Automatic Mesh Adaptivity for Hybrid Monte Carlo/Deterministic Neutronics Modeling of Difficult Shielding Problems

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INTRODUCTION

Over the last decade, the role of neutronics modeling has been shifting from analysis of each component separately to high-fidelity, full-scale analysis of the nuclear systems’ entire domains. The high accuracy associated with minimizing modeling approximations by including more physical and geometric details is now feasible because of advancements in computing hardware and development of efficient modeling methods. The hybrid Monte Carlo (MC)/deterministic techniques CADIS [1] and FW-CADIS [2] dramatically increase the efficiency of neutronics modeling, but their use in the accurate design analysis of very large and geometrically complex nuclear systems has been restricted by the availability of computing resources for their preliminary deterministic calculations and the large computer memory requirements of their final MC calculations.

To reduce the computational time and memory requirements of the CADIS and FW-CADIS methods while maintaining their efficiency improvements, three automatic mesh adaptivity algorithms were developed and added to the AutomateD VAriaNce reducTion Generator (ADVANTG) code [3]. First, a macromaterial (MM) approach [4], which mixes the materials for the deterministic calculations in the SCALE [6] shielding analysis sequence MAVRIC. By querying the MC model for the material at more than one point and creating a homogenized mixture for each mesh element, the MM approach enhances the accuracy of the material volumes. The MM approach was added to ADVANTG and used in the deterministic mesh refinement algorithm.

ALGORITHMS

Macromaterials Approach

The traditional process of defining the materials in deterministic models of CADIS and FW-CADIS simulations uses a cell-centered (CC) approach. With the CC approach, the material of each mesh element in the deterministic model is set to the material located at the center point of the element in the MC model. This approximation is simple, but it does not conserve relevant physical quantities such as material volumes.

The MM approach [4] was developed for improving the material definitions in the deterministic calculations in the SCALE [6] shielding analysis sequence MAVRIC. By querying the MC model for the material at more than one point and creating a homogenized mixture for each mesh element, the MM approach enhances the accuracy of the material volumes. The MM approach was added to ADVANTG and used in the deterministic mesh refinement algorithm.

Deterministic Mesh Refinement

In all current implementations of CADIS and FW-CADIS, the deterministic mesh must be manually created. Even with the automation of the material specifications, developing an efficient mesh for the deterministic calculations can be very difficult for large and complicated problems. A deterministic mesh refinement algorithm was developed to create deterministic meshes that capture as much geometric detail as possible without exceeding a maximum number of mesh elements that is usually determined by the availability of computing resources.

The deterministic mesh refinement algorithm uses a mesh potential function describing the materials’ heterogeneity in each mesh element. During the MM calculations, the constituents of each mesh element are internally stored in a vector of volume fractions. Each component in the vector represents the volume fraction of one of the materials in the MC model. The heterogeneity parameter used in developing the mesh potential function of the deterministic mesh refinement algorithm is...
\[ h_{ijk} = (\sigma_{\text{max}} - \sigma_{ijk}) V_{ijk}, \quad (1) \]

where \( h_{ijk} \) is the heterogeneity parameter of the mesh element defined by the three indices \( i,j, \) and \( k; \sigma_{ijk} \) is the standard deviation of the fractions in the vector consisting of the material fractions and the void fraction of the mesh element; \( \sigma_{\text{max}} \) is the maximum possible standard deviation of this vector; and \( V_{ijk} \) is the volume of the element.

Like many discrete-ordinates (S\(_N\)) deterministic codes, Denovo [7] performs calculations on an orthogonal, simply connected mesh in which each element face adjoins one and only one neighbor. Because Denovo is the preferred deterministic code for ADVANTG, the implementation of the mesh refinement algorithm in ADVANTG was constrained by preserving the connectivity of the orthogonal Cartesian mesh. A “block heterogeneity parameter” was defined for each \( X, \ Y, \) or \( Z \) block as the sum of the heterogeneity parameters of all the elements that belong to each block:

\[ H_l = \sum_{j,k} h_{ijk}, \quad H_j = \sum_{i,k} h_{ijk}, \quad H_k = \sum_{i,j} h_{ijk}. \quad (2) \]

Starting from a coarse user-defined mesh (initial guess), the steps of the deterministic mesh refinement algorithms can be summarized as follows:

1. Calculate the heterogeneity parameter of each mesh element using Eq. (1).
2. Calculate the block heterogeneity parameter of each \( X, \ Y, \) and \( Z \) block using Eq. (2).
3. Modify the mesh by inserting an extra plane at the midpoint between the two bounding planes of the \( X, \ Y, \) or \( Z \) block with the maximum heterogeneity parameter.
4. Recalculate the heterogeneity parameter for each of the new elements added by the extra plane insertion.
5. Recalculate all block heterogeneity parameters.
6. Repeat steps 3, 4, and 5 until a user-specified total number of mesh elements is reached or until the sum of the heterogeneity parameters of all the mesh elements becomes zero.

For Cartesian meshes, the sum of the heterogeneity parameters of all the mesh elements can only be zero for underlying geometries with only rectangular cross-sectional areas. The maximum number of mesh elements is specified using a refinement parameter representing the ratio between the total number of elements in the final and initial meshes.

### Weight-Window Coarsening

Both CADIS and FW-CADIS use the deterministic adjoint fluxes to calculate a biased source and WW parameters for the MC calculation. The MC calculation will stop if the MC code cannot allocate enough memory to store the WWs. The problem will be more pronounced with parallel processing because the current production-level MC codes (e.g., MCNP [8]) depend on replication of the MC data (geometry, cross sections, WWs, etc.). Because the WWs are traditionally generated using the same mesh and energy group structure as the deterministic calculations, the size of the WW maps poses a very restrictive limit on the deterministic mesh resolution in CADIS and FW-CADIS simulations of large and complicated problems. Decoupling the WW and deterministic meshes is necessary to allow the use of finer deterministic resolutions without increasing the storage size of the WW maps. An efficient algorithm for reducing the storage size of the WW maps should minimize the penalty in the MC efficiency that is expected because of the loss of fidelity due to storage size reduction.

The WW coarsening algorithm uses a flux-weighted average of the adjoint fluxes, represented by

\[ \phi_{ijkg} = \frac{\sum_g \sigma_{ijkg} \phi_{ijkg} \sigma^+_{ijkg} V_{ijk}}{\sum_g \sigma_{ijkg} \phi_{ijkg} \sigma^+_{ijkg}} \quad (3) \]

In Eq. (3), the \( i,j,k \) and \( g \) summations on the RHS include all the fine space-energy elements that compose the coarse space-energy element determined by the spatial indices \( I, J, \) and \( K \) and the energy group index \( G; \sigma_{ijkg} \) is the volume of element \(ijk\) in the fine grid; \( V_{ijk} \) is the volume of element \( IJK \) in the coarse grid; \( \phi_{ijkg} \) and \( \phi_{ijkg}^+ \) are the fluxes and adjoint fluxes of the fine grid; and \( \phi_{ijkg}^+ \) is the coarse grid adjoint flux. By using a flux-weighted average of the adjoint flux, the adjoint flux of the coarse element is controlled by the adjoint fluxes of the fine elements with higher real (forward) fluxes. Furthermore, the adjoint fluxes calculated from Eq. (3) conserve the contribution flux [9], represented by the forward flux multiplied by the adjoint flux, of the fine mesh deterministic calculations. Because the contribution flux identifies the potential response contribution of each region [9], the coarse mesh adjoint flux, calculated by Eq. (3), preserves the expected response calculated using fine mesh deterministic calculations.

Because most of the MC computational efforts are spent in tracking the particles, achieving a high figure of merit (FOM) requires focusing the MC particles in important phase-space regions. The use of fine meshes increases the fidelity of CADIS and FW-CADIS deterministic calculations, and can consequently increase the MC FOM. To minimize the decrease in the MC FOM that is expected with the mesh coarsening necessary to reduce the size of the WW maps, it is desirable to preserve the mesh fidelity in the regions of highest contribution flux in CADIS and FW-CADIS simulations. Therefore, mesh elements with lower contribution fluxes
should be collapsed before mesh elements with higher contributon fluxes.

Because only structured, simply connected WW maps can be used in MCNP without modification, the removal of the space-energy elements in ADVANTG WW maps was restricted to the removal of spatial (X, Y, or Z) blocks or energy groups. The WW coarsening algorithm used “block contributon parameters,” representing the space and energy summations of the product of the contributon fluxes and the volumes of all the space-energy elements belonging to each X, Y, or Z block or to each energy group. As an example, the block contributon parameter for one X block is expressed as

\[ C_i = \sum_g \sum_{j,k} \phi_{ijk,g} \phi_{ijk,g} V_{ijk}. \quad (4) \]

The steps of the WW coarsening algorithm can be summarized as follows:

1. Calculate the block contributon parameters for all blocks and energy groups.
2. Calculate the average adjoint fluxes (Eq. (3)) for all the space-energy elements of the spatial block or energy group \((B_{\text{min}})\) with the lowest block contributon parameter and the corresponding space-energy elements of the neighboring block or energy group \((B_{\text{neighbor}})\).
3. Update the adjoint fluxes in all the space-energy elements of \(B_{\text{neighbor}}\) by replacing them with the calculated average.
4. Update the forward fluxes and the volumes of the space-energy elements of \(B_{\text{neighbor}}\) by adding the corresponding forward fluxes and volumes of \(B_{\text{min}}\) to the corresponding values in \(B_{\text{neighbor}}\). No volume changes will occur if \(B_{\text{min}}\) represents an energy group.
5. Update the block contributon parameter of \(B_{\text{neighbor}}\) by adding the block contributon parameter of \(B_{\text{min}}\) to it.
6. Remove the forward and adjoint fluxes of all the space-energy elements of \(B_{\text{min}}\) and remove the block contributon parameter of \(B_{\text{min}}\).
7. Repeat steps 2–6 until the total number of space-energy elements reaches a user specified value.

\(B_{\text{neighbor}}\) should be the neighboring block or group with the lower block contributon parameter except boundary blocks with only one neighbor. The user should determine the total number of space-energy elements in the final WW mesh according to the computer memory available for the MC calculations. The desired number of elements in the final WW map is specified using a collapsing parameter that represents the ratio between the total number of space-energy elements in the fine deterministic mesh and the total number of space-energy elements in the coarse WW mesh.

**RESULTS**

For this analysis, the three algorithms were combined to increase the efficiency of a FW-CADIS simulation of the prompt dose rate throughout the entire ITER experimental facility. The original calculation, described in Ref. [10], used a Cartesian mesh tally with uniform cubic elements, 10 cm on a side, to calculate the total (neutrons + photons) prompt operational dose rates throughout the ITER experimental facility. The efficiency and reliability improvements provided by each of the three algorithms individually have been demonstrated in Ref. [11] for several CADIS and FW-CADIS simulations.

**ITER Prompt Dose Rate**

Figure 1 shows the cumulative distribution functions (CDFs) of the mesh tally relative uncertainties \((R_s)\) of two 10-day MCNP runs that used two WW maps developed by two FW-CADIS cases. The WW maps of both cases had similar sizes and occupied about 0.2 GB of hard disk space. The first FW-CADIS case did not use any of the three algorithms. The Denovo model in this case used a uniform mesh with elements of side lengths between 50.8 cm and 51.43 cm. The total number of space-energy elements in the Denovo model in this case was \(16.4 \times 10^6\). For the second FW-CADIS case, the Denovo model, which had \(528.0 \times 10^6\) space-energy elements, was created using the deterministic mesh refinement algorithm and used the MM approach for materials definitions. To reduce the size of the WW map in the second case, the WW coarsening algorithm was used to collapse the adjoint fluxes from the structure of the Denovo calculations to a structure with only \(16.3 \times 10^6\) space-energy elements.

![CDFs of mesh tally R](image)

*Fig. 1. CDFs of mesh tally R for 10-day MC calculations of two FW-CADIS cases.*

The use of the three algorithms increased the fraction of nonzero scoring mesh tally elements from 79.3% to 97.8%. This is equivalent to 501,477 more elements with calculated MC answers. The average relative variance of the mesh tally elements, which is used in assessing the efficiency of global MC problems [12], increased by a
factor of 3.4 due to the use of the three algorithms. This high increase in the MC efficiency, which was not accompanied by any increase in the memory requirement, can greatly facilitate performing such a difficult MC simulation with parallel-processing.

CONCLUSION

The MM approach, which improves the material representation in the deterministic models of CADIS and FW-CADIS simulations, was used to develop the deterministic mesh refinement algorithm in ADVANTG. By automatically refining a coarse initial mesh, the deterministic mesh refinement algorithm generates deterministic models that provide a good representation of the underlying MC geometries and can greatly simplify the difficult and error-prone process of manually developing meshes suitable for CADIS and FW-CADIS simulations of large and complicated problems.

The WW coarsening algorithm decouples the space-energy mesh of the WW maps from the space-energy mesh of the deterministic calculations. Because the deterministic meshes do not have to be constrained by the size of the WW maps, the WW coarsening algorithm allows the use of finer mesh resolutions in CADIS and FW-CADIS simulations. By only removing the elements of least importance to the MC calculations, the WW coarsening algorithm minimizes the reduction in the FOM that is expected with any collapsing scheme because of the loss of fidelity of the fine mesh deterministic calculations.

When the three algorithms were combined to speed up the calculation of the prompt dose rate throughout the ITER experimental facility, they significantly enhanced the MC efficiency and increased the regions where the dose rate calculation was possible.

ENDNOTES

4 In this work, the contributon flux was approximated as the product of the scalar forward and adjoint fluxes. A quadrature integration of the angular moments can be used to improve the accuracy if the flux is strongly anisotropic.

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