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The SIP Program for the Evaluation of Neutron Scattering Experiments.

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Summary. This computer program aims to make the evaluation of the count-rate and resolution of neutron scattering experiments a routine task. The Shelter Island Program (SIP) was conceived to estimate the performance of new neutron sources, new instruments and new experiments in a realistic way. Its data bases and default parameters include the performance characteristics of the 18 principal existing and proposed reactor and pulsed sources, typical instrumental configurations for the 10 most common elastic and inelastic instruments, and the tables of neutron cross-sections for the elements. Given the sample atomic or weight fraction, the most common scattering laws are evaluated analytically. These include the small-angle defect, liquid hard sphere, Bragg, Einstein oscillator, phonon, magnon and crystal field cross sections.

Neutron beam time represents an expensive resource. This program aims to optimise its utilisation by the evaluation of experimental count-rates and resolution before an experiment is performed. It aims to avoid both the waste of beam time resulting from extravagant statistical precision, as well as the possible failure of an experiment caused by too low a count-rate or resolution. The prudent experimenter *SIP's* before he drinks. The program was conceived for the Shelter Island Workshop set up to evaluate the relative performance of the new reactor and pulsed neutron sources proposed for the United States. Comparisons of performance are only realistic if made in terms of the count-rate expected for particular experiments at given values of the scattering vector Q and energy transfer $\hbar\omega$ and their resolutions ΔQ and $\Delta\hbar\omega$. The comparison of count-rates using different methods at the same resolution was the original aim of the program.

The program works simultaneously in two modes. The experimenter can specify an *actual* instrument configuration, and evaluate the corresponding count-rate and resolution for a given value of Q,ω and experimental cross-section. At the same time he is requested to specify the required Q,ω value and the resolution $\Delta Q,\Delta\omega$ and is given the *best* possible count-rate consistant with this resolution. Simple matching methods are used to specify the corresponding best values of intrumental parameters such as the flight paths and

collimations. A serious approximation is that no consideration is taken of focussing. A comparison between the *Actual* and *Best* values enables a judgement to be made of the degree of optimisation of the present instrumental configuration.

The data-bases accessed by the program contain a parameterisation of the flux-distribution and pulse width of 9 reactor and 9 pulsed sources. Both include Maxwellian and epithermal terms specified in the conventional way as the energy-integrated Maxwellian flux $cm^{-2}s^{-1}$, and the epithermal flux from the whole moderator surface at 1 eV $s^{-1}sterad^{-1}eV^{-1}$. A novel method is used to specify the performance of the most commonly used instruments on neutron steady and pulsed sources. The final count-rate is expressed as a product of 5 terms:

1. The moderator flux in $s^{-1}sterad^{-1}eV^{-1}$ units.
2. A generalised *monochromator element* expressing in units of sterad eV the fraction of neutrons transmitted to the sample in terms of the incident solid-angle and energy window.
3. The sample macroscopic cross-section expressed in units of $sterad^{-1}eV^{-1}$.
4. A generalised *analyser element* expressing in units of sterad eV the fraction of neutrons transmitted from the sample to the counter.
5. The counter efficiency.

The 10 instruments chosen include the small angle, reactor crystal monochromator and pulsed time-of-flight diffractometers, and for inelastic scattering, the reactor triple axis, the pulsed source rotor, crystal analyser, crystal monochromator, beryllium filter and resonance detector spectrometers. These instruments have many monochromator and analyser elements in commmon. For example the same crystal monochromator element is used for a reactor diffractometer, triple axis and pulsed crystal monochromator instruments. The *actual* monochromator element for a crystal monochromator is defined by the program in the conventional notation as

$$E_M^A = 2E_0 \cot\theta_M \frac{\alpha_I \alpha_0 \eta_M}{\sqrt{(\alpha_I^2 + \alpha_0^2 + 4\eta_M^2)}} x \frac{\beta_I \beta_0}{\sqrt{(\beta_I^2 + \beta_0^2 + 4\sin^2\theta_M \eta_M^2)}} x R$$

where R is the crystal reflectivity, which is evaluated from a data base containing the properties of the most common analyser crystals. The *best* value for the monochromator element is evaluated using the value of the incident wavelength resolution $R_0 = \Delta k_0/k_0$ where the wavevector resolution Δk_0 is calculated from either the specified scattering vector resolution ΔQ or the energy resolution $\Delta\hbar\omega$, which ever gives the lowest value.

$$E_M^B = 2E_0 \tan\theta_M R_0^2 \beta_I \; x \; R$$

For time-of-flight experiments in either direct or inverted geometry the program evaluates the count-rate per *resolution element* . This is roughly the counts per time channel integrated over a resolution broadened peak in the time-of-flight spectrum. Many time-of-flight instruments can employ many resolution elements along the time-of-flight scan, and possible many counters simultaneously. The number of useful resolution elements (*publishable points*) must be evaluated separately for any given experiment and used to multiply the count-rate per element to give an overall count-rate before comparing with say a single counter triple axis count-rate.

The program has been checked successfully against several well documented experiments. It was developed on a Sinclair QL home computer but uses standard IBM PC BASIC code of some 13000 lines. At present an extensive manual is being prepared. This will include the extensive set of equations relating the final count-rate for the most common types of experiment to the source, instrumental and sample variables — all specified in a consistent set of units with appropriate default values. It is hoped that these will prove valuable in other calculations.