1
# OutF: Out put file name
guiFitLog
# ProcN: Total process number (int)
1
# ParamN: Fitting parameter number (int)
3
# Pguess: Fitting parameter guessed values (real/double)
1.5E+00 -0.5E+00 0.23E+00
# NmodN: Number of TV modified (int)
2
# Nypair: TV index1 (int), value1 (int), index2, value2, IV(17): Max# of funct
ion evaluations, IV(18): Max# of iterations allowed
17 200 18 150
# NmodN: Number of V modified (int): no modification according to user input fo
r now
2
# Npar: V index1 (int), value1 (real/double); index2, value2, V(39): the real
e vector D init value (=0), V(57): The init value of all components of D0 vecto
r (=0);
38 0. 37 1.0
# End
```

Run on TeraGrid



Visualize from portal

Student opportunities at conferences



➤ Student Volunteer for SC

- Travel
- Attend presentations
- Attend exhibits
- Networking

Student opportunities at conferences



- **Student research contests**
 - Present work
 - Attend science and/or computing sessions
 - Networking