How to use Powder 4 to merge files….
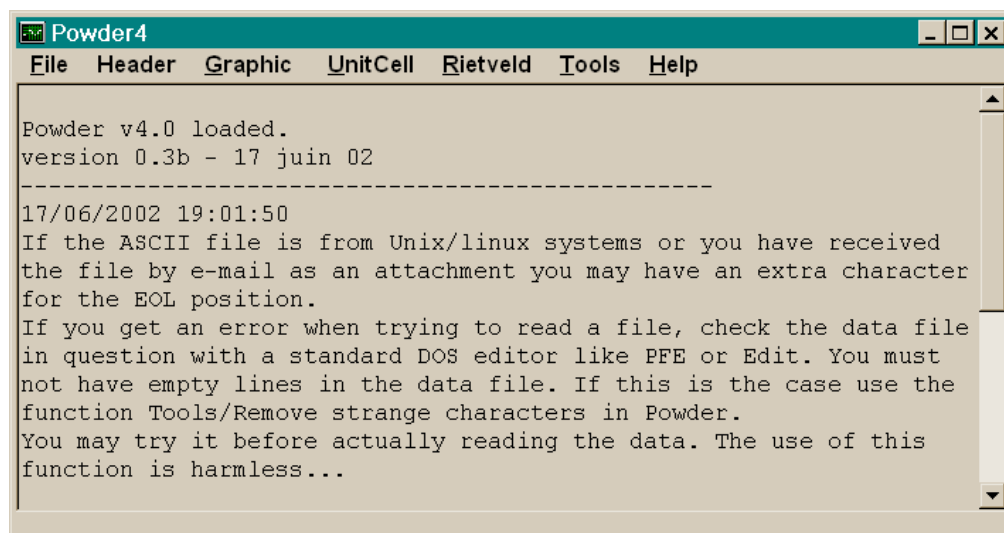

Here are few tips on how to use the latest Powder4 (i.e. version 0.3b) if you want to merge files. WARNING: this is a dangerous operation, do not massage your data; make sure you know what you are doing….

First open the program (which is downloadable from CCP14 web sites) and make sure you have the latest version. You should have a window something like this:


Few instructions are listed on this panel ; read this from time to time, it contains some useful hints on what's going on.

We are going to merge three files named d_per1.dat, d_per2.dat and d_per3.dat. These files are included in the distribution files (for training purposes; they are truncated version of one acquisition of some double perovskite).
All these three files have a title (one line of comments), so we'll have to "tell" the program how to handle this. First, we click on Header/I don't have a header (this is optionally here but in many cases it's important to instruct the software that there is no header to look for). Then we click on Header/Ignore menu, just like in the following picture:
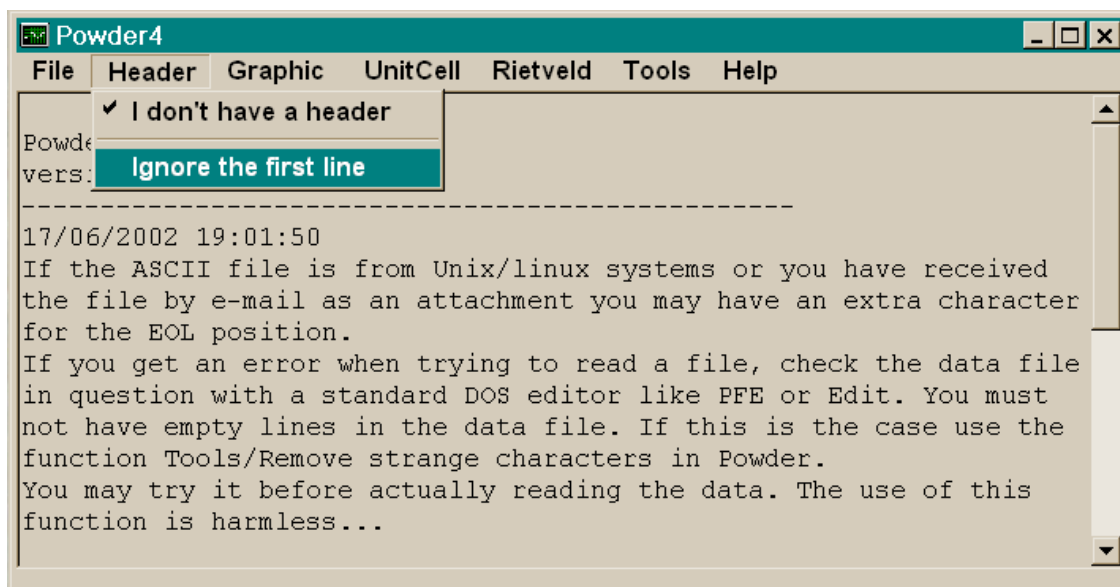
Now this is important : you have to instruct the program to ignore the first line otherwise you'll get a mess. Alternatively you can delete all the comments from the file but it's better to keep the original header in place…(do not mix up the files…!!!).
A small window will appear in which you insert (an integer) how many lines will be ignored.
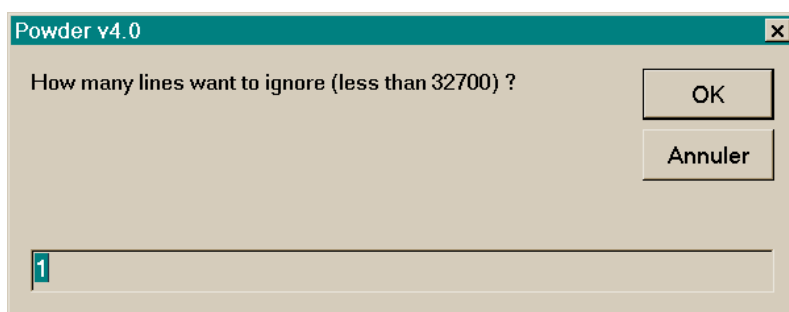

Cancel or 0 have the same effect.

After that you can see listed in the menu Header/Ignore how many lines are going to be ignored. By line I mean everything up to an EOL character.
You may imagine now that Merging files required all files to have the same format (the same number of comments, the same step, the same wavelength…). It is not necessary to have overlapping ranges, you may as well just add to files say one having data from 20 to 90 the other from 90 to 120….
There are two possibilities for merging files: either XY ascii files or XYZ ascii files. For the first case the ESD will be computed internally; then everything is the same.
Let's merge the three files : we choose File/Merge XY files then the following window will appear:
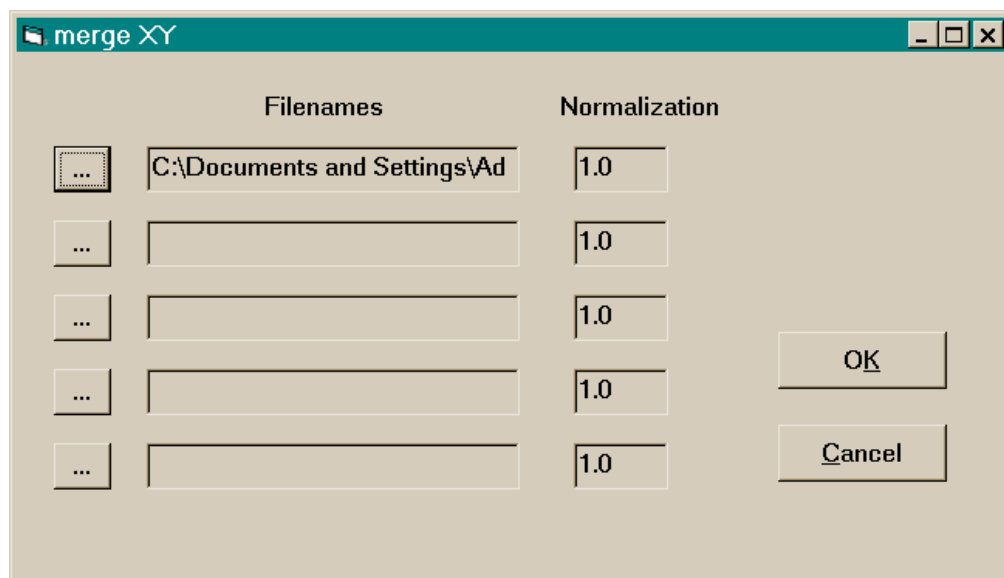
You need 2 to 5 files. By clicking on the small button on the left you can select the file location; it will then be listed adjacently. In the normalization field you need to insert a standard monitor count…Let s consider this case as having true CPS values…
After selecting the three files we choose OK and if everything is OK we get this message:
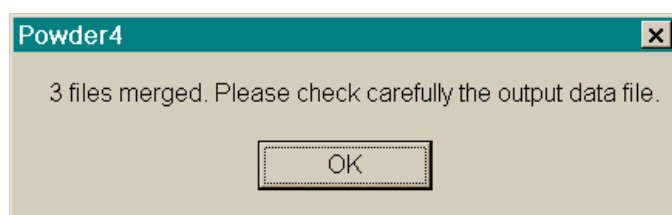

If we don t have this message then something is wrong : first look at the panel where all the errors are listed, then try to correct the problem (the most frequent error is an extra char for the EOF or empty lines..)

Let's see what was obtained. We can read the output files, directly the 3rd column. That will give us an ideea of the ESD values…In order to do this (after ignoring the 1st line) we select Open/Custom.
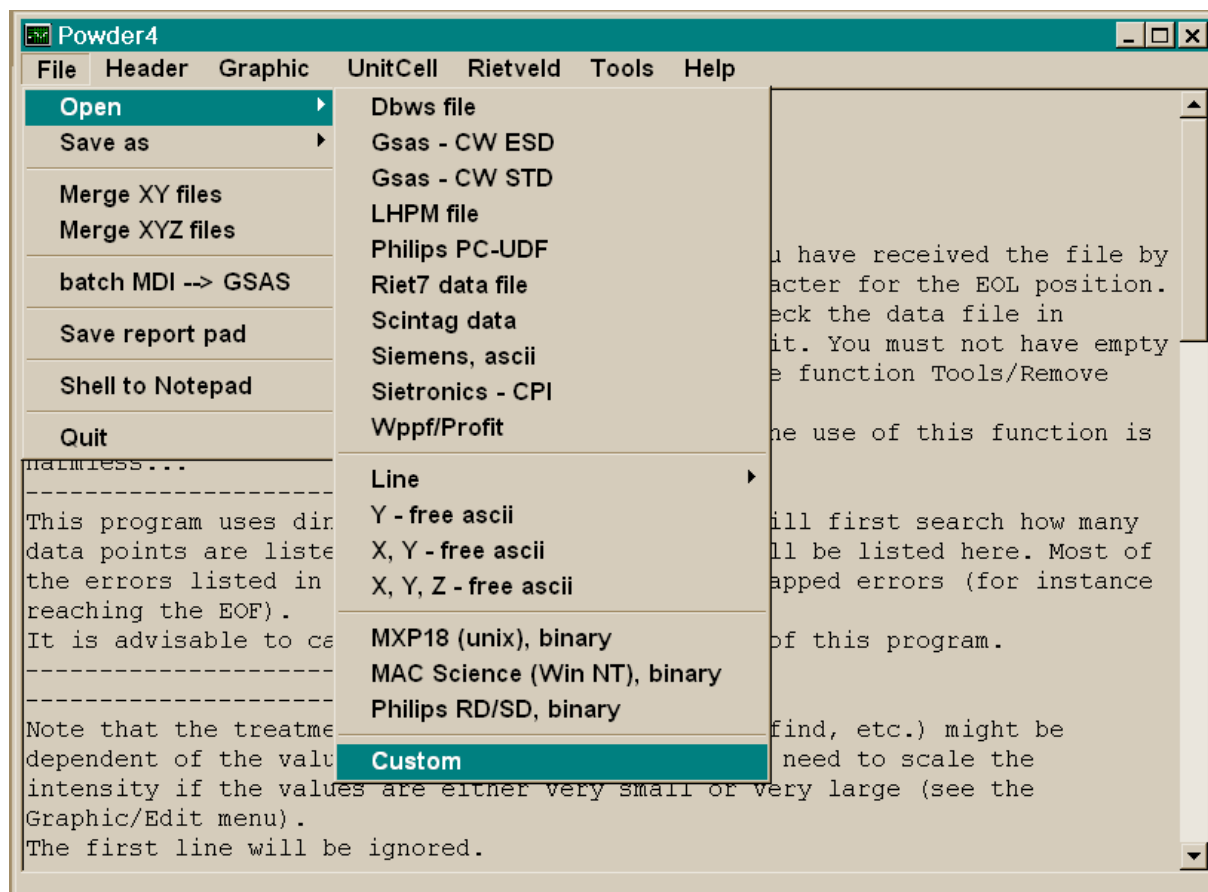
Then we have to select which column : in the X, Y, ESD output from the merging files one can select : read the 3rd value then ignore 2. This is equivalent to reading the 3rd column only.
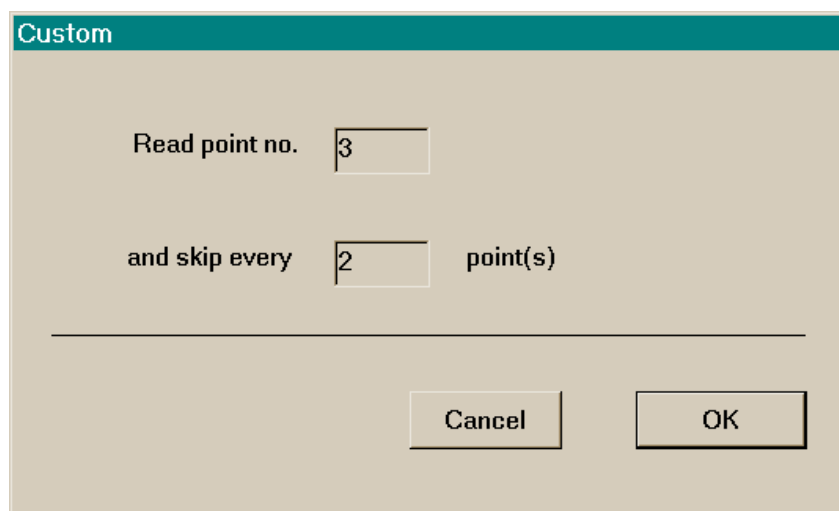

Then we can inspect the data graphically ; by selecting Graphics we get this indication :
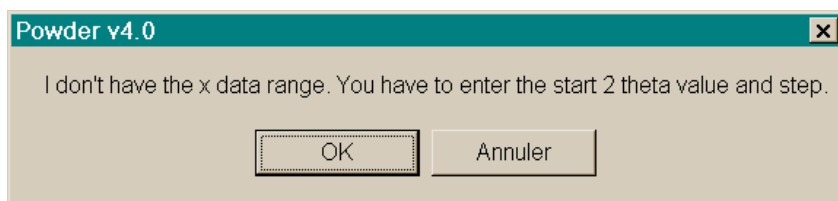
The program asks for X range since we read only one column (of Y). We insert 15 and 0.02 for step (the starting 2theta is 15, we can see this in the merge.dat file). 2 theta must be the same for all files to be mixed…

Then we get this image: note that this is the ESD function of 2theta (it is normal that looks like any diffractogram)…

Note the discontinuity at 35 and at 75: this is normal since the second file was from 35 to 119.96; the 3rd was from 75 to 119.96. The last point is at 119.98 (it has the "normal" ESD, it was not averaged)
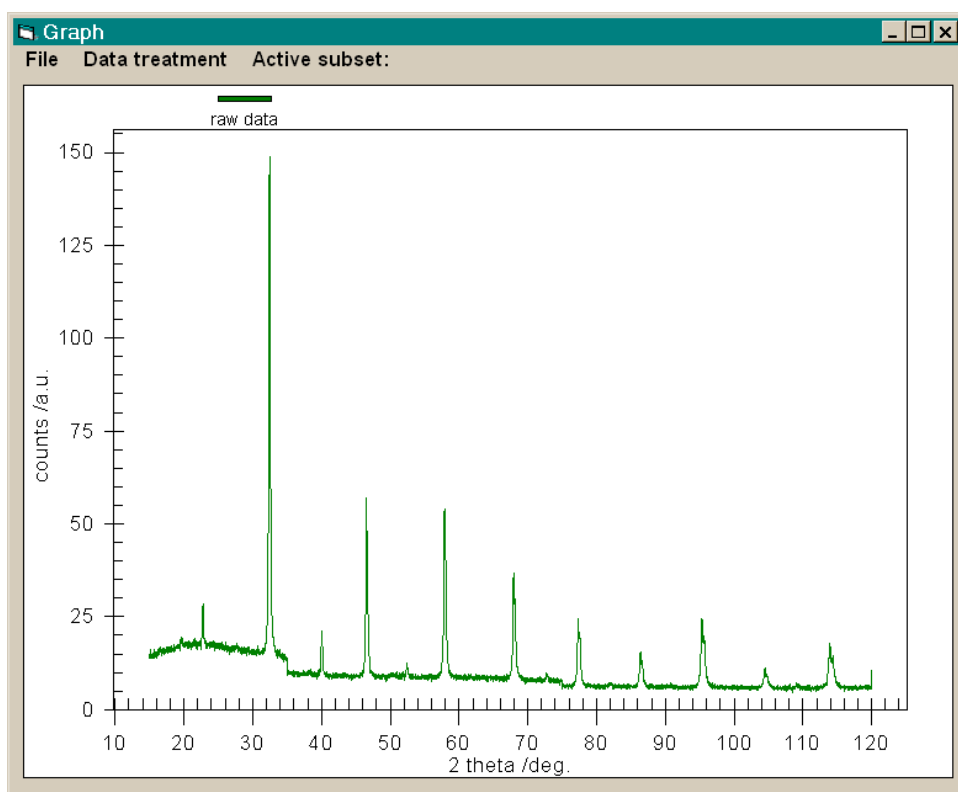
If we want to look at the output file we can open it as a column (2nd column) or as XYZ ascii file. Here is the output file.
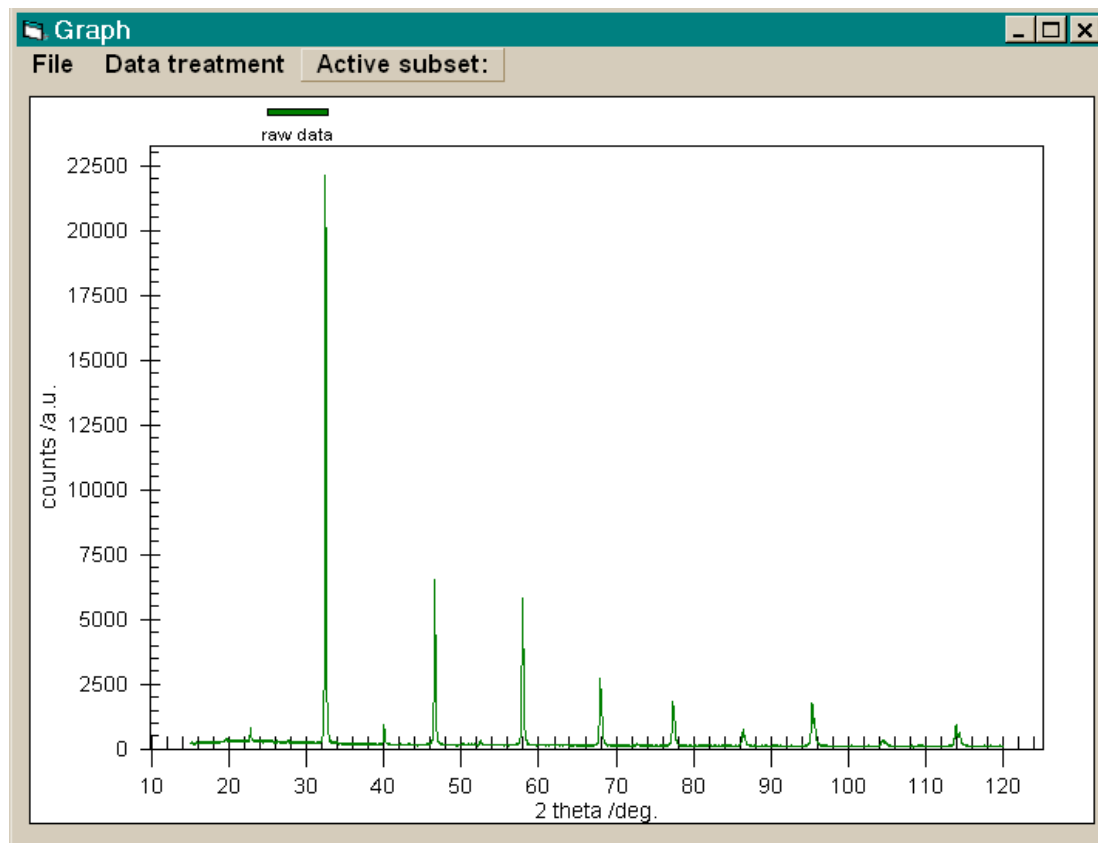
The Y are averaged (in this case there was nothing to average, they all have the same values..).
Anyway, normally you shouldn't see any steps in Y after merging files (probably that the
background noise will shrink little by little by averaging…but this is normal, there is no
massaging but just more info then better statistics). We can check that the background in this
case doesn't change:
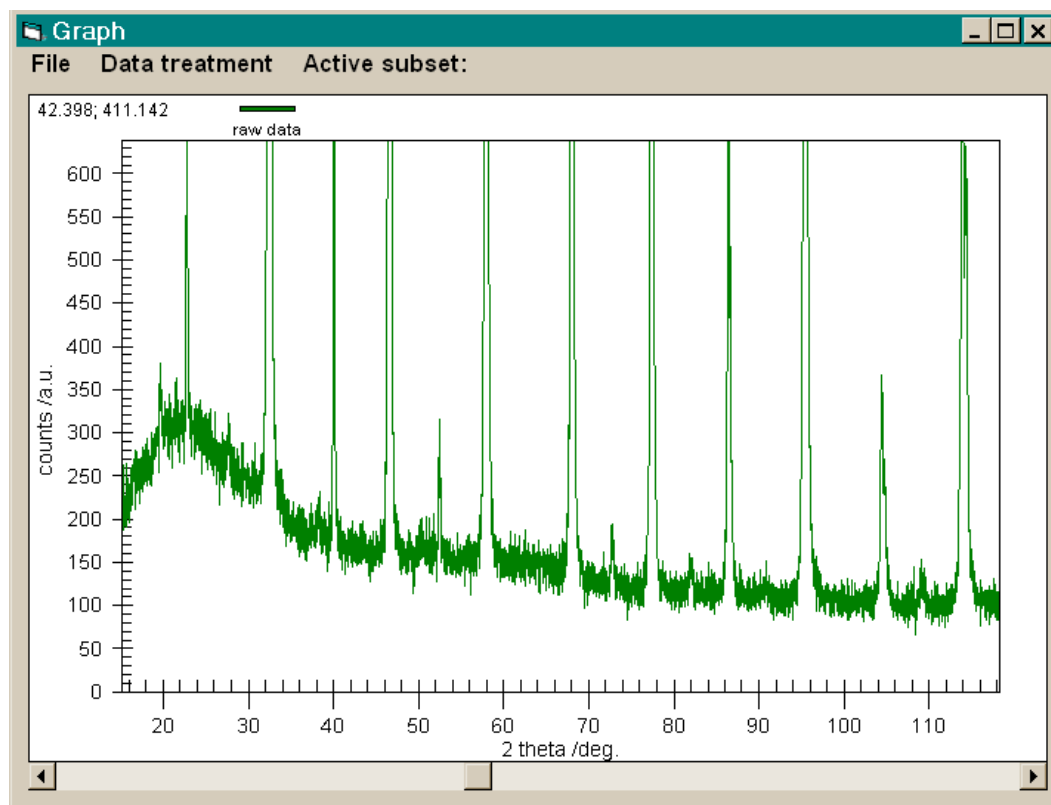
Concerning the algorithm, it is listed on the ccp14 pages as well:

http://www.ccp14.ac.uk/solution/summing_diffraction_files.html

Good luck !

PS Hope to get more input on how this is working..