

Monte Carlo Code Comparisons for a Model Instrument

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Introduction

Because modern neutron scattering instruments are expensive to construct, it is essential to optimize designs. Several Monte Carlo simulation codes are available for this purpose. The user community, however, is rightfully skeptical of using these codes as “black boxes,” since the code authors may be overly confident. A project is underway to compare the code results for a relatively simple well-specified instrument. This report is a continuation of the work reported at the International Conference on Neutron Scattering held in Munich from September 9–13, 2001 (unpublished).

The instrument chosen was the Triple-Axis Spectrometer formerly installed on beamline H8 of the High Flux Beam Reactor at Brookhaven National Laboratory, because this instrument was most familiar to Larry Passell, who initiated the project. The layout is shown in Figure 1; a description with dimensions of the components is available [1]. We expect purely geometric elements to give the same answers with all codes. In particular, the Soller collimators are taken to be ideal, with no internal reflections or penetration of blades. On the other hand, the different algorithms used for the mosaic crystals and for vanadium scattering may cause variations. The only standard imposed between the codes is that the rocking curve for the crystals should match the measurement of Shapiro and Chesser [2], made with horizontal and vertical beam divergences of $20'$, giving $fwhm = 0.6^\circ$ and peak reflectivity 70%.

The results with five codes have been compared: RESTRAX (RESolution of TRiple-AXis spectrometer [3], MCSTAS (Monte Carlo Simulation of Triple-Axis Spectrometer) [4], NISP (Neutron Instrument Simulation Package) [5], VITESS (Virtual Instrumentation Tool for ESS) [6], and IDEAS® (Instrument Design and Experiment Assessment Suite) [7]. Some features of the codes are discussed briefly below, with descriptions of the mosaic crystal and vanadium scattering algorithms as applied to the present simulation.

RESTRAX: <http://omega.ujf.cas.cz/restrax/index.html>

Unlike the others, this code is specific to a particular form of instrument: the triple-axis spectrometer (TAS). It includes parts of the older codes RESCAL [8] and TRAX [9] for analytical calculation of the TAS resolution matrix and adds a highly optimized Monte Carlo ray-tracing code for alternative simulation of the resolution function and for Monte Carlo convolution with non-linear scattering function $S(\mathbf{Q}, \omega)$. This function can be defined by users in a shared library and used to fit experimental data. Recently, the original ray-tracing code of RESTRAX has been upgraded to simulate the spectrometer components more realistically and to allow for higher flexibility. Though RESTRAX uses a fixed set of components, it also permits simulation of other configurations (powder and strain-scanning diffractometers and neutron guides), and monitoring of the neutron beam at dif-

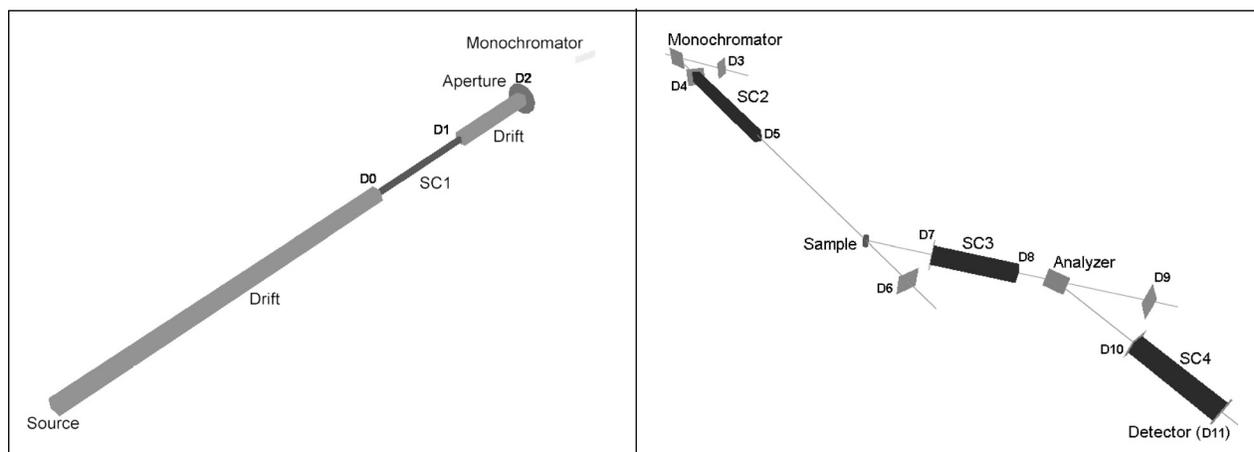


Figure 1. Layout of the H8 Triple-Axis Spectrometer, pre-monochromator (left) and post-monochromator (right). SC1, SC2, SC3, and SC4 are Soller collimators. D0 through D11 represent beam monitors; note that D3, D6, and D9 are transmitted rather than reflected or scattered beams, and D11 is the final detector. The takeoff angle from the bent (vertically focusing) PG002 monochromator is 41.18° for neutron energy 14.7 meV. The sample is a vanadium cylinder. The analyzer is a bent (vertically focusing) PG002 crystal. The figures were generated by NISP.

ferent positions along the TAS. For input, the code uses command lines and configuration files. The code is written in F90 (or F77 with extensions) for Unix operating systems and requires the free PGPLOT library [10] for graphical output.

The vertically focusing PG crystals are simulated by assemblies of thirty-one tilted segments with corresponding radius (tilt angle depends on the vertical coordinate y of the segment center as $\Delta\phi = y/R$). The reflection at the PG crystals is simulated as a random walk in each segment, with the mean-free-path corresponding to the scattering probability for a given neutron direction and local lattice orientation. Each event is weighted by a transmission factor, including neutron capture and incoherent scattering [11] and considering actual path-length through the crystal. The intrinsic mosaicity and primary extinction factor were set to give the required rocking curve.

Scattering by the vanadium sample was simulated by sampling the neutron path in the sample from an exponential law using the scattering cross-section of 0.362 cm^{-1} . Each event was weighted by the attenuation factor for the absorption cross section, 0.476 cm^{-1} , for the total path length of the neutron in the sample (before and after the reflection).

MCSTAS: <http://neutron.risoe.dk/mcstas/>

This code has expanded from its “triple axis” origin, to be a general code for all reactor and spallation instruments. It was designed at Risø and is actively maintained at Risø, the ILL, and ANSTO. An instrument is written as an ordered list of components in a text file using macros from a dedicated meta-language. Each component instance includes position,

orientation, shape, and physical parameters as required for the algorithm. The instrument description file is processed by MCSTAS (including library components and additional user code in C), resulting in a source file to be compiled in standard C. The preprocessing and compilation tasks are performed automatically so that the final instrument appears as a single executable program that prompts for input, runs the simulation, and produces various output files. The user interface is written in PERL. The code is provided as sources, and is portable to Unix and Linux, and runs partly on Windows and Macintosh.

Each of the vertically focusing PG crystals was expressed as fifty tilted flat slabs. The algorithm assumes an infinitesimally thin crystal and uses a small-mosaicity approximation. (Reflection geometry is assumed, but it is possible to track the transmitted beam instead of the reflected.) The in-plane angle of a single crystallite orientation is selected from a Gaussian distribution. If the scattering succeeds, an out-of-plane component is added using an independent Gaussian distribution. For this problem, the mosaic spread (isotropic) and peak reflectivity were chosen to give the specified rocking curve.

Physical processes included in the vanadium sample are incoherent scattering and absorption. The position of the interaction is selected from a linear (rather than exponential) distribution. Every neutron hitting the sample scatters into a specified solid angle; i.e., trajectories are aimed in the appropriate exit direction. The statistical weight is adjusted for scattering probability, the solid-angle restriction, and absorption in the incident and scattered path lengths.

NISP: <http://strider.lansce.lanl.gov/NISP/Welcome.html>

The core of NISP is a library of subroutines (MCLIB [12]) written in F90 (or F77 with extensions) and supplied as source code. At present, these routines support about forty region types, as well as magnetic field configurations that can overlay physical regions. In this library, the geometry of neutron transport is treated separately from the contents of a region. Unlike the other codes in this project, which are linear, regions are connected through a *matrix* and neutrons are *not* required to pass through a specific list of elements. This allows beam splitting (for instance, for polarization), treatment of unexpected trajectories, and shielding efficiency.

The other two components of NISP are the execution code (MC_Run, supplied as source to be compiled and linked with the library, or for certain operating systems as an executable), and a graphical user interface (MC_Web) that runs only on the server [13]. Communication between MC_Web and the executable code is by means of an editable text file. It is simple to add new algorithms to MCLIB, and straightforward to link region objects to the new methods by updating the OPERATE procedure in MCLIB. (It is not necessary to modify MC_Run, except to link to the revised library.) However, no tools are yet available for a user to add a new element to the Web application in the server. Instead, the user calls for an instance of an element that has appropriate geometry and then enters the required intrinsic parameters of the new region type as a list of values.

The algorithm for mosaic crystals is described elsewhere [14]. It takes fixed steps, with random crystallite orientation and d spacing selected from Gaussian or Lorentzian distributions at each step. The broadest of the three distributions is applied as the mosaic factor in the analytic solution of the Darwin equations [15], which determines reflection, transmission, absorption, and incoherent scattering probabilities. This is continued until the neutron reaches some surface of the crystal (or undergoes an incoherent scatter). An odd number of internal reflections results in a reflected neutron. The mosaic spreads and reflectivity coefficient per step were adjusted to give the required rocking curve (the d -spacing distribution was a δ -function for this case).

When the scattering solid angle is restricted, the incoherent scattering sample type in NISP does *not* include separate absorption and scattering cross sections, nor multiple scattering. To simulate the correct transmission and the interaction depth, it is necessary to use the *total* cross section, 0.838 cm^{-1} , which overestimates the scatter. A portion of the statistical weight of the neutron is transmitted, and the remaining weight is split into several parts for which independent penetration depths are selected from the truncated exponential distribution. The statistical weight is reduced by the accepted fraction of the sphere. A short run with absorp-

tion and full multiple scattering into 4π showed that a factor of 0.382 ± 0.007 must be applied to D7 and all downstream detectors.

VITESS: <http://www.hmi.de/projects/ess/vitess/>

A simulation in VITESS comprises one or more sequential modules called using a command-line pipe: Each module passes its neutron data to the following one, without necessarily storing the intermediate results in an external file. If an intermediate file is written, it may be used to describe the neutron beam in full detail at that position. Generation of the standard batch command file is facilitated by a graphical user interface (GUI) that can control up to thirty modules per pipe. It is also possible to write the control files directly without the GUI. To obtain full portability of the program package, the GUI is implemented in Tcl/Tk, which is available for most platforms commonly in use. The computationally demanding modules are implemented in Ansi-C. In addition to the large range of existing modules, non-VITESS executables can also be included using an “external command” module.

The monochromator-analyzer module is described elsewhere [16]. In this simulation the cylindrical mosaic crystals were each represented by twenty flat slabs. Every neutron finds a crystallite with the specified d -spacing (the d -spacing distribution width was zero) on which it is forced to be reflected. The cone of all possible mosaic orientations conforming to the Bragg condition is determined, and a random orientation is selected which is close (i.e., within a specified range factor) to the maximal probability line. The statistical weight of the neutron is adjusted according to anisotropic Gaussian mosaic distributions, and multiplied by a peak reflectivity factor. (For accurate intensity comparisons, a renormalization procedure is suggested.) The mosaic spreads and peak reflectivity were adjusted to match the required rocking curve.

The elastic isotropic scattering sample used in the VITESS calculation does not include multiple scattering or self-shielding. Each neutron is scattered once at one linearly chosen random position along the path. The microscopic scattering probability is proportional to the incoherent cross section multiplied by the local area density seen by the neutrons. Absorption is treated as attenuation along the incident and exit paths. The scattering is into a specified solid angle, and the statistical weight is multiplied by the ratio of accepted solid angle over 4π (as well as by scattering probability and attenuation).

IDEAS: <http://www.sns.anl.gov/components/montecarlo.html>

IDEAS is a general-purpose computer program for simulating neutron scattering instruments. The simulation pro-

gram utilizes a linear approach in which self-contained subroutine modules, each of them simulating the interaction of a neutron with a particular instrument component (e.g., a guide), are arranged in series to form an instrument with single or multiple beam paths. During a simulation, a set of parameters that specifies the state of a neutron is passed sequentially to the series of components or modules. Each module modifies the neutron parameters subject to the physics of the interaction. The codes of the subroutine modules are pre-compiled and loaded dynamically at run time. The use of pre-compiled modules and the dynamic loading of instrument setting allows rapid prototyping of an instrument. An integrated user interface has been implemented for Windows platforms, which reduces the work for the inclusion/deletion of a component and the change of component parameters to virtually the click of a button. IDEAS has adopted standard specifications for both the neutron parameters and the subroutine interface structure. This not only ensures a smooth passage of data between the modules, but also guarantees the reusability of existing modules. In addition, users can readily incorporate their own instrument components coded in C or Fortran.

The focusing crystals were modeled with a curved continuous surface. The algorithm for the mosaic crystal was based on the idea of Wildgruber and Passel [17]. Once a neutron hits the crystal, Monte Carlo sampling is carried out on the Bragg cone formed by the surface normal of all mosaic blocks that satisfy the Bragg condition for the incident neutron. The reflected neutron is weighted by the probability of the sampled mosaic block and the peak reflectivity. In the current module, the mosaic blocks are assumed to follow a Gaussian distribution, with different mosaic spreads in the horizontal and vertical scattering planes.

The incoherent scattering of the vanadium sample was simulated as follows. First, the neutron path through the sample was determined. Next, a scattering spot was randomly chosen (linearly) along the beam path. Finally, the direction of the scattered neutron was chosen within the specified solid angle. The scattered neutron was weighted by the solid angle and the attenuation of neutrons within the sample, which includes both the absorption and incoherent scattering. Partial correction for multiple scattering was also included.

Intensity comparisons

The first level of comparison between the codes is the absolute intensities determined at as many of the monitor positions (indicated in Figure 1) as possible. The results are shown in Figure 2. (Note that the scale changes by a factor of 10^6 after the sample.) As expected, there are no significant differences through the first collimator and aperture. Because of the variety of mosaic crystal algorithms, there are differences at D4; these differences are kept small because of the

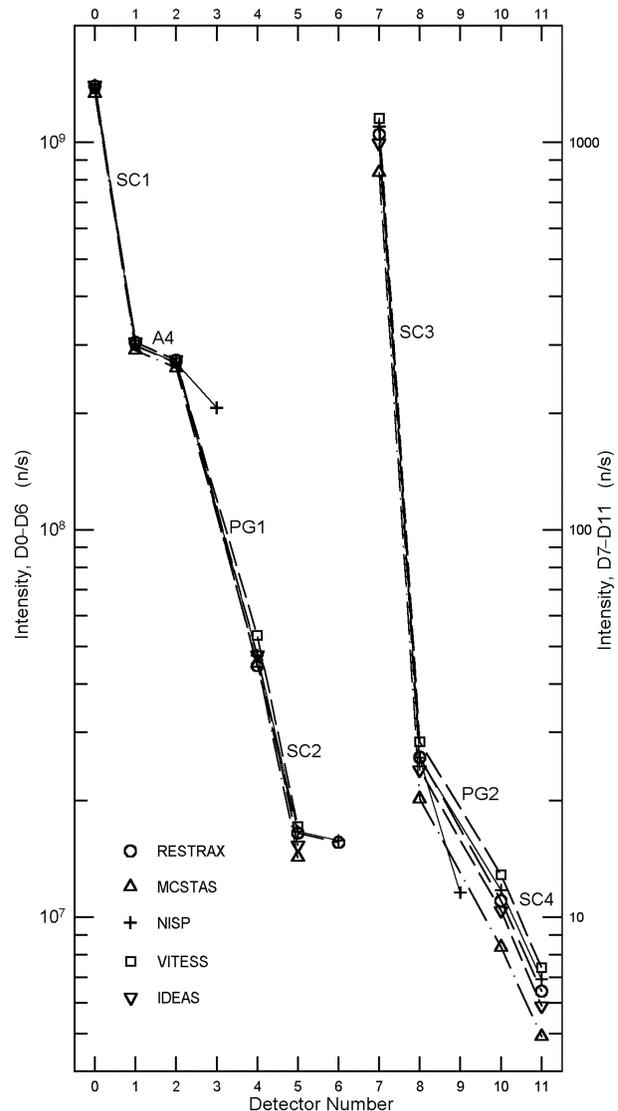


Figure 2. Comparison of integrated intensities. The horizontal axis is detector numbers from Figure 1. Note that D3, D6, and D9 are not in the principal beam and not all codes report them.

requirement to adjust model parameters to fit a specified rocking curve.

Much larger differences between codes occur for the vanadium scattering algorithm as seen at D7. The average of the five programs at D7 (which is the input area of SC3) is 1027 ± 121 n/s. The relative loss of neutrons beyond that point is essentially the same for all codes. The ratio of counts of D11 to D7 is 0.00613 ± 0.00023 . That is, the (unbiased) relative standard deviation at D7 is 12%, but for the ratio D11/D7 it is reduced to 3.7%. This is surprisingly good agreement!

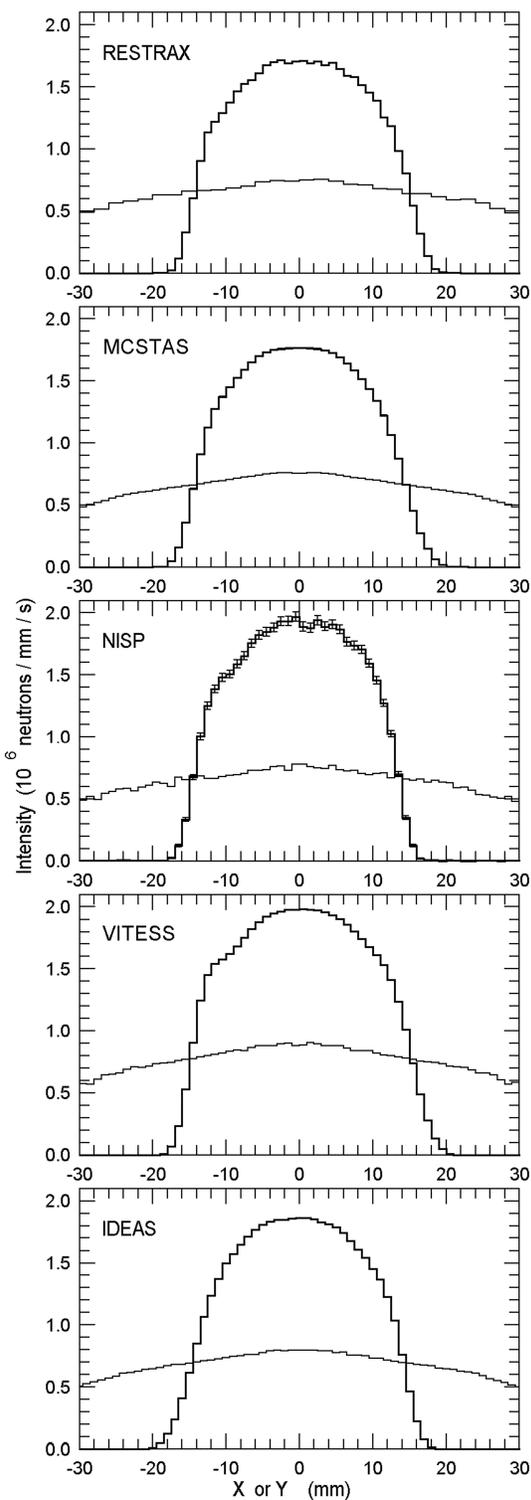


Figure 3. Horizontal and vertical beam profiles at D4 (after PG1).

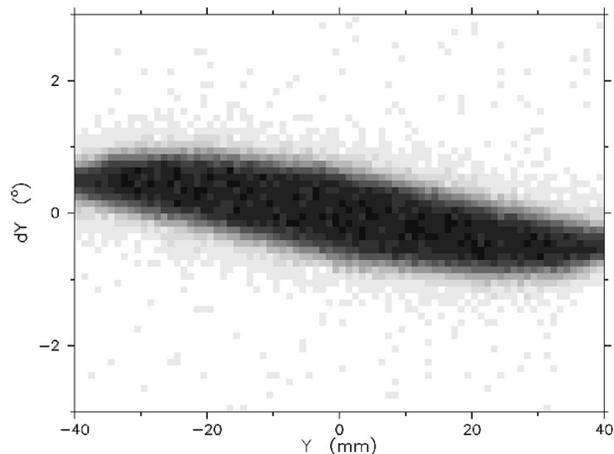


Figure 4. Vertical acceptance diagram at D4. The negative slope illustrates the focusing effect of the curved monochromator. Monte Carlo acceptance diagrams show density fluctuations in addition to outlines. The gray scale is proportional to the square root of the intensity, with the lightest shade being 0.4% of the maximum.

The intensity distributions at D4 (monochromator output) are compared in Figure 3. The heavy lines are horizontal and the lighter lines are vertical distributions, and error bars are shown on the horizontal data when provided by the programs. It is seen that the vertical distribution is very tall. By making a vertical acceptance diagram as in Figure 4, we see that the slope is inverted: Neutrons that are high on the detector have downward trajectories. Thus we can see the focusing effect of the curved crystal. Notice that acceptance diagrams produced by Monte Carlo show variations in phase-space density (such as fuzzy edges). This plot (made by NISP) also shows the background due to incoherent scatter from PG1. A report with a full set of acceptances and profiles for this simulation, along with examples of other information that can only be obtained by Monte Carlo, is available at ftp://strider.lansce.lanl.gov/pub/NISP/document/H8sim_Jan29.doc.

Execution times

The time it takes to prepare the data for a simulation is totally dependent on the familiarity of the user with the particular package being used. Likewise, the time spent on the “learning curve” of a package is very subjective, and no attempt will be made to quantify it. We can make some statements about execution time, but even that is difficult to compare because of different computer speeds and different

statistical precision for the various runs in this study. Furthermore, times are highly dependent on the problem, and on details (such as solid angle to be sampled), which were not optimized in the model definition used in this study. All times have been adjusted to represent a statistical precision (standard deviation) of 1% in the final detected count rate, assuming the variance is inversely proportional to the length of the run. (In some cases, the times have been reduced to represent more optimized conditions.) The results are: RESTRAX, 6.0 minutes (500 MHz Alpha); MCSTAS, 90 minutes (667 MHz Alpha); NISP, 23 minutes (600 MHz Pentium III); VITESS, 10.5 minutes (667 MHz Alpha); and IDEAS, 58 minutes (600 MHz Pentium III). The real significance of these times is that reasonable statistics can be obtained with any current package on today's computers in times less than an hour. Thus parametric studies to optimize instrument designs are practical.

Conclusions

When this project was first reported at the ICNS 2001 meeting in Munich, there were significant differences in the monochromator efficiency (D4). This was largely due to variations in the way mosaic spread is applied. By adjusting parameters so that all codes produce the same rocking curve, the *rms* spread was reduced from 13% to 6.5%. The largest remaining difference between codes is the treatment of absorption and multiple scattering in the vanadium sample.

We are now very satisfied with the level of agreement between these programs. The next step should be to compare the results to actual experiments. Unfortunately, the H8 instrument is not available for measurements, and study of the log books did not uncover an absolute calibration of the instrument. Thus, the next step involves selecting an instrument that is well defined and available for calibration measurements. Possibilities are IN3 or IN12 at ILL.

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