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Working document on time-of-flight data reduction within the Bastille project

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1. Gather run numbers for different Conditions: Sample (F), Empty (E), Vanadium (V), Empty- Vanadium (G), and possibly Cadmium (Cd).
   - Done: Loaders IN4, IN6.
   - IN5 should be OK. To check!
2. Read and add data files for each Condition.
   - Done: MergeRuns
   - Issues with background or noisy data resulting in a different elastic peak channel →Solved using a reference file in the call to Load.
   - XML file to select properties that must be consistent.

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3. Check consistency for added files.
   - To be done (refs. Stunault and Glyde). Caveat: Not automatic procedure. User intervention?
   - Will be a separate utility.
4. Extract integrated intensity and position of the peak in the monitor spectrum. The peak position is used on some instruments to calibrate the incoming energy. Various levels of sophistication exist to extract these quantities.
   - Done: NormalizeToMonitor. GetEiMonDet v2.
   - Shall we fit the peak in monitor to a Gaussian and subtract the background to get normalizing intensity?
   - Give integration range in call?
5. Extract integrated intensity and position of the elastic peak (if present) from the sample for each pixel i, j. In unambiguous cases, the sample position x, y can be extracted by a fit to the peak position of all pixels. In such cases, the sample-detector distance for each pixel can be determined. By comparing (normalized) intensities with some specified criteria, the detector mask could be updated.
   - Done: Loaders. Individual sample-detector distance for each pixel.
   - Not done: Refine sample position. Caveat: Need to define method how to do this. Unambiguous cases?
   - Not done: Automatic masking. How should be done? Dangerous?

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6. Determine the “flat” background away from the elastic peak for each pixel.
   - Done: CalculateFlatBackground
   - If Cd measurement given, use this as purely instrumental (sample-independent) background. OK?
7. Correct for frame overlap (if necessary). This is a difficult task in the general case, as frame overlap depends on the physics of the sample.
   - To be done: Method?
8. Determine the energy transfer for each pixel and time channel. It is important to keep channel information along the data reduction.
   - Done: ConvertUnits. Each detector pixel has its own energy axis.
   - Not done: *“There are various algorithms and approximations that can be used here. If the true/measured sample-pixel distance has been determined as outlined above, a more sophisticated algorithm can be used (see e.g. Ref. [3])”* Really need another method? [3] is a private communication of A. Stunault.
9. Calculate statistical counting errors (one) based on Poisson statistics.
   - Done.
   - Need to check error propagation?

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10. Correct data (and vanadium, and possibly empty can) for absorption or self-shielding, as a function of pixel and time (or energy transfer). Correction for standard sample geometries such as slabs (both transmission and reflection) and cylinders (including annular geometry) are required. Since some of these calculations are non-analytical and hence time consuming, interpolation procedures may be necessary. Computing time may be substantially reduced if the corrections can be saved for subsequent data sets.
    - Done: FlatPaalmanPingsCorrection and CylinderPaalmanPingsCorrection algorithms compute the needed corrections and ApplyPaalmanPingsCorrection apply them during the basic data reduction (step 12).
    - CylinderPaalmanPingsCorrection is very slow (python algorithm). Need to accelerate it (C++ or MC integration)
    - Develop algorithms for other more strange geometries? Some already exist in Mantid. Can be adapted to compute the correction factors in a similar way to the PaalmanPings algorithms and then apply them using again ApplyPaalmanPingsCorrection?
11. Normalize data to the beam monitor (this can also be done under point 4). In some cases normalization to measurement time (or something else) might be better.
    - Done. Default: Normalization to monitor, but possible to normalize to time.

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12. Perform the basic data reduction, i.e., (F − eE)/(V − gG).
    - Done: ApplyPaalmanPingsCorrection or Minus / Divide.
    - UI: Possibility to give sample info to compute PaalmanPings corr or simply transmissions for Minus/Divide
13. Correct for the detector efficiency, which is a function of the final energy. It is customary to use η(E)/η(E = 0), assuming that the width of the elastic peak is negligible for the vanadium run (this might not be true on D7?).
    - Done: DetectorEfficiencyCorUser . Equations implemented at present?
    - More accurate expressions? IN5?
    - Need to implement possibility of having 2 or more different formulas for an instrument.
14. Absolute normalization of data.
    - Done: Divide / Vanadium normalization?
    - More accurate expressions to calculate Debye-Waller factor for vanadium?
    - Absolute units: $S_{ij} = \frac{F_i I_{ij}^s}{I_i^{el}}$ with $I_i^{el} = \rho_N V_i^N \sigma_N \frac{1}{4\pi} S_N(k_i) \Delta\Omega_i$, $I_{ij}^s = \rho_s V_i^s S_{ij} \Delta\lambda_i \Delta\Omega_i$, $F_i = \frac{\rho_N V_i^N \sigma_N S_N(k_i)}{4\pi \rho_s V_i^s \Delta\lambda_i}$
      and $\Delta\lambda_i$ is the width of the time-of-flight channel on wavelength scale. Requires additional information about the normalization (vanadium?) sample. Ref. Verkerk and vanWell (1985).

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15. Convert the intensities from time of flight $I(\Omega_{ij}, t)$ to energy transfer $I(\Omega_{ij}, E)$. Note that in the general case, different detector pixels will not have a common energy array.
    - Done: Not specific conversion needed. Mantid can define a workspace as an histogram or a distribution.
    - Each pixel has its own energy array.
16. Optionally, the data $S(\Omega_{ij}, E)$ could be rebinned to equidistant (or smart [user-provided] non-equidistant energy bins E) so that all spectra have a common energy array.
    - Done: Using Regroup +
17. On some instruments, detectors with the same but different can be grouped together for powder samples (sumbank).
    - Not done. Needed? Bin to theta axis?
18. For powder samples, optionally transform $S(\Omega_{ij}, E)$ to S(Q,E).
    - Done: SofQWNormalisedPolygon. Better avoid using SofQWCentre and SofQWPolygon, as they may be faster, but are less precise (according to the documentation) and tests show strange results.
    - Not done: *"I note in this context an alternative method employed successfully in mslice, where $S(\Omega_{ij}, E)$ is not transformed to S(Q,E) but instead is plotted on a regular Q–E grid along curved detector trajectories."*

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19. For single crystals, transform $S(\Omega_{ij}, E)$ to $S(\mathbf{Q}, E)$. This requires knowledge of the sample orientation in the beam (described by the 3×3 UB matrix).
    - Not done: Vates / Horace.
20. Optionally, transform S(Q,E) to the imaginary part of the dynamic susceptibility ''(Q,E) or to the symmetrized (classical) $\hat{S}(Q,E)$, or simply check the detailed balance condition. Phonon density-of-states calculations and a few other special transformations [such as $S(Q,E) \cdot E/Q$] are also of interest.
    - Done: ComputeIncoherentDOS. Detailed balance: ApplyDetailedBalance, Symmetrise?
    - To do: Dynamic susceptibility, S(Q,E) x E/Q
21. Cuts are of great physical and diagnostics importance: $S_Q(E)$, $S_E(Q)$.
    - Done. Any need beyond standard Mantid plotting tools?
    - To do: Normalization of cuts. Standard/general method?
22. Multiple scattering corrections are outside the scope of this treatise.
    - Done? Need to check current work being done (mainly at ISIS?).

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23. Resolution calculations are also outside the scope of this treatise.
24. Smoothing should be avoided as much as possible, as it severely correlates neighboring data in an often uncontrolled way. Binning is in most cases a better alternative.
    - OK. Goes well with the philosophy applied.
25. Visualization of both 2D and 1D data using standard graphical interfaces (e.g. matlab) is an absolute requisite. Graphics should also be easily printed and saved in files that are as small as possible. It is worth the effort to push the fine-tuning of the visualization in the direction to produce figures that are essentially ready for publication.
    - OK. Need to worry about size of output graphic files?
    - Are Mantid graphics of publication quality?

- Output files: Define needed formats.
- Single crystal:
  - Same data treatment up to 18.
  - Transformation using UB matrix outside workflow (Vates / Horace)?
  - If so, data format for Horace? $I(\theta_i, \phi_i, E_j$ + sample rotation?)

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Three basic principles guide the data reduction described in this note:

(1) NEVER remove any pixels. Pixels that should not be retained for treatment should instead be listed in a mask file. Such a mask file could already be provided by the instrument, and updated during the treatment. ✓ But intensity of masked pixels set to 0!

(2) Introduce as little correlations as possible between pixels as late as possible. ✓

(3) The different routines that constitute the data reduction should be independent, well documented, and do just what they are supposed to do. *Reasonably the case?*

Efforts are also required in order to assure complete scripting of the data reduction, in order to reduce the influence of human errors on the result. Scripting is best done using simple ascii files that can be edited using any text editor (✓ python!), but graphical interfaces (that produces such ascii scripts) are probably also needed. Of equal importance is that the data reduction produces a log file that tells what was done and which parameters were used, to assure a complete record of the data reduction (✓ log?).

Requirements / desired UI?

Practical problems: Installation in instrument machine (admin permission?)

Data access (reading from rawdata / writing to processed) ✓

Interface Ideas

Global options

Hard detector mask:

Normalization: monitor

Incident energy calibration

IndexType: Detector ID

Monitor: 0

Detectors: 1-100

Reductions

Add row | Clone row | Erase row

ID	Type	Inputs	Cd	EC	Vana	EPPTable	MonEPPTable	FlatBkg	FlatBkg scale	FlatBkg window	Transmission	Binning in W
1	Vana	016821							0.9			
2	EC	92-017							0.9			
3	Sam	82-017		2	1	1	1		0.9		0.91	
4	Sam	34-018		2	1	1	1	3	0.95		0.88	-10,0.05,25

Process

Property editor

Cd	
EC	2
Vana	1
EPPTable	1
FlatBkg	3
FlatBkg scale	0.95
FlatBkg window	
Transmission	0.88
Binning in W	-10,0.05,25

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