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

 dévelop 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

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

- Added to SNS portal (neutronsrs.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

Please Verify or Enter All Required Parameters,
Then Press the 'Submit' Button to Perform the Simulation Operation.
(* = Required Fields)

Submit  Close  Reset to Defaults  Clear All Values  Save Config As...

Job Parameters  Model Parameters  Code Parameters

Number of CPUs *: 10
Input Filename *:
Add Selected File
Number of Data Points *: 1000
Number of X-Values Per Data Point *: 1
Model *: (Select Instrument)
Fitting Code *: (Select Code)
Output Filename *:
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<th>Max</th>
<th>Min</th>
<th>Vary</th>
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<td>IV(outlev)</td>
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<td>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.</td>
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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
Sequence

Choose a service

Configuration File

Data to portal

Visualize from portal

Run on TeraGrid

Visualize from portal

Managed by UT-Battelle
for the Department of Energy
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


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Jim Kohl - XML software
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TeraGrid/NSF group
Mark Hagen

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