Fusion Engineering and Design 89 (2014) 1875–1879

Contents lists available at ScienceDirect

Fusion Engineering and Design

journal homepage: www.elsevier.com/locate/fusengdes

Assessment of fusion facility dose rate map using mesh adaptivity enhancements of hybrid Monte Carlo/deterministic techniques

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HIGHLIGHTS

- Calculate the prompt dose rate everywhere throughout the entire fusion energy facility.
- Utilize FW-CADIS to accurately perform difficult neutronics calculations for fusion energy systems.
- Develop three mesh adaptivity algorithms to enhance FW-CADIS efficiency in fusion-neutronics calculations.

ARTICLE INFO

Article history:
Received 11 September 2013
Received in revised form 10 February 2014
Accepted 20 February 2014
Available online 20 March 2014

Keywords:
Hybrid Monte Carlo/deterministic
Neutronics shielding
ITER prompt dose

ABSTRACT

Three mesh adaptivity algorithms were developed to facilitate and expedite the use of the CADIS and FW-CADIS hybrid Monte Carlo/deterministic techniques in accurate full-scale neutronics simulations of fusion energy systems with immense sizes and complicated geometries. 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 geometric 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 and 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. Additionally, because of the significant increase in the efficiency of FW-CADIS simulations, the three algorithms enabled this difficult calculation to be accurately solved on a regular computer cluster, eliminating the need for a world-class super computer.

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1. Introduction

Assessment of the dose rates throughout ITER is necessary to determine personnel accessibility, ensure occupational safety, and guide possible design changes for the reactor building. The biological shield (bioshield) of ITER, which has a thickness of 2 m, is designed to provide ~7 orders-of-magnitude attenuation in the absence of penetrations. However, many penetrations are necessary to route hydraulic, electrical, and other systems through the bioshield. During operation of the reactor, radiation streaming through these penetrations is expected to play a dominant role in increasing the dose rates outside the bioshield. Three dimensional (3-D) analysis is necessary to accurately predict the effect of these penetrations. Due to the immense size and complexity of the ITER structure, calculation of the radiation dose rates outside the bioshield has always depended on coupling the final 3-D analysis with simplified 1-D and/or 2-D analyses [1], which ignore critical inner geometric details such as the large diagnostics ports. A full-scale 3-D neutronics analysis of the entire ITER reactor is needed to determine the important effects of these penetrations on the dose rates outside the ITER experimental facility [2]. Fig. 1 shows a schematic view of the ITER bioshield and the ITER ports.

The Consistent Adjoint Driven Importance Sampling (CADIS) [3] and Forward-Weighted CADIS (FW-CADIS) [4] hybrid Monte Carlo (MC)/deterministic techniques have demonstrated dramatic

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http://dx.doi.org/10.1016/j.fusengdes.2014.02.046
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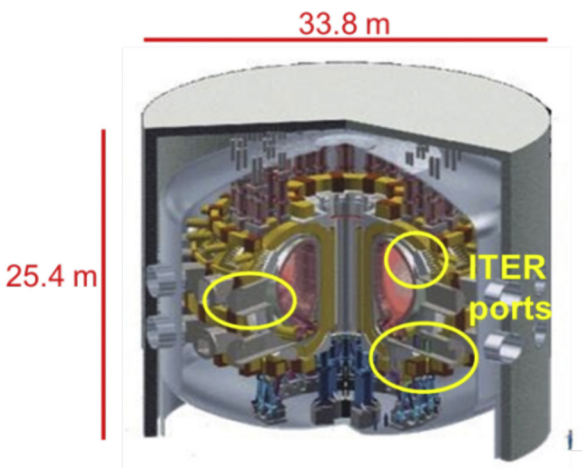

Fig. 1. ITER bioshield and ports.

improvements in the efficiency of full-scale analyses of problems with physical sizes similar to and larger than ITER [5]. These methods use approximate deterministic calculation(s), generally discrete ordinates (S_N), to create the source biasing and weight-window (WW) parameters needed for efficient MC simulations. In a previous analysis, the prompt dose rate throughout the entire ITER experimental facility was calculated using the FW-CADIS method [2]. Despite the remarkable success of the FW-CADIS method in accurately and efficiently determining the dose rates outside the ITER bioshield, the MC tally results in this analysis still had high uncertainties, especially at the inboard (IB) regions of ITER. Because of the limited computing resources available for the preliminary deterministic calculations and the limited computer memory available for storing the WW parameters of the final MC calculation, a nonuniform mesh was used in the deterministic calculations of the FW-CADIS simulation described in Ref. [2]. This mesh was manually structured to enhance the MC calculation efficiency for the outboard ITER regions at the expense of the MC efficiency for the IB ITER regions.

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 [6]. First, a macromaterial (MM) approach [7], which mixes the materials for the deterministic calculations, enhances the fidelity of the deterministic models without requiring mesh refinement. 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 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. In this work, the three algorithms were applied to the FW-CADIS calculation of the ITER global prompt dose rate calculation described in Ref. [2].

2. Algorithms

2.1. 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 [7] was developed for improving the material definitions in the deterministic calculations in the SCALE [8] 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 fidelity of the material volumes. The implementation of the MM approach in ADVANTG replaced the SCALE/MAVRIC point-testing method with a ray-tracing technique. Unlike the point-testing method, which samples the materials using a series of test points, the ray-tracing method shoots rays from the mesh boundaries and determines the material fractions along the path of each ray until it leaves the mesh [9].

The MM approach was used in the deterministic mesh refinement algorithm.

2.2. Deterministic mesh refinement

In all previous 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 [10] uses a mesh potential function describing the material 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

$$h_{ijk} = (\sigma_{max} - \sigma_{ijk})V_{ijk}, \tag{1}$$

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

Like many S_N deterministic codes, Denovo [11] 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:

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

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 [12]) depend on replication of the MC data (geometry, cross sections, WWs, etc.) on all processors. 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 [10] uses a flux-weighted average of the adjoint fluxes, represented by

$$\phi^{+}_{IJK,G} = \frac{\sum_g \sum_{ijk} \phi^{+}_{ijk,g} \phi_{ijk,g} V_{ijk}}{\sum_g \sum_{ijk} \phi_{ijk,g} V_{ijk}} \tag{3}$$

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*, and *K* and the energy group index *G*; V_{ijk} is the volume of element *ijk* in the fine grid; and $\phi_{ijk,g}$ and $\phi^{+}_{ijk,g}$ 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 contributon flux [13], represented by the forward flux multiplied by the adjoint flux,[1] of the fine mesh deterministic calculations. Because the contributon flux identifies the potential response contribution of each region [13], the coarse mesh adjoint flux, calculated by Eq. (3), preserves the expected response calculated using fine mesh deterministic calculations.

In previous works, it has been theoretically proven [14] and demonstrated [10] that the CADIS and FW-CADIS methods tend to populate the MC particles according to the contributon flux. Regions with high contributon fluxes, which should have a high population of MC simulated particles, are expected to have a higher impact on increasing or decreasing the MC figure of merit (FOM) than regions with lower contributon fluxes. 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 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 contributon flux in CADIS and FW-CADIS simulations. Therefore, mesh elements with lower contributon fluxes should be collapsed (lose fidelity) 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

$$C_i = \sum_g \sum_{j,k} \phi^{+}_{ijk,g} \phi_{ijk,g} V_{ijk} \tag{4}$$

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

$C_{neighbor}$ should be the neighboring block or group with the lower block contributon 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.

[1] 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.

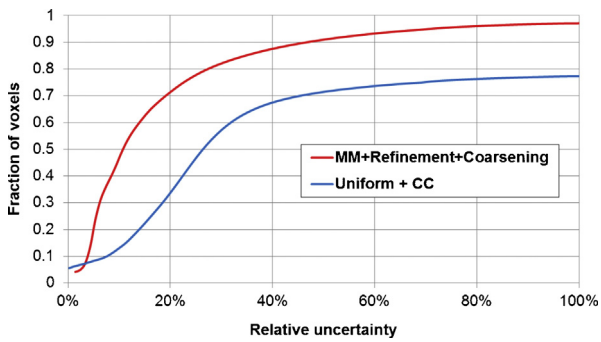

Fig. 2. CDFs of mesh tally relative uncertainties for 10-day MC calculations.

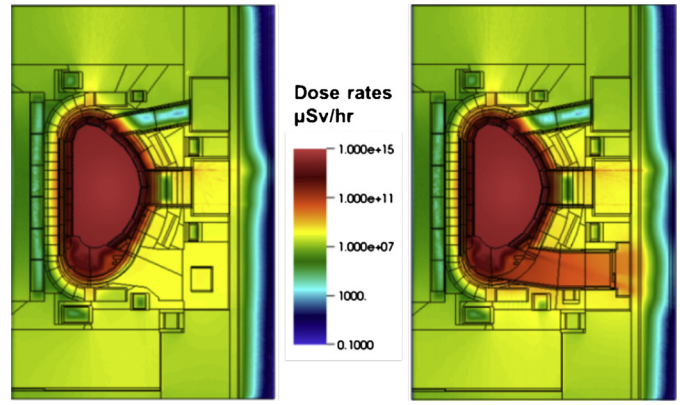

Fig. 3. Dose rate map on central plane and on plane rotated 20° from central plane.

3. Results

3.1. Effects of the three algorithms

The efficiency and reliability improvements provided by each of the three algorithms individually have been demonstrated in Ref. [10] for several CADIS and FW-CADIS simulations. For the present analysis, the three algorithms were combined to increase the efficiency of an FW-CADIS simulation of the prompt dose rate throughout the entire ITER experimental facility. The original calculation, described in Ref. [2], 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.

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.

Fig. 2 shows the cumulative distribution functions (CDFs) of the mesh tally relative uncertainties 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 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 and used the CC approach for defining the materials. The total number of space-energy elements in the Denovo model in this case was 16.4×10^6. For the second FW-CADIS case, the Denovo model, which had 528.0×10^6 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 16.3×10^6 space-energy elements.

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. For assessing the efficiency of global MC problems, an FOM based on the average relative variance of the mesh tally elements can be used [15]. This FOM 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.

3.2. Global prompt dose rate calculation with parallel processing

The large reduction in the size of the WW map for the automatically refined FW-CADIS case enabled performing a 940 processor-day MCNP calculation by parallel processing on the UNIX computer cluster of the University of Wisconsin-Madison Department of Engineering Physics. For this calculation, 92.7% of the mesh tally elements had relative uncertainties below 10%. From all of the mesh tally elements (2,676,552) that lie within the 40° sector of the MCNP model, only 19 elements did not have MC scoring in this calculation.

Fig. 3 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. 4.

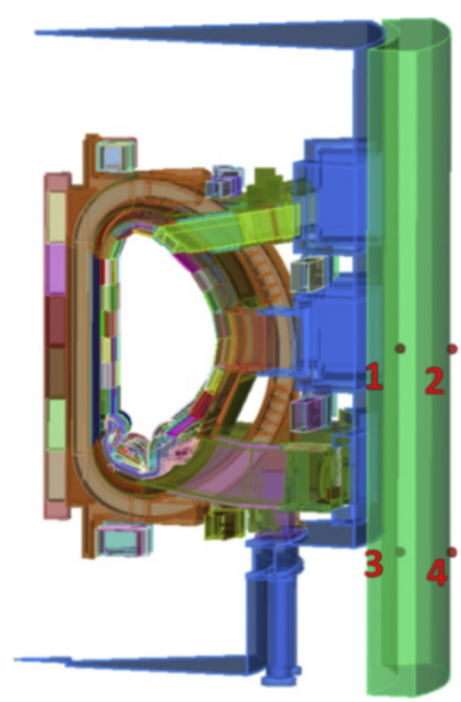

Fig. 4. Positions of the four points used in validation of ITER prompt dose rate global MC calculation.

Table 1
Dose rates calculated at four points for ITER global prompt dose rate problem.

Points	Mesh tally (μSv/h)	Point detector (μSv/h)	Denovo (μSv/h)
1	$2.0 \times 10^7 \pm 7.0\%$	$2.8 \times 10^7 \pm 5.5\%$	2.2×10^7
2	$17 \pm 6.3\%$	$15 \pm 4.4\%$	14.2
3	$4.2 \times 10^6 \pm 0.6\%$	$5.3 \times 10^6 \pm 2.1\%$	4×10^6
4	$2.8 \pm 14.0\%$	$2.3 \pm 2.8\%$	1.8

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 with a stand-alone Denovo calculation that used a spatial mesh with 1.34 billion elements, a 46 neutron/21 gamma energy group FENDL2.1 cross-section library, and 1.6×10^{15} total unknowns. This high-performance-computing (HPC) calculation was performed on 33,552 cores of the ORNL supercomputer Titan. 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. Table 1 shows the dose rates calculated at the four points using the mesh tally, the point detectors, and the HPC Denovo calculations.

Considering the 13–14 orders-of-magnitude attenuation between the source region and points 2 and 4 as well as the 7–8 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 40.0%, while the maximum relative difference between the global MC results and the Denovo results is 35.7%. 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. Conclusion

Three mesh adaptivity algorithms were developed to enhance the efficiency of CADIS and FW-CADIS simulations of fusion energy systems, which usually have immense sizes and complicated geometries. The three algorithms reduce the memory requirements of CADIS and FW-CADIS simulations without sacrificing their efficiency improvements. 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. Comparison of two FW-CADIS calculations, both using similar amounts of memory, but one employing all three algorithms described in this paper while the other used none of these algorithms, demonstrated that the use of all three algorithms increased the regions for which MC results were calculated by 23.3%. Additionally, the efficiency of the MC calculation using the algorithms described in this paper increased by a factor of 3.4 for a 10-day MCNP simulation of the prompt dose rate throughout the entire ITER facility. 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 accurate simulation of this difficult shielding problem using parallel processing of MC calculations. The global MC results from this FW-CADIS calculation agreed well with a localized FW-CADIS calculation of the dose rates at four points and with the dose rates calculated deterministically. The three algorithms developed in this work are currently being added to the production version of ADVANTG.

Acknowledgments

This manuscript has been authored by UT-Battelle, LLC, under contract DE-AC05-00OR22725 with the U.S. Department of Energy. The United States Government and the publisher, by accepting the article for publication, acknowledges that the United States Government retains a nonexclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this manuscript, or allow others to do so, for United States Government purposes.

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