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GSAS

GENERAL STRUCTURE ANALYSIS SYSTEM

Allen C. Larson & Robert B. Von Dreele
LANSCE, MS-H805
Los Alamos National Laboratory
Los Alamos, NM 87545

GSAS Introduction

Welcome to the General Structure Analysis System (**GSAS**). **GSAS** is a set of programs for the processing and analysis of both single crystal and powder diffraction data obtained with x-rays or neutrons. It is capable of handling all of these types of data simultaneously for a given structural problem. In addition, it can handle powder diffraction data from a mixture of phases refining structural parameters for each phase. **GSAS** is designed to be easy to use and features a menu driven editor (**EXPEDT**) equipped with help listings and error trapping features. **EXPEDT** is used to prepare all input for the main calculation programs in **GSAS**. The entire **GSAS** system is written in FORTRAN and uses some system callable features. The current distributions of **GSAS** are available for both VMS and UNIX operating systems (VAX/VMS, Alpha/OpenVMS, Silicon Graphics Irix, DecStation Ultrix and Hewlett-Packard UX). An integral part of **GSAS** is the facility for interactive graphics display which is based on the Common Graphics System (CGS) of Los Alamos National Laboratory. **GSAS** supports many standard graphics terminals including X-windows work stations as well as Tektronix type terminals and DEC ReGIS terminals. It also supports various hard copy graphics devices (PostScript printers, DEC LA50 dot matrix printer, DEC laser printers, Hewlett-Packard printers and plotters, and CGS metafiles). This manual consists of three sections; this introduction, a training manual and a technical manual.

GSAS Installation

In this section we give the instructions for obtaining and installing a **GSAS** distribution kit for the DEC Alpha/OpenVMS and Silicon Graphics Irix (UNIX) operating systems from an anonymous ftp account at Los Alamos. Other distribution kits are available from the same source; detailed instructions are available in a file "readme.1st" located in the home directory of the anonymous ftp account. This manual is also available from this source in formats suitable for printing from both VMS and UNIX platforms on Postscript printers.

An Anonymous FTP Server for **GSAS** on DEC Alpha/OpenVMS Codes

The **GSAS** distribution kit for DEC Alpha/OpenVMS contains two large files which are kept in a compressed form that is approximately 50% smaller than the original. Also stored in this directory are the executable forms of the programs for compression and decompression of any file. These files need to be transferred in binary format. There are also two smaller command files and a document file describing the compression routines along with this "readme" file. These latter files are transferred in ASCII format.

GSAS Installation from ftp files:

System Requirements: Alpha/OpenVMS Version 1.5 or later,
SYS$LIBRARY:DECW$XLIBSHR must be an installed image.

To ensure that the file structure and command files for **GSAS** are set up appropriately on your Alpha, we have provided an installation procedure and a command file. These instructions cover both the initial installation of **GSAS** on an Alpha as well as the replacement of an old version of the system. If there is an existing **GSAS** to be replaced the first step is omitted and the entire directory structure for **GSAS** will be replaced. Thus it is not advisable to use any of the **GSAS** directories for any other files. This installation scheme is used if you obtain the installation files by ftp file transfer from Los Alamos.

1. Set up a subdirectory named [.GSAS] or a main directory [GSAS]. Sufficient disk space to hold the system should be made available (ca. 25000 blocks).

2. Set the current directory to the directory created in step 1 (e.g. SET DEF [GSAS]).

3. Initiate contact with the distribution machine at Los Alamos:

```
ftp mist.lansce.lanl.gov
```

This is a DEC Alpha/OpenVMS machine. When you get a MIST.LANSCE.LANL.GOV> prompt, type:

```
login anonymous
```

When you get the prompt for a password, type your e-mail address. To get general information concerning the files, type (but not the stuff in parentheses)

```
ASCII             (to set the mode of transfer)
get readme.1st    (to transfer the file)
cd [.alphavms]    (to change to the alpha distribution directory)
get alphagsas.ftp (to transfer this readme file)
```

These files should be read off-line; they contains general information about the versions of **GSAS** that are currently available as well as this instruction file. If you wish to obtain a new version of **GSAS** for DEC Alpha/OpenVMS, type the following commands:

```
binary            (set the mode of transfer)
mget *.lz         (transfer the compressed files)
```

If the decompression routines are not already available, type:

```
mget lz*.exe      (transfer lzcmp.exe and lzdcmp.exe)
```

which transfers the compression and decompression utilities. The executables were linked under OpenVMS V1.5 and should run on all Alpha/OpenVMS systems. To complete the file transfer, type:

```
ASCII             (set the mode of transfer)
mget *.com        (transfer the files)
mget *.doc
quit              (exit ftp)
```

The file, IMPORT.COM, is the installation routine for **GSAS**. It will process the other files and produce a working version of **GSAS** on your machine. Details of its operation are given below. The file, LZSOURCE.COM, is a self-unpacking archive file. If you desire source code for the compression routines and you have a C compiler, then issue an @SOURCELZ command, followed by an @LZBUILD command to create the new compression executables. LZCOMP.DOC is documentation for the compression utilities.

4. Run the import command file. (e.g. @IMPORT). After this completes you are in the subdirectory [GSAS.COM].

While running IMPORT.COM you will be asked about the names of batch queues. **GSAS** requires that your Alpha have at least one batch queue and will support up to three queues. You can use the default of SYS$BATCH but a better sharing of resources can be obtained with queues for fast, medium and slow jobs. If the queues are not yet determined you can change them later by editing the file [GSAS.COM]GSASDEF.COM and inserting the queue names. The command file asks four questions to determine the portions of **GSAS** you desire and will submit up to 36 batch jobs to SYS$BATCH. (Currently none of the LANSCE specific parts of **GSAS** are operational on Alpha/VMS.) In this way the executable versions of the **GSAS** programs are created for your version of the VMS operating system. After these batch jobs complete, you may wish to free ca. 10000 blocks of disk space by deleting the libraries which are contained in the directory [GSAS.LIB]. Before the command file finishes it will inform you of the symbol definition for **GSAS** that should be placed in either a system wide login file or else each user login file.

An Anonymous FTP Server for **GSAS** SGI Irix Codes

The **GSAS** distribution kit for Silicon Graphics Irix contains a single large file which is kept in a compressed form that is approximately 50% smaller than the original. This file needs to be transferred in binary format. There is also this "readme" file which is transferred in ASCII format.

GSAS Installation from ftp files:

System Requirements: SGI Irix 4.x or 5.x with f77 and XWindows. For Irix 5.x, an additional file will need to be transferred which contains the executables.

To ensure that the file structure and command files for **GSAS** are set up appropriately on your SGI we have provided below an installation procedure and an "install" script file. This installation scheme is used if you obtain the installation files by ftp file transfer from Los Alamos.

1. Set up a directory named "gsas" in a convenient location on your file system. (e.g. "mkdir ./gsas"). Note that sufficient disk space (ca. 50Mb) to hold the all the **GSAS** files is needed in the file system.

2. Set the current directory to the directory created in step 1 (e.g. type "cd ./gsas"). Make a note of the full name of this directory (e.g. type "pwd"); you will need this name for step 4, below.

3. Initiate contact with the distribution machine at Los Alamos:

    ftp mist.lansce.lanl.gov (This is a DEC Alpha/OpenVMS machine.)

When you get a prompt for "Name", login as:

    anonymous

(If you get an ftp> prompt, type "user anonymous"). When you are prompted for a password, type your e-mail address.

To get general information concerning the files, type the following (without the stuff in parentheses).

ASCII	(to set the mode of transfer)
get readme.1st	(to transfer the file)
cd [.sgiunix]	(to change to the SGI distribution directory)
get sgigsas.ftp	(to transfer this readme file)

(Read these files off-line; they contain general information about the versions of **GSAS** that are currently available as well as this instruction file. To obtain a new version of **GSAS** for your SGI, type the following commands:)

binary	(set the mode of transfer)
get GSAS.TARZ	(transfer the compressed file)

If you are running Irix 5.x, you will need to transfer the following:

get GSASEXE.TARZ	(transfer the compressed file of executables)

Then exit ftp by

quit	(exit ftp)

Next rename the file GSAS.TARZ and GSASEXE.TARZ files so that the decompression routine will properly convert it, decompress it to create file gsas.tar and then restore the **GSAS** files. Use the following commands to do this:

mv GSAS.TARZ gsas.tar.Z	(rename the compressed file)
mv GSASEXE.TARZ gsasexe.tar.Z	(if necessary)
uncompress gsas.tar	(creates gsas.tar from gsas.tar.Z)
uncompress gsasexe.tar	(if necessary)
tar -xvf gsas.tar	(creates all the gsas files)
tar -xvf gsasexe.tar	(creates the executables for Irix 5.x)

You may now delete gsas.tar to save ~13Mb of disk space.

rm gsas.tar	(delete file)

The script file, "install", completes the installation for **GSAS** on Irix 4.x; it is not needed on Irix 5.x. It uses the f77 command to load the executables for **GSAS** from all the object files it finds in ./gsas/gsasmain and puts the .exe files into the directory ./gsas/exe. After it finishes you may delete the files libgsas.a and the contents of ./gsas/gsasmain to save ~6Mb of disk space. The commands are:

install	(load the gsas executables)
rm libgsas.a	(delete the library)
rm gsasmain/*	(delete the object files)

4. Finally you need to edit your .cshrc file to include an alias like

    alias gsas /usr/gsas/gsas

to point at the path for the script file gsas (replace "/usr/gsas" with the location you chose for gsas (see step 2).

You are now ready to use **GSAS**. Everything that is in the present **GSAS** manual will work as in the VMS versions except that UNIX style file paths must be used for the exercises. For example, use "/usr/gsas/gsas_exercises/NICKEL.RAW" for the data set name in the first exercise. (Your path will be different depending on where you put the directory gsas.)

If there are any problems or questions call:

Bob Von Dreele (505)-667-3630 e-mail: VONDREELE@LANL.GOV
Allen Larson (505)-667-2942 e-mail: ALARSON@LANL.GOV

GSAS Problem Reporting

If you experience any difficulties with the operation of **GSAS**, find any errors or want to suggest any changes please use the form found on the next page for reporting them.

Submit to: GSAS Manager, Los Alamos National Laboratory, LANSCE, MS H805, Los Alamos, NM 87545 USA

GSAS Problem Report

Title:		ID: Date:
Module name:	Link date:	Problem type ( ) Software ( ) Documentation ( ) Other
Problem Description:		
Enclosures (documenting hardware/software context of the problem): [ ] On-line listings [ ] Off-line listings		
Date problem was first noticed:	Were you able to recover?	Is the problem repeatable?

DO NOT WRITE BELOW THIS LINE

Remarks/Analysis:

ACTION	BY	DATE
Received		
Analyzed		
Acted on		
Notified		

GSAS Organization

GSAS is organized into several main programs each designed for specific types of tasks or types of crystallographic calculations. They are listed below in alphabetic order with a brief description of their features. The various **GSAS** specific files generated by these programs are given in single quotes; they are described in the technical section of this manual. All of these programs as well as a number of utility routines are accessed through the **GSAS** shell which is invoked by entering **'GSAS'** on your terminal. This shell is capable of filtering the **GSAS** commands from other VMS/UNIX commands so that all terminal operations can be done from within the shell. In other words, you are able to do virtually any VMS or UNIX command from within the **GSAS** shell.

BIJCALC - Thermal Motion Analysis

BIJCALC is an interactive routine that analyzes the anisotropic thermal motion parameters and prints some information derived from the values on the list file.

CAD4RD - Input Enraf-Nonius Single Crystal Data

CAD4RD is an interactive routine for reading data measured on the Enraf-Nonius CAD4 instrument, extracting the unit cell information, examining the standard reflections and writing the reflection data into the 'reflection file' with corrections for crystal decay, etc. as indicated by the standard reflections. It also copies the ψ scan data into the 'experiment file' for use in absorption correction calculations.

CLLCHG - Unit Cell Transformation Routine

CLLCHG is an interactive routine for transforming a unit cell and its contents to a different description associated with a, for example, second order phase transition.

DISAGL - Bond Distance and Angle Computation

DISAGL is a batch program to calculate interatomic distances and angles. By using the variance-covariance matrix it also determines estimated standard deviations for these values.

EXPEDT - GSAS Editor

EXPEDT is the interactive editor for **GSAS.** It is generally the first program in **GSAS** run by the user. All input of structural data, program controls and other non-diffraction data is handled interactively by **EXPEDT**. Program control within **EXPEDT** is from a nested series of menus. The choices in the first layer of menus determine what kind of calculation is to be setup; choices in each succeeding menu layer determine finer detail in the setup. Each menu has a help listing associated with it which can be displayed as one of the menu options, thus **EXPEDT** is largely self documenting. **EXPEDT** also has graphics facilities for displaying powder patterns on a graphics terminal to facilitate editing of certain parameters. The second section of this manual contains training exercises which take you through the sequence of steps for running **EXPEDT** during the course of some crystallographic problems. **EXPEDT** modifies the experiment specific control file as the user makes menu selections and inputs data. In **GSAS** this file is known as the 'experiment file' and has the name 'somename.EXP'. It is fully described in the technical section of this manual. During the operation of **EXPEDT** an updated version of the experiment file is created which then becomes the input for any succeeding program in **GSAS**. In the case of VMS systems multiple versions are retained (depending on how "VERSION_LIMIT" is set on your machine). For UNIX systems only one previous version is retained; it has the name 'somename.OLD'.

FITSPEC - Fitting of Incident Spectra

FITSPEC is an interactive routine used to fit the incident spectra from a particular instrument to a variety of functions. It is generally needed only for TOF neutron data. The results are output to an 'instrument parameter file'.

FORSRH - Fourier Peak Search

FORSRH is an interactive Fourier peak search routine. It lists the positions and heights of the peaks found on the 'Fourier map file' and places them in the 'experiment file' for inclusion in distance and angle calculations.

FORPLOT and PLOTTER - Fourier Map Display

FORPLOT and **PLOTTER** are two interactive Fourier map display programs. They are capable of producing on various graphics devices (same as those supported by **EXPEDT**) single map slices, stereo views or interpolated oblique slices of maps generated by **FOURIER** and stored on 'Fourier map files'.

FOURIER - Fourier Map Calculations

FOURIER is a batch oriented standard Fourier map generation program. It can produce xy, xz or yz sections of Patterson, F_o, F_c or ΔF maps. The output is mainly a 'Fourier map file' intended for input to the peak search routine, **FORSRH**, and the graphics display programs, **PLOTTER** and **FORPLOT**. As an option it will produce a numerical map in the list file.

FPRIME - Calculate X-Ray Anomalous Dispersion Coefficients

FPRIME is a modified version of the program written by D. T. Cromer (Acta Cryst. 18,17-23, 1965) which calculates the X-ray anomalous dispersion coefficients and absorption coefficient for any energy. This interactive program will perform these calculations for up to seven energies or wavelengths for a single element using one of three possible methods (method 2 is recommended). It reads the tables of atomic cross sections from the file [GSAS.PARM]XSECT.NDAT. It operates independently of the **GSAS** file structure.

GENLES - General Least Squares

GENLES is a batch oriented least squares refinement program derived in part from a program by the same name written by Allen C. Larson. It constructs a single full least squares matrix and vector using multiple data sets. A mixture of powder diffraction and single crystal data for a given structural problem can thus be processed simultaneously. It also has facilities for constructing linear constraints between parameters, rigid body constraints for molecular fragments and can include bond length observations as 'soft constraints'. **GENLES** outputs a summary of the least squares results on a list file and generates an updated version of the 'experiment file'.

GEOMETRY - Calculate Molecular Geometry

GEOMETRY is an interactive program which will produce on the list file and on the terminal the results of several kinds of molecular geometry calculations. These include the orientation and position of a selected string of atoms as a rigid body, application of thermal motion corrections to selected bonds, hydrogen atom generation from carbon atom positions and calculation of specific torsion angles.

HKLSORT - Reflection Lister for Publication

HKLSORT is an interactive program which will produce on the list file a sorted list of structure factors in a form suitable for deposit with a journal. This list can be structured to have any one of the indices *hkl* as the fast running index and another as the slow running index. Thus, all six cases of *hkl* tables are permitted.

HSTDMP - Powder Pattern Lister

HSTDMP is a powder pattern data listing program. It can list interactively sections of a 'histogram file' or produce a list file of the entire powder pattern in a form suitable for deposit with a journal.

ISTATS - Intensity Statistics

ISTATS is an interactive program used to help determine the space group by creating a list of the average value of $F^2/\sigma(F^2)$ for the various parity classes of reflection sets such as *h00*, *hk0*, etc.

KUMARD - Input KUMA Single Crystal Data

KUMARD is an interactive routine for reading data measured on the KUMA single crystal instrument, extracting the unit cell information, examining the standard reflections and writing the reflection data into the 'reflection file' with corrections for crystal decay, etc. as indicated by the standard reflections. It also copies the ψ scan data into the 'experiment file' for use in absorption correction calculations.

ORTEP - Crystal Structure Plotting

ORTEP, written by Carroll Johnson (ORNL Report 5138), has been modified to adhere to the **GSAS** style with menus and interactive graphics. The current version implements most of the original ORTEP-II instructions through menu responses.

P3R3DATA - Input Siemens P3R3 Single Crystal Data

P3R3DATA is an interactive routine for reading data measured on the Siemens P3R3 single crystal instrument, extracting the unit cell information, examining the standard reflections and writing the reflection data into the 'reflection file' with corrections for crystal decay, etc. as indicated by the standard reflections. It also copies the ψ scan data into the 'experiment file' for use in absorption correction calculations.

POWPLOT - Powder Pattern Plotting

POWPLOT is an interactive graphics program for displaying powder diffraction patterns on various graphics devices. It is capable of displaying observed, calculated and difference curves with reflection markers at the user's option. It can also analyze the weighted differences and produce normal probability plots. In order to use **POWPLOT** on a particular powder pattern, **POWPREF** must have been run at least once. This program also has the ability to calculate the Fourier transform of the residuals to determine the radial distribution function of an amorphous phase, if one is present.

POWPREF - Powder Data Preparation

POWPREF prepares powder diffraction data for subsequent least squares analysis. The major tasks of **POWPREF** are to associate the position, channel or step width, incident intensity, refinement weight and a list of contributing reflections with each observation in a powder pattern. Additional flags are set for excluded regions, reflection markers, etc. for each point. Thus, **POWPREF** generates the full list of unique reflections from the lattice parameters and space group information for each phase in the sample; systematic extinctions and reflection multiplicities are automatically determined. There is a set of reflections generated for each powder pattern in the data set. **POWPREF** outputs a brief summary of its work on a list file and produces a 'reflection file' and a 'histogram file' for each powder data set processed.

PROFTEST - Display of Powder Profile Shapes and Derivatives

PROFTEST displays individual computed powder profile shapes for any of the profile functions available in **GSAS**. The profile shapes may be varied by adjustment of the profile coefficients and peak position (2Θ or TOF). Numerical and analytic derivatives of the profiles with respect to profile coefficients may also be displayed. It operates independently of the **GSAS** file structure and is generally used for diagnostic purposes.

PUBTABLES - Preparation of Tables for Publication

PUBTABLES prepares tables of structure factors and atomic parameters which are suitable for publication purposes.

RAWPLOT - Plotting of Powder Patterns

RAWPLOT is a graphics routine for displaying powder diffraction data in either d-spacing or data collection units (2Θ or time-of-flight). The input data must be in the **GSAS** standard raw data file format and an 'instrument file' is also required.

RCALC - Analysis of Structure Factor Residuals

RCALC is an interactive program which can be used to determine R-indices for the various parity classes of reflections. It also can be used to generate plots of residuals vs. a number of data parameters, such as d^*, F_{obs}^2, etc.

REFLIST - Reflection Data Lister

REFLIST is a reflection listing routine. It is capable of listing on either the terminal screen or on the listing file some or all of the reflections associated with each histogram.

REFLTOASCII - Conversion Of Reflection File to ASCII

REFLTOASCII converts **GSAS** reflection files (single crystal or powder) into an ASCII form suitable for transfer between VMS and UNIX machines. The ASCII files may also be read by nonGSAS crystallographic software (e.g. MULTAN). (See REFLTOBIN below).

REFLTOBIN - Conversion of ASCII Reflection File to GSAS Binary

REFLTOBIN converts ASCII files created by **REFLTOASCII** back to **GSAS** reflection file format.

RDUCLL - Cell Reduction Routine

RDUCLL is a unit cell reduction routine originally written by Yvon LaPage. It finds the conventional representation of the cell and detects any possible pseudosymmetry. It operates independently of the **GSAS** file structure.

SCABS - Single Crystal Absorption Calculations

SCABS is a batch oriented program for making absorption corrections to single crystal data from either X-ray or neutron single crystal instruments.

SCMERGE - Single Crystal Data Sort and Merge

SCMERGE is a batch oriented program for merging single crystal reflection data into a unique set with standardized reflection indices which are written to a new 'reflection file'. The space group extinct reflections are omitted and the Friedel related reflections are flagged and written adjacent to the standard reflection in the output 'reflection file'.

SPCGROUP - Interpretation of Space Group Symbols

The interactive program **SPCGROUP** interprets space group symbols to give a table of the equivalent positions and will do this for any setting of the 230 three dimensional groups except that trigonal, rhombahedral, tetragonal and hexagonal space groups must have the c-axis as the unique axis. Optionally it will determine the site symmetry rules for any location in the unit cell. It will also process spin flip assignments for magnetic symmetry and display a stereo pair drawing showing the resulting pattern of magnetic moments. The routines in **SPCGROUP** are those used elsewhere in **GSAS** for space group symbol interpretation.

SXTLDATA - Generalized Input of Single Crystal Data

SXTLDATA is a generalized structure factor input routine for single crystal data from an ASCII file which is then put into a standard **GSAS** format reflection file.

TDPLT - Drawing of Ball and Stick Models

TDPLT is an interactive program for generating views of the crystal structure. Several options are available for determining the space included in the drawing, namely, a sphere about a point in the unit cell, rectilinear blocks of space, and parallelogram blocks terminated by unit cell edges. Thermal ellipsoids are represented by plotting only the principal ellipses. Bonds are represented only by lines, but can have the bond length plotted in the center of the bond. Two classes of bonds are represented as either solid lines or dotted lines. There is no hidden line elimination.

UNIMOL - Assembling of Unique Molecules

UNIMOL is an interactive program for assembling unique molecules from the atoms in the 'experiment file'. The current version is rather crude in that it does nothing to maintain the continuity of a string of atoms, but only insures that all atoms in the molecule are in a contiguous set in the 'experiment file'. One however has the option of rearranging the atom list to suit their needs.

Other Programs in GSAS

In addition to the 36 programs listed above there are an additional 20 which are specific to crystallographic data processing at LANSCE which are only available for the VAX/VMS version of **GSAS**. They include routines for display of LANSCE data, preliminary data reduction, pole figure analysis from SCD data and various other routines.

Utility Routines in GSAS

There are a number of utility routines in **GSAS** that simplify many routine operations with **GSAS** list files, etc. as well as provide easy access to some of the data files within **GSAS**.

ATOM - Display of Atomic Scattering Factor Data

The **ATOM** facility displays for the selected chemical element (e.g. ATOM TI) all the information stored on the file ATOMDATA.DAT for that element.

ELST, DLST, SLST, TLST - List File Utilities

ELST is for editing the list file using the system standard editor; **DLST** is used to delete the list file, **SLST** is used to search the list file for a string and **TLST** will display the list file on the terminal.

PEXP, TEXP, DEXP, SEXP, LSEXP, EDEXP - Experiment File Utilities

PEXP (VMS only) is used to purge the experiment files, **TEXP** is used to list the experiment file on the terminal, **DEXP** (UNIX only) is used to delete all files for the experiment except the experiment and raw data files, **SEXP** is used to search the experiment file for a string, **LSEXP** (UNIX only) is used to list the names of all experiment files in the directory, and **EDEXP** is used for editing by hand (not recommended) the experiment file.

EXPNAM, NEXT, SELECT, PREV - Experiment Selection Utilities

EXPNAM is used to set a particular experiment name to be used for subsequent **GSAS** operations. **NEXT** and **PREV** (UNIX only) select the next (or previous) experiment in alphabetical order. **SELECT** (VMS only) lists the available experiments in the directory and prompts for your selection.

TLOG, DLOG - Log File Utilities (VMS only)

TLOG displays the log files for the current experiment on the terminal; **DLOG** deletes these log files.

DBCH - Batch File Utility (VMS only)

DBCH is used to delete batch files. This utility is most commonly used when a batch job fails with a system error leaving a number of uncompleted batch files in the directory which must be deleted before **GSAS** will allow further work on that experiment.

Program Execution in GSAS

The programs in **GSAS** are either executed in interactive mode (e.g. **EXPEDT**) or optionally in batch mode (e.g. **GENLES**). For each program request in **GSAS** the shell will determine whether it is interactive or possibly batch.

For **GSAS** on VMS systems, the shell will examine the command line looking for additional batch routines to be set up as a sequence. For example the command line **'POWPREF GENLES FOURIER FORSRCH DISAGL'** will cause the five batch routines to be executed in sequence as separate jobs. For each one the shell will request from you the appropriate batch queue and instructions for handling the log file and then produce a "batch" file. The batch files are named 'EXPNAME$PGMNAME.BCH'. The first one is submitted to the requested queue; as it finishes it submits the next one to be executed and then deletes itself. If a program aborts with an error the remaining routines are not executed and the remaining batch files will still exist in your current directory. They will have to be deleted before any **GSAS** routine can be run on the experiment (use the utility **DBCH** to remove them).

On UNIX systems, all the programs in **GSAS** are assumed to be run interactively although **POWPREF**, **GENLES** and some others may optionally be run in the background. Unlike VMS, input of multiple programs on one command line is not allowed and will generate an error.

GSAS Program and File Layout

The layout of the programs in **GSAS** and the interconnecting files for powder calculations is shown in the following figure. The program names, which are not inclusive, are shown in boldface; the arrows indicate the direction of input and/or output by each program.