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Overview of Monte Carlo radiation transport codes

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ABSTRACT

The Radiation Safety Information Computational Center (RSICC) is the designated central repository of the United States Department of Energy (DOE) for nuclear software in radiation transport, safety, and shielding. Since the center was established in the early 60's, there have been several Monte Carlo (MC) particle transport computer codes contributed by scientists from various countries. An overview of the neutron transport computer codes in the RSICC collection is presented.

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1. Introduction

The Radiation Shielding Information Center (RSIC) was established in 1963 in response to the Weinberg Report titled "Science, Government, and Information". In 1996, RSIC became RSICC to reflect the scope of technical coverage and to keep up with changing computational technology. RSICC is charged by United States government agencies to collect, test, package, and disseminate computational tools used in radiation shielding, transport, and protection. RSICC is the custodian of more than 1700 computational tools gathered from national and international laboratories, educational institutions, and private industry. Together with the Nuclear Energy Agency Data Bank in Paris, France, RSICC serves as an international resource for nuclear computational tools.

Since its inception, RSICC has collected over 200 computer codes involving the Monte Carlo method. A few of them in the area of neutron transport are described in the write-up.

2. Historical Monte Carlo software

2.1. O5R

One of the earliest neutron transport code was the Oak Ridge Random Research Reactor Routine (O5R). O5R was originally written in FORTRAN Assembly Program (FAP) for the IBM 7090.

The O5R (Coveyou et al., 1965) code system was designed to calculate, by Monte Carlo methods, any quantity related to neutron

transport in reactor or shielding problems. The system consisted of O5R-STATEST which calculates the neutron flux, for various energy bins, at various points by statistical estimation; and O5R-K which calculates the multiplication constant of a chain-reacting system. Sources may have arbitrary spatial, energy, and angular distributions via a subroutine written by the user. Arbitrary three-dimensional geometries bounded by quadric surfaces may be treated. Anisotropic scattering can be included for both elastic and inelastic processes. Fissionable as well as non-fissionable media can be treated. Several variance reduction techniques are available.

O5R was followed by another RSICC software package O6R and later by MORSE.

2.2. O6R

The O6R (Thompson and Straker, 1969) code system consists of modifications and extensions made to O5R, designed to calculate any quantity related to neutron transport in reactor or shielding problems. The system solves the integral Boltzmann transport equation in general phase space for the collision density of neutrons in the system. By using the appropriate analysis routines, quantities of interest such as the flux, absorption rate, neutron lifetime, and slowing down density can be estimated. A wide variety of problems in the areas of radiation shielding, reactor analysis and design, criticality safety, and neutron scattering experiments can be solved with the O6R system. The O6R-ACT1FK prototype permits simultaneous neutron transport and analysis, the specific features slanted toward the application to calculations of shields rather than reactors. It embodies all the features of O5R and ACT1FK-analysis codes with substantial improvements.

2.3. MORSE

Originally released as MORSE in 1971, MORSE-CGA (Emmett, 1985) is a general purpose of Monte Carlo multi-group neutron and gamma ray transport code with array geometry capability. It was developed at Oak Ridge National Laboratory, Oak Ridge, Tennessee and is written in Fortran 77 with some IBM assembler language for the IBM 3090 version; Cray, VAX, PC, and Unix workstations.

MORSE-CGA was developed to add the capability of modeling rectangular lattices for nuclear reactor cores or for multipartitioned structures. It thus enhances the capability of the MORSE code system. The MORSE code is a multipurpose neutron and gamma ray transport Monte Carlo code. It has been designed as a tool for solving most shielding problems. Through the use of multi-group cross-sections, the solution of neutron, gamma ray, or coupled neutron—gamma ray problems may be obtained in either the forward or adjoint mode. Time dependence for both shielding and criticality problems is provided. General three-dimensional geometry may be used with an albedo option available at any material surface. Isotropic or anisotropic scattering up to a P16 expansion of the angular distribution is allowed.

2.4. MICAP

MICAP (Johnson and Gabriel, 1988) is a Monte Carlo code for the analysis of ionization chamber responses. MICAP was developed at Oak Ridge National Laboratory, Oak Ridge, Tennessee. MICAP was written in Fortran IV and Assembler Language for the IBM 3033.

MICAP includes neutron transport and coupled electron-photon transport capabilities. For cross-sections, ENDF/B-V data, pre-processed through the RESEND5-LINEAR/SIGMA1 programs so that all cross-section data are linearly interpolated over the entire energy range, are included in the package for the following nuclides: hydrogen, carbon, nitrogen, oxygen, fluorine, aluminum, argon and calcium

MICAP was developed to determine the response of a gas-filled cavity ionization chamber or other detector type (plastic scintillator, calorimeter) in a mixed neutron and photon radiation environment. In particular, MICAP determines the neutron, photon, and total response of the detector system. The applicability of MICAP encompasses all aspects of mixed field dosimetry analysis including detector design, pre-experimental planning and post-experimental analysis. MICAP is a modular code system developed to be general with respect to problem applicability. The transport modules utilize combinatorial geometry to accurately model the source/detector geometry and also use continuous energy and angle cross-section and material data to represent the materials for a particular problem.

3. Current Monte Carlo software

3.1. TART

TART2005 (Cullen, 2005) is a coupled neutron-photon, 3-D, combinatorial geometry, time dependent, Monte Carlo transport code. It was developed at Lawrence Livermore National Laboratory (LLNL), Livermore, California. TART2005 is written in Fortran and C and runs under Windows and Linux for PCs and MACs.

Neutron and photon sources as well as neutron-induced photon production can be tracked. TART2005 uses ENDF/B-VI, Release 8 data. It uses continuous energy neutron cross-sections, in addition to its traditional multi-group cross-sections. For neutron interaction, the data are derived using ENDF-ENDL2005 and include both continuous energy cross-sections and 700 group neutron data

derived using a combination of ENDF/B-VI, Release 8, and ENDL data. The 700-group structure extends from 10 to 5 eV up to 1 GeV. Presently nuclear data are only available up to 20 MeV, so that only 616 of the groups are currently used. For photon interaction, 701-point photon data were derived using the Livermore EPDL-97 file. The new 701-point structure extends from 100 eV up to 1 GeV, and is currently used over this entire energy range.

3.2. COG

COG is a multi-particle Monte Carlo code for shielding and criticality safety applications. COG was developed at Lawrence Livermore National Laboratory, Livermore, California. COG is written in Fortran 77 and C. COG uses Monte Carlo methods to solve the Boltzmann transport equation for particles traveling through arbitrary 3-D geometries. Neutrons, photons, electrons, and protons can be transported. Electron transport uses the Electron Gamma Shower (EGS) transport kernel.

For neutron libraries, COG uses:

- ENDFB6R7 Data pre-processed from the Brookhaven ENDF/B-VI Release 7 nuclear database.
- ENDL-90 The LLNL ENDL-90 nuclear database.
- RED2002 A hybrid ENDFB/ENDL database developed by Red Cullen at LLNL.
- COGSAB Thermal scattering database using $S(\alpha, \beta)$ model.

For photon libraries, COG uses the COGGXS LLNL evaluated Photon Data Library (EPDL) photon database.

For charged particles, COG uses:

- elossr Proton stopping powers
- Landau Proton straggling data

COG is a modern, full-featured Monte Carlo radiation transport code which provides accurate answers to complex shielding, criticality, and activation problems. COG is fully 3-D, uses pointwise cross-sections and exact angular scattering, and allows a full range of biasing options to speed up solutions for deep penetration problems. Additionally, a criticality option is available for computing $k_{\rm eff}$ for assemblies of fissile materials. ENDL or ENDFB cross-section libraries may be used. COG can use either the LLNL ENDL-90 cross-section set or the ENDFB-VI set. Analytic surfaces are used to describe geometric boundaries. Parts (volumes) are described by a method of Constructive Solid Geometry. Surface types include surfaces of up to fourth order, and psuedo-surfaces such as boxes, finite cylinders, and figures of revolution. Repeated assemblies need to be defined only once. Parts are visualized in cross-section and perspective picture views.

Source and random walk biasing techniques may be selected to improve solution statistics. These include source angular biasing, importance weighting, particle splitting and Russian roulette, path length stretching, point detectors, scattered direction biasing, and forced collisions. COG will compute $k_{\rm eff}$ by transporting batches of neutrons through the system for criticality calculations. For activation, COG can compute gamma ray doses due to neutron-activated materials, starting with just a neutron source. COG can solve coupled problems involving neutrons, photons, and electrons.

COG will transport neutrons with energies in the range of 10–5 eV to 150 MeV, protons with energies up to hundreds of GeV, and photons with energies in the range of 10 eV–100 GeV. (COG's energy ranges are limited by the available cross-section sets and physics models). Using the EGS4 electron transport kernel, electrons in the range of 10 keV to a few thousand GeV can also be transported.

3.3. MCNP5/MCNPX

MCNP5/MCNPX is a Monte Carlo N—Particle transport code which includes MCNP5 1.51 and MCNPX 2.6.0 and data libraries. It is developed at Los Alamos National Laboratory (LANL), Los Alamos, New Mexico. MCNP5 (Briesmeister, 2000) can be used for neutron, photon, electron, or coupled neutron/photon/electron transport, including the capability to calculate eigenvalues for critical systems. MCNPDATA contains the standard neutron, photoatomic, photonuclear, and electron data libraries for MCNP5 and MCNPX.

Some of the new features of MCNP5 1.51 include:

- Variance reduction with pulse height tallies
- New VAR input card added to control variance reduction methods
- Annihilation gamma tracking
- Doppler broadening added to the MAKXSF utility code
- Improved $S(\alpha, \beta)$ thermal scattering
- Large lattice enhancements
- Direct RSSA file reading for distributed multiprocessing
- Improve Compton scattering PSC calculation for detectors & DXTRAN
- Web-based documentation

The MCNP5 code treats an arbitrary three--dimensional configuration of materials in geometric cells bounded by firstand second-degree surfaces and fourth-degree elliptical tori. Pointwise cross-section data are used. For neutrons, all reactions given in a particular cross section evaluation (such as ENDF/B-VI) are accounted for. Thermal neutrons are described by both the free gas and $S(\alpha,\beta)$ models. For photons, the code accounts for incoherent and coherent scattering, the possibility of fluorescent emission after photoelectric absorption, and absorption in electron-positron pair production. Electron/positron transport processes account for angular deflection through multiple Coulomb scattering, collisional energy loss with optional straggling, and the production of secondary particles including K Xrays, knock-on and Auger electrons, bremsstrahlung, and annihilation gamma rays from positron annihilation at rest. Electron transport does not include the effects of external or self-induced electromagnetic fields. Photonuclear physics is available for a limited number of isotopes.

Important standard features that make MCNP very versatile and easy to use includes powerful general source, criticality source, and surface source; both geometry and output tally plotters; a rich collection of variance reduction techniques; a flexible tally structure; and an extensive collection of cross-section data. Energy ranges are from 10^{-11} to 20 MeV for neutrons with data up to 150 MeV for some nuclides, 1 keV to 1 GeV for electrons, and 1 keV to 100 GeV for photons.

MCNPX (MCNP eXtended) (Hendricks et al., 2008; Pelowitz, 2008), an extension of MCNP, is a Fortran-90 Monte Carlo radiation transport computer code that transports many particles over a broader range of energy than MCNP. It is a superset of MCNP4C3 and has many capabilities beyond MCNP4C3. MCNPX is a production computer code that models the interaction of radiation with matter. Newer capabilities and enhancements of MCNPX include:

- Depletion and burnup;
- Heavy-ion (*Z* > 2) transport;
- Long file names;
- Delayed-particle emission;
- Criticality source convergence acceleration;
- Energy-time weight windows;

- Spherical mesh weight windows;
- Charged ions from neutron capture in table range;
- Muon capture physics.

MCNPX began in 1994 as a code-merger project of MCNP 4B and LAHET 2.8. In 2002, MCNPX was upgraded to MCNP 4C, converted to Fortran 90, enhanced with 12 new features, and released to the public as version 2.4.0. The release of version 2.6.0 includes many new features described in the "MCNPX extensions version 2.6.0" document which is provided with the MCNPX distribution. The depletion/burnup capability is based on CINDER90 and MonteBurns. MCNPX depletion is a linked process involving steadystate flux calculations in MCNPX and nuclide depletion calculations in CINDER90. Currently, the depletion, burnup, and transmutation capability is limited to criticality (KCODE) problems. Physics improvements include a new version of the Cascade-Exciton Model (CEM), the addition of the Los Alamos Quark-Gluon String Model (LAQGSM) event generator, and a substantial upgrade to muon physics. Current physics modules include the Bertini and ISABEL models taken from the LAHET Code System (LCS), CEM 03, and INCL4. Many new tally source and variance reduction options have been developed. MCNPX is released with libraries for neutrons, photons, electrons, protons and photonuclear interactions. In addition, variance reduction schemes (such as secondary particle biasing), and new tallies have been created specific to the intermediate and high-energy physics ranges. The 'mesh' and 'radiography' tallies were included for two- and three-dimensional imaging purposes. Energy deposition received a substantial reworking based on the demands of charged particle high-energy physics. An auxiliary program, GRIDCONV, converts the mesh and radiography tally as well as standard MCTAL-file results for viewing by independent graphics packages. The code may be run in parallel at all energies via PVM or MPI.

Energy ranges covered by MCNPX include:

- All standard MCNP neutron libraries over their stated ranges (~0-20 MeV).
- Neutrons in the LA150 library from 0 to 150.0 MeV in tabular range for 42 isotopes (except for 9 Be at 100 MeV).
- Neutrons from 1.0 MeV in the physics model regime.
- Photons from 1 keV to 100 GeV.
- Photonuclear interactions from 1.0 to 150.0 MeV in tabular range for 12 isotopes.
- Photonuclear interactions from 1.0 MeV in the CEM physics model.
- Electrons from 1 keV to 1 GeV.
- Protons from 1.0 to 150.0 MeV in tabular range for 41 isotopes.
- Protons from 1.0 MeV in the physics model regime.
- Pions, muons, and kaons are treated only by physics models.
- Light ions from 1 MeV/nucleon in the physics model regime.
- Heavy ions from 3 MeV/nucleon in the LAQGSM physics model.

3.4. VIM

VIM (Blomquist, 2009) is a continuous energy neutron/photon transport code. It is developed by Argonne National Laboratory (ANL), Argonne, Illinois. The current version, VIM 5.1, is written in Fortran 90 with a few subprograms in C. The geometry visualization program, Slicer, is written in C++. VIM runs on Linux PC, Sun, and Mac Pro.

VIM is a continuous energy criticality, reactor physics, and shielding code. It solves the transport problem for neutrons or photons, includes thermal neutron scattering effects, either in the eigenvalue mode or for photon or neutron fixed source. VIM features flexible geometry and neutron physics data carefully

constructed from ENDF/B data. Special neutron physics capabilities in VIM include unresolved resonance probability tables, and direct treatment of resolved resonances described with Reich—Moore parameters. It has been extensively benchmarked, using both experiments and other accurate codes.

VIM solves the steady-state neutron or photon transport problem in any detailed three-dimensional geometry using either continuous energy dependent ENDF nuclear data or multi-group 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, and 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 VIM 5.1 (April 2009) release includes data from ENDF/B-IV, ENDF/B-V, ENDF/B-VI and ENDF/B-VII.O. ASCII data libraries and a convenient means to convert them to binary on a target machine are included.

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 $k_{\rm eff}$ is determined by the optimum linear combinations of two of the three eigenvalues estimates analog, collision, and track length. Resonance and smooth crosssections are specified pointwise with linear interpolation, frequently with many thousands of energy points. Unresolved resonances are described by the probability table method, which allows the statistical nature of the evaluated resonance crosssections to be incorporated naturally into the representation of selfshielding effects. Neutron interactions are elastic, inelastic and thermal scattering, (n,2n), fission, and capture, which includes (n,γ) , (n,p), (n,α) , etc. Photon interaction data for pair production, coherent and incoherent scattering, and photoelectric events are taken from MCPLIB. Trajectories and scattering are continuous in direction, and anisotropic elastic and discrete level inelastic neutron scattering are described with probability tables derived from evaluated nuclear data. 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. Groupwise 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 PN elastic scattering. The serial correlation of eigenvalue estimates is computed to detect underestimated errors.

The maximum number of isotopes in one calculation is 100. The maximum mumber of splitting surfaces is 60. All other problem characteristics are accommodated by variable dimensioning.

3.5. TRIPOLI

TRIPOLI (Petit et al., 2008) is a coupled neutron, photon, electron, positron, 3-D, time dependent, Monte Carlo, transport code. TRIPOLI is developed by the Commissariat à l'énergie atomique, CEA/SACLAY, Cedex, France. TRIPOLI is written in Fortran 77 and C and runs on SUN, IBM, Digital, Compaq and Linux based PCs.

The data libraries are GALILEE 0.2 processed libraries in a TRIPOLI-4 specific format based on JEFF-31, FENDL-21, JENDL-33, ENDFB7R0, and EPDL-97.

TRIPOLI uses the Monte Carlo method to simulate neutron and photon behavior in three-dimensional geometries. The main areas of applications include but are not restricted to: radiation protection and shielding, nuclear criticality safety, fission and fusion reactor design, nuclear instrumentation. In addition, it can simulate electron-photon cascade showers. It computes particle fluxes and currents and several related physical quantities such as, reaction rates, dose rates, heating, energy deposition, effective multiplication factor, perturbation effects due to density, concentration or partial cross-section variations.

Neutron cross-sections are available for the following nuclear evaluations: JEFF-3.1, ENDF/B-VII.0, JENDL-3.3, and FENDL-2.1. NJOY-99.259 and CALENDF-2005 were used in GALILEE 2, which was used to process the libraries. Cross-sections and probability tables are given at 294 K. The bound nuclei cross-sections are given at every temperature available from the evaluation. Gamma cross-sections are all given from the EPDL-97 evaluation. Additional data libraries distributed with the TRIPOLI-4 include:

- ENDFB6R4: neutron, gamma data library
- ENDL: gamma data library
- JEF2: neutron, gamma data library
- Mott-Rutherford: electron, positron cross-section library
- Q-fission: energy release during fission library

Particle energies in TRIPOLI are:

Neutrons: 0–150 MeVGamma: 0–100 MeV

• Electrons/positron: 1 MeV — several GeV

3.6. SHIELD

SHIELD (Dementyev and Sobolevsky, 1994) is a Monte Carlo transport code for simulating interaction of high energy hadrons with complex macroscopic targets. SHILED is developed at the Institute for Nuclear Research of the Russian Academy of Science (RAS), Moscow, Russia. It is written in Fortran 77 for the Sun, IBM PC, and VAX.

The SHIELD code considers interaction of high-energy particles with condensed matter, including hadron-nucleus interactions inside the target, generation and transportation of secondary particles, deposition of energy and production of radionuclides in the target. The modern version of the SHIELD code allows simulation of the transfer of nucleons (including low-energy neutrons), pions, kaons, antinucleons, and muons in energy range up to 1 TeV. Recently, the transfer of ions (arbitrary A,Z-nuclei) was added. The ionization loss and straggling (optionally) are taken into account as well as the main modes of the mesons decay. The transfer of neutrons (En < 14.5 MeV) is simulated on the basis of the 28-group neutron data system BNAB. A special interface allows one to use the known EGS4 code for simulation of electromagnetic (EM) showers initiated by products of meson decay. Programs for simulation of nuclear reactions, included in the hadron-nucleus generator of the SHIELD code (Many Stage Dynamical Model-MSDM), were elaborated by N.S.Amelin, K.K.Gudima and V.D.Toneev, Joint Institute for Nuclear Research, Dubna, and by A.S.Botvina, Institute for Nuclear Research RAS, Moscow.

The SHIELD code allows one to simulate transfer of nucleons (including low energy neutrons above thermal energy), pions, kaons, antinucleons, and muons in energy range up to 1 TeV at arbitrary configuration and chemical composition of the target.

Within this scope any limitations are practically absent. The only restriction involves the transport of neutrons below 14.5 MeV. The BNAB neutron data library, used in SHIELD, includes near 40 chemical elements, but not the whole Mendeleev's Periodical Table.

3.7. MONACO/MAVRIC

Monaco is integral to the Standardized Computer Analysis for Licensing Evaluation (SCALE, 2009) code. Monaco (http://www.ornl.gov/sci/scale/news/SCALENews_Jan2008.pdf; http://www.ornl.gov/sci/scale/news/SCALENews_Jan2009.pdf) is a fixed source, 3-D generalized geometry, multi-group Monte Carlo radiation transport code. It is developed at Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Monaco is based on the same physics as MORSE but uses the SCALE Standard Composition Library and the SCALE Generalized Geometry Package (SGGP) that is used by KENO-VI. For difficult shielding problems, the MAVRIC (Monaco with Automated Variance Reduction using Importance Calculations) sequence has been developed to provide automated 3-D variance reduction by automatically creating space/energy importance maps and biased source distributions for Monaco. A new ENDF/B-VII 200 neutron group and 47 gamma group library is included in SCALE 6. Monaco is the result of a modernization effort combining the multi-group neutron and photon physics of MORSE with the flexibility of the second order surface SGGP. Major efforts have been made in bringing the coding style up to modern Fortran 95 standards so that future development can be more easily continued. Monaco is much more flexible than MORSE. Users can construct a source by specifying the separate spatial, energy, and directional distributions. Available tallies in Monaco include point detectors, region-based flux tallies and mesh tallies (a set of region tallies defined on a mesh that overlays the physical geometry). Any Monaco tally can be convolved with a response function, either user defined or from a standard list available with each SCALE cross-section library. Mesh tally values and uncertainties can be viewed with a special Java viewer that works on Windows, Unix, Linux, and Mac.

For radiation transport, MAVRIC can be optimized to calculate one specific detector response at one location using the Consistent Adjoint Driven Importance Sampling (CADIS) methodology or to calculate multiple responses/locations with roughly the same relative uncertainty using forward weighted CADIS (FW-CADIS) (Wagner et al., 2007). For calculating mesh tallies of fluxes or dose rates, MAVRIC also uses FW-CADIS to help balance the Monaco Monte Carlo calculation such that low-flux voxels are computed with approximately the same relative uncertainty as high-flux voxels.

3.8. MONK/MCBEND

MONK and MCBEND (http://www.sercoassurance.com/ANSWERS/index.php) are commercial computer codes and are distributed and actively supported by Serco in the United Kingdom (UK), as part of its ANSWERS Software Service. The development of MONK started about forty years ago. MCBEND has evolved over thirty years of development.

MCBEND is a computer program written to solve problems of radiation transport in sub-critical systems using the Monte Carlo method. MCBEND started as a basic shielding code for simple geometries. It is now capable of modeling realistic geometries in great detail and is applicable to an extensive range of problems involving the transport of neutrons, gamma rays and charged particles.

MONK is a code written for both criticality safety and reactor physics depletion problems. It uses superhistory powering to accelerate the source convergence. It is supplied with validation data taken from the International Criticality Safety Benchmark Experiments Program (ICSBEP) handbook.

Both codes use Simple Body Geometry input to construct the main components of a model through the use of a hierarchy of PARTS that can be independently modeled. This extremely versatile geometry system is further enhanced with HOLE geometries based on Woodcock tracking that uses simple generic input to provide greater flexibility with repeating structures and additional detail for systems such as bent fuel pins, PBMR, dropped fuel rods and many others. A range of nuclear data libraries is available based on JEF, ENDF and JENDL evaluations.

4. Conclusion

Monte Carlo computer codes continue to be important in radiation transport, shielding and detection studies. The update of software is essential in ensuring that the computational tools today are in-line with the progress in nuclear science and technology.

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