

**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

61

**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

62

**4.1 Create new GSAS experiment**

The image shows three sequential screenshots illustrating the process of creating a new GSAS experiment:

- Step 1:** A file selection dialog titled "Experiment file" showing a list of files in the directory "/private/tmp". The file "SIM" is selected and circled in yellow.
- Step 2:** A "File Open Error" dialog box with the message "File SIM.EXP does not exist in /private/tmp. OK to create?". The "Create" button is circled in yellow.
- Step 3:** An "Input title for experiment /private/tmp/SIM.EXP" dialog box. The text "test simulation" is entered in the input field, and the "Set" button is circled in yellow.

63

**4.2A Add Phase**

The image shows the EXPGUI interface with the "Add Phase" dialog box open. The "Powder Xtal" menu option is circled in yellow and labeled with a "4". The "Add Phase" button in the dialog is circled in yellow and labeled with a "5". The dialog contains fields for phase name, type, ref/damp, fractional coordinates (a, b, c, alpha, beta, gamma), and unit cell parameters.

### 4.2B Add Phase

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### 4.2C Add Phase

10 Spend a minute to make sure the symmetry makes sense

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Check the symmetry operators in the output below

Space group R -3 c
The lattice is centric R-centered trigonal Laue symmetry 3bar1
Multiplicity of a general site is 36
The symmetry of the point 0,0,0 contains 1bar

The equivalent positions are:
( 1)  X  Y  Z ( 2)  -Y  X-Y  Z ( 3)  Y-X  -X  Z
( 4)  Y-X  Y  1/2+Z ( 5)  -Y  -X  1/2+Z ( 6)  X  X-Y  1/2+Z

Lattice centering vectors
0.00  0.00  0.00
0.33  0.67  0.67
0.67  0.33  0.33
    
```

11 Continue Redo

#	Atom type	Name	x	y	z	Occ	Uiso	Use Flag
1	Al	Al1	0.0	0.0	0.34	1.0	0.025	<input type="checkbox"/>
2	O	O1	0.33	0.0	0.25	1.0	0.025	<input type="checkbox"/>

12 Add Atoms Cancel Import atoms from: Crystallographic Information File (CIF)

### 4.3A Add Histogram

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### 4.3B Add Histogram

15 Dummy Histogram

16 Select File Edit file

19 Data range: min max step degrees  
 (2Theta) 5 150 0.05  
 20 2901 points, D-space range: 0.80-17.65 Å, Q: 0.36-7.88/Å

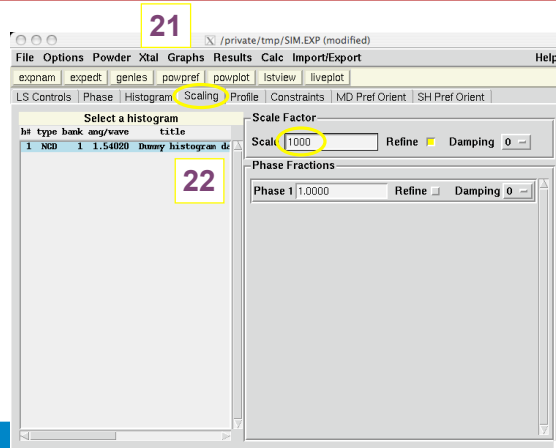
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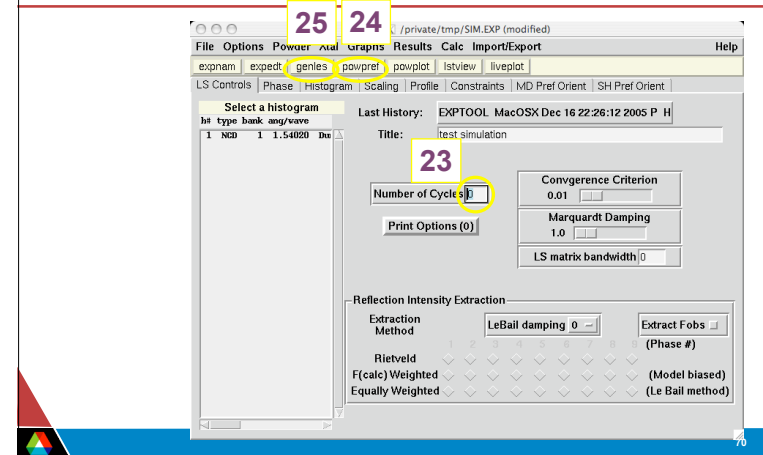
#### 4.4 Change Scale Factor to Reasonable Value (optional)

##### 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

