13 June 2017 Mantid Users Workshop

Direct Geometry Inelastic

Comment on Mantid 4.0 – Yes (in principle)! Must be done: change GUI; To be worked on: renaming algorithms, move toward API implementation – what is the longer term plan and what is the cost?

**Summary**

1. Completion of crystal fields to cope with multisite, and any outstanding bug fixes
2. Complete Mslice GUI and features
3. Mslice command line and publication quality graphics
4. Continue GetPhononDOS developments
5. Detector calibration
6. Prototype python–workspace interface layer (?) Impact for history?

Other discussion notes -

What is covered in Mantid?

ISIS: Use a Mantid workspace in future work (MDworkspace?) but it isn’t necessarily fundamental to new developments e.g. for distributed computing; Resolution, fitting outside scope; Visualization based on current capabilities (small port to matplotlib)

ORNL: Use Mantid as a package feeding into something to handle resolution corrections, fitting; Visualization in Mantid that handles MDworkspace (some there, but DAVE Mslice workflow isn’t a clear implementation)

ESS: Data structure not conducive to command line manipulations. Does mantid.math cover all needs?

1. Powder
   1. Mslice replacement
      1. Finish effort as defined now
      2. Python scripting
      3. Enable additional features
         1. Corrections – multiple scattering, absorption, multi-phonon, …
         2. Phonon DOS
         3. Hooks for new application areas, e.g.
            1. Crystal field
2. Single crystal
   1. Focus on one application for data visualization with full features
      1. Subsets of data – 3D to 2D to 1D – done “correctly”
   2. Resolution convolution of models