Problem 4: How to Use GSAS for Quick Simulations: Test Your Idea Before Doing the Experiment!

- GSAS is a great tool for simulating diffraction patterns. An experimentally rigorous pattern can be generated in a minute or two.
- CMPR, etc. can be used to compare results from different possible models

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4.1 Steps to simulate a diffraction pattern

- Prerequisites
  - a prototype instrument parameter file
  - Coordinates, preferably in electronic form
    - *For example, a CIF (supplementary materials or database export)*
- Steps:
  - Create new GSAS experiment

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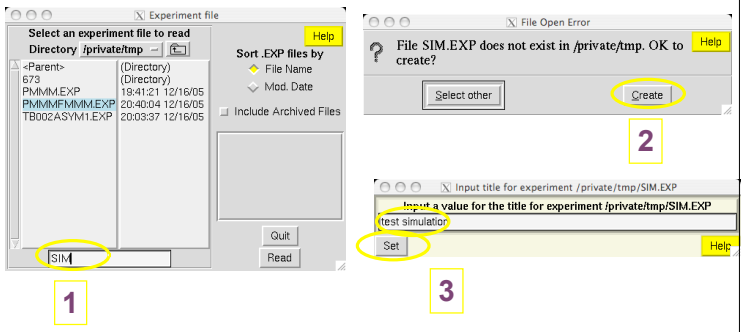
4.1 Create new GSAS experiment



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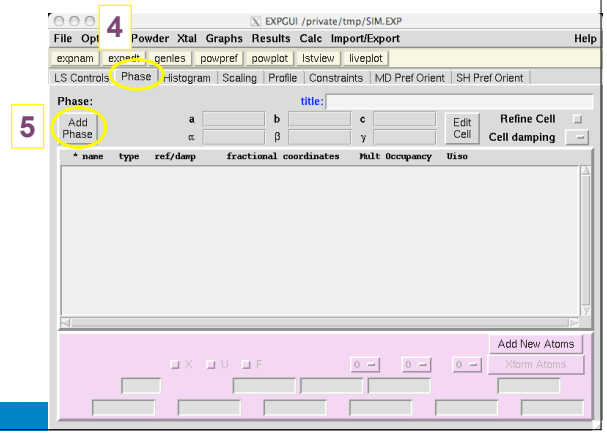
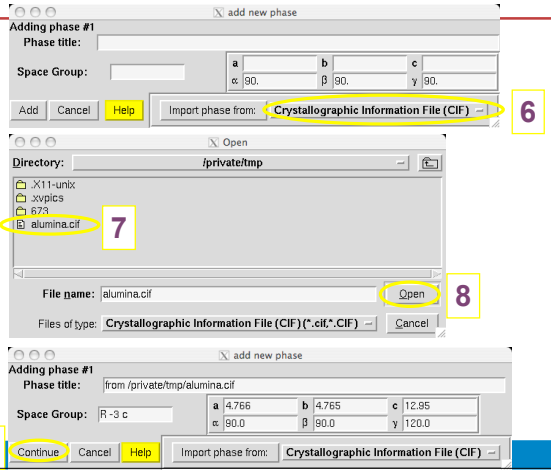
4.2A Add Phase

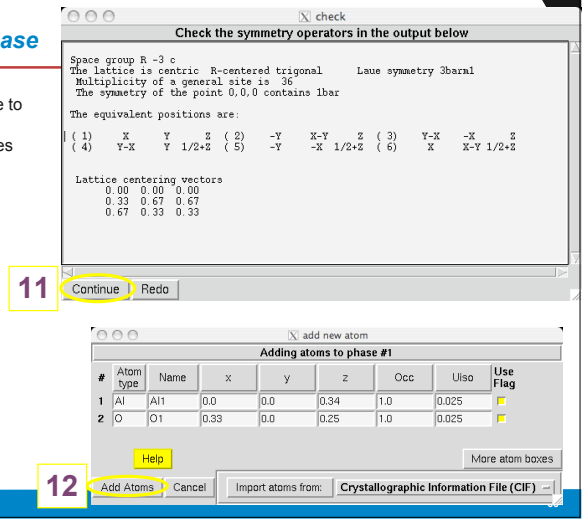


4.2B Add Phase

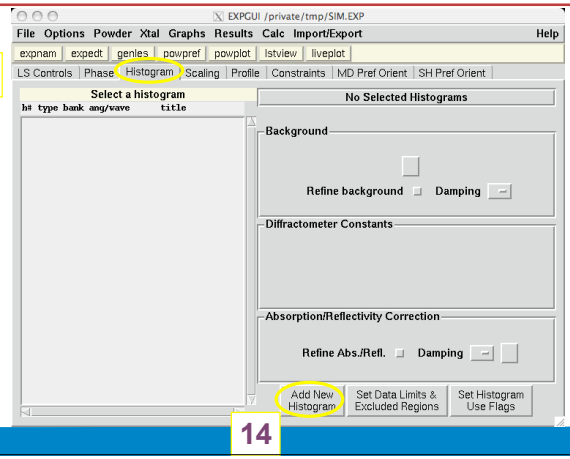


4.2C Add Phase

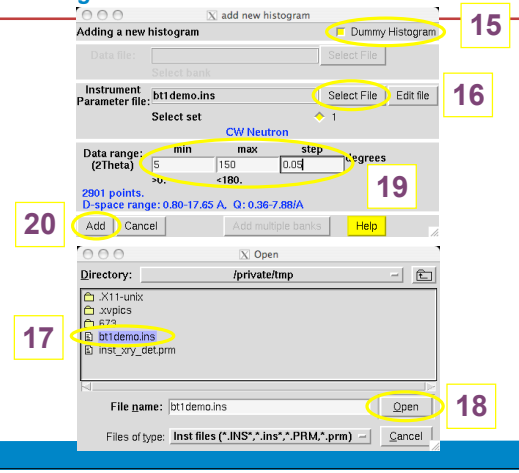
10 Spend a minute to make sure the symmetry makes sense



4.3A Add Histogram



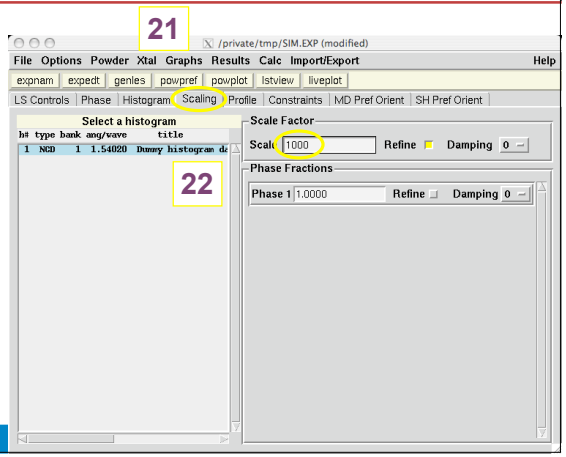
4.3B Add Histogram



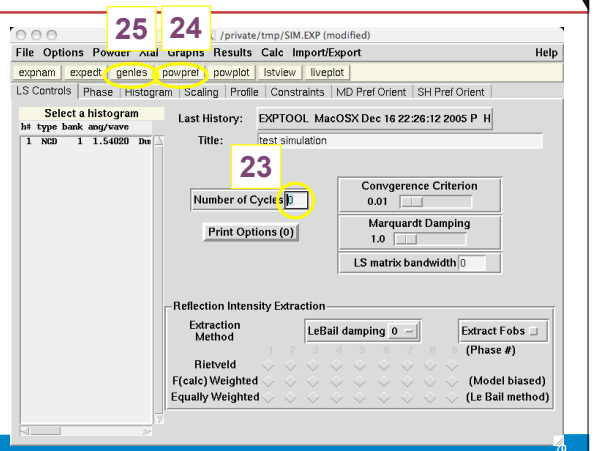
4.4 Change Scale Factor to Reasonable Value (optional)

Why?

GSAS adds simulated noise to simulated "experimental" pattern. Noise is not very realistic when intensity scale ranges from 0 to 0.1 counts



4.5 Change cycles to zero; run POWPREF & GENLES



4.6 Pattern Simulation: Summary of actions

- Push buttons: 19 times.
- Type 31 characters in 7 boxes.
- Think -- once.
- ***Provides a realistic simulation of an instrumental result***