

10. Miscellaneous tips & "cute EXPGUI tricks/tools"

- Tip & "cute EXPGUI tool": use "print summary of shifts"
- Trick: "Change Profile Type" window shows profile defaults
- Trick: Detachable menus
- Tool: COMPOSITION utility
- Tool: EXCLEDT excluded region/data limits tool.

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10.1 Tip: always turn on "Print Summary of Shifts"

Why? Because it makes it easy to determine what parameters are "blowing up" in a refinement

- Below, note 1 5PF 3 (phase 1, histogram 5, profile term #3 has shifts that are getting larger each cycle -- not a good sign.

The screenshot shows the 'Print Options (256)' dialog box with several options checked, including 'Print summary shifted data after last cycle (256)'. Below it is a window titled 'View TB002ASYM1.LST' showing a table of refinement parameters.

Profile	Phase	Term	Value	StdDev	Weight
1	2PF	2	0.46	0.62	0.45
1	2PF	2	0.12	0.45	0.62
1	2PF	2	-0.54	-0.52	0.00
1	3PF	2	0.00	0.00	0.00
1	3PF	2	0.00	-0.01	0.00
1	3PF	3	0.00	0.70	0.00
1	4PF	3	0.65	0.87	0.66
1	5PF	3	-0.50	-1.10	-1.23
1	6PF	3	0.09	0.07	0.05
1	7PF	3	0.25	0.33	0.23
1	8PF	3	-0.44	-0.55	-0.44
1	9PF	3	-0.30	-0.31	-0.30
1	10PF	3	-0.09	-0.13	-0.10
1	11PF	3	0.00	0.00	0.00

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10.2 Tool: Working with Summary of Shifts Data in LSTVIEW

- LSTVIEW can jump to the summary of shifts at the end of each run
- LSTVIEW can plot shift/s.u. or R-factors vs. cycle

The screenshot shows the 'View TB' window with the 'Summary of Shifts' table and a 'plot' window showing a line graph of shifts vs. cycle. The 'Show Plot' button in the 'View TB' window is highlighted with a yellow circle, and an arrow points to the 'plot' window.

Shift	Final var	StdDev	Weight	
1	1U1S0	0.13	-0.07	-0.12
1	2U1S0	0.03	-0.05	-0.08
1	2X	-0.02	-0.02	-0.03
1	3U1S0	0.03	-0.03	0.04
1	4U1S0	-0.14	0.05	0.04
1	00000	1.10	1.10	0.74

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10.3 Trick: Detachable Menus Make Repetitive Menu Access Easy

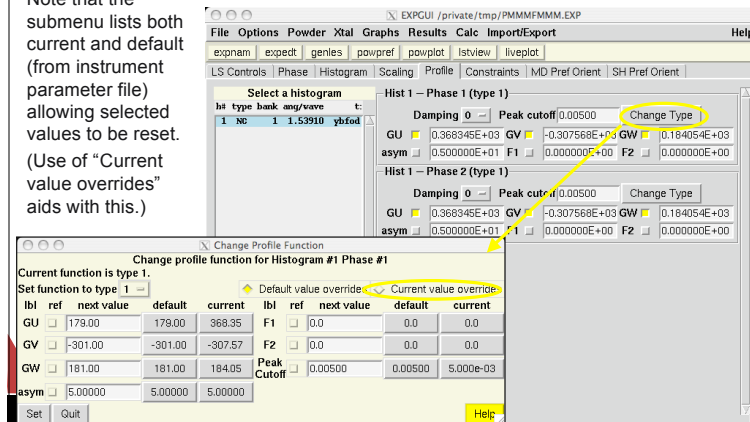
- Anywhere in EXPGUI where a menu contains a dashed line, clicking on that line creates a separate window providing the contents of that menu

The screenshot shows the 'Import/Export' menu with a dashed line under 'Coord Export'. A yellow circle highlights this dashed line, and an arrow points to a separate window titled 'Coord Export' which is a detachable sub-menu containing options like 'gsas2cif', 'coords-only CIF', etc.

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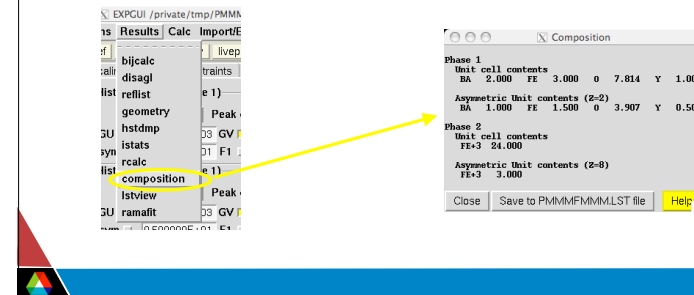
10.4 Trick: The Profile Panel's Change Profile Type Menu is Good For More Than Changing Profiles Types

Note that the submenu lists both current and default (from instrument parameter file) allowing selected values to be reset. (Use of "Current value overrides" aids with this.)



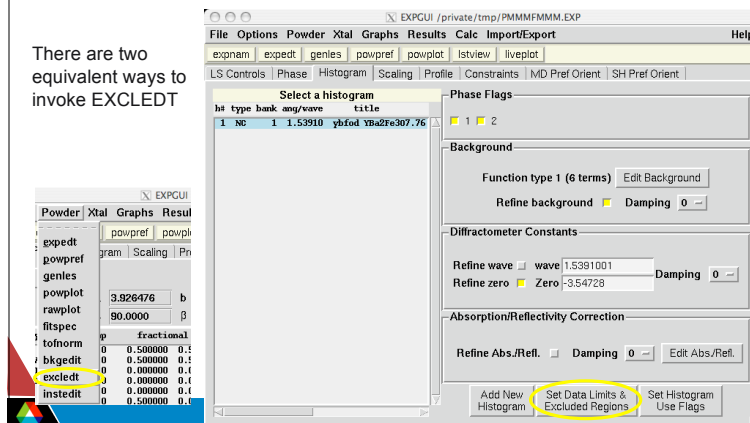
10.5 Tool: Compute Unit Cell Contents With COMPOSITION

- Computes the number of atoms in the unit cell & asymmetric unit (Z determination is a bit weird)
 - Assumes listed multiplicities are correct (if coordinates are edited in phase panel, use "Reset Multiplicities" in "Xform Atoms" window)



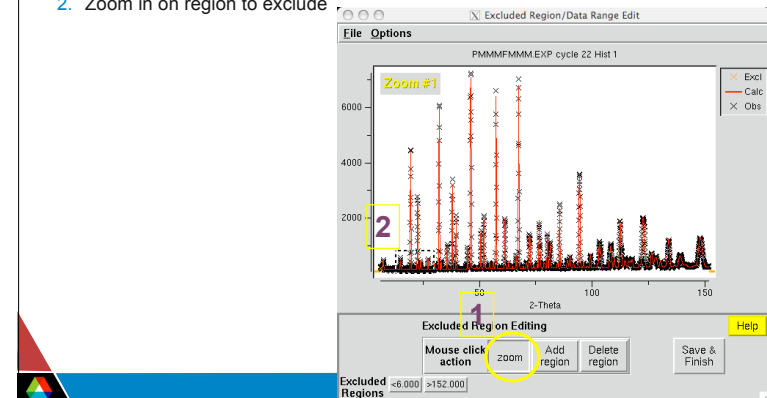
10.6A Tool: Change Data Set Range & Set Excluded Regions With EXCLEDT

There are two equivalent ways to invoke EXCLEDT



10.6B Using EXCLEDT to Add an Excluded Region

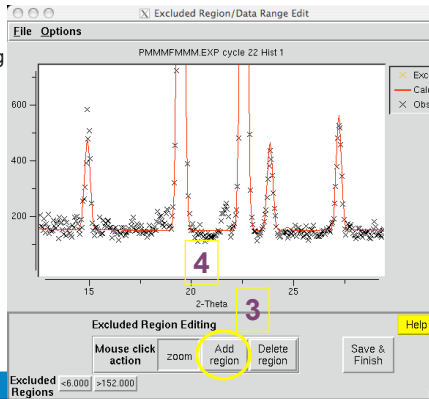
- Set mode to "zoom"
- Zoom in on region to exclude



10.6C Using EXCLEDT to Add an Excluded Region

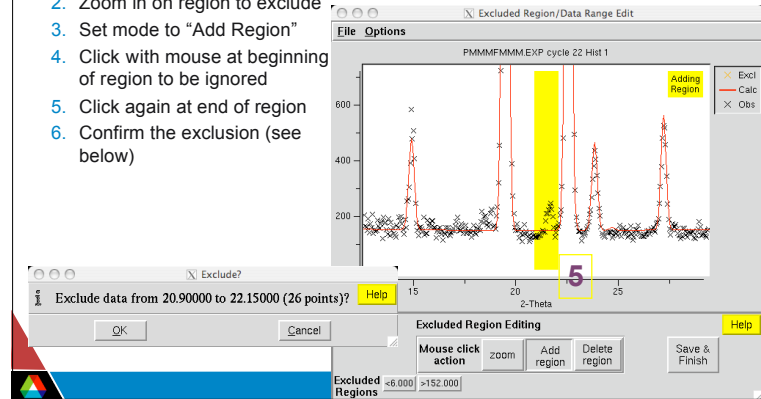
1. Set mode to "zoom"
2. Zoom in on region to exclude
3. Set mode to "Add Region"
4. Click with mouse at beginning of region to be ignored

Note that arrow keys can be used to move zoom region around



10.6D Using EXCLEDT to Add an Excluded Region

1. Set mode to "zoom"
2. Zoom in on region to exclude
3. Set mode to "Add Region"
4. Click with mouse at beginning of region to be ignored
5. Click again at end of region
6. Confirm the exclusion (see below)

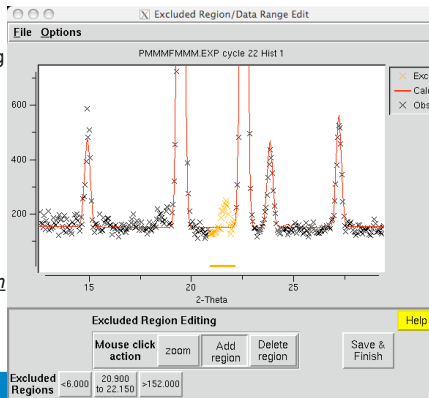


10.6E Using EXCLEDT to Add an Excluded Region

1. Set mode to "zoom"
2. Zoom in on region to exclude
3. Set mode to "Add Region"
4. Click with mouse at beginning of region to be ignored
5. Click again at end of region
6. Confirm the exclusion (see below)

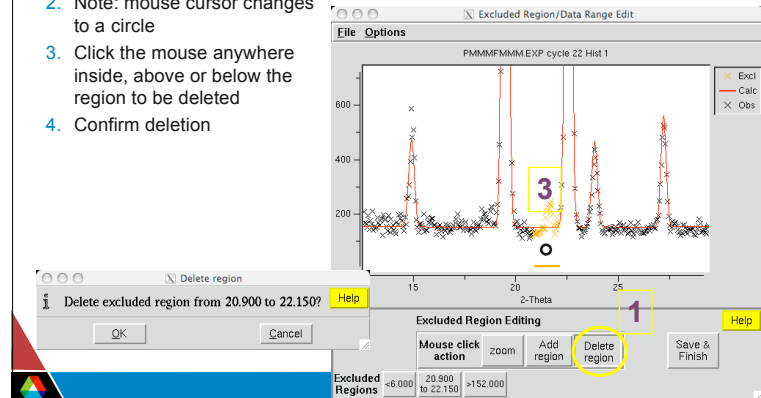
Note change in appearance of excluded points and addition of orange line

You should not attempt to publish a result unless you understand why a region is being excluded



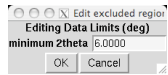
10.6F Using EXCLEDT to Delete an Excluded Region

1. Set mode to "Delete Region"
2. Note: mouse cursor changes to a circle
3. Click the mouse anywhere inside, above or below the region to be deleted
4. Confirm deletion



10.6G Using EXCLEDT to change data range

- To change upper or lower data limits, click on boxes at lower line. (Can do the same with excluded regions). Edit window will open, as below.



POWPREF must be run after changes to the data limits and excluded regions. EXPGUI will "encourage" you to do this.

