**Focus of the mantid user meeting** <https://www.mantidproject.org/Category:Users_Workshop_2018>

1. To present on progress on the items raised at the 2017 Scientific steering committee
2. To capture and discuss the requirements of the scientific groups over the next 1-2 years.
3. To discuss planned strategic and technical developments, including Mantid 4.0
4. To share best practice and encourage collaboration.

**Suggestions:**

*General Plotting*

Interactive Graphic User Interface (GUI) for 1D profile, 2D slice and 3D volumetric data. This was suggested at the 2017 Scientific steering committee, but it has yet to be done.

*Single Crystal Diffraction*

A Graphic User Interface (GUI) for visualizing and indexing of both satellite and main Bragg peaks from single crystal neutron time-of-flight Laue diffraction. Implement algorithms that have been developed for data reduction of modulated structures (Collaboration between ORNL and ISIS by Shiyun Jin, Vickie Lynch and Xiaoping Wang @ORNL & by Sam Jackson and Pascal Manuel @ISIS)

**Appendix**

**Index and refine (3D+n) modulation wave factors from neutron single crystal data measured on TOF Laue instruments** (Shiyun Jin, Vickie Lynch and Xiaoping Wang)

1. **Index satellite and refine *q*-vector from find peaks**.

[Steps 1-4 can be done with existing mantid algorithms]

1. Search for strong peaks from the data set (mantid FindPeaksMD).
2. Find subcell based on the strong reflections.
3. Search for all peaks to include the weak reflections
4. Index all the peaks with fractional hkl (mantid IndexPeaks).
5. Group all the h, k, l into [n-0.5, n+0.5] brackets.
6. Caculate the distance for each h, k, l to the closest integer number (if a certain h lies in the bracket [n-0.5, n+0.5] where n is an interger number, ∆h=h-n)
7. Plot histogram of ∆h, ∆k, and ∆l respectively.
8. Inspect (visually or algorithmically) the histograms to see if there are any peaks other than the one at 0. If two peaks (or more) appears symmetrically around the zero peak, that means satellite reflections are observed.
9. Alternatively, plot a three dimensional histogram in space (∆h, ∆k, ∆l), (not for visualization), and look for peaks symmetrically appear around the center (0, 0, 0) peak
10. The position of the additional frequency peaks (δh, δk, δl) is the q-vector of the satellite reflection, (there are two options, choose the (δh, δk, δl) with least negative value)
11. If more than one pair of peaks appears in the three dimensional histogram, let user select q-vector manually, sort the options by descending frequency.
12. Sort all the found peaks into main reflections, satellites, and outliers. Let user enter threshold, or automatically choose standard (i.e. 2sig)
13. Let user manually select the maximum order of the satellites n, reindex all the reflections. Where main reflection (h,k,l) would be reindexed as (h,k,l,0) (round to intergers), and satellite reflections (h+δh, k+δk, l+δl) would be reindexed as (h,k,l,1) and (h-δh, k-δk, l-δl) as (h,k,l,-1). For all the outliers, test if the fall within the area of (h+iδh, k+iδk, l+iδl) i=-n,-n+1…n-1,n), if they do, index as (h,k,l,i) (h,k,l,i are integers)
14. Refine the q-vector using the sorted satellites
15. After integration, re-refine the q-vector with satellites weighed by their intensities.
16. **Predict satellites and integrate**
17. User input q-vector (δh, δk, δl) for satellites and maximum order n
18. For all the possible Bragg reflections within the range (h,k,l), generate satellite positions (h+δh, k+δk, l+δl), (h-δh, k-δk, l-δl), (h+2δh, k+2δk, l+2δl), (h-2δh, k-2δk, l-2δl)… (h+nδh, k+nδk, l+nδl), (h-nδh, k-nδk, l-nδl)
19. Integrate the satellite peak based on predicted positions (current integrateElipsoid should do the work, but it seems to round the q-vectors to only 0.01, may need to calculate the satellite position in q-space with the generated miller indices to predict accurate satellite positions)
20. For each satellite reflections, (h+mδh, k+mδk, l+mδl), generate new Miller Indices for satellite (h,k,l,m)
21. Refine the q-vector based on observed satellites during the integration if possible.