Status of the VIM Monte Carlo Neutron/Photon Transport Code

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SUMMARY
Recent work on the VIM Monte Carlo code has aimed at advanced data libraries, ease of use, availability to users outside of Argonne, and fission source convergence algorithms in eigenvalue calculations. VIM is one of three US Monte Carlo codes in the USDOE Nuclear Criticality Safety Program, and is available through RSICC and the NEA Data Bank.

I. BACKGROUND

VIM solves the steady-state neutron or photon transport problem in any detailed three-dimensional geometry using either continuous-energy ENDF/JEF nuclear data or multigroup cross sections. VIM has been in use and under development at ANL since the 1970s, and has been applied extensively for benchmarking more approximate transport methods and codes used in reactor experiment analysis, as well as in criticality, reactor, and shielding analyses of systems with irregular geometries or dramatic neutronic heterogeneities.

II. DESCRIPTION

Neutron transport is carried out in a criticality mode or in a fixed source mode (optionally with subcritical multiplication), while photon transport is fixed source. Trajectories and scattering are continuous in direction, and anisotropic elastic and discrete level inelastic neutron scattering are described with probability tables derived from ENDF/B data. The code is written in FORTRAN 77 with minor FORTRAN 90 extensions.

A web-based user's guide has been developed that is now part of the export package. It allows easy navigation among the sections on the guide, and includes information on the nuclear data libraries, the auxiliary codes, complete input specifications, about twenty sample inputs, sample job scripts, and some algorithm details.

A. Geometry

The fundamental geometry options are infinite medium, plate lattice (where each zone is rectangular), and combinatorial geometry[1]. Reactor lattices can be constructed using cells built with combinatorial geometry, repeating in cell assignments in hexagonal or rectangular arrays. Boundary conditions include vacuum, specular and white reflection, and periodic boundaries for reactor cell calculations.

A new input geometry visualization code, SLICER, is used to verify and debug geometry. Written in C++, SLICER generates two-dimensional PostScript snapshots of nearly all possible geometric configurations. Any two attributes of each point in the plot domain (e.g., composition, edit region, source guess region, lattice cell, or zone) can be simultaneously displayed in one plot using both color fill and text labels (Figure 1)

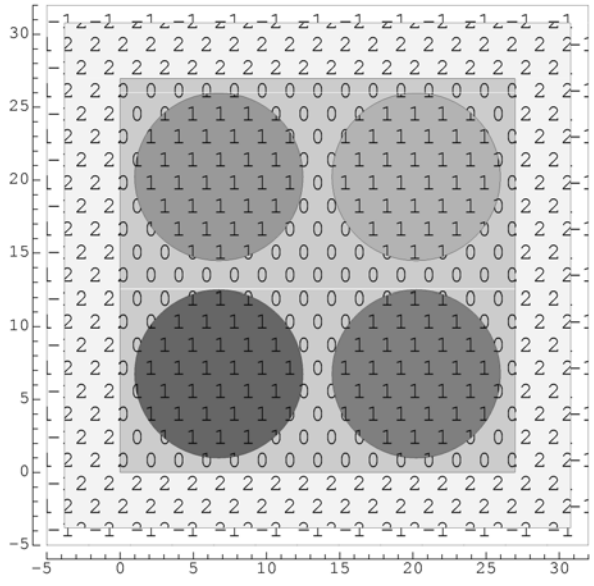

Figure 1. Sample SLICER snapshot (zones in greyscale, compositions identified by number).

B. Variance Reduction
Optional variance-reduction techniques include geometric splitting/Russian roulette and non-terminating absorption with non-analog weight cutoff energy. Absorption events are used in lieu of collision events to spawn potential fission sites in order to reduce the variance arising from variable numbers of collisions in high-scattering fissionable compositions.

The multiplication factor (k_{eff}) is determined by the optimum linear combinations[2] of two of the three eigenvalue estimates - absorption, collision, and track length. A restart capability is available to enable user-directed statistical convergence.

Several auxiliary codes are used to evaluate statistical properties of tallies. One, REBATCH, regroups generation-by-generation tally records to reduce or eliminate the effects of serial correlation of reaction rate and flux estimates. A second, RETALLY, repeats the statistical analysis of tally data, optionally with group condensation and/or spatial homogenization, or skipping early generations. A third, KEFCODE, repeats the statistical analysis of k_{eff} tallies with rebatching or omitting additional settling generations.

C. Tallies
Eigenvalues are estimated using three estimators: absorption, collision, and track length. The serial correlation of eigenvalue estimates is computed to correct underestimated eigenvalue uncertainties from correlated sequences[3]. Eigenvalues are provided for each generation, cumulatively for each generation, and for each possible number of additional skip generations. The eigenvalue estimates from the first and last halves of the calculation are compared for statistically significant differences indicative of insufficient source convergence.

In addition to eigenvalue estimates, track-length or collision estimates of reaction rates are automatically tallied by nuclide, energy group and edit region. Group-wise edits include isotopic and macroscopic reaction rates and cross sections, group-to-group scattering cross sections, volume-integrated net currents, and scalar fluxes. The reaction rates include fission, fission production, absorption, capture, elastic scattering, inelastic scattering, and (n,2n) reaction rates.

Particle pseudo-collisions can be used to estimate microscopic group-to-group (n,2n), inelastic, and P_N elastic scattering rates and cross sections. A utility that converts the principal cross sections and the scattering matrices produced by VIM to ISOTXS format is in use at ANL. Cross sections through order P_1 produced in this way have been used at ANL in physics analyses of systems so heterogeneous that no fundamental mode spectrum can be assumed in many important regions.

C. Benchmarks
VIM and its associated ENDF/B-IV,- and ENDF/B-V-based nuclear data files have been benchmarked extensively against a variety of critical experiments. These include many of the small unreflected and moderated criticals, but most notably the well-characterized Zero Power Reactor and Zero Power Physics Reactor critical series. In these tests, k_{eff}, fluxes and spatial reaction rate distributions have been compared with measurements. Furthermore, k_{eff}, regionwise group reaction rates (and ratios), effective group cross sections, and group fluxes have been compared in detail with those from codes using other data libraries and transport methods.

D. Parallel Algorithm
The parallel version uses a message-passing master-slave algorithm that incorporates natural load balancing on multiple-instruction multiple-data architectures with distributed memories, e.g., a network[4]. The master performs the input processing and provides each slave processor with a complete set of input data arrays. The master process assigns a task (a subset of the histories within a generation) to each of the slave processors and then provides additional tasks to any processor that has completed its assigned work, until all the tasks are assigned. In this way, with appropriately set generation and task sizes, processors with different speeds or interactive loads are accommodated with minimal efficiency penalties. At the end of each generation, source sites are sent to the master, which then constructs the source vector for the next generation. Tally transmittal can be accomplished after each batch of generations to reduce message traffic. Depending on network loads, the algorithm is scalable when using tens of nodes on a busy network, and over a hundred nodes on a dedicated parallel machine, e.g., IBM SP2[5].

The source code includes MPI-standard coding for both parallel and serial implementations that is selectively switched on or off before compilation for the nine subroutines for which parallel and

serial versions are very similar. Only three subroutines have independent serial and parallel versions, and another three are used only in the parallel version. The master and slave both run the same executable.

III. NUCLEAR DATA LIBRARIES

The VIM nuclear data libraries are produced using locally developed or enhanced codes that are completely independent of commonly used continuous-energy processing codes, e.g., NJOY. The detail in the evaluated cross section data is faithfully preserved. Neutron interactions that are explicitly included are elastic, inelastic and thermal scattering, (n,2n), fission, and capture, which includes (n,t), (n,p), (n,alpha), etc.

Resonance and smooth cross sections are specified pointwise[6] with linear-linear interpolation, usually with many thousands of energy points. The method used for Reich-Moore data is taken from the WHOPPER code[7]. Doppler broadening is accomplished using a "time-dependent" algorithm in which temperature is incremented in lieu of time. Since 1972, unresolved resonances have been described by the probability table method[8], which allows the statistical nature of the evaluated resonance cross sections to be incorporated naturally into the representation of self-shielding effects. In this implementation, each total cross section is partitioned into its constituent reactions in proportion to the conditional means of the constituent reactions. Thermal scattering law data is represented as double-P_1 kernels integrated to form a scattering matrix.

Currently, ENDF/B Version IV (106 nuclides), Version V (121 nuclides), and Version VI[9] (192 nuclides) libraries are available as is a JEF-2.2 library (173 nuclides). Some nuclides have been processed at temperatures above 300(K). Photon interaction data for pair production, coherent and incoherent scattering, and photoelectric events are taken from MCPLIB[10].

An auxiliary code, XSEDIT, edits, or converts between binary and ASCII, processed continuous-energy physics data. A system of shell scripts invoking XSEDIT and other smaller programs is used for inter-library comparisons. This system performs simultaneous cross sections plots for various reactions from two different VIM libraries or between a VIM library and an MCNP library. It also produces a common energy mesh with interpolated data that is used for difference plots and a summary edit of the twenty largest unrelated differences between the libraries. This has become a primary nuclear data quality assessment tool complementing physics benchmarks.

Another auxiliary code, ISOVIM, produces multigroup VIM material files from COMPXS or ISOTXS standard interface files[11] or from ASCII output, e.g., CASMO[12].

IV. SPECIAL APPLICATIONS

Small-scale parallel Monte Carlo depletion calculations have been carried out using a shell script that alternately runs the DRAGON lattice physics code[13] and VIM and interface codes that provide depleted atom densities from DRAGON to VIM and fluxes and cross sections from VIM to DRAGON.

ACKNOWLEDGMENTS

Work supported by the U.S. Department of Energy, Nuclear Energy Program under Contract W-31-109-ENG-38.

The initial version of VIM was written at Atomics International by L. B. Levitt and R. C. Lewis. Major contributions to the present version were made by R. E. Prael. F. B. Brown and D. M. Malon completed much of the parallelization work.

REFERENCES

1. M. O. Cohn et al., "SAM-CE: A Three-Dimensional Monte Carlo code for the Forward Neutron and Forward and Adjoint Gamma Ray Transport Equations," MR-7021, Mathematical Applications Group, Inc. (1971).

2. M. Halperin, "Almost Linearly Optimum Combination of Unbiased Estimates," *Am. Statis. Assoc. Journal*, **56**, p. 36 (1969).

3. D. B. McMillan, "Monte Carlo Confidence Limits for Iterated-Source Calculations," *Nucl. Sci. Eng*. 50, 73 (1973).

4. R. N. Blomquist and F. B. Brown, "Parallel Monte Carlo Reactor Neutronics," *Proceedings of the 1994 Society for Computer Simulation Simulation Multiconference*, San Diego, CA, pp. 182-187 (April 1994).

5. B. Shi and R. N. Blomquist,"Performance Studies of the Parallel VIM Monte Carlo Code," *Trans. Am. Nucl. Soc*. **74**, pp. 169-171 (June 1996).

6. J. M. Otter, "UNICORN-A Program to Calculate Point Cross Sections from Resonance Parameters, NAA-SR-11980, Vol. VI (June 1966).

7. R. N. Hwang, “A Rigorous Pole Representation of Multilevel Cross Sections and Its Practical Applications,” *Nucl. Sci. Eng.* 96, 192 (1987).

8. J. M. Otter, R. C. Lewis, and L. B. Levitt, "U3R, A Code to Calculate Unresolved Resonance Cross Section Probability Tables," AI-AEC-13024 (July 1972).

9. R. N. Blomquist, “VIM: Initial ENDF/B-VI Experience”, *Trans Am. Nucl. Soc.* 76: 327(1997).

10. Los Alamos Monte Carlo Group, "MCNP - A General Monte Carlo Code for Neutron and Photon Transport, Version 2B," LA-7396-M, Revised (April 1981).

11. R. Douglas O'Dell, "Standard Interface Files and Procedures for Reactor Physics Codes, Version IV," USDOE Report LA-6941-MS, Los Alamos National Laboratory (September 1987).

12. M. Edenius and A. Ahlin, "CASMO-3 Users Manual," STUDSVIK/NFA-86/7 (1986).

13. G. Marleau, A. Hebert, and R. Roy, “A User’s Guide for DRAGON”, IGE-174 Rev. 2, Ecole Polytechnique de Monteal (1997)“.

Table 2. ADMT-456 Final Data

Description	One	Two	Three
Cfhdljfd8	128.5	8.66	0.649
Dfjkjicj nmks	147.3	8.58	0.458
Wsf mkdfsi	136.3	9.48	0.547
Kjdejit ji uj	115.4	9.36	0.516

If equations are displayed, they should be centered with one space before and after and Arabic numbered. The equation number should be in parenthesis and flush right.

$$U(x)/U_{\phi} = XYZ^{\Psi} \qquad (1)$$