

Creating a Graphical User Interface for Bayesian Fitting in the Neutron Scattering Portal

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http://wiki.ornl.gov/sites/rams09/a_odutola/Pages/default.aspx

The Spallation Neutron Source (SNS) is an accelerator based neutron source in operation at the Oak Ridge National Laboratory. Through neutron scattering, we are able to study and understand the atomic characteristics of materials. This is valuable because many improvements have been made to indispensable products such as automobiles, planes, and medicine. To increase the efficiency of SNS, a graphical user interface (GUI) will be created and implemented. The GUI will produce inputs using the Rappture software and will be used to submit calculations to a nationwide network of supercomputers (TeraGrid). The purpose of this project is to write XML and TCL files for the Rappture software available in the Neutron Scattering Portal which will create a GUI for the Bayesian fitting program within the portal. Using the Rappture software in the portal, the users can analyze their data with less effort minus the background knowledge of the TeraGrid, Rappture software, or Bayesian fitting program. Input data and output from the Bayesian fit are plotted with Rappture in the GUI so they can be compared. The GUI was successfully completed and presented at the SNS Scientific Computing meeting. The results from the code met the required goals of the project.

Introduction

- Fitting software needed for users of SNS instruments
- Software easy to use, and make available in the portal
- Users can analyze data with less effort and no background knowledge

XML File

```
<?xml version="1.0" encoding="UTF-8" standalone="no" ?>
<gui name="Bayesian Fitting" type="TCL" >
  <title>Bayesian Fitting</title>
  <description>Bayesian Fitting</description>
  <author>Adeola Odutola</author>
  <version>1.0</version>
  <category>Data Analysis</category>
  <tags>Bayesian Fitting</tags>
  <input type="Text" name="input" value="" >
    <description>Input data for Bayesian fitting</description>
  </input>
  <output type="Text" name="output" value="" >
    <description>Output of Bayesian fitting</description>
  </output>
  <command type="TCL" name="fit" >
    <description>Run Bayesian fitting</description>
  </command>
  <plot type="Line" name="plot" >
    <description>Plot of Bayesian fitting results</description>
  </plot>
</gui>
```

Figure 1. XML file used to create the GUI

Future Research

- Customize for all instruments
- Use Rappture to develop GUI for another fitting service
- Improve graphics of Rappture GUI animation of how fitting Improves during run in TeraGrid



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
- Purdue University
- Pittsburg Supercomputing Center
- Indiana University
- Oak Ridge National Laboratory
- National Institute for Computational Sciences

Research Objectives

- Learn to use Linux, Winscp421, PuTTY to access SNS computers
- Create a graphical user interface (GUI) for Bayesian Fitting in the neutron scattering portal
- Plot input data and fit that was calculated in GUI
- Obtain requirements for GUI from instrument scientists and portal developers

Results

- Used Rappture software GUI to submit calculations to a nationwide network of supercomputers (TeraGrid)
- Collaborated with Nick Dexter to obtain final input GUI for code
- Input data and output from Bayesian fit plotted with Rappture GUI comparison

Methods

- Edited XML and TCL files for Rappture software to create graphical user interfaces (GUI)
- Interacted with Nick Dexter and portal developers to input needed for Bayesian fitting program
- Edited TCL file obtain plotting for Bayesian code output

Fitting Service (GUI)

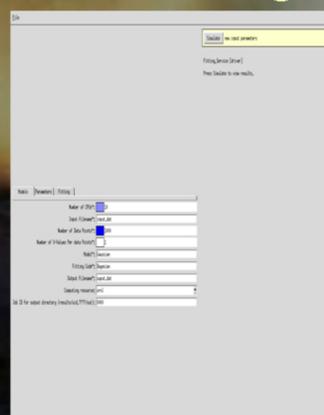


Figure 2. Information page on GUI.

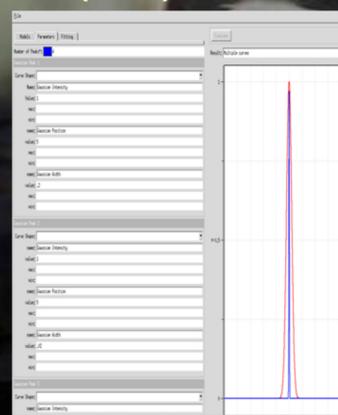


Figure 3. Input page and graph.