

Spallation Neutron Source Data Analysis



TeraGrid™



Presented by

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August 14, 2008
Oak Ridge, Tennessee

Outline

- **Purpose**
 - **Develop graphical user interface (GUI) for fitting code**
 - **Run on TeraGrid**
- **Graphical user interface**
 - **Need for GUI**
 - **Fitting code**
 - **XML**
- **Putting it all together**
 - **Add to Spallation Neutron Source (SNS) portal**
 - **Create GUI**
 - **Write configuration file**
- **TeraGrid**
 - **Explain TeraGrid**
 - **Show TeraGrid facilities**
- **Sequence**
- **Future work**

Purpose

- **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**

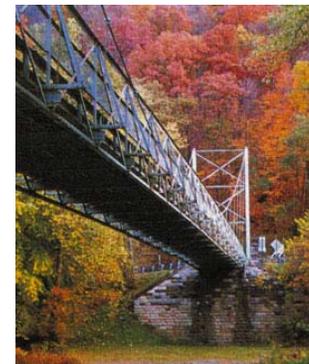
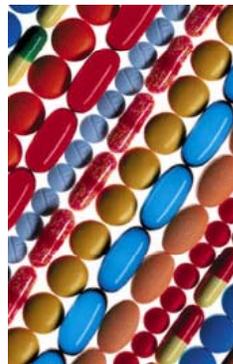
- **Run on TeraGrid from SNS portal**
 - **Add to simulation tab in portal**
 - **Use community account**

Need for Fitting Service

- **Built for use at SNS**
 - Accelerator-based neutron source
 - \$1.4 billion project
 - Most intense pulsed beams in world
 - Need tools for analysis to make data useful
- **Used by scientists to fit experimental data**



Spallation Neutron Source (aerial view)



Fitting Code Behind the GUI

➤ NL2SOL

- “Adaptive non-linear least-square algorithm”
- Jacobian matrix must be provided
- Tested by Meili Chen
- Used to fit fabricated data

➤ NL2SNO

- Computes approximate Jacobian matrix by forward differences

➤ DAKOTA

- Design Analysis Kit for Optimization and Terascale Applications
- Developed by Sandia National Laboratories
- Contains following algorithms for optimization
 - with gradient- and nongradient-based methods
 - parameter estimation with nonlinear least squares methods
 - uncertainty qualification
 - sensitivity/variance analysis

XML File

- **Written detailing components of GUI**
- **Used Faregate**
 - **Unix system**
 - **vi editor**
- **Given examples of McStas and AmorRed**
- **Documentation**

Code

```
<paramgroup name="Job Parameters">  
  <parameter id="cpus" required="yes">  
    <cliname type="text" prefix="-" separator=" ">S|np</cliname>  
    <guirep>  
      <widget label="Number of CPUs">  
        <tooltip>  
          Number of processors on which to run job.  
        </tooltip>  
        <textentrybox default="10" width="8" />  
      </widget>  
    </guirep>  
  </parameter>  
</paramgroup>
```

Putting it all together

- **Added to SNS portal (neutronsr.us)**
- **Anyone with access to portal will have access to this tool**
- **Sudharshan Vazhkudai will write configuration file out of input**
- **Configuration file read by fitting code**
- **Show portal**

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.

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**



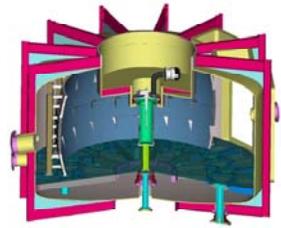
TeraGrid Facilities



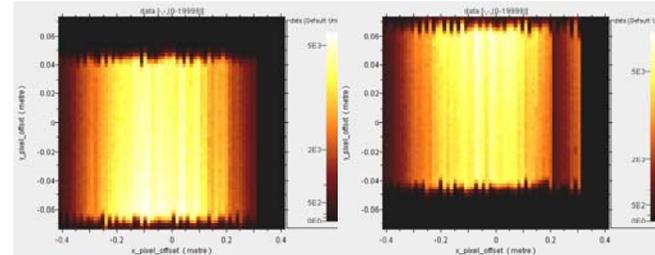
- San Diego Supercomputer Center
- National Center for Atmospheric Research
- Texas Advanced Computing Center*
- National Center for Supercomputing Applications*
- Louisiana Optical Network Initiative
- University of Chicago/ Argonne National Laboratory
- Purdue University
- Pittsburgh Supercomputing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

*sites available for the fitting service

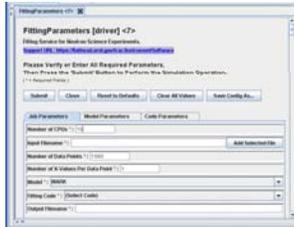
Sequence



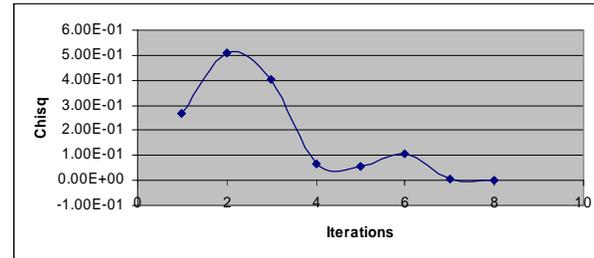
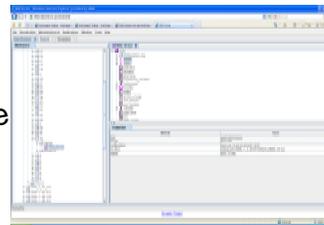
Data to portal



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
```

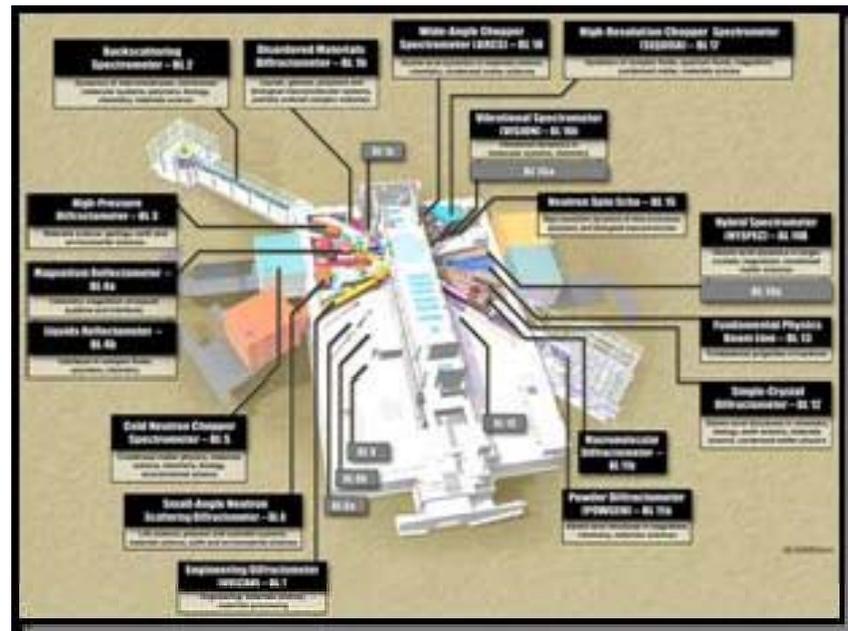
Run on TeraGrid



Visualize from portal

Future work

- Analyze real data from SNS
- Include more instruments as they come online
- Add more models as they become available
- Use more fitting codes (possibly Bayesian fitting)
- Make improvement to GUI and add more features to software



Acknowledgments

The Research Alliance in Math and Science program is sponsored by the Office of Advanced Scientific Computing Research, U.S. Department of Energy.

The work was performed at the Oak Ridge National Laboratory, which is managed by UT-Battelle, LLC under Contract No. De-AC05-00OR22725. This work has been authored by a contractor of the U.S. Government, accordingly, the U.S. Government retains a non-exclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.

George Seweryniak - RAMS sponsor

Vickie Lynch and John Cobb - mentors

Sudharshan Vazhkudai - configuration file

Meili Chen - NL2SOL, NL2SNO, DAKOTA

Jim Kohl - XML software

Neutron Science Portal Development group at SNS

TeraGrid/NSF group

Mark Hagen

<http://teragrid.org/about/> - TeraGrid information

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