Spallation Neutron Source Data Analysis

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http://computing.ornl.gov/internships/rams/rams08/abstracts/index.shtml

Abstract

The Spallation Neutron Source (SNS) portal was developed to give virtual access to SNS data as well as access to tools to reduce, analyze, and visualize that data. The purpose of this project was to make a graphical user interface (GUI) for a fitting service to be added to the SNS portal. An XML file was written describing the components and features of the GUI. That XML file was then added into the SNS portal where it was read by existing software to create the GUI. When submitted, the GUI will provide input for a fitting code (NL2SOL, NL2SNO, or DAKOTA) which will run on the TeraGrid, a nationwide network of supercomputers. The results will then be sent back to the portal where users can visualize the fit data as well as use the output parameters for a new run. This project is useful for developers and users alike in that the developers can easily modify the XML files in the portal and the users can analyze their data at the push of a button without having to know anything about the TeraGrid, XML, or parallel computing.

Project Goals

- Create GUI for fitting service to be added to SNS Portal
- Make GUI useful and attractive
- Add descriptions for components to make more comprehensive for users
- Incorporate suggestions and ideas from SNS instrument scientists to develop GUI into what users want/need

Creation

- Created by an XML file
- Used examples and software documentation to guide development
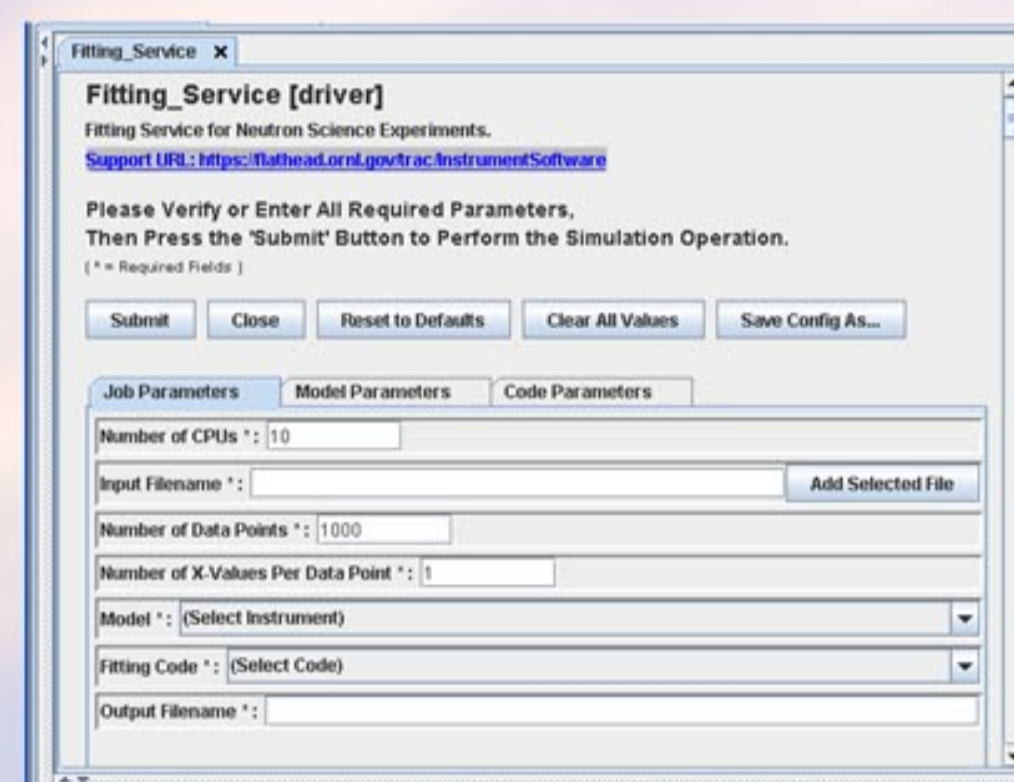- Defaults and other values provided
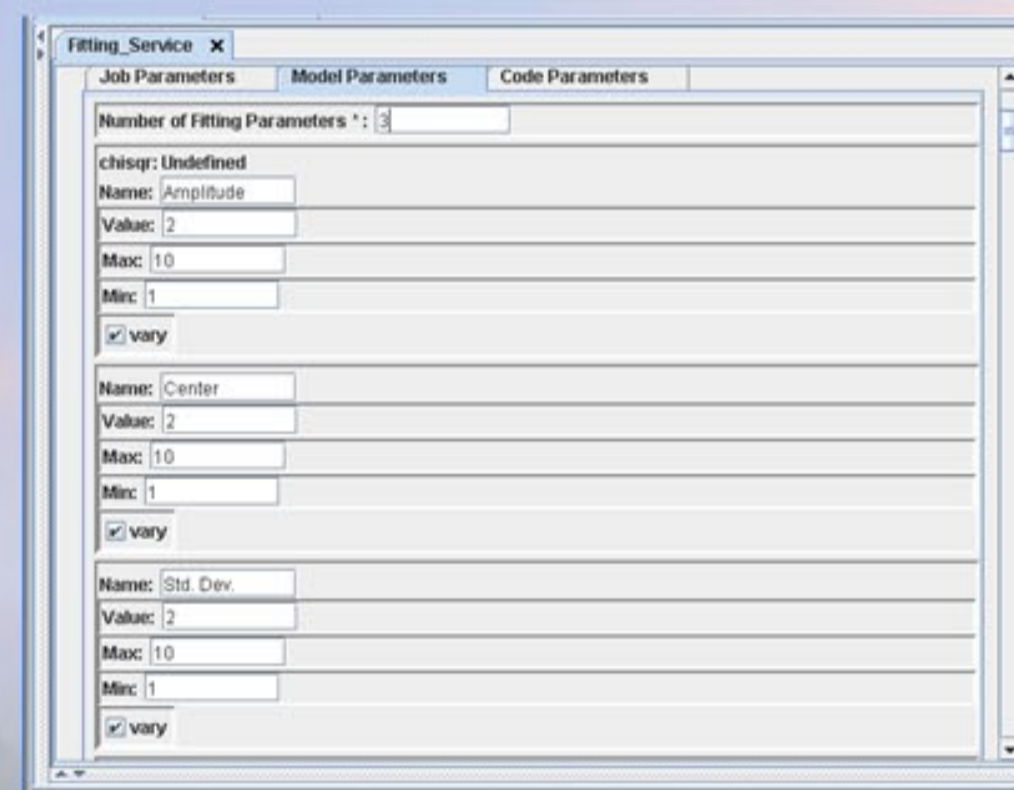
Fitting Service GUI

Figure 1: Input Parameters Page

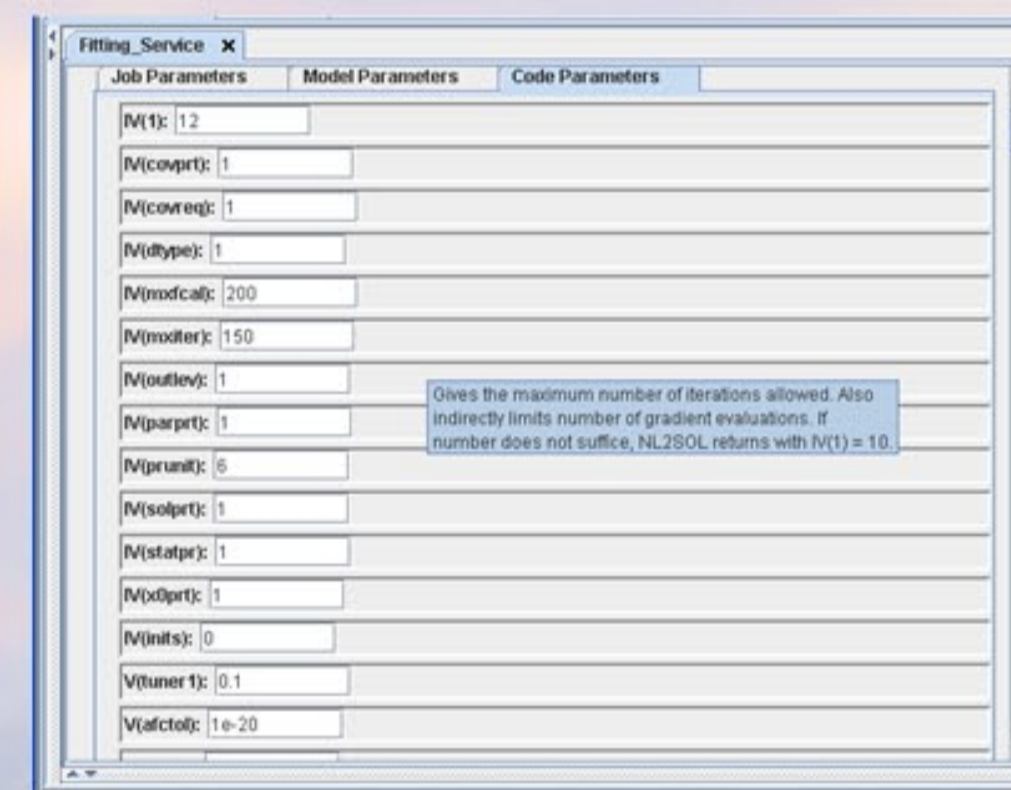Figure 2: Model Parameters Page


Figure 3: Code Parameters Page

GUI Content

- Figure 1: Input Parameters Page
  - User inputs info about data
  - Selection of instrument (Model) sends values to Model Parameters Page.
- Figure 2: Model Parameters Page
  - User selects number of parameters to use
  - Chisqr is calculated when the program runs and is then returned here
  - User sets max and min and decides whether to vary each parameter
- Figure 3: Code Parameters Page
  - Needed by NL2SOL and NL2SNO
  - Descriptions in tooltips

SNS Portal
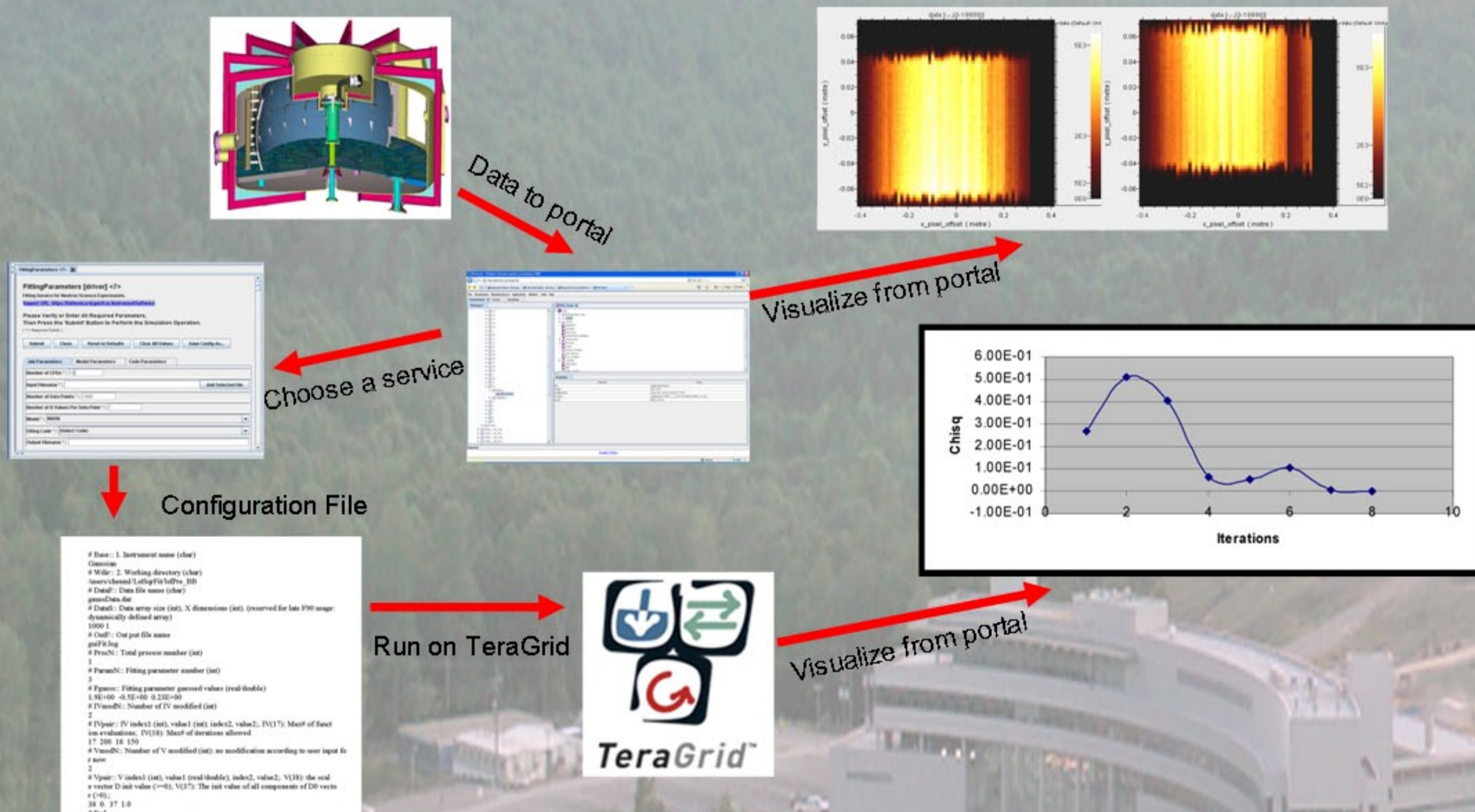
- Ability to immediately see GUI changes in portal helped with design
- Capability to run on TeraGrid
  - Run thru community account- Jimmy Neutron
  - Sent to another machine if run fails

Future Work
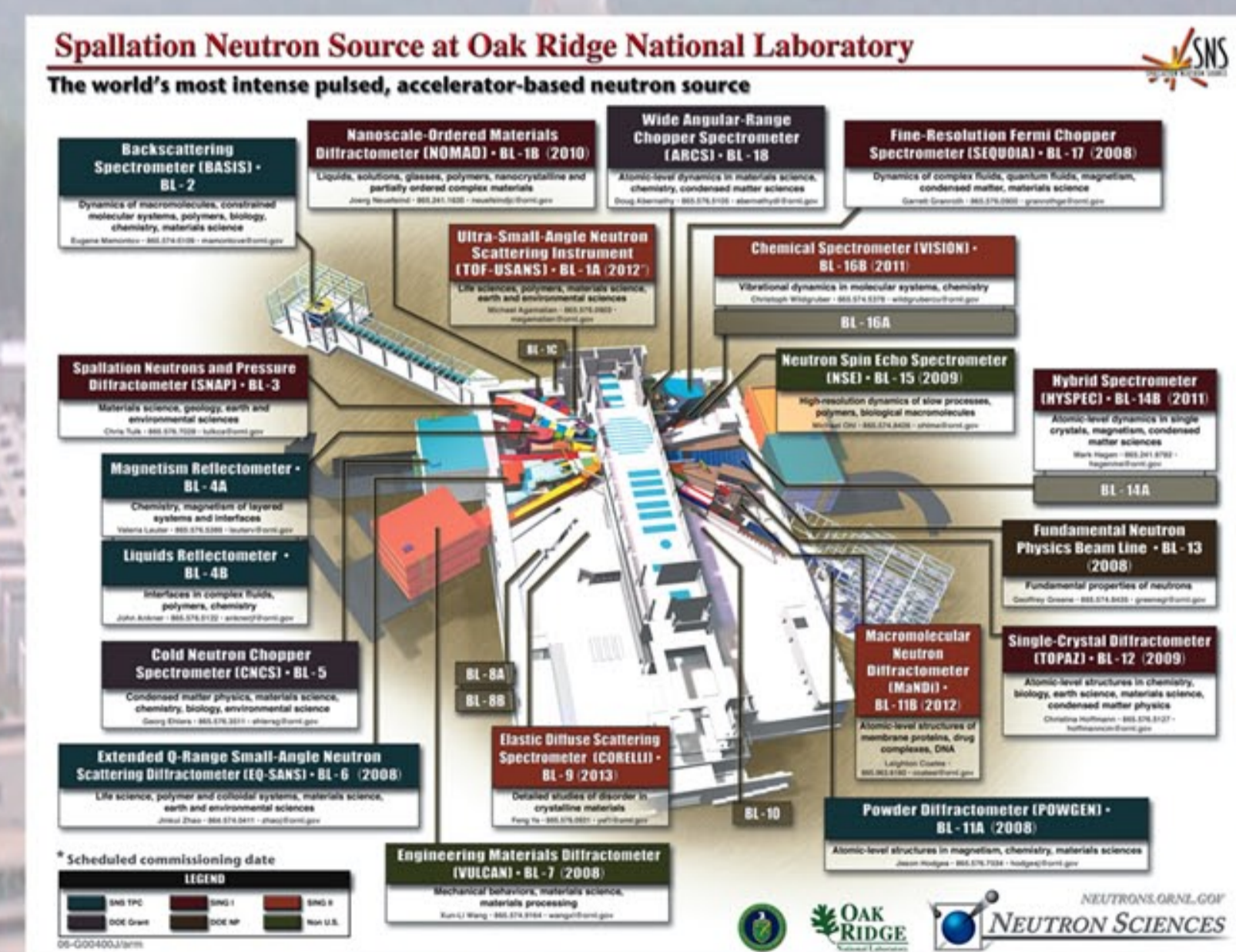
- Test with Gaussian
- Make available on Backscattering Spectrometer when configuration file is completed
- Include more instruments as they come online (see chart above for examples)
- Add more models as they become available
- Use more fitting codes (possibly Bayesian fitting)
- Make improvement to GUI and add more features to software

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