AUTOMATIC MESH ADAPTIVITY FOR CADIS AND FW-CADIS
NEUTRONICS MODELING OF DIFFICULT SHIELDING PROBLEMS

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ABSTRACT

The CADIS and FW-CADIS hybrid Monte Carlo/deterministic techniques 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 limited by the large number of processors
and memory requirements for their preliminary deterministic calculations and final Monte Carlo
calculation. Three mesh adaptivity algorithms were developed to reduce the memory requirements
of CADIS and FW-CADIS without sacrificing their efficiency improvement. First, a
macromaterial approach enhances the fidelity of the deterministic models without changing the
mesh. Second, a deterministic mesh refinement algorithm generates meshes that capture as much
detail as possible without exceeding a specified maximum number of mesh elements. Finally, a weight window coarsening algorithm decouples the weight window mesh and energy
bins from the mesh and energy group structure of the deterministic calculations in order to remove
the memory constraint of the weight window map from the deterministic mesh resolution. The
three algorithms were used to enhance an FW-CADIS calculation of the prompt dose rate
throughout the ITER experimental facility. Using these algorithms resulted in a 23.3% increase in
the number of mesh tally elements in which the dose rates were calculated in a 10-day Monte
Carlo calculation and, additionally, increased the efficiency of the Monte Carlo simulation by a
factor of at least 3.4. The three algorithms enabled this difficult calculation to be accurately solved
using an FW-CADIS simulation on a regular computer cluster, obviating the need for a world-
class super computer.

Key Words: Hybrid Monte Carlo/Deterministic, CADIS and FW-CADIS, ITER neutronics

1. INTRODUCTION

Over the last decade, the role of neutronics modeling of reactor systems has been shifting from
separate analyses of individual components to high-fidelity, full-scale analyses of the entire

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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 Consistent Adjoint Driven Importance Sampling (CADIS) [1] and Forward Weighted CADIS (FW-CADIS) [2] hybrid Monte Carlo (MC)/deterministic techniques dramatically increase the efficiency of neutronics modeling and simulation [3], but their use in the accurate design analysis of very large and geometrically complex nuclear systems has been limited by the large computing resources required for their preliminary deterministic calculations and the large computer memory requirement imposed by the weight window maps generated for 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 [4]. First, a macromaterial (MM) approach [5], which mixes the materials for the deterministic calculations, enhances the fidelity of the deterministic models without changing the mesh. Second, a deterministic mesh refinement algorithm improves the accuracy of structured mesh deterministic calculations by generating meshes that capture as much geometric detail as possible without exceeding some maximum number of mesh elements, usually determined by the availability of computing resources. Finally, a weight window (WW) coarsening algorithm decouples the WW mesh from the mesh of the deterministic calculations in order to remove the memory constraint of the WW map from the deterministic mesh resolution.

The three algorithms were used to increase the efficiency of an FW-CADIS calculation of the prompt dose rate throughout the entire ITER experimental facility. This calculation represents a very challenging shielding problem because of the immense size (cylindrical model with a 40-m diameter and 25-m height) and complexity of the ITER structure and the presence of a 2-m-thick concrete biological shield [6].

2. ALGORITHMS

2.1. Macromaterials

Automating the process of mapping the materials from the MC geometry to the deterministic mesh is necessary for CADIS and FW-CADIS simulations because the manual materials description is an error-prone process that is intractable for geometrically complex problems. Previous implementations of CADIS and FW-CADIS deterministic calculations used a cell center (CC) approach. The CC approach assigns a material for each mesh element in the deterministic model based on the material existing at the center point of this element in the MC model. Despite its simplicity, it is difficult to capture important geometric detail using the CC approach. Furthermore, to decrease the computational and memory requirements of CADIS and FW-CADIS simulations, the mesh used in their deterministic calculations is generally coarser (tens of cms) than the mesh that would typically be used in a stand-alone discrete ordinates calculation. This increases the probability of “missing” important details in the deterministic calculations, which consequently decreases the efficiency and, in some cases, the reliability of the CADIS and FW-CADIS simulations [7].
The MM approach was developed to enhance the geometric representation of the CADIS and FW-CADIS deterministic models without increasing their mesh resolution. It automatically creates a mixture for each mesh element in the deterministic model by homogenizing the materials that coincide with this element in the MC model.

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

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

Because the materials are queried \( p^3 \) times in each mesh element, 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 for reducing the number of materials and hence minimizing the memory requirements; otherwise, the number of materials scales with the number of mesh elements in the original grid.

2.2. Deterministic Mesh Refinement

In all current implementations of CADIS and FW-CADIS, the positions of the planes of the deterministic structured mesh must be manually chosen. Even with automation of the material specifications, developing an efficient mesh for the deterministic calculations can be difficult for large and complicated problems. A deterministic mesh refinement algorithm was developed to create 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

\[
h_{ijk} = (\sigma_{\text{max}} - \sigma_{ijk})V_{ijk},
\]

where \( h_{ijk} \) is the heterogeneity parameter of the mesh element defined by the three indices \( i, j, \) and \( k; \sigma_{ijk} \) is the population 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. The value of the
maximum standard deviation of the materials vector depends only on the number of materials in
the MC model. It corresponds to cells with only one material and no heterogeneities.
Theoretically, the standard deviation can be zero for cells with equal fractions of materials
(including vacuum). These cells have the maximum disparity of materials and should have a high
heterogeneity parameter. By subtracting the standard deviation from the maximum standard
deviation, mesh cells with equal volumes will have maximum heterogeneity parameters if they
have uniform materials fractions, and minimum heterogeneity parameters if they are composed
of only one material. Table I shows a simple example explaining how to calculate $\sigma_{\text{max}} - \sigma_{ijk}$
for four mesh elements with different materials fractions in an MC model with three materials.

<table>
<thead>
<tr>
<th>Materials\Cells</th>
<th>Element 1</th>
<th>Element 2</th>
<th>Element 3</th>
<th>Element 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vacuum</td>
<td>0.25</td>
<td>0.33</td>
<td>0.50</td>
<td>1.00</td>
</tr>
<tr>
<td>Mat 1</td>
<td>0.25</td>
<td>0.33</td>
<td>0.50</td>
<td>0.00</td>
</tr>
<tr>
<td>Mat 2</td>
<td>0.25</td>
<td>0.33</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Mat 3</td>
<td>0.25</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Standard deviations</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_{ijk}$</td>
</tr>
<tr>
<td>$\sigma_{\text{max}} - \sigma_{ijk}$</td>
</tr>
</tbody>
</table>

Like many discrete-ordinates deterministic codes, Denovo [8] performs calculations on an
orthogonal, simply connected mesh in which each element face adjoins one and only one
neighbor. Because Denovo is the deterministic code used by 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 of the elements that belong to each
block:

$$H_i = \sum_{j,k} h_{ijk}, \quad H_j = \sum_{i,k} h_{ijk}, \quad H_k = \sum_{i,j} h_{ijk}. \quad (2)$$

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 that represents the ratio between the total number of elements in the final and initial meshes.

### 2.3. 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 cannot run 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 [9]) 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 as the WW map is coarsened.

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

\[
\phi_{ijkl,g}^+ = \frac{\sum_g \sum_{ijk} \phi_{ijkl,g}^+ \phi_{ijkl,g} V_{ijkl}}{\sum_g \sum_{ijk} \phi_{ijkl,g}^+ V_{ijkl}}. \tag{3}
\]

In Eq. (3), the \(ijk\) and \(g\) summations on the right-hand side include all of the fine space-energy elements that compose the coarse space-energy element determined by the spatial indices \(I, J, K\), and \(G\) and the energy group index \(G\); \(V_{ijkl}\) is the volume of element \(ijkl\) in the fine grid; and \(\phi_{ijkl,g}\) and \(\phi_{ijkl,g}^+\) are the fluxes and adjoint fluxes of the fine grid. While FW-CADIS uses approximate forward and adjoint deterministic calculations, the CADIS method only requires one adjoint deterministic calculation. An extra forward deterministic calculation will be needed to apply the WW coarsening algorithm for CADIS simulations.

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 \([10]\), represented by the forward flux multiplied by the adjoint flux, of the fine mesh deterministic calculations.\(^2\) Because the contribution flux identifies the potential response contribution of each

\(^2\) In this work, the contribution 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.
region [10], the coarse mesh adjoint flux, calculated by Eq. (3), preserves the expected response calculated using fine mesh deterministic calculations.

The use of finer deterministic meshes in CADIS and FW-CADIS reduces the discretization errors in the deterministic calculations, yielding better weight windows, which should increase the MC figure of merit (FOM). Because most of the MC computational effort is spent in tracking the particles, achieving a high MC FOM requires focusing the MC particles in important phase space regions. Consequently, regions with a high population of simulated particles are expected to have higher impact on the MC FOM than regions with a lower MC particles population. 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 contributon flux in CADIS and FW-CADIS simulations. Therefore, mesh elements with lower contributon 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,

\[
C_i = \sum_g \sum_{j,k} \phi_{ij,k,g}^+ \phi_{ij,k,g} V_{ij,k}, \quad C_j = \sum_g \sum_{i,k} \phi_{ij,k,g}^+ \phi_{ij,k,g} V_{ij,k}, \\
C_k = \sum_g \sum_{i,j} \phi_{ij,k,g}^+ \phi_{ij,k,g} V_{ij,k}, \quad C_g = \sum_{i,j,k} \phi_{ij,k,g}^+ \phi_{ij,k,g} V_{ij,k}. 
\]  

(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 flux-weighted average adjoint fluxes (Eq. (3)) for all the space-energy elements of the spatial block or energy group with the lowest block contributon parameter \(B_{\text{min}}\) 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 contribution parameter except for 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 of 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.

3. ITER PROMPT DOSE RATE

The three algorithms described in this work were applied to an FW-CADIS calculation of the ITER global prompt dose rate calculation described in Ref. [6]. The goal of the analysis described in Ref. [6] was to emphasize the importance of the high-fidelity, full-scale modeling of large and complicated systems. In Ref. [6], it was shown that an accurate MC calculation of the prompt dose rate at a single point outside the biological shield (bioshield) would require about 400 processor-years using traditional variance reduction techniques, and the calculation of global prompt dose rates would be even more intractable. Because of the difficulty in completing such a calculation, previous assessments have depended on coupling the final 3-D analysis with 1- or 2-D analyses [11]. These approaches ignore critical geometric details—such as large diagnostics ports—and can overestimate the prompt dose rate by a factor of 100 or more.

3.1. Methodology

The ITER 3-D model, Alite03 (Fig. 1), was used in the form of an MCNP5 input file representing a 40° sector of the ITER device [12]. The MCNP5 input file, which exceeded 19,800 lines of geometry (cell and surfaces) description, was built from the previously used BRAND model [13] and updated using MCAM [14], a CAD-MCNP interface program developed by the Fusion Design Study Team at the Institute of Plasma Physics, Hefei, China. Because of the complexity of the geometry, developing deterministic models that capture the geometric details of the Alite03 model is a very difficult process.

A Cartesian mesh tally with uniform cubic mesh elements with a side length of 10 cm was used to tally the total (neutron + photon) prompt operational dose rates throughout the entire ITER experimental facility.

ADVANTG was used to employ the FW-CADIS method for this analysis. The source biasing parameters were not used because, in some testing cases, they did not change by more than one order of magnitude because the source particles are emitted in vacuum. To optimize the mesh tally, the adjoint source in ADVANTG was defined to include all of the ITER geometry. The group-wise energy spectrum of the adjoint source was defined as the flux-to-dose-rate conversion factors in an energy structure equivalent to that of the multi-group data library of the deterministic calculation.

\[3\] As described in Ref. 6, the single tally MC calculation that did not employ the CADIS method used two traditional MCNP variance reduction techniques, namely, a point detector tally and the implicit capture.
For the forward and adjoint Denovo calculations to be performed within the limited computing resources (32 processors with ~1 GB per processor), the number of mesh elements in all of the Denovo calculations was set to not exceed 8 million cells. A uniform cubic mesh with a side length of 16.36 cm was used. For this uniform mesh, both the CC and the MM approaches were used for the material definitions in two different FW-CADIS cases. The automatic deterministic mesh refinement algorithm was also used to automatically create a mesh with the same total number of mesh elements. An initial mesh with $1.3 \times 10^6$ elements was used for the automatically refined case. This initial mesh had uniform side lengths of 32.7 cm in the Y direction and 35.3 cm in the Z direction. The initial dimensions of the mesh elements were varied in the X direction to capture the flux gradient in the bioshield and the inner shielding layers. After the final mesh was automatically generated using the deterministic mesh refinement algorithm, the MM approach was used for the materials definitions in the Denovo model. The WW coarsening algorithm was also used to collapse the fluxes of the automatically refined FW-CADIS case by factors of 2, 4, 8, 16, and 32.

A 46 neutron group 21 gamma group FENDL 2.1 [15] library was used for the Denovo calculations, and a continuous energy FENDL 2.1 library was used for the MCNP calculation.

### 3.2. Effect of Macromaterials and Deterministic Mesh Refinement

Figure 2 shows the cumulative distribution functions (CDFs) of the mesh tally relative uncertainties ($R_s$) for an analog MC calculation and for the three FW-CADIS cases that did not use WW coarsening. The MCNP running time was fixed at 10 days for each of the four cases. In Fig. 2, a perfect CDF would have a sharp jump to 100% of voxels near relative uncertainty $R = 0$, indicating uniformly well-converged tallies.
Figure 2. CDFs of mesh tally R for 10 day MC calculations of analog MC case and three FW-CADIS cases.

The maximum R for 90% of the mesh tally elements is 72.1% for the CC case, 54.4% for the MM case with no mesh refinement, and 43.8% for the deterministic mesh refinement case. Based on these preliminary calculations, the minimum MCNP computer time required to reduce the relative uncertainty of 90% of the tallies to below 10% for any of the FW-CADIS simulations is about 190 processor-days.

Table II shows the computer time utilized in performing the deterministic calculations for the three FW-CADIS cases. The initialization times include the time spent in generating the Denovo models for the FW-CADIS calculations.

<table>
<thead>
<tr>
<th>Case</th>
<th>Time (processor-hr)</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Initialization</td>
<td>Deterministic</td>
</tr>
<tr>
<td>CC</td>
<td>0.6</td>
<td>195.2</td>
</tr>
<tr>
<td>MM</td>
<td>16.6</td>
<td>1514.7</td>
</tr>
<tr>
<td>Automatic</td>
<td>14.1</td>
<td>222.6</td>
</tr>
</tbody>
</table>

The adjoint Denovo calculation for the FW-CADIS case that used the MM approach but did not use the deterministic mesh refinement algorithm took 56.85 processor-days, which is at least a factor of 9.1 longer than any of the other Denovo calculations. The version of Denovo that was used in this calculation stored all of the homogenized materials on every processor, the effect of
which was to dramatically increase the required memory and the calculation time. In contrast, the current version of Denovo only replicates the clean materials and builds only the mixed materials needed on the remote processors. Both the deterministic and initialization times will be small compared to the computer time required by a more accurate MCNP calculation, which exceeds 190 processor-days. For initialization times of the MM case with no mesh refinement and the automatic mesh refinement case to be close, the MM parameter used for the MM case with no mesh refinement was set to be 5, and the MM parameter of the automatic mesh refinement case was set to be 3.

Table III shows the fraction of the mesh tally elements that had MC scoring and the FOMs defined for the three FW-CADIS cases. The FOMs in Table 3 are based on the average relative variance, a metric sometimes used in assessing the efficiency of global MC problems [16]. This FOM is defined as

$$FOM = \frac{1}{\bar{R}^2 T},$$

(5)

where $\bar{R}^2$ is the mean of the distribution function of the relative-variances ($R^2$) of the mesh tally elements and T is the MC computation time. In Ref. [16], the basic assumption for this FOM was that the user desires as many mesh tally elements having all R below a specific value for the lowest time possible. In MC calculations of large and complicated problems, the calculations frequently need to be stopped before MC scoring occurs in all the mesh tally elements. A typical procedure for calculating $\bar{R}^2$ is to assign $R = 100\%$ for all the elements without MC scoring. The FOM is expected to be overestimated with this assumption because elements with no MC scoring expected to have a slower convergence rate than the tallies with $R = 100\%$. Because the magnitude of the overestimation in this FOM is expected to be lower for the cases with larger fractions of the non-zero scoring elements, this FOM has to be combined with the fraction of non-zero scoring elements. In this analysis, the FOMs were normalized by dividing them by the FOM calculated for the analog case and the $Rs$ of the zero scoring mesh tally elements were considered to be 100%. Because of the meaningless overestimated value of the analog FOM (~75% of the voxels do not have scoring), each normalized FOM in isolation has no meaning, but this FOM is still useful in making comparisons between different biased calculations.

<table>
<thead>
<tr>
<th>Case</th>
<th>Fraction of nonzero elements</th>
<th>Normalized FOM</th>
</tr>
</thead>
<tbody>
<tr>
<td>CC</td>
<td>95.5%</td>
<td>7.2</td>
</tr>
<tr>
<td>MM</td>
<td>97.5%</td>
<td>9.1</td>
</tr>
<tr>
<td>Automatic</td>
<td>98.3%</td>
<td>11.1</td>
</tr>
</tbody>
</table>

Table III: MC FOM and fraction of mesh tally elements with MC scoring for three FW-CADIS cases for ITER prompt dose rate problem
The use of the MM approach in creating the deterministic models increased the fraction of elements with MC scoring by 2.1% (53,000 elements), and using the deterministic mesh refinement algorithm in automatically creating the Denovo models increased the fraction of elements with MC scoring by 2.9% (74,000 elements). The calculated dose rate on the central plane of ITER and on a plane rotated 20° from the central plane are shown in Fig. 3 for the three FW-CADIS cases. The automatically refined case, which also used the MM approach for materials definitions, had more mesh tally elements with MC scoring in the upper diagnostics port, which is plugged by 5 m of shielding materials, and in the equatorial port, which is plugged by 2 m of shielding materials. Because it is difficult for the MC particles to score in the shielding plugs of these ports, the extra scoring in these regions shows that the WW parameters of the automatically refined case are more effective.

![Dose rate map on central plane and on plane rotated 20° from central plane for three FW-CADIS cases.](image)

In addition to more efficient distribution of scores for the MC particles, the FOM of the MM case is 26.4% higher than the CC case, and the FOM of the automatically refined case is 54.2% higher than the CC case.

### 3.3. Effect of Weight-Window Coarsening

Table IV shows the fraction of scoring elements and global MC FOM for 10-day MCNP runs of the automatically refined FW-CADIS case and the five FW-CADIS cases that used the WW coarsening algorithm to reduce the size of the WW map of the automatically refined FW-CADIS
case by factors of 2, 4, 8, 16, and 32. The FOMs were calculated using Eq. (5) and normalized to the analog FOM values. The Rs of the zero scoring elements were considered to be 100%. The computational time of the WW coarsening algorithm was less than 20 hours for each case. Because the amount of time needed to accurately perform this difficult calculation is on the order of hundreds of days, this time of the WW coarsening algorithm was not included in the FOM analysis.

Table IV: MC FOM and fraction of mesh tally elements with MC scoring for FW-CADIS cases with WW coarsening

<table>
<thead>
<tr>
<th>Case</th>
<th>Size of WW file (GB)</th>
<th>Fraction of nonzero elements</th>
<th>Normalized FOM</th>
</tr>
</thead>
<tbody>
<tr>
<td>No coarsening</td>
<td>6.5</td>
<td>98.3%</td>
<td>11.1</td>
</tr>
<tr>
<td>Coarsening 2</td>
<td>3.3</td>
<td>98.3%</td>
<td>11.2</td>
</tr>
<tr>
<td>Coarsening 4</td>
<td>1.7</td>
<td>97.8%</td>
<td>9.0</td>
</tr>
<tr>
<td>Coarsening 8</td>
<td>0.8</td>
<td>97.5%</td>
<td>8.2</td>
</tr>
<tr>
<td>Coarsening 16</td>
<td>0.4</td>
<td>97.6%</td>
<td>9.7</td>
</tr>
<tr>
<td>Coarsening 32</td>
<td>0.2</td>
<td>97.8%</td>
<td>10.1</td>
</tr>
</tbody>
</table>

For all of the cases with the reduced size WW maps, the decrease in the fraction of nonzero scoring mesh tally elements was less than 1%, and the decrease in the MC FOM was less than 26.1%. The systematic reduction in the fraction of elements with calculated MC answers is 0.5%, and the systematic reduction in the FOM is 9%. These reductions in the MC efficiency are offset and easily justified by the large compensatory reduction in the size of the WW map, which in turn greatly facilitates the parallel processing of the MC calculation.

3.4. Combined Effect of Macromaterials, Deterministic Mesh Refinement, and Weight-Window Coarsening

As noted in Sect. 3.2, even with the FW-CADIS method, an accurate and reliable MCNP calculation of a problem with the magnitude and complexity of this system requires hundreds of processor-days. Performing such a calculation without parallel processing is difficult. Because the size of the WW map may constitute the limiting factor on the number of MCNP jobs that can be run in parallel, it is illustrative to compare the MC efficiencies of different FW-CADIS cases with similar WW map sizes.

Figure 4 shows the CDFs of the mesh tally R of two 10-day MCNP runs that used two FW-CADIS cases, both of which had similarly sized WW maps that occupied about 0.21 GB of hard disk space.
The first FW-CADIS case did not use any of the algorithms developed in this work and used the CC approach for defining the materials in the deterministic calculations. The Denovo model for this case used a uniform mesh for which the elements had side lengths of between 40 cm and 42.33 cm. The total number of space-energy elements in the Denovo model for this case was $16.4 \times 10^6$. The second FW-CADIS case used the same automatically refined Denovo model created for the automatic refinement case of Sect. 3.2. This Denovo model contained $528.0 \times 10^6$ space-energy elements. The WW coarsening algorithm was used to reduce the number of space-energy elements in the WW map of this case to $16.3 \times 10^6$.

Table V shows the fraction of nonzero scoring mesh tally elements and the MC FOM of the two FW-CADIS cases. The FOMs were calculated using Eq. (5) and normalized to the analog FOM values. The $R$s of the zero scoring mesh tally elements were considered to be 100%.

Table V: Fraction of mesh tally elements with scoring and the MC FOM of two FW-CADIS cases with 0.206 GB WW map for ITER prompt dose rate problem

<table>
<thead>
<tr>
<th>Case</th>
<th>Fraction of nonzero elements</th>
<th>Normalized FOM</th>
</tr>
</thead>
<tbody>
<tr>
<td>No adaptivity</td>
<td>79.3%</td>
<td>3.0</td>
</tr>
<tr>
<td>Adaptivity</td>
<td>97.8%</td>
<td>10.1</td>
</tr>
</tbody>
</table>

For the FW-CADIS cases with WW maps occupying about 0.21 GB of hard disk space, using the algorithms developed in this work provided a 23.3% increase in the fraction of the nonzero scoring mesh tally elements (about 500,000 elements), and a factor of 3.4 increase in the MC FOM.
The global FOM calculated using Eq. (5) is overestimated, but the magnitude of the overestimation is proportional to the number of replacements in the Rs of the zero scoring mesh tally elements by 100%. Because the FW-CADIS case that used the three algorithms developed in this work had 23.3% nonzero scoring elements, the real (asymptotic) increase in the MC FOM is expected to be higher than the calculated value. As will be shown in the next section, the high increase in the MC FOM significantly reduces the time needed to perform such a difficult MC simulation.

3.5. Reliability of ITER Prompt Dose Rate Calculation

The large reduction in the size of the WW map for the automatically refined FW-CADIS case enabled performing a 460 processor-day MCNP calculation by parallel processing on the computer cluster of the University of Wisconsin-Madison Department of Engineering Physics. For this calculation, 87.5% of the mesh tally elements had relative uncertainties below 10%, and only 1.3% of the tallies were non-scoring. Figure 5 shows the dose rate map on the central plane of the model and on a plane rotated 20° from the central plane.

To develop confidence in the accuracy of this FW-CADIS calculation, the global MC results at four points were compared to the results of two other complementary approaches. The four points represent interesting positions inside and outside the bioshield at the mid-plane and at the bottom of the tokamak. The positions of the four points used in the verification of the global MC calculation are shown in Fig. 6.

![Dose rate map on central plane and on plane rotated 20° from central plane for 460 days of MCNP runs with FW-CADIS and three algorithms.](image)
The results of the global MC calculation at these four points were compared to results from an MC calculation using four point detectors (F5 tallies) at the four positions. It was necessary to use the FW-CADIS method for this calculation because the computer time required for doing such a calculation using conventional MC simulations is too large. Using the FW-CADIS approach was necessary for this calculation because of its difficulty, but the calculation still provided some complementarity from the original global calculation because the convergence of the MC calculations is much faster when the FW-CADIS method is used to optimize only localized tallies. The FW-CADIS calculation used four point adjoint sources with an energy spectrum equal to the flux-to-dose-rate conversion factors in the 46 neutron/21 gamma energy group structure of the multi-group library used in the deterministic calculation. Using the next event estimator of the point-detector tally instead of the track length estimator of the mesh tally provided another sort of complementarity between the two calculations. The dose rates at these four positions were also compared to the dose rates calculated deterministically by a fine-mesh stand-alone Denovo calculation. This high-performance-computing (HPC) calculation was performed on the ORNL supercomputer Jaguar using a 1.34 billion cell model. ADVANTG was used to create the input file for this HPC Denovo calculation. An approximate source that peaked in the plasma zone was used to approximate the ITER source for this calculation. A 46-neutron/21-gamma FENDL2.1 library was used for the HPC Denovo calculation. Table VI shows the dose rates calculated at the four points using the mesh tally, the point-detectors, and the HPC Denovo calculations.
### Table VI: Dose rates calculated at four points for ITER global prompt dose rate problem

<table>
<thead>
<tr>
<th>Points</th>
<th>Mesh tally (µSv/hr)</th>
<th>Point-detector (µSv/hr)</th>
<th>Denovo (µSv/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$1.9 \times 10^7 \pm 7.9%$</td>
<td>$2.8 \times 10^7 \pm 5.5%$</td>
<td>$2.2 \times 10^7$</td>
</tr>
<tr>
<td>2</td>
<td>$17 \pm 8.6%$</td>
<td>$15 \pm 4.4%$</td>
<td>$14.2$</td>
</tr>
<tr>
<td>3</td>
<td>$4.2 \times 10^6 \pm 0.9%$</td>
<td>$5.3 \times 10^6 \pm 2.1%$</td>
<td>$4 \times 10^6$</td>
</tr>
<tr>
<td>4</td>
<td>$2.7 \pm 21.0%$</td>
<td>$2.3 \pm 2.8%$</td>
<td>$1.8$</td>
</tr>
</tbody>
</table>

Considering the 13 to 14 orders-of-magnitude attenuation between the source region and points 2 and 4 as well as the 7 to 8 orders-of-magnitude attenuation between the source and points 1 and 3, the global MC results showed very good agreement with both the point-detector and the HPC Denovo results. The maximum relative difference between the point-detector results and the global MC results is 42.1%, while the maximum relative difference between the global MC results and the Denovo results is 32.6%. Differences like these are expected because the global MC results are averaged across cubical mesh cells with sides of 10 cm, the Denovo results are averaged across cubical mesh cells with sides of 2 cm, and the point-detector results are not averaged.

### 4. CONCLUSIONS

To increase the fidelity of the deterministic calculations used in CADIS and FW-CADIS simulations without exceeding the total number of mesh elements—which determines the computational resource requirements—the MM approach and deterministic mesh refinement algorithm were developed. The MM approach provides a method for homogenizing the materials of each mesh cell in the deterministic models. For a fixed number of mesh elements, the deterministic mesh refinement algorithm seeks an efficient mesh that can minimize the geometry discretization errors that are inevitable for geometrically complex problems. The algorithm takes the guesswork out of developing an appropriate, problem-dependent mesh for the deterministic calculations. By increasing the fidelity of the deterministic models, the MM and the deterministic mesh refinement algorithms increase the accuracy of the deterministic solutions and the efficiency of the MC calculations in CADIS and FW-CADIS simulations.

Using finer mesh resolution is desirable for CADIS and FW-CADIS simulations because it reduces both the truncation and the geometry discretization errors of the deterministic calculations, and consequently increases the CADIS and FW-CADIS simulation efficiency. Due to the one-to-one correspondence of the spatial mesh and energy groups between the deterministic solution and the WW map in the previous implementations of CADIS and FW-CADIS simulations, the deterministic mesh resolution was limited not just by the availability of computing resources but also by the large size of the WW maps generated for the MC calculations. This latter limitation can be very restrictive with parallel processing because current production-level MC codes (e.g., MCNP) depend on replication of the MC data (geometry, cross sections, WW parameters, etc.). Development and use of a WW coarsening algorithm removes this restrictive limitation. The WW coarsening algorithm uses a flux-
weighted average of the adjoint fluxes to decouple the space-energy mesh of the WW maps from the mesh and energy group structure of the deterministic calculations. This flux-weighted average conserves the deterministic estimate of the MC particles as represented by the contribution flux, which was approximated by the product of the space- and energy-dependent scalar forward and adjoint fluxes of each space-energy cell. By conserving the contribution fluxes of the deterministic calculations, the weights generated by the adjoint flux collapsing formula are controlled by the weights of the collapsed mesh elements with higher fluxes. Additionally, the WW coarsening algorithm carefully distinguishes between the space-energy cells with the fewest MC particles (smallest contribution flux) from those of greater importance, and selectively removes them from the data to be processed in order to reduce the computer memory burden. This minimizes the reduction in the MC FOM that is expected with any averaging scheme.

The three algorithms were used in calculating the prompt dose rate throughout the entire ITER experimental facility. This calculation represents a very challenging shielding problem because of the immense size and complexity of the ITER structure and the presence of a 2-m bioshield. Compared to an FW-CADIS calculation with the same storage size of the variance reduction parameters, the use of the three algorithms increased the regions for which the MC results were achieved by 23.3%, and increased the efficiency of the MC calculation by a factor of 3.4 for a 10-day MCNP calculation. Due to significant improvement in the MC efficiency without any increase in the memory requirement, the use of the three algorithms with FW-CADIS enabled the simulation of this difficult shielding problem on the University of Wisconsin-Madison Department of Engineering Physics computer cluster using parallel processing of the MC calculations.

The three algorithms developed in this work are currently being added to the production version of ADVANTG.

5. ACKNOWLEDGMENTS

Research was sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U.S. Department of Energy.

6. REFERENCES


