Notes on isis\_powder routines (Sam Jenkins working on these). Points that require developers' effort highlighted in red.

HRPD:

* almost ready to start running with isis\_powder routines (hope to have time to start testing them in June - if not swamped with upgrade work).
* Initial flat plate/slab absorption correction problems seem to have been resolved; as has spline fitting of vanadium data

GEM:

* Has been using isis\_powder routines for over 1 year now (since Cycle 2017/2).
* A bug in the GEM-specific routines causing the sample absorption correction to fail has recently been fixed (Ron Smith/Sam Jenkins).

Polaris:

* Also has been using isis\_powder routines for over 1 year now (since Cycle 2017/2).
* **Total scattering work is progressing very slowly due to lack of developer effort** (this has been discussed between Helen Playford and Nick Draper)

PEARL:

* Still using own old Mantid routines. New Mantid routines to be tested when there is time.
* Would be good to get Bill Marshall’s Fortran code (for correction for beam attenuation through anvils) ported and modified to work within Mantid.
* Single crystal attenuation from single crystal diamond anvils is required for PEARL.
* Polycrystalline sintered diamond/tungsten carbide anvil attenuation for SXD instrument is required for use on PEARL (Fortran code exists).

Some thoughts about speeding up the isis\_powder routines...

1. When processing a series of files, the background is read and then subtracted from the vanadium each time. The process would be much faster when batch processing multiple runs if this subtraction was done for the first data set and then the "background-subtracted vanadium"stored for subsequent re-use with the other data sets.  
     
   Better still would be if the "background-subtracted-vanadium" was created during the pre-processing (spline smoothing) of the vanadium data set in the "create\_vanadium" method...  
     
   (comment: this current behaviour is probably how Aziz's old routines worked - and which the isis\_powder ones were written to replicate - but it would be good if this could be modified)
2. I believe the absorption correction will behave in a similar way. Could the possibility of the correction being calculated once and then stored in a workspace for re-use be investigated?

Next, a suggestion for improved functionality in batch processing a number of raw files. At present, a range of run numbers may be processed in two ways:

1. "Individual" mode treats each raw file separately and produces a .gsas, .nxs, and .dat files for every run number, or
2. "Summed" mode accumulates all the raw files into one data set and produces a single set of .gsas, .nxs and .dat files

Although it wouldn't take a lot of effort for users to wrap the data focusing procedure in one or more loops to achieve more elegant/complex summing of multiple data sets, it would be nice if something could be incorporated into isis\_powder. Some suggested examples:

* 60 data sets each of 1 minute duration grouped every 5 runs so that each data set had 5 minutes worth of counting statistics (in Aziz's old routines this could be achieved with a run number definition string such as "100001-100060-5").
* extend 1. so that the grouping progressed through the range (attention would need to be paid to what happens with the last few runs):  
  first process 100001-100005; 100006-100010; 100011-100015; ...  
  then process 100002-100006; 100007-100011; ...
* generate sets of grouped files that progressively increase the number of merged runs:  
  first process 100001-100002; 100003-100004; 100005-100006; ...  
  then process 100001-100003; 100004-10006; 100007-100009; ...

Finally - for **absorption corrections**, the isis\_powder routines use the absorption calculation built in to the **Mayers Multiple Scattering correction algorithm**: this is based on code used previously in Genie-2 (VMS) & OpenGenie (Windows) to normalise data on pre-2010 incarnations of Polaris. It was converted into a Mantid algorithm by Martyn Gigg, and as part of its Monte Carlo calculation for the multiple scattering incorporates a numerical integration absorption correction calculation. However, there is still a bug within the code which means that sample details have to be given as the chemical formula and the number density (rather than scattering and absorption cross sections) - actually, giving the formula is probably the easier option anyway...

Nevertheless, absorption correction in Aziz's routines was done using the CylinderAbsorption algorithm. If I understand from a previous report on absorption corrections, the CylinderAbsorption algorithm is faster. It would be good if the isis\_powder routines had this available, both for speed and in order to allow direct comparison between the newer isis\_powder routines and the old (Aziz) ones...

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