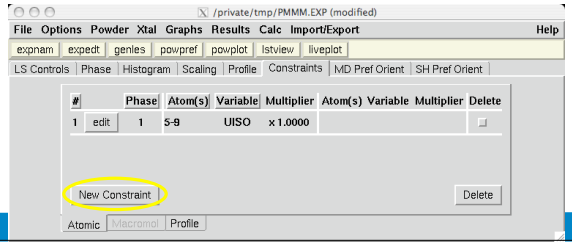
Problem 9: How Do I Constrain Atoms?

- Note that GSAS allows parameters to be grouped using constraints. This reduces the number of refined parameters since all the constrained parameters are now a single variable.
- This is done by specifying a ratio to be applied to the shifts for each of the grouped parameters
  - Note that constraints only apply to the shifts on parameters, not on their values
- Constraints are different from restraints (a.k.a. soft constraints), which apply a penalty function to the refinement to keep parameters in bounds.
- EXPGUI has some options useful for setting up commonly-needed atom constraints
- *Note that a parameter may not appear in more than one constraint equation -- EXPGUI will warn if you try to do this.*

9.1A Example: Constrain Two Atoms Sharing a Site So the Sum of Their Occupancies Stays Constant

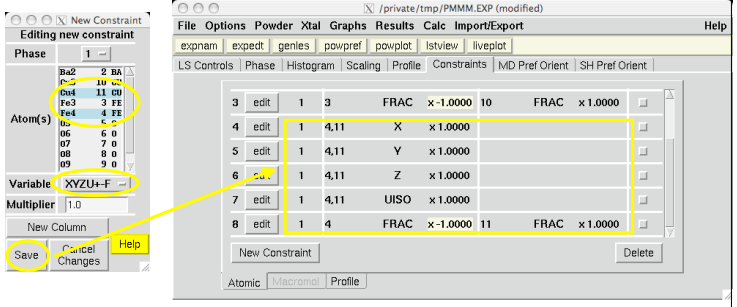
	name	type*	ref/damp			fractional coordinates			Mult	Occupancy	Uiso
2	Ba2	BA	XO	UO	0	0.500000	0.500000	0.173345	2	1.0000	0.01185
10	Cu3	CU	XO	UO	0	0.000000	0.000000	0.000000	1	0.5000	0.01000
11	Cu4	CU	XO	UO	0	0.000000	0.000000	0.339000	2	0.5000	0.01000
3	Fe3	FE	XO	UO	0	0.000000	0.000000	0.000000	1	0.5000	0.01000
4	Fe4	FE	XO	UO	0	0.000000	0.000000	0.339000	2	0.5000	0.01000

- Cu4 & Fe4 share a site (same for Cu3 & Fe3)
  - Need to constrain shifts on z, Uiso & to be the same, shifts on Frac to be opposite.



9.1B Example: Constrain Two Atoms Sharing a Site So the Sum of Their Occupancies Stays Constant

- Constraint can be set up in a single step in EXPGUI
  - Note constraints on x & y are not needed, but cause no problems.



9.2 Other ways to group parameters

- XYZU constrains the selected atoms to translate as a group (use a rigid body where group rotation is needed) and share the same shifts on Uiso.
- Uxx constrains the shifts to be the same on anisotropic displacement parameters