Title: Monte Carlo Code for Neutron Scattering Instrument Design and Analysis

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Monte Carlo Code for Neutron Scattering Instrument Design and Analysis

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Abstract
This is the final report of a one-year, Laboratory-Directed Research and Development project at the Los Alamos National Laboratory. The development of next-generation, accelerator-based neutron sources calls for the design of new instruments for neutron scattering studies of materials. It will be necessary, in the near future, to evaluate accurately and rapidly the performance of new and traditional neutron instruments at short- and long-pulse spallation neutron sources, as well as continuous sources. We have developed a code that is a design tool to assist the instrument designer model new or existing instruments, test their performance, and optimize their most important features.

1. Background and Research Objectives

Next-generation (greater than 1 MW) spallation neutron sources are currently being studied worldwide. The motivation behind the present flurry of activity stems partly from the desire to overcome the intensity “barrier” that presently limits many neutron scattering experiments, and partly from the rapidly increasing demand for neutrons as a tool for basic studies in many disciplines ranging from condensed matter physics to structural biology. In fact, the development of an accelerator-driven, 1-MW, long-pulse, spallation-neutron source for neutron scattering and the upgrade of the short-pulse spallation source (LANSCE 1.5) have been identified as main thrust areas for the Laboratory in the coming years.

Undoubtedly, the design, optimization, and analysis of new instruments for neutron sources is a major issue in the design of next-generation neutron sources. The complexity of these instruments, coupled with the desire to optimize their performance as much as possible, calls for design tools that go beyond traditional ray-tracing techniques. Simultaneously, the development of moderator simulation methods and recent advances in high-performance computing make detailed moderator information (time and energy neutron pulse structure)

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available to the instrument designer. The only way to make use of this information is in a computer simulation.

Many new instruments and families of instruments have been proposed for next-generation spallation sources. It will be necessary to evaluate accurately and rapidly whether these new ideas are viable, and if so, how an instrument would perform at a given source. Following the preliminary design phase, instrument optimization with the Monte Carlo code could lead to substantial additional gains. Finally, even the performance of more traditional instruments in use at neutron sources throughout the world is still not completely understood and could benefit from a detailed analysis with our code.

The objective of this project was to develop a Monte Carlo computer code for the design, optimization, and analysis of arbitrarily complex instruments for neutron scattering. A window-based, mouse-driven user interface facilitates the definition of instrument geometries and the addition of new element types to the code. The code was benchmarked by comparison with experimental data obtained on existing instruments. The code can be used in conjunction with complex models of neutron sources and moderators (e.g., reactor cold and hot sources, coupled and decoupled moderators) to explore the dependence of the performance of neutron scattering instruments at various types of sources. Besides code development, benchmarking, and fundamental understanding of instrument performance at various sources, we simulated several instruments of interest for the LPSS, namely instruments for elastic scattering such as a small-angle neutron scattering diffractometer, neutron reflectometer, Laue crystal diffractometer, neutron powder diffractometer, and instruments for inelastic scattering such as a multi-chopper spectrometer and a cold neutron triple-axis spectrometer.

2. Importance to the Laboratory's Science and Technology Base and National R&D Needs

The computer code we have developed and the studies performed with it will directly impact such LANL tactical goals as the neutron laboratory and the science-based stockpile stewardship program. Indeed, the code will be used to design an instrument suite for the LANSCE target upgrade project, to design the short- and long-pulse spallation sources, and to help in the design of critical SBSS experiments at existing and future neutron scattering instruments. The computer modeling and simulation of highly complex experimental equipment (neutron scattering instruments) from simple modules based on the fundamental laws of neutron optics and the study of the resulting performance of these instruments is a scientific premiere. It will lead to significant scientific progress in neutron source design and
use, and will help the Laboratory to remain on the cutting edge of neutron science and technology.

3. Scientific Approach and Results to Date

The code we have developed for instrument design is a Monte-Carlo code for neutron optics. It allows the user to define an instrument by selecting components from a library, to specify the characteristics of these components, and to arrange them in space to form a complete instrument. The code then transports neutrons in the instrument, much in the way in which a real instrument operates (analog Monte Carlo simulation). The detector counts are then analyzed using standard data analysis procedures to extract whatever information is needed.

The implementation of the code is user friendly. We have developed a first prototype of a windows-based user interface that allows the instrument designer, who is an expert in neither nuclear physics nor computer science, to make rapidly mock up an instrument geometry. The interface also allows the expert user to add new instrument components and test their performance easily. The interface is based on the object-oriented paradigm and is easily maintainable and expandable. Its usefulness has been demonstrated by setting up in minutes instrument configurations that previously required several days of coding and thousands of lines of FORTRAN code. A first version will soon be released for use by general users. The interface can also be used to run and control the Monte Carlo simulation itself.

New components have been added to the standard library of instrument elements. We have developed and implemented new physics models for: flat and curved monochromators (isotropic and anisotropic mosaic structure); a general neutron filter; two different types of drum choppers, including a Fermi chopper; a general sample scattering according to an arbitrary scattering law; $S(q, \omega)$; a general powder sample for neutron powder diffractometry (general composition and space group); a general multi-layered sample for neutron reflectometry; a delta function scatterer for inelastic scattering; several types of one- and two-dimensional detectors on flat and curved surfaces; super mirrors; and Soller collimators.

Libraries of new sample scattering kernels were added, as mentioned above, for use with small angle scattering, reflectometry, powder diffractometry, and quasi-elastic scattering.

New moderator source terms were calculated for the future 1-MW LPSS and SPSS cold and hot, coupled and decoupled moderators. Source terms were also produced for the existing target stations at LANSCE. Reactor source terms for the cold sources at ILL and NIST were also obtained. A generic Maxwell-Boltzmann source term was produced to facilitate comparison with simple analytical calculations. Several variations of these source terms were
also calculated to study systematically the effect of varying certain neutron pulse features (rise time, long tails, repetition rate, etc.).

Code benchmarking comparisons were made between existing instruments at LANSCE (LQD, SPEAR, NPD) and calculations done with the Monte Carlo code. Reasonable to good agreement was observed in most cases. More refined models and better source terms should help improve the agreement between experimental results and simulations.

We modeled a number of existing instruments (LQD, NPD, and SPEAR at LANSCE; the NIST reflectometer; and the IN5 multi-chopper spectrometer at ILL), one instrument under construction (the cold neutron triple-axis spectrometer at NIST), and several proposed instruments for the LPSS (reflectometer, small-angle scattering, and a multi-chopper spectrometer).

The recent Berkeley workshop on neutron instrumentation for long-pulse spallation sources, which was organized jointly by LANL and LBNL and attended by representatives from all main neutron scattering centers (ANL, BNL, ORNL, Missouri, NIST, ISIS, PSI, KENS, ILL, KFA-Juelich, Hahn-Meitner Institute), has further clarified the type of instruments that could perform well at a LPSS. Preliminary Monte Carlo results for small-angle neutron scattering and reflectometry were presented and reviewed in great detail. As a result, the workshop participants endorsed the Monte Carlo method wholeheartedly and encouraged us to pursue its development and application, particularly to determine the performance of complex instruments for inelastic neutron scattering (e.g., cold neutron triple-axis spectrometer, PRISMA-type machine) and to investigate specific problems that are difficult to address with ray-tracing techniques (e.g., effect of "long tails" in the neutron pulse, chopper jitter effects). It was pointed out that in many cases, the Monte Carlo technique is likely to be the only way to design portions of instruments as complex as, for instance, the double analyzer system in the secondary spectrometer of PRISMA at ISIS. Many participants indicated their desire to start using the code at their home institution as soon as a first version becomes publicly available.

**Acronyms Used**

ANL - Argonne National Laboratory
BNL - Brookhaven National Laboratory
ILL - Institut Laue Langevin
ISIS - Rutherford Laboratory Neutron Facility
KENS - KEK (Japan High-Energy Physics Laboratory) Neutron Source
KFA - Kernforschunganlage
LANL - Los Alamos National Laboratory
LANSCE - Los Alamos Neutron Scattering Center
LANSCE 1.5 - Los Alamos Neutron Scattering Center, intermediate upgrade configuration
LBNL - Lawrence Berkeley National Laboratory
LDRD Laboratory Directed Research and Development
LPSS - Long Pulse Spallation Source
LQD - Low Q Diffractometer
NIST - National Institute of Standards and Technology
NPD - Neutron Powder Diffractometer
ORNL - Oak Ridge National Laboratory
PRISMA - Multianalyzer Spectrometer
PSI - Paul Scherrer Institute
SBSS - Science-Based Stockpile Stewardship
SPEAR - Surface Profile Analysis Reflectometer
SPSS - Short-Pulse Spallation Source