VIM: A CONTINUOUS ENERGY MONTE CARLO CRITICALITY CODE

Roger N. Blomquist
Argonne National Laboratory
9700 S. Cass Ave.
Argonne, IL 60439-4803
RNBlomquist@anl.gov
(630)-252-8423

ABSTRACT

1. Program Name and Title: VIM: A continuous energy neutron and photon transport code.

2. Computer for which Program is Designed and Other Machine Versions Available: RSICC Packages are available for Sun SPARC Station (Solaris) and other UNIX workstations, including IBM RS6000 (AIX). Has also run on Apollo, IBM SP 128-node parallel system (AIX); Cray (COS, UNICOS) and IBM mainframes (MVS).

3. Problem Solved: VIM[1] solves the steady-state neutron or photon transport problem in any detailed three-dimensional geometry using either continuous energy-dependent ENDF nuclear data or multigroup cross sections. Neutron transport is carried out in a criticality mode, or in a fixed source mode (optionally incorporating subcritical multiplication). Photon transport is simulated in the fixed source mode. The geometry options are infinite medium, combinatorial geometry [2], hexagonal or rectangular lattices of combinatorial geometry unit cells, and rectangular lattices of cells of assembled plates. Boundary conditions include vacuum, specular and white reflection, and periodic boundaries for reactor cell calculations.

The code is one of the three criticality safety codes comprising the Analytical Methods and Benchmarking task areas of the Department of Energy's Nuclear Criticality Safety Program [3]. The ZPR-9 Assembly 34, ZPR-6 Assembly 9 and other Criticality Safety benchmark experiments [4] have been analyzed with VIM, and it has also been applied to the NEA Pu recycle[5], Burnup Credit[6], and Power Distribution Within Assemblies[7] benchmarks. The code has been used in a variety of criticality safety analyses, including a utility spent fuel storage fuel, the IPNS booster target, etc. It is currently a testing platform for the application of stratified sampling techniques to problems with slow and unpredictable fission source convergence.

VIM was developed originally as a reactor criticality code. Its tally and edit features are very easy to use, and automatically provide fission, fission production, absorption, capture, elastic scattering, inelastic scattering, and (n,2n) reaction rates for each edit region, edit energy group, and isotope, as

well as the corresponding macroscopic information, including group scalar fluxes. Microscopic and macroscopic cross sections, including microscopic P_N group-to-group cross sections are also easily produced. 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. A comprehensive validation bibliography is available. In addition to normal quality control check, the ENDF/B-VI and JEF2.2 VIM libraries have been benchmarked computationally.

4. <u>Method of Solution</u>: VIM uses standard Monte Carlo methods for particle tracking with several optional variance-reduction techniques. These include splitting/Russian roulette, non-terminating absorption with nonanalog weight cutoff energy. The multiplication factor (k_{eff}) is determined by the optimum linear combinations[8] of two of the three eigenvalue estimates — analog, scoring $\nu\Sigma_f/\Sigma_a$ at each absorption; collision, scoring $\nu\Sigma_f/\Sigma_t$ at each collision; and track length, scoring $\nu\Sigma_f \ell$ on each track segment.

Resonance and smooth cross sections are specified pointwise with linear - linear interpolation[9], Frequently with many thousands of energy points. Unresolved resonances are described by the probability table method [10], which allows the statistical nature of the evaluated resonance cross sections to be incorporated naturally into the representation of self-shielding effects. Neutron interactions are elastic, inelastic and thermal scattering, (n,2n), fission, and capture, which includes (n,t), (n,p), (n,α), etc. Photon interaction data for pair production, coherent and incoherent scattering, and photoelectric events are taken from MCPLIB.[11] 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.

Recent development work has been aimed at upgrading the nuclear data libraries. ENDF/B-VI and JEF-2.2 data have been processed, accommodating the Reich-Moore formation in the resolved range and the intermediate structure data in the unresolved range. Processing is now much faster because a single supervisory shell script controls all of the cross section processing codes. An automated plotting package has been developed that produces plots of all cross sections secondary energy distribution, scattering angle distributions, and unresolved resonance probability tables. Large libraries of ENDF/B-IV, V, VI and JEF-2.2 data have been processed.

VIM has an automatic restart capability to permit user-directed statistical convergence. In eigenvalue calculations, the beginning source sites are from a random (flat) guess, or can be provided via ASCII input, or from a previous calculation. The starting neutrons for each subsequent generation are randomly selected from the potential fission sites in the previous generation.

Track-length or collision estimates of reaction rates are automatically tallied by energy group and edit region to facilitate comparison to other calculations. Group edits include isotopic and macroscopic reaction rates and cross sections, group-to-group scattering cross sections, net currents, and scalar fluxes. Particle pseudo-collisions are used to estimate microscopic group-to-group (n,2n), inelastic, and P_N elastic scattering rates. The serial correlation of eigenvalue estimates is computed to detect underestimated errors.

Recently, a depletion capability has been developed in which a shell script alternatively runs VIM to produce fluxes and cross sections for the DRAGON physics code, which in turn solves the depletion equations.

Other recent developments include a web based User's Guide, the capability to mix libraries (e.g., ENDF/B-V ^{235}U with an ENDF/B-VI library) at run time.

Auxiliary codes allow post-Monte Carlo group collapse, spatial homogenization, and statistical re-analysis of eigenvalue, reaction rates, group cross sections, and scalar fluxes.

Recently, a version of the code has been developed for parallel execution on MIMD distributed memory architectures such as heterogeneous networks of workstations and scalable multi-processor computers. Speedups of x80 have been attained on a 120-node IBM-SPI [12,13]. A skip-ahead random number generator is used for reproducibility between different machines. A naturally load-balancing parallel algorithm provides high efficiency even when many processors are used. The MPI standard syntax [14] has been used to promote portability.

5. Restrictions on the Complexity of the Problem: The maximum number of nuclides in one calculation is 40. The maximum number of splitting surfaces is 60. Variable dimensioning accommodates all other problem characteristics.

6. Typical Running Time: Varies widely, depending on geometric complexity, the number of isotopes, application of absorption weighting and splitting, overall scattering ratio, and desired statistics. A 6000-zone calculation of the Savannah River LTR-IIa reactor k_{eff} to a one standard precision of 0.3% requires approximately10 minutes on a Sun Sparc 20.

7. Unusual Features: Unresolved resonance probability tables, combined parallel-serial source code, ENDF/B-IV, -V, -VI, and JEF2.2 libraries, depletion capability with the DRAGON physics code.

8. Related and Auxiliary Programs: The RSICC code package includes associated utility codes for re-analysis of tally data, problem library preparation, and input visualization.

9. Status: The code and ENDF/B-IV and –V libraries are available at RSICC.

10. <u>References:</u>

1. R. N. Blomquist, "VIM-A Continuous Energy Monte Carlo Code at ANL," A Review of the Theory and Application of Monte Carlo Methods, Proceedings of a Seminar-Workshop, ORNL/RSIC-44 (April 1980).

2. 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).

3. "United States Department of Energy Nuclear Criticality Safety Program Five Year Plan", August 1999.

4. "International Handbook of Evaluated Criticality Safety Benchmark Experiments", NEA/NSC/DOC (95) 03, OECD.

5. "Physics of Plutonium Recycling", OECD/NEA, Working Party Report, 1995.

6. H. Okuno, et. al., "International Studies on Burnup Credit Criticality Safety by an OECD/NEA Working Group – Calculation Benchmarks for BWR Spent Fuels", Proceedings of the Sixth International Conference on Nuclear Criticality Safety, Versailles, France, September 20-24, 1999.

7. "Benchmark Calculations of Power Distributions within Assemblies", OECD NEA/NSC/DOC (94) 28, 1994.

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

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

10. 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).

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

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

13. 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).

14. M. Snir, et.al., MPI: The Complete Reference, The MIT Press, Cambridge, MA, 1996.

11. Computer Hardware Requirements:

- VIM Executable: 1 Mbyte memory
- Other Executables: < 0.5 Mbytes each
- Base Cross Section Libraries: 100 Mbytes disk
- Run-time Cross Sections (parallel): 8 Mbytes memory
- Run-time Cross Sections (serial): 4 Mbyte memory
- Restart/tally files: Highly problem-dependent

12. Programming Language(s): FORTRAN 77, except for dynamic memory allocation routines which are provided in C for UNIX systems.

13. Operating System (s): UNIX, AIX, UNICOS

14. Other Programming or Operating Information of Restrictions: At RSICC, the system was successfully tested on an IBM RS/6000 model 590 under AIX 4.2 with XLF77 version 3.2.2 and on the Sun Sparc 20 running SUNOS 5.6 (Solaris 2.6) with f77 version 4.2. The proprietary DISSPLA plotting software is called but this coding can be easily removed. VIM produces a PostScript file containing the assembly layout of hex-lattice reactor cores, which may then be printed if a PostScript driver is available. The parallel version includes MPI standard subroutine and function calls.

15. Name and Affiliation of Author or Contributor:

Roger N. Blomquist
Reactor Analysis Division
Argonne National Laboratory
9700 S. Cass Ave.
Argonne, IL 60439-4803
RNBlomquist@anl.gov
(630)-252-8423

16. Material Available: The RSICC package includes the referenced document and either a CD-ROM or tape cartridge with a compressed Unix tar file which contains installation instructions, the User's Guide, Fortran source (VIM, cross section library management codes, post-processing codes, multigroup library production code, and a geometry input checking code), test cases, and binary ENDF/B-IV and -V neutron physics libraries processed at ANL and the associated photon data.

17. Category: B. J. C

Keywords: Neutronics, Criticality, Criticality Safety, Monte Carlo, Neutron Transport, Photon Transport

18. Sponsor: Development was sponsored by U.S. Department of Energy, Office of Nuclear Energy, Science, and Technology. Current development is sponsored by the US DOE Office for Environmental Management for use by the criticality safety community. 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.