

Improving the S_N Adjoint Source and Geometry Representation Capabilities in the SCALE Hybrid Shielding Analysis Sequence

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INTRODUCTION

The hybrid Monte Carlo (MC)/deterministic techniques, CADIS [1] and FW-CADIS [2] have proved to provide a factor of >1000 increase in the efficiency of the neutronics modeling of problems with immense geometry and massive shielding [3,4,5]. These methods use approximate forward and/or adjoint S_N calculation(s) to develop the variance reduction parameters for a subsequent MC calculation. Despite that the deterministic calculation(s) are only used in the primary steps of the modeling sequence, the efficiency of the final MC calculation depends on the accuracy of the results of the S_N calculation(s). The material definitions for S_N calculations have been based on a simple approximation. This work studies the benefits of a new approach which provides a better representation of the MC geometry in the S_N calculation(s).

The effectiveness of the hybrid techniques is measured in their time savings compared to using either the deterministic or the MC methods individually. For saving human and computer time, the deterministic calculation has to be fast and automated. The computer time required by the deterministic calculation has an approximately linear scaling with the total number of mesh elements. Therefore, it is desirable to minimize the number of elements used, while maintaining a mesh that preserves the main geometric features of the problem. The automation of the deterministic input file creation requires an algorithm for defining the material and densities of each deterministic mesh element based on the MC geometry. Prior to this work, the implementation of the hybrid techniques used the cell center (CC) approach, which assigns the materials and densities to the S_N mesh cells based on the MC materials existing at the center points of the mesh cells. This approach did not conserve relevant quantities such as material volumes. The macro-material (MM) approach [6] was developed for better representation of the MC geometry in the deterministic calculation. The approach depends on querying the MC geometry for the materials at multiple points within each mesh element and defining a new material based on the partial volume fractions of the original MC materials.

For the deterministic calculations of CADIS and FW-CADIS an adjoint source, representing the MC tally, has to be defined. The MM approach was implemented in

the adjoint source definition for additive responses such as radiation dose or nuclear heating in mesh elements that include heterogeneities. The materials' responses are weighted by the MM fraction of each mesh cell before summing them to build the adjoint source spectrum representing the response of the tally to be optimized.

The goal of this work is to investigate the effect of using the MM approach in both the materials assignments and in the adjoint source definition on the time and memory requirement of the deterministic calculation and on the figures of merit (FOM) of the final MC calculation.

DESCRIPTION OF THE ACTUAL WORK

The MM approach was implemented in the SCALE [7] shielding analysis sequence, MAVRIC. It will be available in SCALE 6.1. MAVRIC uses the S_N code Denovo [8] for the deterministic calculation and the code Monaco for the MC calculation.

The steps of the MM approach can be summarized as follows:

1. Construct a sub-grid over each of the user-supplied mesh cells. The number of subdivisions, p , in each dimension is supplied by the user and hence the total number of sub-voxels is p^3 .
2. Determine the material associated with each sub-voxel using the CC approach.
3. Calculate approximate volume fractions associated with each material to calculate a homogenized material mixture for each mesh cell.
4. Loop through the newly created materials and set materials with similar compositions, within a preset threshold, to be equivalent.

Since the materials are queried p^3 times in each mesh cell, the error in approximating the volume fraction of materials, and thus the mass conservation, decreases as $O((1/p)^3)$. The drawback of the MM approach is the potential creation of a large number of material mixtures. Step 4 is important to reduce the number of materials and hence minimize the memory requirements; otherwise, the number of materials scales with the number of mesh elements in the original grid.

A function that weights the adjoint source strength with the MM material fractions of all the materials in each mesh cell was added to MAVRIC. This function is used with tallies that calculate additive responses such as the nuclear heating which is the sum of all the heatings

generated in the individual materials that exist within the tally volume.

RESULTS

As a preliminary test for MM approach in materials specifications, it was tested with a source-detector problem. The problem represents a 1.22 m thick concrete wall with 5.72 cm diameter steel rebar on 30.48 cm centers in each dimension and 1.27 cm thick steel plates on each side. The objective is to calculate the dose 1 m from the wall from a 1 Ci source of spent fuel photons 1 m on the other side of the wall. The S_N mesh was fixed at 4×10^5 voxels. With a uniformly spaced grid and the CC approach (Fig. 1-A), the steel rebar is completely missed in the S_N mesh. The MM capability (Fig. 1-B) was used with different numbers of cells subdivisions, $p=2,3,4,5$. For comparison, a non-uniform mesh (Fig. 1-C-D) with the same number of voxels was also used. This grid captured all the geometric details and conserved the mass of the rebar.

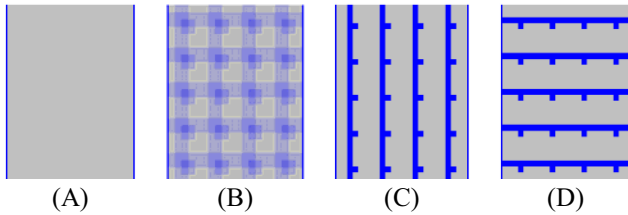


Figure 1: S_N meshes for the concrete/rebar shielding problem

Table I shows the number of materials, the running time for both the S_N and the MC calculations, and the MC figure of merit (FOM) for each case. Each simulation calculated a dose rate of 2.5×10^{-9} rem/hr with a relative uncertainty of less than 0.5%. The FOM of the analog MC (implicit capture only) calculation is estimated to be less than 1×10^{-3} /min, which is $5 \times 10^5 - 1 \times 10^6$ less than the values for the non-analog cases.

Table I: Concrete/rebar shield problems results

	# of Mats	Denovo (min)	Monaco (min)	FOM (/min)
CC testing	2	20.9	186.4	514
MM testing: 2^3	5	20.6	184.7	1079
MM testing: 3^3	5	21.7	183.8	906
MM testing: 4^3	5	20.9	186.6	1031
MM testing: 5^3	5	21.3	187.8	1007
Non-uniform grid	2	21.4	182.5	877

The use of the MM capability did not affect the running time of the Denovo calculations. The MM

capability clearly improves (~double) the MC figure of merit. The non-uniform grid did not perform as well as the MM because the mesh elements within the concrete were larger in size than those used in the uniform grid.

An example problem showing the effect of using MM in the construction of the adjoint source will be presented. The FOM of the final MC step will be compared to the corresponding one using the CC approach in the adjoint source definition.

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