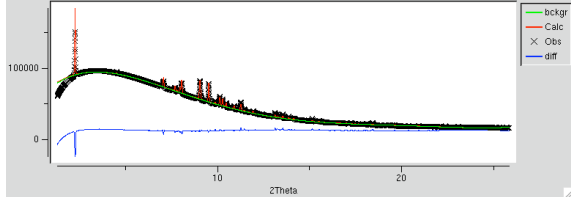


Problem 5: How to Fit Tough Backgrounds

- When backgrounds are large it can be hard to fit them without a good model and it can be hard to get a good model without a good background fit
- With Le Bail fits, background fitting can be unstable or even arbitrary
- Use of fixed points to define backgrounds is not a good idea (IMHO)
 - Good for initial stages, but can prevent final optimization
 - Prejudices results
 - Artificially turns off interaction between background & U_{iso} 's
- Solution: fit a function to fixed points and refine the function in the late stages of the fit (if possible)
 - Use routine BKGFIT

5.1 Example of problem

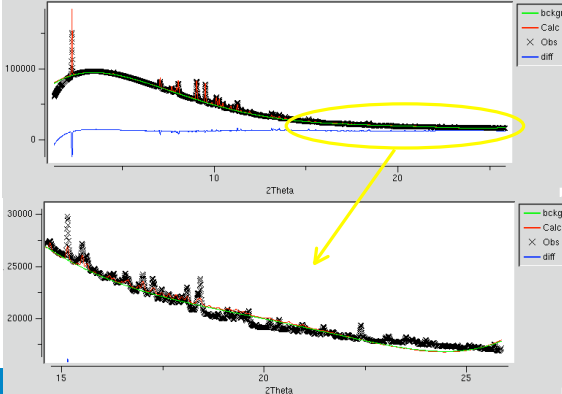
- Superficially: fit looks reasonable



5.2 Example of problem

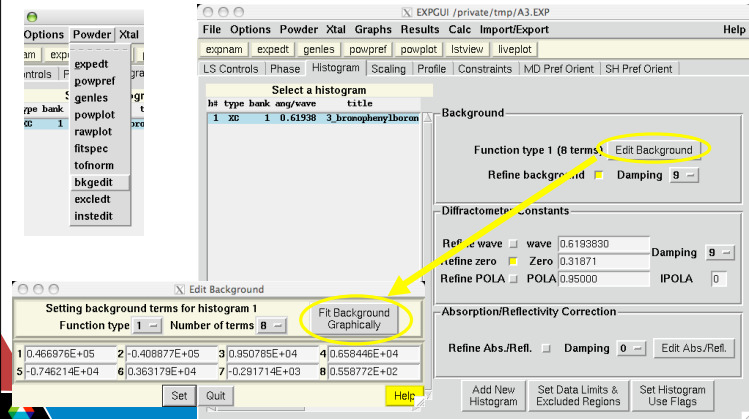
- Superficially: fit looks reasonable

In reality:
Fit is poor & not likely to improve without a better background.
Background is not likely to improve without a better model!



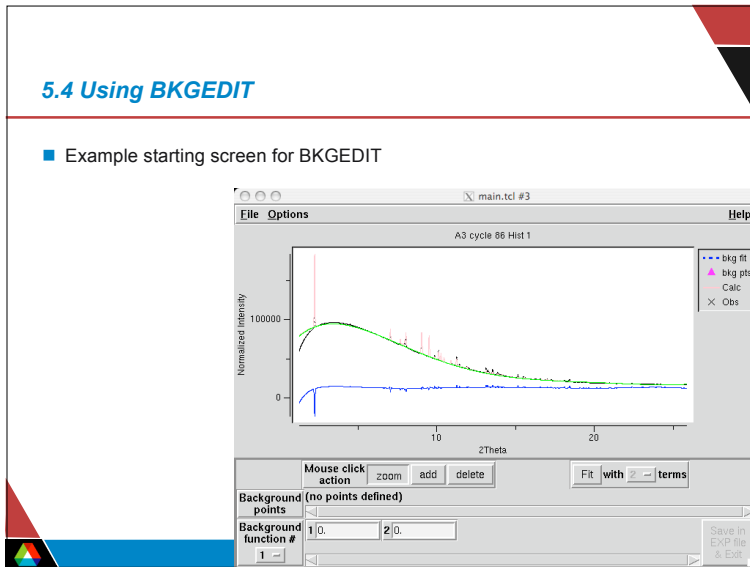
5.3 BKGEDIT to the rescue!

- Find BKGEDIT in the Powder menu or in "Edit Background" window



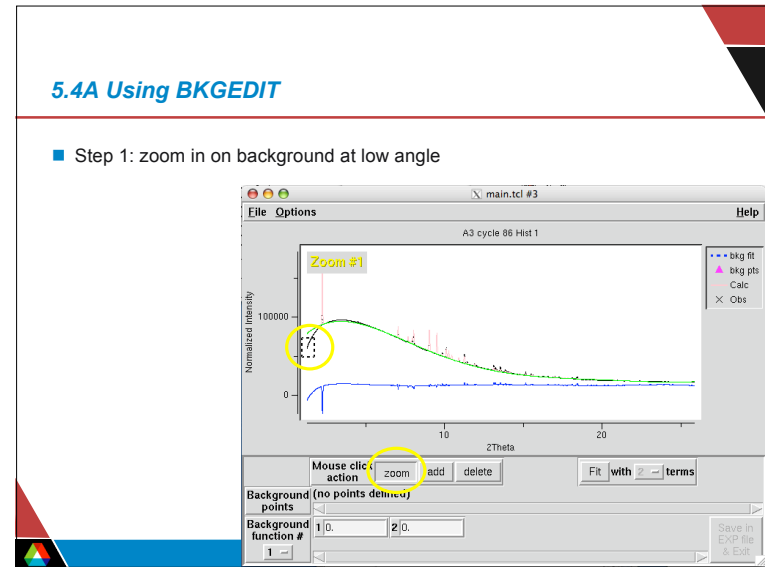
5.4 Using BKGEDIT

- Example starting screen for BKGEDIT



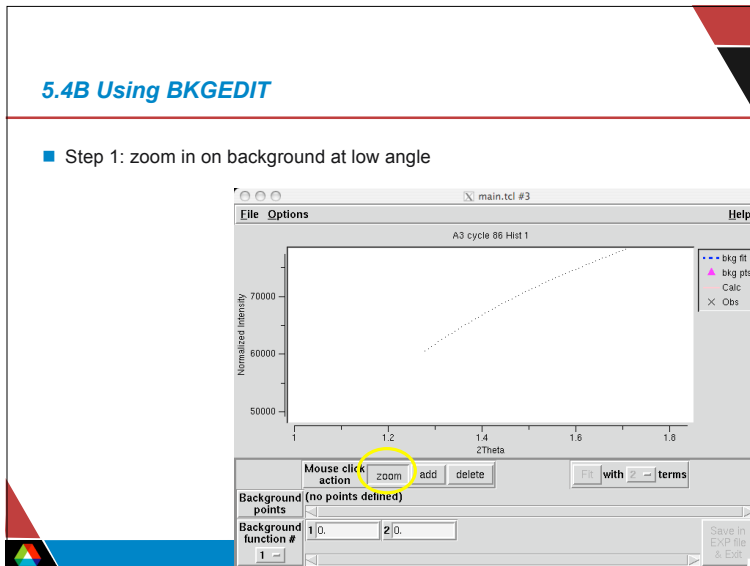
5.4A Using BKGEDIT

- Step 1: zoom in on background at low angle



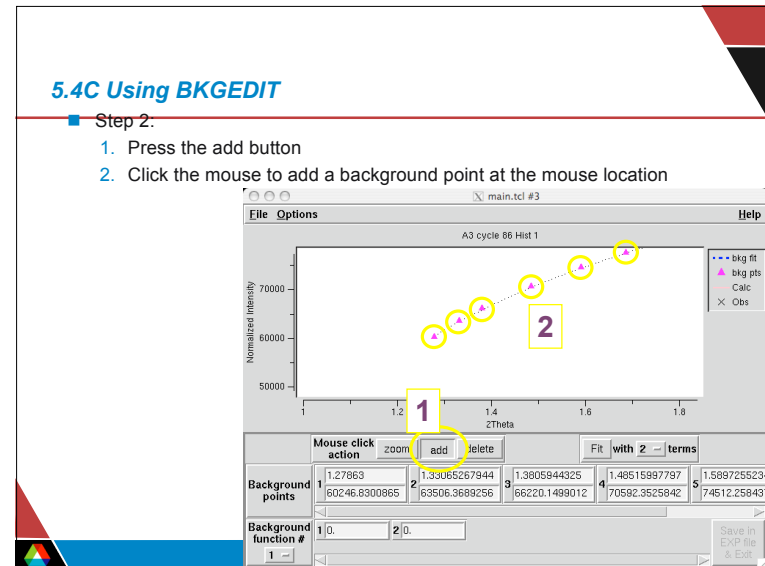
5.4B Using BKGEDIT

- Step 1: zoom in on background at low angle



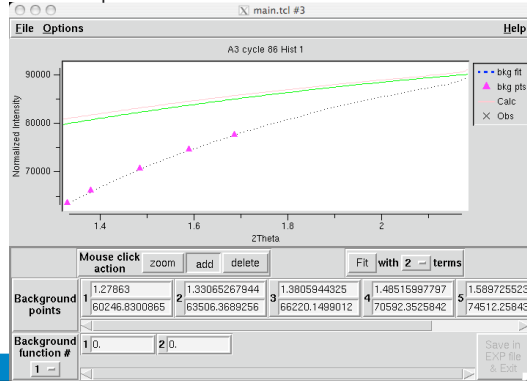
5.4C Using BKGEDIT

- Step 2:
 1. Press the add button
 2. Click the mouse to add a background point at the mouse location



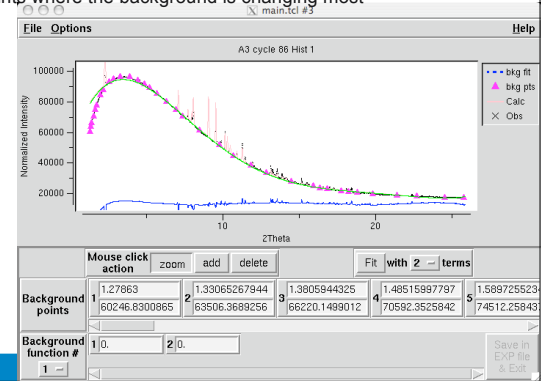
5.4D Using BKGEDIT

- Step 3: Use the up/down & right/left arrow keys to move follow the diffraction data and enter more points



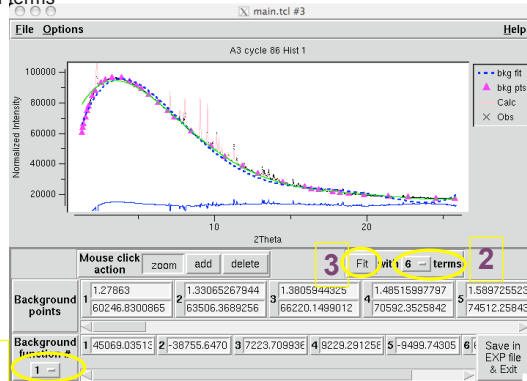
5.4E Using BKGEDIT

- Keep adding points across the entire pattern
 - Use lots of points where the background is changing most



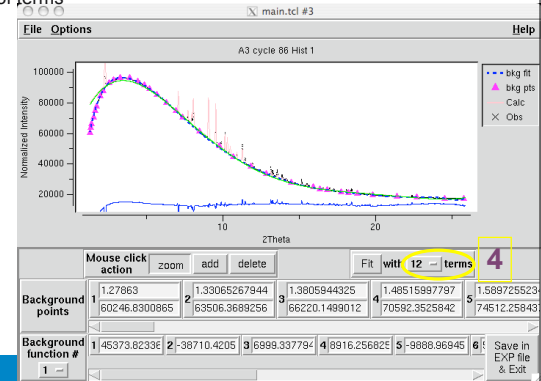
5.4F Using BKGEDIT

- Select a background function
- Select a number of terms
- Press fit



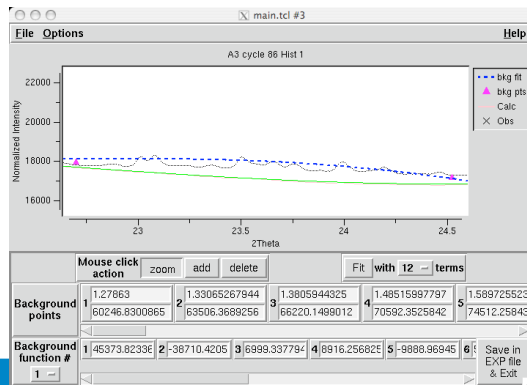
5.4G Using BKGEDIT

- Select a background function
- Select a number of terms
- Press fit
- Add terms until fit improves
- In some cases more background points are needed



5.4H Using BKGEDIT

- Zooming in is a good idea to check the quality of the fit



5.4I Using BKGEDIT

- Press Save in EXP file & Exit when you are satisfied
 - Background refine flag will be turned off; don't turn back on until fit is in good shape

It is possible to experiment with different functions (#1 usually works as well as any others)

Note: the fitted background need not be perfect, as you will refine the terms later.

