MANTID @ ILL by December 2017

Goals:

- Use as standard data reduction tool in 9-10 instruments
      TOF (IN4, IN5, IN6), BS (IN16B), REF(D17, Figaro), DIF (D20, D1B+D2B+D4?)

- Workflow / interface SANS (D11, D22, D33)

- Solution for scanning instruments (D2B, D4, D16, D7) defined

- Organise training for ILL scientists and users

Challenges:

- Mantid constraints (project size, dependence on work done at other facilities e.g. Instrument 2.0, multiple revision cycles, …)

- No immediate need and no clear perception of advantages

- Expectations that Mantid should replace old soft even to treat old data

MANTID January-April 2017

- **Cycle 2017-1 (19 Jan – 8 Mar)**
  - Use/feedback from IN16B *(GV+MG)*
  - Use/feedback from IN4 *(AS+MG)*
  - Mid-Feb (?) → Use/feedback from IN5B/IN6

- **PMC meeting (13 March)** **Note change of date!** **→ Scientific Council 6-7 April**
  - (Good) news from use 'in vivo'
  - Prototype interface for TOF & BS *(AS+GV)*
  - Reflectometry:
    - Able to treat D17 data (at least script) *(VR)*
    - Interface (ISIS one adapted? Or think what is needed) *(VR)*
    - Plan to treat polarized data *(VR + T. Saerbeck)*
  - Powder Difraction:
    - Loader D20 / D1B (NeXuS meeting end January, if not use ASCII?) *(GV)*
  - Scanning instruments / Instrument 2.0:
    - Status and planning *(IB)*
    - Schedule for D2B, D4, D16, D7 *(IB)*

SINE 2020 – WP 10 (Data Treatment Software)

Tasks:

10.1 Dissemination and management (ESS)

10.2 Guidelines and standards (STFC, ILL as observer)
- To enable different software to be interoperable
- Based on work in the Mantid project + previous projects

10.3 **Converging on Mantid for continuous sources** (**ILL**, partners FZJ and PSI)

2 PY

10.4 Interoperable data treatment software

- Phase I
    - SANS → SasView (ESS)
    - Reflectometry → BornAgain (FZJ)
    - Imaging → MuhRec & KipTool (PSI + CEA, ISIS, ESS)

- Phase II

    - **QENS → Mantid** (ISIS + **ILL**, FZJ)
        - More user-friendly interfaces
        - Extension of model fitting functions

    - **Atomistic modelling → MDANSE / ASE & DFT** (**ILL** + ESS, ISIS, PSI, Parma)
        - Extension to convert LD (and MC?) to scattering curves
        - Muon spectroscopy

2 PY

Meetings / workshops & related work

- **SINE 2020 – WP10 workshop II @ ILL (24-25 April)**
  - Present progress & status of Mantid at ILL
  - Meet with FZJ and PSI partners
  - Plan next work on QENS & atomistic modelling (likely to be done in Mantid or keeping strong contacts with Mantid)

  - (Hopefully) recruit someone to work during two years in these tasks.
  - Training and inclusion in working team

- **Mantid workshop (14th – 16th June)**
  - Mantid V4 (Developers: ISIS 2, SNS 2, ESS 1, **ILL 1/n**)
  - Instrument 2.0

MANTID May-December 2017

Cycles 2017-2 (1 Sep – 18 Oct) + 2017-3 (3 Nov – 21 Dec)

- Refine TOF & BS *(AS + GV)*
- Reflectivity: Deploy / test in D17 and Figaro *(VR → AS)*
- Powder diffraction: Deploy / test in D20 and D1B *(GV)*

- Scanning instruments: Loaders D2B, D4, D16, D7 *(IB)*
  - Workflow D4 (liquids & amorphous)
  - Workflow D7 (full polarization analysis)
  - Cases D16 (D4-like, SANS, REF)

- SANS: Loaders D11, D22, D33 *(?)*
  - SANS workflow
  - SANS interface
  - D33 case (5 detector panels, monochromatic + TOF mode)

Next spring meetings

Current status of corresponding technique and establish list of objectives for next technique meeting

Monday 30 January   Status backscattering (Gagik + Tilo)

Monday 6 February   Status TOF and discussion/plans for interface (Antti+ Bjorn)

Monday 13 February   Progress with reflectometry (Verena + Thomas S.)

Weeks 8/9[*]   Diffraction / scanning instruments (Ian, Gagik, Gabriel, Thomas H.)

Monday 6 March   Summary and preparation for PMC meeting

Monday 13 March   PMC meeting

Weeks 12/13/14/15   Cycle BS / TOF / REF/ DIF

[*] 20-21 Feb   Meeting at Copenhagen to discuss use of ASE for Task 10.4 in SINE2020-WP10
   20 Feb – 6 March   School holidays