

## **PROGRESS WITH THE GSAS-II SOFTWARE PACKAGE FOR CRYSTALLOGRAPHY**

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GSAS has been a major success story in crystallographic analysis. It was started as an analysis package for single crystal and powder diffraction data from the Los Alamos spallation source, but soon expanded to use both laboratory and synchrotron powder diffraction data. GSAS is unique in that it can be used to analyze all types of diffraction data: powder and single crystal, neutron or x-ray, constant wavelength or energy dispersive (EDX or TOF) and can be used to fit models ranging from simple inorganics to proteins. GSAS was originally developed for VAX computers, but now runs on all common computing platforms. The EXPGUI package was developed to provide a graphical user interface for some of the features in GSAS and has eased distribution of the software by providing easy-to-install packages as well as making the software more novice-friendly. The impact of these programs has been huge: GSAS has been cited at over 5,000 times and EXPGUI has been cited nearly an additional 1,000 times.

The age of GSAS shows under the hood. While the software was developed with modular programming concepts that had yet to become popularized, it is still a set of monolithic Fortran programs where code is difficult to reuse and where extension is complex to perform. While the EXPGUI program is extensible, it offers access to only a small fraction of the total capabilities of GSAS.

To develop a new versatile and comprehensive crystallographic package, the authors have started a new project, called GSAS-II. This will eventually incorporate all the capabilities of GSAS, but will have the top-level code developed in Python, while speed-sensitive computations will be performed in packages such as SciPy or Fortran routines. This will allow expert users to adapt and add new functionality to GSAS-II in a way that is not possible with compiled software. Central to the development of GSAS-II is graphical interaction with the user, both through GUI controls and extensive plotting capabilities.

This talk will discuss some of the development work that is in progress on GSAS-II. This includes new strategies for code distribution that have been implemented in GSAS & EXPGUI, as well as the development of capabilities not available in GSAS: data reduction, peak fitting, and pattern indexing. Structure solution tools are also anticipated soon.