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SHAMGAR's *OXGOAD*: A New Approach to the Problem of Resolution Corrections for Triple-Axis Neutron Inelastic Scattering Data using Parallel Processors

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Abstract

One problem in the analysis of triple-axis neutron inelastic scattering data is the large numerical computations involved in applying full resolution corrections, which in one extreme involves an often-repeated four-dimensional numerical integral. A program called *SHAMGAR* has been written for an ICL Distributed Array Processor that will both calculate the full convolution of a model scattering function with the resolution function and allow refinement of the model simultaneously to many sets of experimental data by a non-linear least-squares fit. Sample results and performance figures are given.

1. Introduction

Typically, a neutron inelastic scattering experiment is designed to measure the scattering function $S(\mathbf{Q}, \omega)$, which contains information concerning the microscopic static and dynamic properties of the system under study ($\mathbf{Q}$ is the wavevector transfer of the neutrons and ω is the energy transfer). Generally, some part of the analysis of scattering data will involve the fitting of a model for $S(\mathbf{Q}, \omega)$ to the experimental measurements. However, strictly speaking what is measured is a convolution of $S(\mathbf{Q}, \omega)$ with some experimental resolution function over momentum and energy transfer. The form of the resolution function for a triple-axis neutron spectrometer is well understood, both generally (Cooper & Nathans, 1967) and also in the limit of small scattering angle (Mitchell, Cowley & Higgins, 1984). In many cases the resolution correction can be considered to affect only the energy transfer, and this convolution is straightforward. But, in other cases, this simple approximation is not valid and will lead to spurious results from model fitting. In this case the full convolution, involving a full four-dimensional integral, may be required. Such calculations can prove to be very time consuming, certainly much longer than practical for the purposes of model parameter fitting.

Early attempts to implement such convolution programs on serial computers, based on the Cooper–Nathans resolution function, were pursued both at Brookhaven (Samuelsen, Hutchings & Shirane, 1970; Samuelsen, 1971) and Studsvik (Pynn & Werner, 1971; Werner & Pynn, 1971). They were successful in giving the desired results, but were too slow for routine use, especially in interactive mode. Subsequent developments of the original Brookhaven program (*RESFLD*) have produced a fitting version (*FITSQW*), which is widely used at AERE Harwell in batch mode (Hutchings, Als-Nielsen, Lingard & Walker, 1981). Similar developments at Brookhaven have produced three similar programs, *FIT3AX* (Tarvin, 1977; Heilmann & Tarvin, 1977), *CONSTE* (Heilmann & Tarvin, 1978) and *DICEFIT* (Youngblood, 1978), which also require batch operation. The last of these uses Monte Carlo integration instead of a grid method, but requires more computer time to achieve comparable results.

A new route was explored by a joint Harwell–ILL Grenoble project (*PKSIM*), which employed various devices to accelerate the integration and which has achieved the speed necessary for incorporation into a fitting routine (Paul, 1984). However, this program is not general enough to be able to handle some of the integrals required. This lack of reliability may well be an inevitable result of using 'highly efficient' integration schemes, although there may yet be found ways of improving the generality without sacrificing efficiency.

Another solution to this problem is to write efficient conventional programs to run on some of the very large mainframe computers currently in operation, such as those of the CRAY or CYBER series. However, general access to such machines is often limited. Alternatively, there is a trend (in the computing world) towards the use and development of parallel processes (PP), which can perform parallel operations on multiple data streams simultaneously (Hockney & Jesshope, 1981). Such machines are relatively inexpensive, and we anticipate a growing proliferation of them so that in the near future any interested user will have ready access. Accordingly, we have written a program, called *SHAMGAR*, for the calculation of the convolution of a model $S(\mathbf{Q}, \omega)$ with the full resolution function that will also allow parameter

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fitting by non-linear least-squares fitting. In the following sections we describe the operation of the PP for which the program has been written, together with details of the functioning of the program and of some of the parallel algorithms. We conclude by presenting some illustrative results.

2. Parallel processors

A PP consists of a number of separate processing elements (PE) that are hard-wired together to form a grid that allows for the transfer of information between the separate PE's. Each PE will contain a certain amount of memory storage, and the PP operates by performing operations on a number of sets of data stored on each PE. Thus, whereas a normal serial computer operates by performing a string of identical operations in sequence, a PP will perform all of the identical operations simultaneously. The present work uses the Distributed Array Processor (DAP) that was built by ICL (Great Britain). The DAP consists of 4096 PE's, connected onto a 64×64 square grid, each with 512 bytes of memory. The programming language that has been developed for the DAP is an extension of Fortran IV, called DAP-Fortran, and because of this it is not particularly difficult for the new user to write programs for the DAP for himself. It should also be noted that in operation the DAP is attached to a mainframe computer, and runs as a dedicated device.

At the present time the DAP is but one machine among several in the world (but the only one at the present time to which the scientific community in Great Britain has general access), and possibly the language DAP-Fortran will not be used for the other PP's being developed. However, many of the ideas and results presented here will be of general importance.

3. Description of the program

SHAMGAR has been written to calculate the full convolution of a model form of $S(\mathbf{Q},\omega)$ with the experimental resolution function, and to fit this model together with a model background function to the experimental data by non-linear least-squares fitting. One feature of the program is that it is able to refine 'global' parameters for several different sets of data simultaneously. *SHAMGAR* deals with four different cases of the scattering function, which are permutations of broad or narrow frequency widths of the excitations and large or small scattering angle [using the Cooper & Nathans (1967), CN, or Mitchell, Cowley & Higgins (1984), MCH, resolution functions respectively]. The four versions are: version 1: sharp excitations with MCH resolution function; version 2: broad excitations with MCH resolution function; version 3: sharp excitations with CN resolution function; and version 4: broad excitations with CN resolution functions. Because of storage requirements, the four versions are compiled into four separate object files, called respectively *OXGOAD*1 *etc.* Version 3, which is for narrow line widths and large scattering angles, corresponds to measurements of sharp phonon or magnon dispersion curves and has been programmed to allow for the existence of excitations from several different branches of the dispersion curves. The background function may be any function of the nominal wavevector transfer $\mathbf{Q}_0$, the nominal energy transfer ω_0, temperature, and up to sixteen other parameters, and has been represented in tests of the program as a Gaussian peak in energy, typically centred around zero energy transfer, with a polynomial sloping background and a wavevector-dependent intensity. The structure of *SHAMGAR* is such that all of these models have been coded as small DAP-Fortran functions that are called by the main routines of the program. As such, they can be readily reprogrammed to incorporate any model required by the user, this facility being one of the principal design features of *SHAMGAR*.

The version of *SHAMGAR* for use with the Cooper–Nathans resolution function and a 'broad' scattering function (version 4) requires a four-dimensional numerical integral, and this is set up in $\mathbf{Q}$–ω space in the frame in which the resolution function is diagonal. An 8^4 mesh is set up and the integrand is evaluated at all of the grid points so established, and a cut-off is introduced on the ellipsoid surface at which the resolution falls to e^{-3} of its maximum value (this cut-off is used in all four cases). The integral is computed by simply summing the integrand at each of the included grid points. The case of the 'sharp' scattering function (version 3) is dealt with by projecting the resolution function perpendicular to the energy axis and setting up a 16^3 mesh in $\mathbf{Q}$ space in the frame in which the projected resolution function is diagonal. The integrand is evaluated at each point, having first calculated the corresponding excitation energy associated with the dispersion relation, taking the product of the full resolution function and the weight function associated with the dispersion relation. Both energy gain and loss have been included in the convolution integral.

The small-angle resolution function of Mitchell, Cowley & Higgins reduces the dimensionality of the problem by one in both cases, by recognising the linear dependence of two components in the resolution function. The integrals are thus to be evaluated only in three and two dimensions for the 'broad' (version 2) and 'sharp' (version 1) cases respectively, and so 16^3 and 64^2 meshes are used in these cases. All of the above meshes are readily mapped onto the 64^2 hardware grid of the DAP.

The calculation of the numerical integral of the

resolution-function convolution is performed as a parallel operation, with serial looping over the data points. The differentials required in the fitting routine are calculated numerically by forward and backward difference, and those associated with the background function can be calculated in parallel.

The non-linear least-squares fitting routine incorporated into *SHAMGAR* is straightforward, using a system-supplied routine for efficient full inversion of the Hessian matrix (the matrix that contains the products of the derivatives of the calculated function with respect to the refined parameters). Many aspects of this fitting routine, such as the changing of parameter values, involve parallel computations. *SHAMGAR* incorporates a new method of error analysis that takes account of known uncertainties in the values of parameters that are not allowed to vary in the least-squares fitting routine (*e.g.* measured background), and also takes account of uncertainties in the values of individual nominal spectrometer settings as well as the usual uncertainties in the corresponding measured intensity values. The extension of the normal least-squares method to incorporate these features is given in the Appendix.

We stress that *SHAMGAR* has been written taking account of both efficiency and simplicity. Because of the power of the DAP it has been unnecessary to incorporate any potentially troublesome time- or storage-saving features. In addition, the structure of the program has been arranged to make user-required alterations as easy as possible. Because of this flexibility it has already been possible to adapt the code to accept measured resolution parameters instead of calculating them. In particular, this has been applied to X-ray diffuse scattering measurements, with appropriate adjustments to account for the effective integration over all energies performed by the X-rays (Gibaud & Cowley, 1985).

4. Results

The program has been subjected to a series of tests to check that it is handling the rather subtle aspects of the resolution function correctly, and to evaluate its performance and usefulness. Some of the early tests, which set out to establish merely whether the focusing properties were correct, actually revealed errors in the standard Cooper–Nathans routine used in this and other programs. These errors were associated with the orientation of the resolution function, and were absent in the first and second quadrants of the scattering coordinates, but were present in the third and fourth quadrants. Having ironed out these problems, we now are confident that the calculations are performed correctly.

Four examples will follow, illustrating the four modes of operation. In each case we quote the computer time taken in the running of the program in order to indicate its efficiency. All tasks have been performed interactively rather than in batch mode, the ability to do this being one of the prime motivations in writing the program, and thus, when the host computer is heavily loaded there may be lapse times of a few minutes in each case that arise primarily as a result of data transfer from file store.

Version 1: *sharp excitations with small-angle resolution function*

The first example is taken from a recent experiment on the cold-source triple-axis spectrometer IN12 at the ILL, Grenoble (Mitchell & Paul, 1985*a*) on small-wavevector spin waves in the ferromagnetic disordered alloy Pd–1%Fe. Fifteen different scans were included in the data set, with a total of 265 data points obtained under four different resolution conditions (four 'fixed k_I' values between 1.1 and 1.85 $Å^{-1}$) over the range of $\mathbf{Q}$ from (0·01, 0·01, 0·01) to (0·035, 0·035, 0·035) and energy transfers (losses and gains) up to 0·16 THz, and at temperatures from 5 up to 44 K ($T_c = 56$ K). Sixteen parameters were used to specify the background, largely because different widths were needed to account for the elastic scattering at different incident wavevectors, and because the intensity of this scattering was highly q dependent. However, the spin waves were characterized by only three parameters. The spin wave energy ε was given by

$$\varepsilon = D(T)|\mathbf{Q}|^2$$

with

$$D(T) = D(0)[1 - (T/T_c)^2]^{1/2}$$

and the intensity contained a term proportional to $\exp(-\alpha|\mathbf{Q}|^2)$ to account for giant-moment form-factor effects. The third variable parameter, along with $D(0)$ and α, was an overall scale factor. The changes in the resolution volume within each scan and between various resolution conditions and changes in the monitor efficiencies are all handled within the program along the lines specified by Mitchell, Cowley & Higgins (1984).

The performance figures for the program are 6·35 s CPU time for the host and 129 s for the DAP for three refinement cycles to reach convergence. One of the fifteen scans is illustrated in Fig. 1.

Version 2: *broad excitations with small-angle resolution function*

This example also uses data from IN12, but in this case from an experiment on Ni_3Al (Bernhoeft, Lonzarich, Mitchell & Paul, 1985). The data were fitted to a Lorentzian form in energy, taking into account the energy widths and wavevector-dependent susceptibilities, which vary appreciably over the resolution volume. Only one scan was used in this example, and this is illustrated in Fig. 2. There are 31 points and five

variable parameters (three that define the background and two that define the quasi-elastic scattering). The analysis used 2.6 s host CPU time and 23 s of DAP time, and convergence was reached after seven cycles of refinement.

Version 3: sharp excitations with the Cooper–Nathans resolution function

This example is taken from an experiment performed on the thermal-neutron beam spectrometer IN3 at the ILL (Mitchell & Paul, 1985*b*) on pure nickel. High-resolution conditions were used (PG_{004} monochromator and analyser, and 30′, 20′ and 30′ horizontal collimation after the monochromator, sample and analyser, respectively). The data inevitably include both longitudinal acoustic phonon scattering and the spin-wave scattering, which is of interest in the experiment. The complicated observed line shapes may be accounted for by inclusion of both phonons and magnons in the model, and one scan is shown in Fig. 3. The phonon velocity was measured separately and fixed in this analysis at the measured value, so there are four variable parameters (flat background, spin-wave stiffness, spin-wave intensity and phonon intensity) in the fit to three scans (45 points in total). The analysis used 3·26 s host CPU time and 108 s of DAP time, convergence being reached after eight cycles.

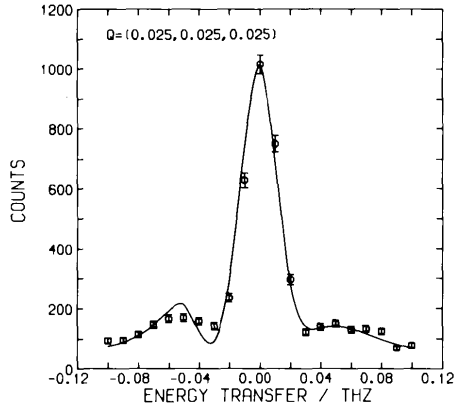

Fig. 1. One representative scan from 15 fitted simultaneously using version 1. The sample was a single crystal of Pd – 1% Fe, and the measurement was a constant-**Q** scan with the sample at 35 K. The circles represent the raw data points, and the solid curve is the computed fit as described in the text.

Version 4: broad excitations with the Cooper–Nathans resolution function

This example involves no experimental data, but is a comparison between *SHAMGAR*'s *OXGOAD*4 and *FITSQW*, where the present program was used to fit a model function to a corresponding model profile generated by *FITSQW*. [This has been made possible by kind permission of M. T. Hutchings of AERE Harwell, who also made available the source code and output from *FITSQW* (Hutchings, 1984).] The scattering function is defined as a combination of lightly damped inelastic spin-wave scattering and a broad quasi-elastic line due to critical fluctuations, and requires nine input parameters including an overall scale factor. Only this last factor has been allowed to vary in fitting the results of the present program to those of *FITSQW*, and reasonable agreement is obtained (Fig. 4).

The computer times taken by *SHAMGAR* to produce one set of intensity values were 5·2 s host CPU time and 2 s DAP time. The corresponding time used by *FITSQW* was 24·3 s CPU time on the Harwell IBM 3081 K.

A few comments on the differences between the two sets of output are perhaps in order. *FITSQW* used an

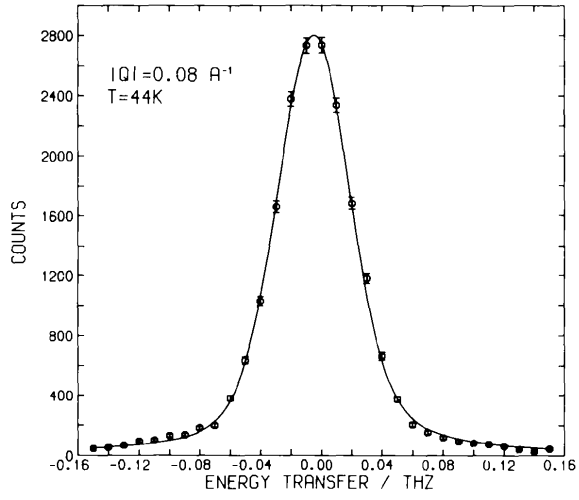

Fig. 2. Constant-|**Q**| scan from a polycrystalline sample of Ni_3Al just above T_c. The solid line is the fit as computed by version 2 of the program (see text).

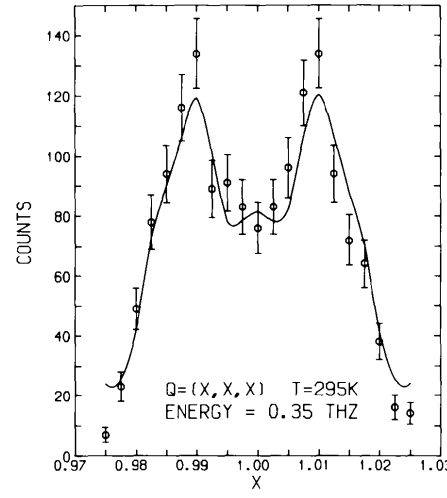

Fig. 3. Constant-energy scan for nickel near 111, analysed allowing for the presence of sharp LA phonons as well as sharp spin-wave scattering. The solid curve is the fit computed by version 3.

integration grid of $4 \times 6 \times 16 \times 10$ points (total of 3840) suitably constructed on the diagonalized resolution function, with the grid dimensions specially chosen for this application. On the other hand, *SHAMGAR* uses a standard $8 \times 8 \times 8 \times 8$ point grid (total of 4096 points), which is not so suitable in this particular case. In fact, the raw values generated in this way show small oscillations owing to the graininess of the integration grid, and these have been smoothed out using a simple triangular weighted smoothing function at each point, using two neighbouring points either side. This has the inevitable side effect of broadening and reducing the height of the spin-wave peak at about 0.02 THz energy gain. The differences that remain after this procedure has been applied are no larger than the typical statistical errors encountered in real data from an experiment of this kind (often about 10% of the values, see Fig. 1–3).

If the above explanation for the discrepancies is accepted, this comparison lends weight to the view that *SHAMGAR* is capable of producing reliable simulations of observed data from models for $S(\mathbf{Q}, \omega)$ that are accurate at least to within the statistical accuracies of measurements obtained from neutron inelastic scattering experiments and which are suitable for parameter fitting. It should be stressed that the problems outlined above could be easily avoided by the use of more appropriate grid dimensions. *SHAMGAR* can be readily adapted by the user to take account of specific requirements; the programmed grid and smoothing facility simply add the desirable feature of generality.

5. Discussion and summary

We have described the operation of a program that will fit model functions of neutron inelastic scattering intensities to corresponding experimental data, taking explicit account of full resolution corrections. The new direction that is represented by this work is the use of parallel processors, and this has meant that a problem that was widely considered to be too large for routine computation is now reduced to a normal data reduction procedure that is suitable for interactive use. The version that was used in all of the tests described in the preceding section was designed and written with the aim of making it of general applicability, but any changes that could improve its accuracy in special cases could easily be made.

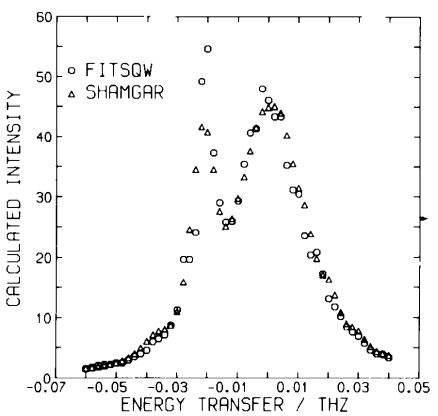

Fig. 4. Comparison of the model curves generated by *FITSQW* (circles) and *SHAMGAR* (triangles). Details are given in the text.

The work presented here is clearly directly relevant for only one particular machine namely the ICL DAP. However, as other similar machines are being developed and purchased by academic institutes, we hope that one result of this work will be to encourage other workers in the field of neutron scattering to use such machines in the routine analysis of data. This may involve either of two courses of action. The user who will not have immediate access to a PP should be able to make arrangements to use the DAPs based in Edinburgh or elsewhere *via* the now well established national and international computer communications networks. Alternatively, the user who has access to a PP may adapt the program *SHAMGAR* to his own system. Thus, copies of the program are available from the authors, who are also agreed to give advice if needed. It is the contention of the authors that the relatively small time and financial costs required to implement the use of *SHAMGAR* or a related program compared with those expended in the process of experimental preparation and data acquisition mean that the types of calculation described in this paper should soon be widely considered to be routine.

APPENDIX

(i) Incorporation of uncertainties in fixed parameter values

The uncertainty of a parameter value that is determined by the fitting procedure depends on the uncertainty of the other variable parameters if they are at all correlated. We estimate the uncertainties of the parameter values by computing the changes in the parameters that would increase the value of χ^2 from its minimum (convergence) value χ_0^2 by one standard deviation of the χ^2 distribution. The change δp_i in parameter p_i is calculated in the following way:

$$\delta p_i = [(H^{-1})_{ii}]^{1/2}(2\chi_0^2)^{1/4},$$

where H is the Hessian matrix as defined in § 3.

If there is a well known uncertainty in one of the fixed parameters in the fitting procedure, *SHAMGAR* allows the input of this information and, if any such errors have been specified, it incorporates them in the final estimates of the varying parameter errors. Once the best parameter set has been found, each such parameter is included, one at a time, as a variable, and

the Hessian matrix is recalculated. The resulting parameter errors are all scaled by a factor that sets the error on the fixed parameter equal to its input value, and the equivalent errors on all of the varying parameters are added in quadrature to the errors estimated from the fitting procedure:

$$\sigma(p_i)^2 = \sigma(p_i)_f^2 + \sigma(p_i)_1^2 + \sigma(p_i)_2^2 + \ldots,$$

where $\sigma(p_i)$ is the estimated error on the variable p_i, $\sigma(p_i)_f$ is the estimated error of the variable p_i as obtained from the initial fitting procedure, and $\sigma(p_i)_1$ *etc.* is the estimated error on p_i induced by the known errors on the fixed parameter 1 *etc.*

(ii) Spectrometer setting errors

In a typical triple-axis experiment, the changes of spectrometer angles between successive points of a scan are between 0·1 and 0·5°. Since the precision of the equipment is frequently of the order of 0·01–0·04°, the uncertainty or 'setting error' in the spectrometer settings can be a significant fraction of the step size. When the scattering intensity is changing rapidly across a scan, as for example in a well focused phonon scan, then the error in the measured intensity that arises because of the setting error can be as large as, or even larger than, the statistical or counting error. In this case the appropriate value to use in the weighting of the least-squares sum is not the counting error, but the counting error and the derivative of the line-shape function multiplied by the setting error, added in quadrature:

$$\sigma_i^2 = I + [(\partial I/\partial x)\Delta x]^2.$$

where σ_i is the standard deviation to be used in the calculation of χ^2,

$$\chi^2 = \sum_i (y_i - I_i)^2/\sigma_i^2,$$

I is the calculated intensity (number of neutrons) and x is the scan variable (typically an energy or wavevector).

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