

LM-06K144
January 9, 2007

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THE MC21 MONTE CARLO TRANSPORT CODE

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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 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. This paper describes various aspects of the code, including the neutron physics and nuclear data treatments, the geometry representation, and the tally and depletion capabilities.

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. This paper provides an introduction to the neutron-transport aspects of MC21 and the related parts of CMCDT. The next section describes the neutron physics treatments. The nuclear data system is described in Section 3. Section 4 contains a discussion of the geometry representation. The tally capabilities are outlined in Section 5. The CMCDT system links MC21 with a depletion solver, and this is described in Section 6. A few miscellaneous features are mentioned in Section 7, and eigenvalue results obtained for a model of the Advanced Test Reactor are presented in Section 8.

2. NEUTRON PHYSICS TREATMENTS

MC21 uses continuous-energy neutron and cross section methodologies over the energy range from 10^{-5} eV to 20 MeV. Each nuclide employs its own unique energy mesh on which the cross sections for all reactions for that nuclide are tabulated. The total and elastic cross sections are tabulated at every mesh point, while other reactions are only tabulated over the range of mesh points for which they have non-zero values. The energy dependence of the cross sections between the tabulated points is assumed to be linear, and the mesh spacing is made sufficiently fine that linear interpolation leads to negligible error.

The unresolved resonance energy range (URR) is treated using the probability table method [1,2,3]. In this method, the range of possible total cross section values is divided into a number of bands, and associated with each band is a probability giving the likelihood that the total cross section lies within the band. Resonance factors (ratios of band-average to dilute-average cross sections) for the total and various partial cross sections are also tabulated for each band. Whenever a neutron undergoes a source or scattering event for which the post-event energy lies within the unresolved resonance range of a nuclide, a band is randomly sampled using the band probabilities for that nuclide. The resonance factors associated with the sampled band are then applied to the corresponding continuous-energy dilute-average cross section values. These modified cross sections are then used by that neutron until it undergoes its next scattering event. The probability tables are tabulated on an energy mesh independent of that of the continuous-energy cross sections, and are statistically interpolated between energy mesh points.

For the purpose of scattering kinematics, nuclides are classified as either moderators or non-moderators. Those nuclides for which tabulated thermal-range scattering data are available are considered moderators, while all other nuclides are considered non-moderators. Within the moderator class, bound protons are treated slightly differently than the other nuclides in the class. Table I shows the mechanisms used to determine the post-collision energy and scattering angle in each of three energy ranges for the various classes of nuclides. The table entries are discussed below.

Table I. Ranges of Applicability of Scattering Mechanisms

Energy Range	Bound ^1H	Other Moderators	Non-Moderators
400 kT – 20 MeV	SCT	TAR	TAR
$E_{\text{th}} - 400 \text{ kT}$		SCT	FG
$10^{-5} \text{ eV} - E_{\text{th}}$	incoherent inelastic, incoherent elastic, coherent elastic		

Under certain circumstances, scattering kinematics calculations may be significantly simplified by treating the target as a free nucleus at rest in the laboratory reference frame. For this target-at-

rest (TAR) approximation to be valid, several conditions must be met [4]. One condition is that the pre- and post-collision neutron energy must be much greater than kT , where T is the temperature of the material. In addition, there may be an additional condition on the pre- and post-collision de Broglie wavelength of the neutron. For target nuclei that are part of molecules the wavelength must be much smaller than the linear dimension of the molecule. Similarly, for target nuclei in a crystalline material the wavelength must be much smaller than the lattice spacing. The relative simplicity of the TAR scheme makes for efficient kinematics calculations, so MC21 uses this method whenever the approximations involved would result in negligible error.

For elastic and level-inelastic scattering from a target at rest, a scattering cosine in the center of mass system, μ_c , is sampled from a tabulated probability distribution function (PDF). The scattering cosine in the laboratory reference frame is then given by

$$\mu = \frac{\gamma + \tau\mu_c}{\sqrt{\gamma^2 + 2\tau\gamma\mu_c + \tau^2}} \quad (1)$$

and the post-collision energy by

$$E' = E \frac{\gamma^2 + 2\tau\gamma\mu_c + \tau^2}{(\gamma + 1)^2}, \quad (2)$$

where γ is the ratio of the mass of the neutron to that of the target nucleus,

$$\tau = \sqrt{1 + \frac{1 + \gamma}{E} Q}, \quad (3)$$

and $-Q$ is the amount of energy absorbed by the target nucleus [5]. For elastic scattering $Q = 0$ and hence $\tau = 1$. For other reaction types that result in a neutron ((n,2n), (n,3n), (n,4n), etc.), the post-collision quantities are determined from individual PDFs for the energy and scattering cosine or from joint energy-cosine PDFs. Regardless of the scattering mechanism employed, the PDFs are generated with the highest possible fidelity from the ENDF-6-formatted¹ data [6]. Statistical interpolation is used to interpolate PDFs between energy points and, when appropriate, is combined with unit base transformation [7].

In the thermal energy range the conditions required for the TAR approximation to be valid are not met. Therefore, in this range nuclides classified as moderators employ three types of tabulated thermal range scattering data: incoherent inelastic ($S(\alpha, \beta)$), incoherent elastic, and coherent elastic (Bragg) [6]. These data are used to determine the scattering in the energy range between 10^{-5} eV and E_{th} – the (nuclide-dependent) maximum energy for which the data are

¹ The term ENDF-6-formatted is used to refer to any nuclear data file that uses the ENDF-6 format. These include ENDF/B, JEFF, JENDL, CENDL, and BROND.

available. In the case of $S(\alpha, \beta)$ scattering law data, MC21 uses a direct sampling algorithm to determine the scattering kinematics [8]. In this method, the raw ENDF $S(\alpha, \beta)$ data is converted into a set of cumulative distribution functions (CDFs) for the dimensionless parameters α and β , based on incident neutron energy. For each collision in the range of the $S(\alpha, \beta)$ data, values of α and β are sampled from the appropriate CDFs. These values are then converted into a scattering cosine, μ , and exiting particle energy, E' , respectively.

For neutron energies higher than E_{th} but not sufficiently high that the motion of the target nuclei can be neglected, scattering from moderators is treated using the short-collision-time (SCT) approximation [6]. For all moderators except bound protons, the SCT approximation is used between E_{th} and $400 kT$, while above $400 kT$ the TAR approximation is used. Since a neutron scattering from a free proton at rest can lose all of its energy, however, TAR kinematics are never used for scattering from bound protons. Instead, for scattering from bound protons the SCT approximation is used for all energies above E_{th} .

In the SCT approximation the velocity distribution of the target nuclei, $M(\mathbf{V}|T^*)$, is modeled as a Maxwellian at an effective temperature T^* , and the scattering cross section is assumed to be independent of the relative velocity. Given that a neutron with velocity \mathbf{v} has collided with a moderator, the target nucleus velocity is thus sampled from the PDF

$$p(\mathbf{V}) = C |\mathbf{v} - \mathbf{V}| M(\mathbf{V}|T^*), \quad (4)$$

where C is a normalization constant [9]. The neutron-nucleus system is then translated to a coordinate system in which the target is at rest by a vector subtraction of the sampled target velocity. After determining the pre-collision neutron energy and direction vector in the TAR system, TAR kinematics calculations are performed to obtain the post-collision energy and direction. Finally, there is a translation of these TAR-system post-collision values back to the laboratory reference frame by a vector addition of the sampled target velocity. These operations yield 'provisional' post-collision values for the neutron energy \hat{E} and direction $\hat{\Omega}$. The reason that these quantities are referred to as provisional is that a rejection scheme is employed that adjusts the amount of upscattering so as to satisfy detailed balance [4,9]. If \hat{E} is less than or equal to the incident energy E (i.e., the neutron has down-scattered), then the provisional post-collision values are retained as the final post-collision values, i.e. $E' \leftarrow \hat{E}$ and $\Omega' \leftarrow \hat{\Omega}$. If $\hat{E} > E$, however, then the provisional post-collision energy and direction are only retained as the final values with probability

$$\rho = \exp \left[-(\hat{E} - E) \left(\frac{1}{T} - \frac{1}{T^*} \right) \right], \quad (5)$$

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 non-moderators, TAR kinematics are used above 400 kT while the free gas (FG) approximation is used for lower energies [10]. The FG approximation is similar to the SCT approximation but with two differences. First, the target nucleus velocity is assumed to be distributed according to a Maxwellian distribution at the ambient temperature T rather than at an effective temperature T^* . Second, the rejection step is omitted since the ambient temperature is used for sampling the target velocity.

3. NUCLEAR DATA

Nuclear data required for MC21 are provided by the NDEX (Nuclear Data Extractor) system of codes. NDEX extracts and processes nuclear data primarily from ENDF-6 and ACE (A Compact ENDF) [11] formatted source files. These data are processed and arranged to meet the specific requirements of MC21, and then written to a file named ND_LIBRARY that can be read by MC21. A schematic is shown in Fig. 1.

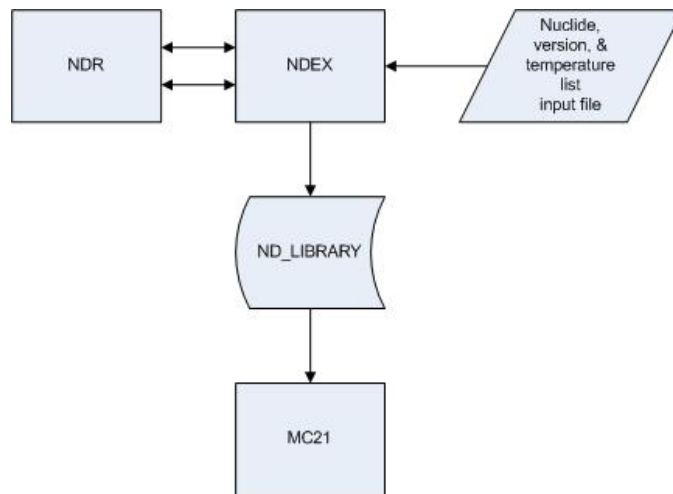


Figure 1: CMCDD Nuclear Data System Schematic

NDEX is intended to be used in conjunction with a Nuclear Data Repository (NDR), which is used to store essential files for specific versions of nuclides. The NDR is constructed using a UNIX directory hierarchy as shown in Figure 2. This structure allows for multiple versions of each nuclide. The lowest level directory specific to a nuclide and version number contains the ACE- and ENDF-6-formatted files, as well as MC21-specific thermal scattering law data files and URR probability tables.

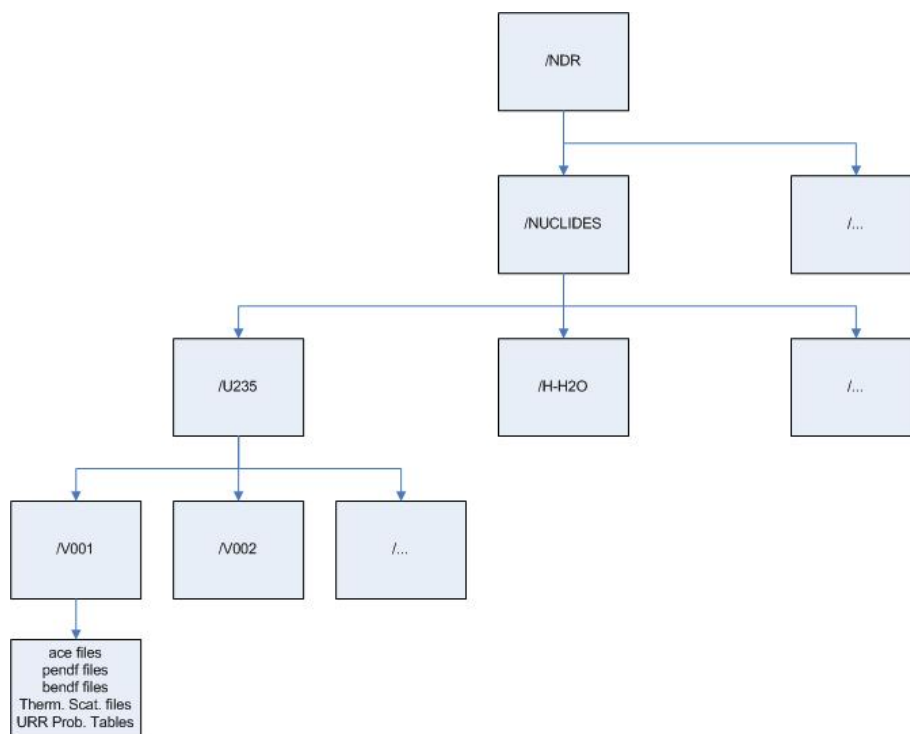


Figure 2: The NDR file structure.

To create a job-specific ND_LIBRARY file, NDEX reads an input file which contains a list of the desired nuclides, version numbers, and temperatures. Multiple versions and temperatures may be specified for each nuclide. NDEX then extracts the necessary data from the NDR and writes it to the ND_LIBRARY file. If a requested data set is not present in the NDR, NDEX will first populate the NDR with the necessary data.

NDEX relies heavily on the NJOY code system [11], extracting microscopic cross sections and secondary angular and energy distribution data from NJOY-generated ACE files. Currently, NDEX supplies the total cross section, plus cross sections for elastic scattering, discrete level inelastic scattering, the inelastic continuum, all (n, xn') reactions, fission, and neutron production due to fission ($v\Sigma_f$). Energy- and isotope-dependent prompt, delayed and total fission spectra, probability tables for URR cross section shielding factors, and moderator thermal scattering data are also processed in NDEX by native routines.

Nominally, the ENDF/B-formatted source data and point-wise cross sections are stored in the NDR. This includes the point-wise 0 K cross sections from RECONR (pendf), the 293.6 K Doppler broadened file (bendf.0294) and the ACE file (ace.0294). If necessary, Doppler broadening of the fast point-wise cross sections is handled by executing an NJOY BROADR job from NDEX, “bootstrapping” from the bendf.0294 file to the desired temperature.

NDEX has native routines that process the ENDF moderator data files into a form that allows for direct sampling of $S(\alpha, \beta)$ data to determine the scattered neutron energy and momentum,

similar to methods used in the RACER code [8]. Coherent elastic and coherent inelastic scattering are also accounted for in the moderator scattering cross section. As previously mentioned, this file is generated only once for a specific version of a nuclide and written to the NDR. Subsequent requests for thermal data for this specific version of a nuclide read the previously generated file, thus reducing the time to generate the ND_LIBRARY.

Unresolved resonance parameters are extracted from ENDF-6-formatted files directly. NDEX controls the execution of the PROTAB code [3] to generate probability tables for shielding factors at multiple temperatures. The files are written to the NDR for later use. As is in the case of thermal scattering data, subsequent requests for that nuclide and version read the previously generated probability tables, thereby greatly reducing the time to generate ND_LIBRARY files.

Fission spectra in MC21 are always based on linear-linear interpolation of PDFs tabulated as a function of incident neutron energy. NDEX reads the prompt and delayed fission spectra directly from the ENDF-6-formatted source data, along with the delayed neutron yields and average number of neutrons released from fission for both delayed and prompt neutrons. Regardless of how the fission spectra are represented in the ENDF-6-formatted files, NDEX converts them to linear-linear interpolable PDFs. Depending on what data are available, NDEX creates total, prompt, and delayed spectra. The delayed spectrum is a linear combination of the spectra for each of the precursor groups weighted by their respective yields. The total spectra are linear combinations of the prompt and delayed spectra, weighted by the delayed neutron fractions at the corresponding incident neutron energy. Conversion of fission spectra in the ENDF-6 format to the MC21 format can be time consuming. Therefore—as is the case with the probability tables and the thermal scattering data—once a fission spectrum has been created for a specific version of a nuclide it is written to the NDR for future use.

4. GEOMETRY

MC21 possesses a highly flexible three-dimensional (3-D) combinatorial geometry capability coupled with a dedicated two-dimensional (2-D) geometry kernel [12]. MC21's combinatorial geometry and use of geometric hierarchy is similar to that of MCNP [10], while the 2-D constructs are based on similar structures in RCP01 [13] and RACER [14]. 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.

The five main geometric constructs of MC21 are: *surface*, *component*, *grid*, *2Dlattice*, and *ellipse*. General quadratic surfaces are the building blocks of components. Reduced forms of the general quadratic equation are available to reduce storage and take advantage of increased tracking efficiency relative to general quadratics. Boundary conditions are assigned to surfaces, and MC21 supports reflective, rotational periodic, translational, escape, and transmission boundary conditions. Components, which are generally equivalent to cells in MCNP, are volumes defined by union and/or intersection sets of surface half-spaces. In addition to their half-space definitions, components can be further specified hierarchically with respect to other components. Through this hierarchical definition, components can be constrained to exist only within another component and may contain other components.

Any component can possess additional internal geometric detail in the form of a grid, with the constraint that the component volume must be completely filled by the grid. Component boundaries and the boundaries of the contained grid do not have to be coincident—any portion of the grid that is outside of the component is effectively truncated. The three available grid types are: spherical (r), cylindrical (r,z) and Cartesian (x,y,z). The Cartesian grid is a non-uniform mesh consisting of lines parallel to the x- and y-axes. The angle between the x- and y-axes may be arbitrary. In the z direction (perpendicular to the grid's x-y plane), the x-y mesh planes are given an arbitrary number of axial separations of varying extents.

A Cartesian grid has a number of grid cells equal to $n_x \times n_y \times n_z$, where n_x is the number of separations between x mesh lines, etc. Each grid cell of the Cartesian grid may contain an x-y $2Dlattice$ which repeats in the grid cell and has the same axial extent as the grid cell. The x-y $2Dlattice$ has the same angle between the x and y axes as the Cartesian grid it resides within. Finally, each $2Dlattice$ element may contain a series of ellipses. These ellipses may be nested, tangent, or disjoint, but for tracking efficiency may not intersect within the lattice element.

Region properties are assigned at the innermost level of geometry. The currently available region properties are: the material or depletion composition index, the edit-region index, and the spatial importance index. If a component contains no grid, it is assigned region properties. Similarly, if a grid cell contains no $2Dlattice$, it is assigned region properties. A $2Dlattice$ element is always assigned region properties for the background area, and each ellipse is also assigned region properties.

5. TALLY CAPABILITIES

Tallies are based on the familiar collision and track-length estimators [15] used in other Monte Carlo particle transport codes. These types of estimators are especially well-suited for calculating integral quantities of the form

$$X = \int d\mathbf{r} \int d\Omega \int dE f(\mathbf{r}, \Omega, E) \phi(\mathbf{r}, \Omega, E) \quad (6)$$

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. (6) 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. (6) gives the absorption rate in uranium. To continue this example, if the limits of the integration over energy are adjusted so that $0 \leq E \leq E_{\text{thermal}}$ then Eq. (6) gives the thermal neutron absorption rate in uranium.

The tally system takes advantage of the generality of Eq. (6) to provide users with the maximum flexibility when defining tally edits. Individual edits are configured by defining two parameters: 1) a filter parameter that determines which particles are allowed to score to the edit, and 2) a score parameter that specifies the appropriate scoring function for the edit. The first parameter effectively controls the limits of integration for Eq. (6). 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. The code allows both volume and surface type edits. For volume edits, 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

For surface edits, MC21 includes surface and angular direction filters, as well as a specially designed leakage filter. The leakage tally allows users to filter particles based on their phase state both before and after a surface crossing event. Leakage tallies are defined by specifying a “leaving” and “entering” condition for the particle. For example, a simple leakage filter might allow all particles leaving material 2 and entering material 3 to score. More complex tallies may involve groups of material or region identifiers as well as filters based on the type of surface boundary condition (e.g. reflecting, periodic, etc) encountered by the particle. This tally format allows a convenient way to define many different types of leakage edits without requiring the specification of individual bounding surfaces.

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.

In addition to the user-defined tallies, MC21 offers several predefined tally sets and global edits. The predefined edits are specially designed to interface with other CMCDDT code modules—such as the depletion module. When a user specifies that a job is a depletion simulation, MC21 automatically defines the required reaction rate tallies over all depletable compositions. The depletion module can then directly access and modify the reaction rates and number densities in memory, eliminating the need to write intermediate files to exchange data between modules.

For criticality calculations, MC21 always estimates values for a small set of global quantities for the model. Currently, these global edits include: the system eigenvalue, the total particle leakage from the problem space, the total energy deposition per starting neutron, and β_{eff} . For eigenvalue estimates, three separate statistical estimators are used: collision, track-length, and absorption. During the simulation batch-wise values of the collision estimator are sent to the output stream so that the user can monitor the progress of the simulation. At the end of the job, all three eigenvalue estimates are printed, along with minimum variance combinations of the estimators [16]. The final eigenvalue estimate provided by MC21 is the minimum variance combination of all three eigenvalue estimates.

In addition to flexibility, the MC21 tally system was also designed with performance in mind. The tally system has been specially optimized to maintain a high level of efficiency, even as the number of edit regions becomes very large. In general, Monte Carlo simulations containing many tallies (>1000) can spend a significant amount of total run time searching for and scoring individual edit bins. This is a particular concern for large detailed depletion simulations, which may require hundreds of millions of individual edits. In problems containing many edits, the Monte Carlo code must determine which edit bins to score for every particle collision or surface crossing event. As the number of edits increases, this search process slows down accordingly. In MC21, the tally system uses a series of hashed arrays to increase the efficiency of the edit bin search. In tests this hashed search algorithm has proven to be efficient and robust, allowing simulations with over 300 million edits to be run routinely.

6. DEPLETION

A constant flux depletion process has been implemented in CMCDT by directly coupling MC21 with a stand-alone depletion code. The depletion process is controlled by a depletion feedback module which makes the appropriate calls to both MC21 and the depletion code, and handles all necessary data transfers. Reaction rates are generated in the steady-state MC21 calculations and passed to the depletion solver. The depletion system also requires information that describes the system of equations to be solved. The system of equations can be tailored by the user as to the amount of detail to include.

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 ODE solver [17]. VODE uses variable-coefficient Backward Differentiation Formula (BDF) multistep methods for stiff matrices as taken from the older solvers EPISODE [18] and EPISODEB [19]. Additional accuracy and efficiency issues have also been incorporated into VODE. For maximum efficiency, users supply the Jacobian of the coefficient matrix which VODE allows to be stored in sparse matrix format (only in the Fortran version of VODE). Since depletion systems exhibit a high degree of sparsity, significant computer storage and run time reductions are evident for large systems, such as a complete actinide and fission product model (> 1500 nuclides).

Due to its ability to handle very stiff systems of equations, VODE eliminates the need to precondition the coefficient matrices by chain contraction as is done in the ORIGEN code. Also, since the coefficient matrix accounts for all coupling between nuclides, VODE has an inherent advantage over linear chain solution solvers (e.g., CINDER [20]) since it is very difficult to automate chain generation when neutron absorption effects are incorporated and ensure all contributions are accounted for.

Parallelism has been achieved by having multiple depletion code processes running simultaneously, one for each depletable composition.

7. MISCELLANEOUS FEATURES

MC21 is written in free-source-form Fortran 95 using an object-based style [21]. 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. The CMCDT/MC21 system also has the capability to automatically adjust the position of control devices so as to attain a target k_{eff} .

8. RESULTS

Figure 3 shows a view of an Advanced Test Reactor (ATR) MC21 model that was built by converting an existing MCNP model. The similarities in MC21 components and MCNP cells make this conversion straightforward. This MC21 model contains no grids and all geometric detail is in the form of components. This model was created as a k_{eff} benchmark for comparison to MCNP5. Table 2 gives MC21 and MCNP5 k_{eff} results for this model, which are in very close agreement. For these calculations, both codes used ENDF/B-VI.8 cross sections. This very basic comparison of the MC21 and MCNP5 eigenvalues for this large and complex model demonstrates the successful integration of the multiple subsystems and nuclear data models in MC21. MC21 also has the capacity to generate very large quantities of detailed tallies as discussed in §5. However, a thorough examination and comparison of detailed edits is beyond the scope of this paper.

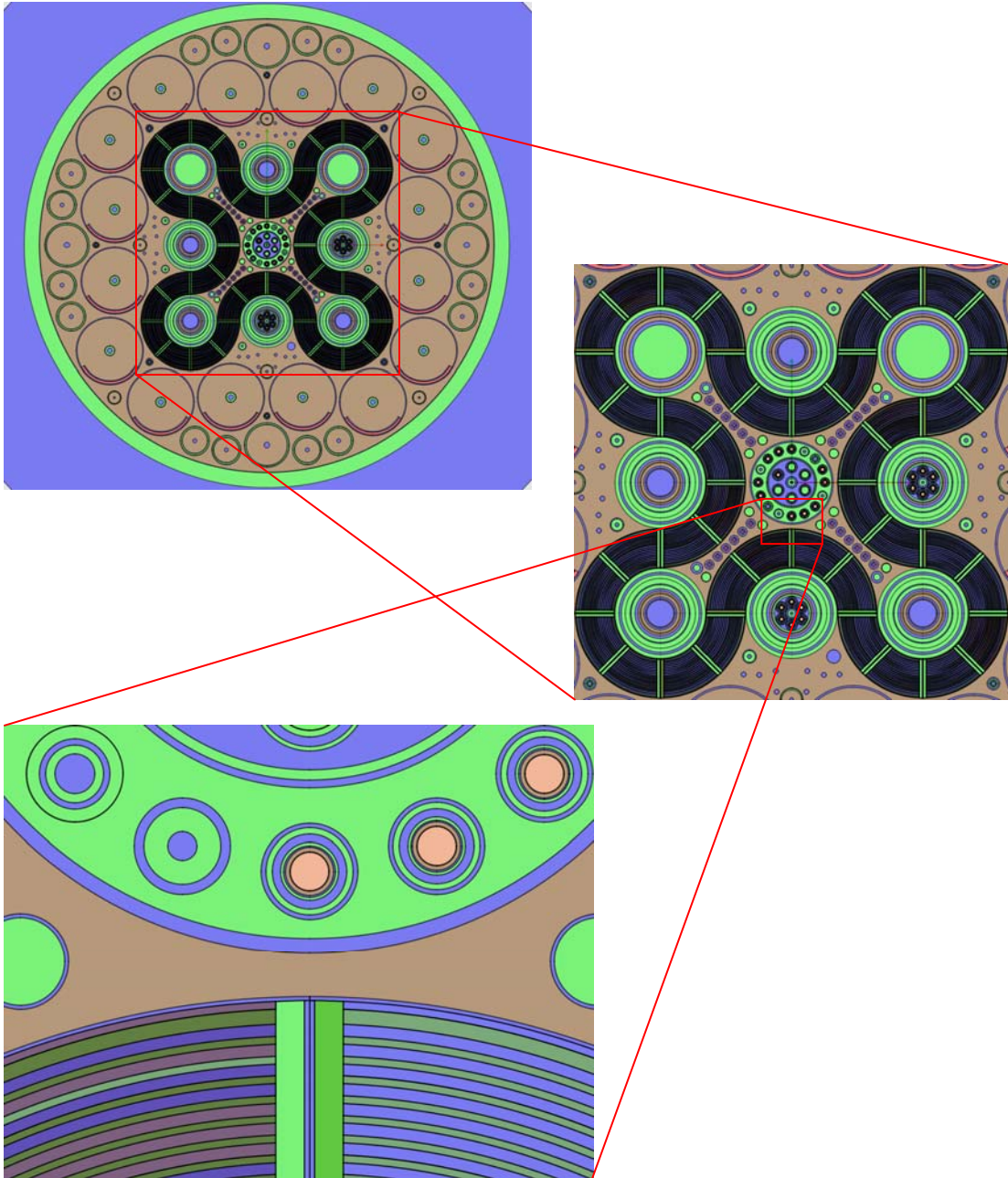


Figure 3: An x-y Slice Through an MC21 Advanced Test Reactor Model

Table 2: ATR k_{eff} Results

Code	k_{eff}
MC21	0.9958 \pm 0.0002 (95% confidence interval uncertainty)
MCNP5	0.9959 \pm 0.0002 (1 Standard Deviation uncertainty)

ACKNOWLEDGEMENTS

The authors wish to thank D. J. Kelly and C. M. Rodenbush for their support in the ATR benchmark model generation and analysis.

REFERENCES

1. M. N. Nikolaev, A. A. Ignatov, N. V. Isaev, and V. F. Kokhlov, "The Method of Subgroups for Considering the Resonance Structure of the Cross Sections in Neutron Calculations (Part 1)", *Atomnaya Energiya*, **29**, pp. 11-16 (1970).
2. L. B. Levitt, "The Probability Table Method for Treating Unresolved Neutron Resonances in Monte Carlo Calculations", *Nucl. Sci. Eng.*, **49**, pp. 450-457 (1972).
3. T. M. Sutton and F. B. Brown, "Implementation of the Probability Table Method in a Continuous-Energy Monte Carlo Code System", *International Conference on the Physics of Nuclear Science and Technology*, Long Island, New York, Oct. 5-8, Vol. 2, pp. 891-903 (1998).
4. E. M. Gelbard, "Epithermal Scattering in VIM", Argonne National Laboratory Report FRA-TM-123 (1979).
5. A. F. Henry, *Nuclear-Reactor Analysis*, MIT Press, Cambridge, Mass., USA (1975).
6. V. McLane, ed., "ENDF-102: Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6", Brookhaven National Laboratory Report BNL-NCS-44945 (1997).
7. R. J. Doyas and S. T. Perkins, "Interpolation of Tabular Secondary Neutron and Photon Energy Distributions", *Nucl. Sci. Eng.*, **50**, 390 (1973).
8. C. T. Ballinger, "The Direct $S(\alpha, \beta)$ Method for Thermal Neutron Scattering", *Proceedings of the International Conference on Mathematics and Computation, Reactor Physics, and Environmental Analysis*, Portland, Oregon, April 30–May 4, Vol. 1, pp. 134-143 (1995).
9. G. I. Bell and S. Glasstone, *Nuclear Reactor Theory*, Robert E. Krieger, Malabar, Fl. (1985).
10. X-5 Monte Carlo Team, "MCNP – A General Monte Carlo N-Particle Transport Code, Version 5", Los Alamos National Laboratory Report LA-UR-03-1987 (2003).
11. R. E. MacFarlane and D. W. Muir, "The NJOY Nuclear Data Processing System: Version 91", Los Alamos National Laboratory Report LA-12740-M (1994).
12. T. Donovan and L. Tyburski, "Geometric Representations in the Developmental Monte Carlo Code MC21", *PHYSOR-2006: Advances in Nuclear Analysis and Simulation*, Vancouver, BC, Canada, Sept. 10-14 (2006).
13. L. A. Ondis II, L. J. Tyburski and B. S. Moskowit, "RCP01—A Monte Carlo Program for Solving Neutron and Photon Transport Problems in Three Dimensional Geometry with

- Detailed Energy Description and Depletion Capability”, Bettis Atomic Power Laboratory Report B-TM-1638 (2000).
14. T. M. Sutton, F. B. Brown, F. G. Bischoff, D. B. MacMillan, C. L. Ellis, J. T. Ward, C. T. Ballinger, D. J. Kelly and L. Schindler, “The Physical Models and Statistical Procedures Used in the RACER Monte Carlo Code”, Knolls Atomic Power Laboratory Report KAPL-4840 (1999).
 15. E. E. Lewis and W. F. Miller, *Computational Methods of Neutron Transport*, American Nuclear Society, La Grange Park, Illinois, USA (1993).
 16. M. Halperin, “Almost Linearly-Optimum Combination of Unbiased Estimates”, *American Statistical Association Journal*, **56**, pp. 36-43 (1961).
 17. P. N. Brown, G. D. Byrne and A. C. Hindmarsh, “VODE: A Variable-Coefficient ODE Solver”, *SIAM J. Sci. Stat. Comput.*, **10**, pp. 1038-1051 (1989).
 18. A. C. Hindmarsh and G. D. Byrne, “EPISODE: An Experimental Package for the Integration of Systems of Ordinary Differential Equations”, Lawrence Livermore National Laboratory Report UCID-30112 (1975).
 19. A. C. Hindmarsh and G. D. Byrne, “EPISODEB: An Experimental Package for the Integration of Systems of Ordinary Differential Equations with Banded Jacobians”, Lawrence Livermore National Laboratory Report UCID-30132 (1976).
 20. T. R. England, “CINDER—A One-Point Depletion and Fission Product Program”, Bettis Atomic Power Laboratory Report WAPD-TM-334 (August 1962, revised June 1964).
 21. V. K. Decyk, C. D. Norton and B. K. Szymanski, “Introduction to Object-Oriented Concepts using Fortran90”, Rensselaer Polytechnic Institute SCOREC Report 1996-10 (1996).