Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C + SNA 2007)
Monterey, California, April 15-19, 2007, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2007)

THE MC21 MONTE CARLO TRANSPORT CODE

T. M. Sutton, T. J. Donovan, T. H. Trumbull, P. S. Dobreff and E. Caro
Lockheed Martin
P. O. Box 1072
Schenectady, NY 12301-1072
sutton@kapl.gov

D. P. Griesheimer, L. J. Tyburski, D. C. Carpenter and H. Joo
Bechtel Bettis, Inc.
P. O. Box 79
West Mifflin, PA 15122

ABSTRACT

MC21 is a new Monte Carlo neutron and photon transport code currently under joint development at the Knolls Atomic Power Laboratory and the Bettis Laboratory. MC21 is the Monte Carlo transport kernel of the broader Common Monte Carlo Design Tool (CMCDT), which is also currently under development. The vision for CMCDT is to provide an automated, computer-aided modeling and post-processing environment integrated with a Monte Carlo solver that is optimized for reactor analysis. CMCDT represents a strategy to push the Monte Carlo method beyond its traditional role as a benchmarking tool or "tool of last resort" and into a dominant design role. In the full paper we will give a thorough introduction to MC21 and the related parts of CMCDT. In this summary, we focus on the areas of neutron scattering physics and tallies.

Key Words: MC21, CMCDT, Monte Carlo

1. INTRODUCTION

MC21 is a new Monte Carlo neutron and photon transport code currently under joint development at the Knolls Atomic Power Laboratory and the Bettis Atomic Power Laboratory. MC21 is the Monte Carlo transport kernel of the broader Common Monte Carlo Design Tool (CMCDT), which is also currently under development. The vision for CMCDT is to provide an automated, computer-aided modeling and post-processing environment integrated with a Monte Carlo solver that is optimized for reactor analysis. CMCDT represents a strategy to push the Monte Carlo method beyond its traditional role as a benchmarking tool or "tool of last resort" and into a dominant design role. In the full paper we will give a thorough introduction to MC21 and the related parts of CMCDT. In the next two sections of this summary, we focus on the neutron scattering physics and tally capabilities. In Section 4 various other aspects of the code are very briefly described. Further expansion of these and other aspects of the code will be provided in the full paper.

2. NEUTRON PHYSICS TREATMENTS

MC21 uses continuous-energy neutron and cross section methodologies. The energy dependence of the cross sections is represented using tabulated energy/cross section pairs and linear interpolation between the tabulated points. Resonance self-shielding in the unresolved range is treated using the probability table method [1]. Table I shows the mechanisms used to determine the post-collision energy and scattering angle in each of three energy ranges for different types of nuclides. In all cases the post-collision energy and scattering angles are determined from distribution functions generated with the highest possible fidelity from the ENDF/B data [2].

Table I. Sample Ranges of Applicability of Scattering Mechanisms

Energy Range	bound ^{1}H	other moderators	all other nuclides
400 *kT* – 20 MeV	SCT	TAR	TAR
E_{th} – 400 *kT*		SCT	FG
10^{-5} eV – E_{th}	$S(\alpha,\beta)$	$S(\alpha,\beta)$, Bragg and/or elastic incoherent	

Scattering from protons bound in molecules (e.g., water) is modeled using $S(\alpha,\beta)$ scattering law data between 10^{-5} eV and E_{th} (the maximum energy for which the data are tabulated). Above E_{th} the scattering kinematics are determined using the short collision time (SCT) approximation [3]. MC21 implements the SCT approximation by sampling the target nuclide velocity from a Maxwellian distribution at an effective temperature T^*, translating to a coordinate system in which the target is at rest and performing the usual kinematics calculations, and then translating back to the laboratory reference frame to obtain a 'provisional' post-collision energy E' and scattering cosine. If the provisional post-collision energy is less than or equal to the incident energy E, then the provisional values are retained as the actual values. If provisional post-collision energy is greater than the incident energy, however, then a detailed balance method [4] is employed in which the provisional energy and scattering cosine are only accepted with probability $\exp\left[-(E'-E)\left(\frac{1}{T}-\frac{1}{T^*}\right)\right]$, where T is the ambient temperature. If the provisional values are rejected, then a new target velocity is sampled and the entire process is repeated.

For other nuclides (i.e., moderators) for which tabulated thermal scattering data (i.e., $S(\alpha,\beta)$, Bragg and/or incoherent elastic) are available, the process is the same except that target-at-rest (TAR) kinematics are employed if the incident energy is greater than 400 *kT*. The TAR approximation avoids the computation involved in sampling a target velocity and performing the necessary coordinate transformations by simply neglecting the target motion altogether.

For nuclides for which tabulated thermal scattering data are not available, then TAR kinematics are used above 400 *kT* while the free gas (FG) approximation [4] is used for lower energies. The FG implementation is similar to the SCT implementation but with two differences: the target velocity is sampled from a Maxwellian distribution at the ambient temperature T rather than from one at an effective temperature T^*, and the rejection method to implement detailed balance is not employed.

3. TALLY CAPABILITIES

Tallies are based on the familiar collision and track length estimators [5] used in other Monte Carlo particle transport codes. These types of estimators are especially well-suited for calculating integral quantities of the form

$$X = \int d\mathbf{r} \int d\mathbf{\Omega} \int dE\, f\left(\mathbf{r}, \mathbf{\Omega}, E\right) \varphi\left(\mathbf{r}, \mathbf{\Omega}, E\right) \tag{1}$$

where f is an arbitrary function and φ is the angular neutron flux as a function of position, direction, and energy. By selecting an appropriate scoring function f and adjusting the limits of integration, Eq. (1) can produce many important quantities for nuclear design and analysis. For example, if f is defined as the macroscopic absorption cross section for uranium, then Eq. (1) gives the absorption rate in uranium. To continue this example, if the limits of the integration over energy are adjusted so that $0 \le E \le E_{\text{thermal}}$ then Eq. (1) gives the thermal neutron absorption rate in uranium.

The tally system takes advantage of the generality of Eq. (1) to provide users with the maximum flexibility when defining tally edits. Individual edits are configured by defining two parameters: 1) which particles are allowed to score to the edit, and 2) the appropriate scoring function for the edit. The first parameter effectively controls the limits of integration for Eq. (1). This parameter is set by applying a series of one or more phase filters to the tally. The phase filters restrict which particles are allowed to score to a particular edit bin. MC21 allows users to filter particles based on spatial region, material, direction, surface, birth region, and both pre- and post-collision energy. By selecting appropriate combinations of phase filters, MC21 allows users to define edits over very specific phase volumes. Advanced filters, such as birth region and post-collision energy, allow users to quickly and easily set up complex tallies to estimate fission and energy transfer matrices

The second tally parameter, the scoring function f, determines the scoring contribution from each particle at every event—such as a collision or surface crossing. By selecting different scoring functions, different physical quantities can be estimated. Scoring functions in MC21 are divided into two categories: macroedits and detailed edits. Macroedits allow users to quickly request common reaction types such as average flux, total reaction rate, average mean free path and total absorption, fission and production rates in the current material. Detailed edits give the user more flexibility by allowing them to specify individual nuclides and reaction types to score. In general, MC21 allows users to request any nuclide in the problem and any ENDF reaction type. The code also supports grouping results from different nuclides or reaction types into a single edit bin.

4. MISCELLANEOUS FEATURES

MC21 is written in free-source-form Fortran 95 using an object-based style [6]. Objects are used, for example, to represent geometric components, neutron scattering laws, and tally

definitions. MC21 is parallelized using both message-passing (i.e., MPI) and shared-memory (i.e., OpenMP) methods. Message passing parallelism may be used between nodes or between processors on the same node, while shared-memory parallelism is used only by processors residing on the same node. Application-level checkpoint/restart is used to enhance fault tolerance.

MC21 may be used for both fixed-source and k_{eff} calculations. Fixed sources may originate at a single point or be spatially distributed, may be isotropic or monodirectional, and may be monoenergetic or have an energy spectrum. A stochastic method based on the fixed-source algorithm is available for computing the volumes of arbitrarily shaped geometry components.

MC21 possesses a highly flexible three-dimensional (3-D) combinatorial geometry capability coupled with a dedicated two-dimensional (2-D) geometry kernel [7]. MC21's combinatorial geometry and use of geometric hierarchy is similar to that used in MCNP [8], while the 2-D extruded constructs are based on similar structures in RCP01 [9] and RACER [10]. This combination permits MC21 to model complex 3-D systems and also ensures that the highly detailed 2-D extruded geometries commonly encountered in reactor analysis models can be compactly represented and efficiently tracked.

NDEX is a system of codes within CMCDT that generates nuclear data libraries for MC21. NDEX uses NJOY [3], PROTAB [1], and other CMCDT-specific routines to process nuclear data files in ENDF/B format. Significant computational effort can be required to create some components of an MC21 nuclear data library, including the unresolved resonance range (URR) probability tables, thermal scattering law distributions, and Doppler-broadened cross sections. To minimize the computational burden, NDEX maintains a nuclear data repository. When NDEX needs to produce a nuclear data library for MC21, it first looks to see if the data corresponding to the desired nuclides, temperatures, and versions are in the repository. Data already in the repository are simply copied to the library. Data not in the repository are generated and placed in the repository as well as in the library being created.

A constant flux depletion process has been implemented in CMCDT by directly coupling MC21 with a depletion code. In the depletion code, the system of ordinary differential equations (ODEs) describing the reaction rates and decay processes are assembled as a single matrix and solved using the VODE [11] variable-coefficient ODE solver. The depletion system is parallelized by having multiple depletion code processes running simultaneously, one for each depletable composition.

5. CONCLUSION

Further detail of each of the areas mentioned above will be provided in the full paper. In addition, benchmark problem results obtained using MC21 will be compared to those obtained using other codes such as MCNP5 [8].

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