Advancements in Generalized-Geometry Discrete Ordinates Transport for Lattice Physics Calculations

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Abstract

This paper describes the generalized-geometry capabilities of the two-dimensional NEWT transport solver, used within the TRITON depletion sequence of the SCALE code system for lattice physics calculation. With the release of SCALE 5.1 in 2006, NEWT will introduce a new automated grid generation procedure based on simple body specifications, using an input format based on the SCALE Generalized-Geometry Processor. The paper will contrast the discretization techniques against those used in other unstructured grid treatments; illustrate the ease of model development, features, capabilities; and demonstrate the unique adaptability of NEWT for a wide range of fuel configurations.

KEYWORDS: NEWT, TRITON, SCALE, extended step characteristics, arbitrary grid

1. Introduction

The radiation transport equation, a linearized derivative of the Boltzmann equation, provides an exact description of a neutral-particle radiation field in terms of the position, direction of travel, and energy of every particle in the field. Both stochastic and deterministic forms of the transport equation have been developed and are heavily utilized in nuclear applications. Each approach has its strengths and weaknesses. Stochastic approaches are extremely effective for problems with complex geometries where the calculations of integral quantities such as radiation dose and neutron multiplication factors are desired. However, calculations to obtain accurate differential information such as the neutron flux as a function of space and energy can be difficult and inefficient at best, and prone to inaccuracies (even if the integral quantity is correct). Deterministic techniques are better suited for problems where differential quantities such as the neutron flux as a function of energy or space are desired. Hence, there exists a need for a deterministic transport solver that can match Mote Carlo methods in terms of geometric flexibility, while simultaneously remaining computationally efficient.

First publicly released with SCALE 5.0 in June 2004, the NEWT [1] transport solver provides a two-dimensional, unstructured-mesh discrete-ordinates solution for multigroup neutron transport calculations for a wide variety of applications. NEWT employs a mesh defined by arbitrary polygons; extended step characteristic (ESC) discretization is applied to calculate transport between sides within each computational cell [2,3]. Using the ESC solution method, computational cells are developed in the form of arbitrary polygons, which are further divided into trapezoids as a function of angle for

a number of angles in a quadrature set. While similar in concept to the Method of Characteristic (MOC) class of discretization, ESC provides a more rigorous spatial representation of bodies and allows significantly more control of spatial mesh refinement.

Grid-generation within NEWT is automated, and models are developed by the placement of simple bodies. With the release of Version 5.1 of SCALE, a new input specification paradigm and grid generation algorithm have been employed in NEWT. The input format has been adapted from the SCALE Generalized-Geometry Processor (SGGP). This combinatorial input format is employed by SCALE's KENO VI Monte Carlo criticality code and is being implemented in the MONACO Monte Carlo Shielding code. The use of a common input format will reduce the learning curve in model development for SCALE users. Although limited to two dimensions, the use of the SGGP input format provides virtually all the geometric flexibility of Monte Carlo for a deterministic solution. It also allows a means for direct comparison of Monte Carlo vs deterministic methods. Using the same cross section data and virtually identical geometric configurations, differences in results can be attributed to differences in the two transport techniques.

Within the SCALE code system, the TRITON sequence [4] is used to couple NEWT (or KENO) with ORIGEN-S for depletion calculations. This functionality has been extended over the last 4 years to be able to use NEWT to produce burnup-dependent lattice physics parameters for use in nodal analyses and includes a branching capability at each depletion state point. This work has been performed under contract with the U.S. Nuclear Regulatory Commission (NRC) to provide NRC staff with a high-fidelity lattice physics capability for the analysis of mixed-oxide (MOX) fuel assembly designs. [5]

With the evolution of fuel assembly designs for current-generationlight water reactors (LWRs), along with anticipated MOX loadings in some core designs and with potential departure from traditional LWR designs in Gen IV, existing (or newly developed) methods must be verified against independent rigorous methods that have the ability to accurately model complex and nonstandard fuel lattice designs. NEWT provides such an analysis capability.

This paper will provide a demonstration of the geometric capabilities of NEWT and will describe some of the features and functionality of the code for various types of transport analysis and lattice physics calculations.

2. Extended-Step Characteristic Discretization

The transport solution algorithm within NEWT is based on Extended-Step Characteristic (ESC) discretization. ESC discretization is a short characteristic implementation of the characteristic form of the transport equation, as opposed to Method of Characteristics (MOC) approaches that rely on long characteristics. The characteristic form of the transport equation,

$$\frac{d\psi(s)}{ds} + \sigma_t(s)\psi(\mathrm{s}) = Q(s)\,, \qquad (1)$$

in which Q(s) is the neutron source, may be easily solved assuming a "step approximation" in which properties and sources are assumed constant; the angular flux at any position *s* measured in a single angular (characteristic) direction is then found to be

$$\psi(s) = \psi_0 e^{-\sigma_t s} + \frac{Q}{\sigma_t}\left(1 - e^{-\sigma_t s}\right), \tag{2}$$

where ψ_0 is the known angular flux at $s = 0$. Some approaches use a linear characteristic approximation, in which Q is assumed to vary linearly with *s*, which gives a somewhat more complex solution.

The distinction between the long characteristic (e.g., MOC) and short characteristic (e.g., ECS) approaches is the length of the ray over which the formulation is applied. Long characteristic solutions perform transport calculations along a set of characteristic rays with a given angular orientation across the entire problem domain, whereas a short characteristic approach defines rays with the same angular orientation but only within the extent of a single computational cell. In both methods, a unique set of rays is defined for a number of angular orientations, with resulting angular fluxes integrated to obtain scalar fluxes.

3. Comparison of ESC to the Method of Characteristics

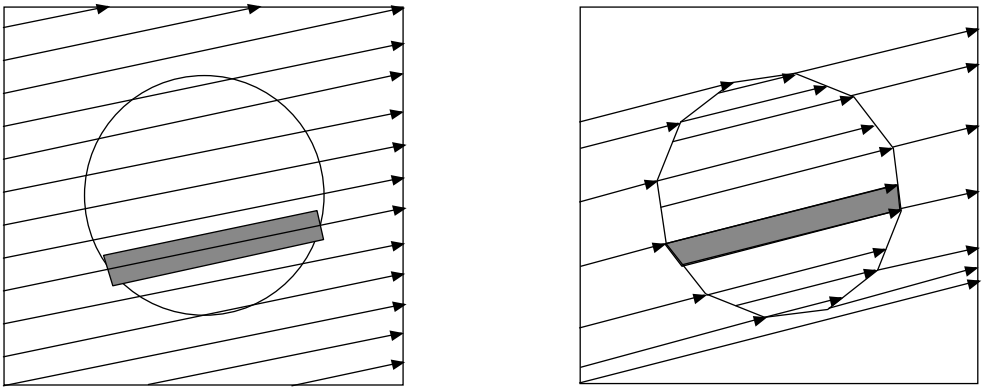
MOC methods have become a popular approach for unstructured mesh calculations [6-9] and are extremely powerful. However, the short characteristic approach used in ESC discretization offers improved resolution in space along with a more flexible form of ray placement that allows "localized" ray refinement.

The "step" approximation in the step characteristic approach is the assumption of a constant source. The source term, Q, comprised of scattering and fission neutrons, will clearly vary spatially. In the limit, as *s* goes to zero, the solution becomes exact. However, for relatively short distances, it is reasonable to assume that Q(s) can be approximated by an average, $\overline{Q}$. Hence, discretization of the spatial domain becomes necessary such that Eq. (2) is integrated over a reasonable track length. In MOC methods, individual bodies are used to define a track length; within a body, properties are constant, and it is assumed that the source term along a ray moving in a given direction may be well represented by an average. A volume is associated with each ray, based on the ray-to-ray spacing. The treatment of the body is exact, but the treatment of internal volumes effectively replaces the body with a series of effectively one-dimensional (1-D) parallel rectangles (i.e. no transverse leakage) in which volume is conserved via fixup factors. Rays are placed globally for each of a finite set of angles, but rays are broken into shorter segments at each body intersection. Conversely, in the ESC approach, all bodies are approximated as polygons with an equivalent volume. Within a computational cell, rays are defined by the vertices of each region. A volume is defined by the four-sided polygon enclosed by the rays, and the average angular flux across the volume is calculated using Eq. (2). No fixups are necessary – the set of polygons comprising each body will always exactly match the volume of the body. Furthermore, the solution within a cell is truly 2-D. Average angular fluxes on outgoing sides are calculated as a function of angular flux contribution from all incoming sides, which intimately couples all

adjacent cells. In MOC methods, there is no spatial coupling of rays, requiring a very fine mesh of 1-D rays to approximate two dimensions.

These two approaches are best demonstrated with an illustration. Consider a transport calculation for a simple cylindrical fuel element within a square moderator region. In the MOC method, for each of a set of angles, a set of rays are laid over the entire domain, as shown in Fig. 1(a). The volume associated with one ray passing through the fuel is represented by the rectangular shaded area in the figure. Fig. 1(b) illustrates the nature of the set of rays generated in the ESC approach. Rays are generated as needed to capture the detail of the bodies modeled. Effectively, MOC methods integrate a volume using a Simpson's Rule approximation, while ESC performs a Trapezoidal Rule integration. Both are exact as the ray spacing goes to zero, but the ESC approach converges to the limit faster and does not need as many rays for a given level of accuracy.

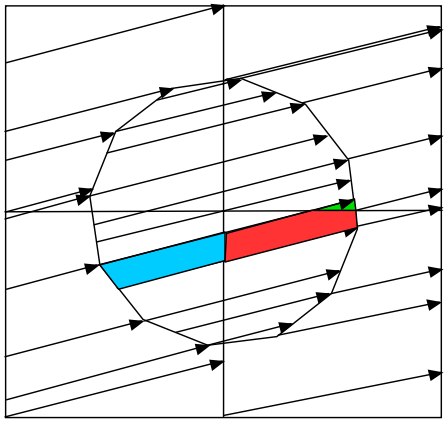
Figure 1. Comparison of ray tracing concepts between (a) MOC and (b) ESC approaches.



(a) (b)

A limitation in standard MOC methods is that the ray spacing must be small enough to provide appropriate sampling (at least one ray) for all bodies. The ESC approach, as implemented in NEWT, automatically places at least one ray in each body, irrespective of angle, and adds rays as necessary to capture the structure of all bodies, no matter what size or shape they may be. Further, this ray refinement is local rather than global, so that a globally fine ray spacing is not necessary to capture locally fine details. NEWT also allows user control over local grid refinement, by adding a rectangular mesh on top of body placement. This mesh reduces cell sizes and thus reduces the volume associated with each ray; it also increases the localized ray spacing. Figure 2 illustrates the addition of an overlaid grid structure, with the corresponding discretization of characteristic rays and computational cells. Within NEWT, the rectangular grid is user controlled and may be easily varied to test convergence. Again, the grid is also locally defined, so refinement may be placed only where needed.

Figure 2. Computational cell refinement by addition of rectangular grid.



4. NEWT Model Development

The SCALE Generalized Geometry Package provides the geometric flexibility necessary to develop extremely complex models for KENO-VI Monte Carlo calculations. Although limited to two-dimensional analysis in an (x-y) plane, the application of the combinatorial SGGP input structure provides the ability to easily develop models for complex configurations in two dimensions. Because it is limited to 2-D, certain bodies (e.g., spheres) cannot be modeled; however, the input flexibility is limited only by the 2-D constraint.

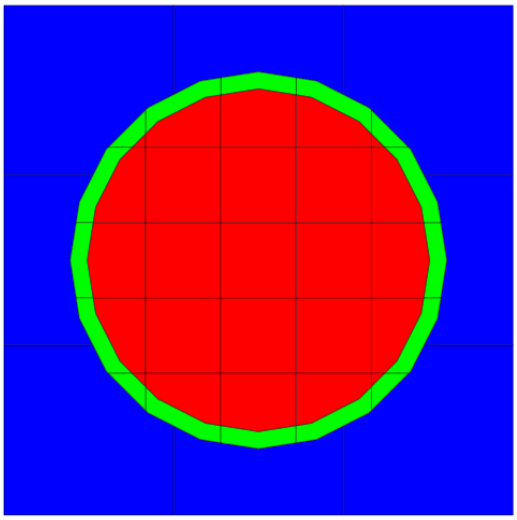
SGGP input is body-based, with bodies placed, rotated, translated, and cut as required for the desired configuration. Bodies are placed into "units," which are basic building blocks for model development. Units may be placed within other units, either in the form of a single placement or in the form of an array; NEWT supports both rectangular and hexagonal array structures.

To this point, the capabilities of the 2-D SGGP implementation in NEWT mirror the capabilities of KENO VI. However, because the ESC methodology is really just an advanced realization of the discrete ordinates method, a grid structure must be introduced. Traditional discrete ordinates methods are based on a grid structure of orthogonal cells in which finite-difference relationships are used to estimate transport across a computational cell. The ESC method uses a short characteristics approach to calculate transport across arbitrary polygons. Diamond-differencing is an approximation in which the derivatives of the flux are assumed to be linear across a computational cell, requiring cell sizes small enough to approximate this assumption. The characteristic solution is an exact representation of transport across a cell; however, approximations are introduced by the calculation of side-averaged fluxes, which limit the length of cell sides such that the variation of the angular flux along a side may be properly represented by an average. Both traditional and ESC discrete ordinates methods are also constrained in size by the assumption of a constant source within the cell. Hence, a grid structure must be introduced to further subdivide the problem domain. In NEWT, this is achieved by the introduction of a rectangular grid; computational cells are defined by the intersection of the rectangular grid and placed bodies. The problem domain is characterized by a largely

rectangular grid which has additional polygonal structure at the intersection of bodies and rectangular cells.

The rectangular grid in NEWT models is imposed at the unit level. An *m* by *n* rectangular grid is assigned to each defined unit. The grid is local to that cell and need not correspond to grid structure in other units. When a unit is place within another unit, the underlying grid of the container unit is removed in favor of the grid associated with the placed unit.

Figure 3. Global grid structure for a unit with one grid refinement placed within another with a more coarse grid structure.



```
unit 1
cylinder 10 0.5
cylinder 20 0.55
media 1 1 10
media 2 1 20 -10
boundary 20 5 5
global unit 2
hole 1
cuboid 10 4p0.75
media 3 1 10
boundary 10 3 3
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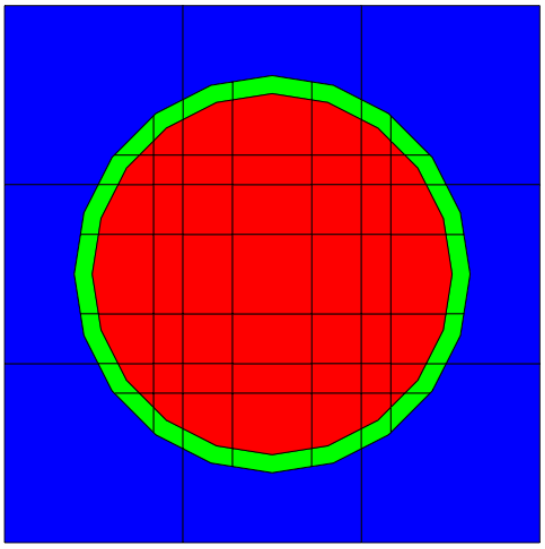
Figure 3 illustrates the grid structure developed for a hypothetical pin cell, along with the geometrical specification for this model. This input also specifies mixture placement, indicated by the three colors. Note that in this case, the grid structure for the unit consisting of two cylinders replaces the grid for the cuboid. The grids for the two regions can be individually set according to the needs of the configuration being analyzed.

5. Acceleration on an Arbitrary Grid

As with other discrete ordinates methods, NEWT can be slow to converge, especially in low absorbing media. However, the structure of the NEWT grid was found to be compatible with coarse-mesh finite-difference (CMFD) acceleration. CMFD methods generally require an orthogonal grid structure within which constituent mixtures can be homogenized on a cell-by-cell basis. A lower-order diffusion solution can then be performed using a finite-difference approach. Prolongation of the solution can then be performed to update the source term estimate for each cell on the fine-mesh transport model. Although a NEWT grid is completely arbitrary and does not necessarily contain the required continuous orthogonal grid structure, addition of such structure is easily accommodated. In fact, due to the use of a rectangular grid for the global unit (the outermost unit of a problem that encloses all bodies), a continuous grid is actually always

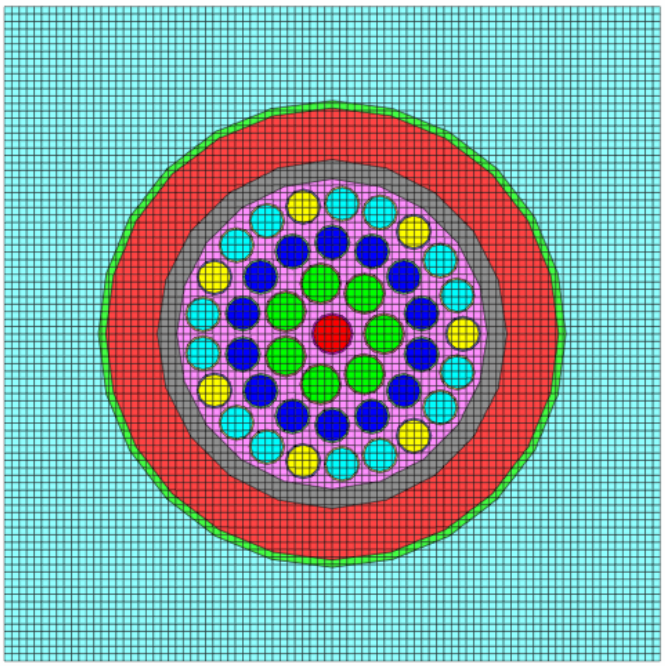
possible. In general, the "background" grid, *i.e.*, the grid associated with the global unit, is suppressed when a different grid structure is imposed on it, as illustrated in Fig. 3. However, it is possible to allow the background grid to "show through," or coexist. Figure 4 illustrates the same pin cell as shown in Fig. 3, but with the background grid retained. This introduces additional computational cells in the fine-mesh (ESC) discretization, but makes CMFD acceleration possible (in this case, on the 3 ×3 base square mesh), which more than offsets the additional work caused by additional transport effort.

Figure 4. Modified computational grid to accommodate CMFD acceleration.



This approach to discretization for a coarse-mesh acceleration makes it possible to apply CMFD to nonorthogonal fuel bundle designs. Consider the ACR-700 fuel bundle with surrounding moderator, illustrated in Fig. 5. Representation of such a configuration is easily accomplished with NEWT, but the large amount of deuterium outside the fuel tube makes the problem extremely difficult to converge. Use of CMFD is essential for problems of this nature, and NEWT makes it possible to combine the power of an arbitrary grid transport solver with the speed and simplicity of a low-order coarse-mesh accelerator.

Figure 5. NEWT model of ACR-700 assembly with surrounding heavy-water moderator.



6. Conclusions

The ESC approach implemented in NEWT provides a unique capability for discrete ordinates calculations on an arbitrary grid. The approach is robust, accurate, and provides mechanisms for localized, user-controlled refinement of spatial grids without necessitating a global refinement.

With the 5.1 release of SCALE, NEWT supports a geometry specification paradigm based on the SCALE Generalized-Geometry Package used by the KENO-VI Monte Carlo criticality code. SGGP is also the basis for geometry definition of the MONACO Monte Carlo shielding code being developed at ORNL. The use of a conceptually identical package within key modules of the SCALE suite of codes facilitates other development efforts (e.g., Graphical User Interface packages) and reduces the training/learning curve burden on users of multiple modules. But most important for NEWT, the SGGP provides a powerful combinatorial geometry input specification that allows complicated model development in simple body-based specifications. Furthermore, the ability to rapidly translate input specifications from KENO-VI to NEWT, and vice versa, provides an excellent methods to cross-check methods (Monte Carlo vs deterministic) in a manner when only the transport solution is different; both codes use identical cross-section data, which can eliminate data-related uncertainties in code-to-code comparisons.

The addition of a coarse-mesh finite-difference accelerator with this release of NEWT improves the efficiency of the solution method, especially for scattering-dominant media. Although NEWT's grid structure supports completely arbitrary

polygons, the use of a rectangular base grid that combines with body shapes to define that grid makes possible the use of a simple CMFD accelerator that can easily exchange information with the arbitrary ESC grid.

NEWT has become the mainstay of a lattice physics package that supports ORIGEN-S-based depletion with branching; this capability is described in a companion paper in this Proceedings [10]. The arbitrary-grid capabilities of NEWT have also been recently combined with the continuous-energy resonance-processing code CENTRM [3] in a proof-of-principle 2-D resonance processing code known as GEMINEWTRN [11]. This code will not be available in the SCALE 5.1 release, but is expected to be prepared for public release in SCALE 6. GEMINEWTRN provides an explicit treatment of 2-D spatial effects in a continuous-energy transport solution that can provide accurate spatially-dependent multigroup cross section weighting for irregular geometric configurations.

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