

# Improving the Mesh Generation Capabilities in the SCALE Hybrid Shielding Analysis Sequence

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## INTRODUCTION

The radiation shielding analysis capabilities in SCALE 6 [1] are embodied in the MAVRIC [2] (Monaco with Automated Variance Reduction using Importance Calculations) sequence, which includes advanced variance reduction methods to enable Monte Carlo (MC) solutions for problems that are otherwise too challenging for standard, unbiased MC simulations. These methods, Consistent Adjoint Driven Importance Sampling (CADIS) [3] and Forward Weighted CADIS (FW-CADIS) [4], have proved to provide a factor of 1000 increase in the efficiency of certain MC simulations. They use approximate forward and/or adjoint fluxes from deterministic calculations to generate source and transport biasing parameters for accelerating MC simulations, and hence are also referred to as hybrid transport methods. The MAVRIC sequence of SCALE uses the discrete ordinates (DO) module Denovo and the MC module Monaco.

Since the deterministic calculations are intended to improve the efficiency of the MC simulation, the computational time required by the deterministic calculation(s) should be a relatively small fraction of the total simulation time. The computer time required by a DO 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 geometric/physics features of the problem. This usually means that the mesh used for a hybrid MC/deterministic calculation is much coarser than the mesh used to solve the problem deterministically. The macro-materials (MM) capability was added to MAVRIC to handle problems with fine details that can be missed with a coarse DO mesh. This feature increases the accuracy of the forward and/or adjoint calculations, which yields better biasing parameters and, consequently, more efficient MC simulations.

## THE CELL-CENTER APPROACH

MAVRIC, in SCALE 6, uses the mesh center points and the MC geometric description to assign materials to the DO mesh elements. While the cell-center (CC) approach does not conserve relevant quantities, such as material volumes/masses, it has proven to be sufficient for several applications [5][6]. Despite the effectiveness of the CC approach, one can readily conceive problems with

geometric details that would not be well represented by this approach; at least not without a very fine mesh. Examples include thin regions (e.g., thermal fins, absorber plates, small ducts) and small spheres or cylinders (e.g., fuel rods) that require fine mesh for accurate representation.

## THE MACRO-MATERIAL APPROACH

The approach used in the MM capability calculates homogenized material mixtures based on volume fractions that are derived from a fine grid representation. In doing that, MAVRIC uses the following steps:

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.

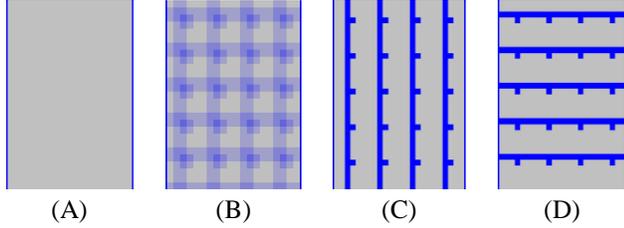
Since the materials are queried  $p^3$  times in each mesh cell, the error in approximating the volume fraction of materials, and thus the mass conservation, decreases as  $O((1/p)^3)$ . The drawback of the MM approach is the potential creation of a large number of material mixtures. Step 4 is important 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.

## TESTING AND RESULTS

### Problem 1

The MM approach was tested with a source-detector problem where the CADIS method is used to optimize the MC calculation of the detector response. 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 DO mesh was fixed at  $4 \times 10^5$  voxels. With a uniformly spaced grid and the CC approach (Fig.

1-A), the steel rebar is completely missed in the DO 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: DO meshes for the concrete/rebar shielding problem**

Table I shows the number of materials, the running time for both the DO and the MC calculations, and the MC figure of merit (FOM) for each case. Each simulation calculated a dose rate of  $2.5 \times 10^{-9}$  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  $1 \times 10^{-3}$  /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**

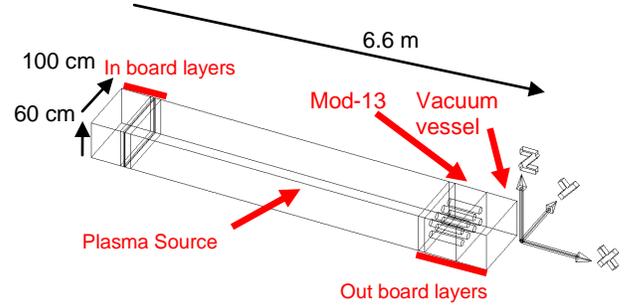
	# of Mats	Denovo (min)	Monaco (min)	FOM (/min)
CC testing	2	20.9	186.4	514
MM testing: $2^3$	5	20.6	184.7	1079
MM testing: $3^3$	5	21.7	183.8	906
MM testing: $4^3$	5	20.9	186.6	1031
MM testing: $5^3$	5	21.3	187.8	1007
Non-uniform grid	2	21.4	182.5	877

The 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.

## Problem 2

The MM capability was also tested on a semi-global problem where the FW-CADIS method is used to control the MC particles distribution to optimize more than one

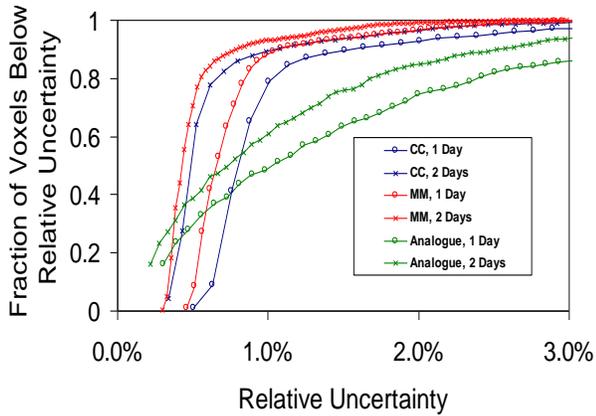
tally, or a mesh tally. The test problem is a simplified model that replicates the overall dimensions and material compositions of the ITER Module-13 problem [6]. Figure 2 shows the geometrical details of the ITER test problem.



**Figure 2: ITER problem geometry**

Mod-13 in the ITER test problem is modeled as a block of a homogenized mixture of the actual mod-13 materials with 10 cm diameter air pipes that penetrate through its whole thickness, as shown in Figure 2. The objective is to find the flux in a uniform mesh tally that overlays all mod-13 as well as the first 8 cm of the vacuum vessel. The mesh tally contained a total of 2880 mesh elements each of  $5 \times 5 \times 5$  cm<sup>3</sup>. The DO mesh used was 10 cm in y, 10 cm in z, and varied along x. The total number of mesh elements in this grid was 31360. The simulations were run for 1 and 2 days using the CC and MM approaches and the results were compared to the analog MC calculations. The CC approach completely missed the air pipes. Setting the number of subdivisions,  $p$ , at 8 resulted in adding only one more material for the DO calculations. This material is composed of mod-13 homogenized mixture with a lower atomic density to account for the existence of the air pipes. The results of the MC simulations based on both the CC and MM approaches for the DO calculations agreed, within the statistical uncertainties, with the analog cases. This provided confirmation that neither the use of the FW-CADIS nor the relatively poor importance estimates based on the DO fluxes computed without the air pipes caused any biasing in the MC calculations. The cumulative distribution functions of the relative uncertainties in the mesh tally voxels are shown in Figure 3.

In the analog cases, the uncertainties in the voxels far from the source region were higher than those close to the source. The use of the FW-CADIS method caused the uncertainties in the mesh tally voxels to be more uniform throughout the region.



**Figure 3: Cumulative distribution function of relative uncertainties in the mesh voxels for the ITER problem**

The fraction of voxels below any specific uncertainty with the MM approach is larger than the corresponding fraction with the CC approach for the same running time. The fractions of the mesh tally voxels with relative uncertainties below 2% is 74.42% for the 1 day analog case, 84.73% for the 2 days analog case, 92.93% with 1 day and the CC approach, 96.39% with 2 days and the CC approach, 96.73% with 1 day and the MM approach, and 99.13% with 2 days and the MM approach.

## CONCLUSION

The MM capability added to SCALE/MAVRIC is effective in increasing the efficiency of the MC runs without increasing the running time required for the DO calculations in hybrid MC/deterministic transport calculations.

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