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The Multi-Step CADIS Method for Shutdown Dose Rate Calculations and Uncertainty Propagation

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INTRODUCTION

Shutdown doses in fission and fusion energy systems result from the decay of neutron-induced activation products in irradiated structural materials. Accurate assessments of shutdown dose rate (SDDR) are critical to support operation, maintenance, and waste disposal planning and to guide possible design changes of critical components in nuclear energy systems. An SDDR calculation involves three steps:

1. a neutron transport calculation to determine the space and energy neutron flux distributions,
2. activation calculations to compute the photon source distribution, and
3. a photon transport calculation for estimating the final SDDR.

Even without considering the second and the third computational steps, SDDR calculations are much more challenging than one-step neutronics calculations, such as the calculation of the prompt dose rate during operation, because detailed space- and energy-dependent neutron fluxes are needed in the neutron transport calculation. In some applications, full-scale SDDR simulations are needed for immensely large systems that involve massive amounts of shielding materials. These simulations require calculating the distribution of radioisotopes everywhere throughout the entire system. For example, SDDR assessments are required everywhere inside the cryostat of the ITER experimental facility to evaluate the required waiting period after the shutdown of ITER and to identify the locations for which human accessibility should be prohibited [1]. The cryostat is a large cylindrical vacuum chamber (~30 m tall and 30 m wide) surrounding the tokomak machine. Determining the effects on SDDR of important factors such as the cross talk (interactions) between the different ports of ITER is only possible through full-scale simulations that involve all the complex inner details of the ITER tokamak machine.

Because discrete ordinates (S_N) methods provide detailed flux information, they may seem more appropriate than Monte Carlo (MC) methods for SDDR neutron transport calculations; however, the truncation errors of S_N methods can adversely affect the accuracy of SDDR predictions. Furthermore, some of the SDDR analyses involve radiation streaming through very narrow solid angles and very complicated pathways, which cannot be appropriately handled by S_N methods. The computational requirements of full-scale structured-mesh S_N simulations of very large and complicated systems such as ITER, which are on the order of tens of processor-years, are only tractable using world-class supercomputers [2]. Even with such expensive requirements, some important geometric features of these complex systems can never be accurately represented using structured-mesh S_N codes. Unstructured-mesh S_N simulations have been used to calculate SDDR at the interspaces of the ITER diagnostics ports; however, these calculations required limited angular discretization and the use of coarse meshes with sizes on the order of tens of centimeters in some regions because of the limited scaling capabilities (up to hundreds of processors) of unstructured mesh S_N codes that were used [3]. These coarse meshes cause severe discretization errors that can be evidenced by the appearance of negative space- and energy-dependent neutron fluxes in the S_N solutions [4].

The rigorous 2-step (R2S) computational system entails Monte Carlo neutron and photon transport calculations coupled with a comprehensive activation step using a dedicated inventory code and library [5]. Accurate full-scale R2S simulations are impractical for large and geometrically complex problems because the calculation of space- and energy-dependent neutron fluxes everywhere in the structural materials is difficult using the MC method. Biasing the neutron MC calculation using an importance function [6] is not straightforward because of the difficulty of explicitly expressing the response function of the neutron calculation, which depends on the next calculation steps. Moreover, typical R2S calculations do not consider the impact of uncertainties in the MC neutron calculation on SDDR uncertainty even though these former uncertainties usually dominate the SDDR uncertainty [7].

The Multi-Step Consistent Adjoint Driven Importance Sampling (MS-CADIS) hybrid MC/deterministic method has been proposed to speed up the SDDR MC neutron transport calculation using an importance function that represents the neutron importance to the final SDDR [8]. This paper provides some valuable insights regarding the MS-CADIS method, including physical interpretations of the MS-CADIS adjoint neutron source and the MS-CADIS adjoint neutron flux. The paper also describes

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the feasibility of using the MS-CADIS adjoint neutron source to calculate the SDDR uncertainty resulting from uncertainties in the MC neutron calculation. A companion paper [9] will provide numerical results that demonstrate the effectiveness of the MS-CADIS method in speeding up SDDR MC simulations and in calculating SDDR uncertainties for problems related to fusion energy systems.

MULTI-STEP CADIS METHOD

SDDR caused by decay photons is defined as[1]

$$SDDR = \langle \sigma_d(\vec{r}, E_p), \phi_p(\vec{r}, E_p) \rangle, \qquad (1)$$

where σ_d represents the flux-to-dose-rate conversion factors at the locations of interest, ϕ_p is the space- and energy-dependent photon flux, and the inner product $\langle \quad \rangle$ also signifies an integration over the entire space and energy domain. If the photon adjoint source is defined to be equal to σ_d, the photon adjoint identity becomes equal to SDDR, as described in Eq. (2),

$$\begin{aligned} SDDR &= \langle q_p^+(\vec{r}, E_p), \phi_p(\vec{r}, E_p) \rangle \\ &= \langle q_p(\vec{r}, E_p), \phi_p^+(\vec{r}, E_p) \rangle, \end{aligned} \qquad (2)$$

where q_p is the decay photon source, q_p^+ is the adjoint photon source defined as σ_d, ϕ_p is the space- and energy-dependent photon flux, and ϕ_p^+ is the adjoint photon flux.

Finding an appropriate adjoint source for the neutron calculation is not as simple as the photon calculation because SDDR is not directly caused by the neutrons but rather is caused by the decay photons of the neutron-activated structural materials. In the Multi-Step CADIS (MS-CADIS) method, we seek an adjoint neutron source whose inner product with the neutron flux is equal to SDDR. This causes the neutron adjoint identity to be equal to SDDR, as expressed in Eq. (3),

$$\begin{aligned} SDDR &= \langle q_n^+(\vec{r}, E_n), \phi_n(\vec{r}, E_n) \rangle \\ &= \langle q_n(\vec{r}, E_n), \phi_n^+(\vec{r}, E_n) \rangle, \end{aligned} \qquad (3)$$

where q_n is the neutron source, ϕ_n is the neutron flux, q_n^+ is the neutron adjoint source, and ϕ_n^+ is the neutron adjoint flux. In [8], a neutron adjoint source that satisfies Eq. (3) was defined as

$$\begin{aligned} q_n^+(\vec{r}, E_n) = \sum_i \Bigg(&\int_{E_p} f_i(E_p) \phi_p^+(\vec{r}, E_p) dE_p \\ &\times \textstyle\sum_x m_{ix}(\vec{r}) \frac{\sigma_{xi}(E_n)}{\sigma_{xi}(\vec{r}) \phi_n^t(\vec{r})} \Bigg), \end{aligned} \qquad (4)$$

where $f_i(E_p)$ is the spectrum of one mass unit of radioisotope i, $m_{ix}(\vec{r})$ is the mass at the end of the irradiation and decay scenario of each radioisotope i that was originally created by the interaction x at $\vec{r}$, $\sigma_{xi}(E_n)$ is the energy-dependent microscopic cross section of the interaction x that leads to the creation of the radioisotope i or its precursor, $\phi_n^t(\vec{r})$ is the total flux at location $\vec{r}$, and $\sigma_{xi}(\vec{r})$ is the one-group cross section of $\sigma_{xi}(E_n)$ that uses $\phi_n(\vec{r}, E_n)$ as the collapsing vector.

The MS-CADIS adjoint neutron source defined in Eq. (4) represents the SDDR resulting from the decay of radioisotopes created through irradiation by a unit neutron flux with energy E_n at location $\vec{r}$. The sum of macroscopic cross sections of the radioisotopes producing interactions represents the intuitive response function (adjoint source) for a neutron-only transport problem. In Eq. (4), $m_{ix}(\vec{r}) \frac{\sigma_{xi}(E_n)}{\sigma_{xi}(\vec{r}) \phi_n^t(\vec{r})}$ represents the microscopic cross section of the radioisotope production reactions multiplied by the mass of each radioisotope existing at the end of the irradiation and decay scenario divided by the interaction rate per atom. This is proportional to the macroscopic radioisotope-production cross section weighted by the fraction of this radioisotope existing at the end of the scenario. The additional weighting function $\int_{E_p} f_i(E_p) \phi_p^+(\vec{r}, E_p) dE_p$ represents the importance of each radioisotope produced in region $\vec{r}$ to the final SDDR.

The physical significance of the MS-CADIS adjoint function can be understood by considering the SDDR at the end of the irradiation and decay scenario caused by a unit neutron source at $\vec{r}_0$ and E_0, $q_{n0} = \delta(\vec{r} - \vec{r}_0)\delta(E - E_0)$. The photon source resulting from the irradiation of this unit neutron source can be represented as

$$\begin{aligned} q_{p_0} = \sum_i \Bigg(&f_i(E_p) \sum_x (m_{ix}(\vec{r}) \\ &\times \frac{\int_{E_n} \sigma_{xi}(E_n) G_n(\vec{r}_0 \to \vec{r}, E_0 \to E_n) dE_n}{\sigma_{xi}(\vec{r}) G_n^t(\vec{r}_0 \to \vec{r}, E_0)} \Bigg) \Bigg), \end{aligned} \qquad (5)$$

where $G_n(\vec{r}_0 \to \vec{r}, E_0 \to E_n)$ is the Green's function neutron transport kernel and $G_n^t(\vec{r}_0 \to \vec{r}, E_0)$ is the neutron transport kernel integrated over neutron energies. By substituting Eq. (5) in Eq. (2), the SDDR caused by irradiation of this unit neutron source can be expressed by

$$\begin{aligned} SDDR_0 = \sum_i \Bigg(&\int_V \int_{E_p} f_i(E_p) \phi_p^+(\vec{r}, E_p) dE_p \\ &\times \textstyle\sum_j m_{ix}(\vec{r}) \frac{\int_{E_n} \sigma_{xi}(E_n) G_n(\vec{r}_0 \to \vec{r}, E_0 \to E_n) dE_n}{\sigma_{xi}(\vec{r}) G_n^t(\vec{r}_0 \to \vec{r}, E_0)} dV \Bigg). \end{aligned} \qquad (6)$$

[1] For simplicity, all the distributions were assumed to be isotropic, but the derivation can be generalized to include the angular variation in a straightforward way.

To find the MS-CADIS neutron adjoint flux $\phi_{n_0}^{+}$ resulting from q_{n0}, the MS-CADIS neutron adjoint source defined in Eq. (4) and the neutron flux kernel must be substituted in the neutron adjoint identity. It can be easily shown that this MS-CADIS adjoint neutron flux is equal to $SDDR_0$. Therefore, the MS-CADIS adjoint neutron flux represents the contribution to SDDR of neutrons produced at $\vec{r}_0$ and E_0. It is this physical interpretation that makes the MS-CADIS adjoint neutron flux well suited to be used in speeding up SDDR MC neutron calculations using the CADIS method [10].

The R2S computational system is based on coupling the activation and MC transport codes and libraries to provide the neutron fluxes calculated from the MC neutron calculation to the activation step and to use the decay photon source in the photon MC calculation. In addition to these calculations, MS-CADIS requires performing (1) a forward (i.e., not adjoint) deterministic neutron transport calculation to estimate $\sigma_{xi}(\vec{r})$ and $\phi_n^t(\vec{r})$, (2) activation calculations for each isotope at each element of the deterministic mesh to estimate $m_{ix}(\vec{r})$, (3) an adjoint deterministic photon transport calculation using an adjoint source equal to the flux-to-dose-rate conversion factors at the position of the SDDR detector, and (4) an adjoint deterministic neutron transport calculation with an adjoint source calculated from Eq. (3). Using the CADIS method, the deterministically calculated adjoint neutron and photon fluxes can be used to calculate the source biasing and weight-window parameters to speed up the R2S neutron and photon MC calculations.

The forward-weighted CADIS (FW-CADIS) method [11] uses the inverse of the responses calculated from a forward deterministic calculation to weight the source of the deterministic adjoint calculation. The MS-CADIS method uses the solution of an adjoint photon deterministic calculation and the estimates of the radioisotope concentrations calculated using a forward deterministic neutron transport calculation coupled with an activation calculation to calculate the adjoint neutron source defined in Eq. (3). Figure 1 shows the difference between the neutron adjoint sources created using the FW-CADIS and MS-CADIS methods for the same simple slab shield problem. The maximum adjoint source strength of the FW-CADIS method is at the extreme corners of the detector side of the steel shield where the forward flux is minimal, while the maximum MS-CADIS adjoint source strength is at the center of the detector side of the steel shield because the activated radioisotopes in this region have the greatest contribution to SDDR at the detector.

MS-CADIS can also be used for speeding up MC calculations of SDDR distributions using mesh tallies or multiple tallies at several locations. Similar to the FW-CADIS method, the source used in the MS-CADIS photon adjoint calculation should be defined as the flux-to-dose-rate conversion factors divided by a deterministic estimate of SDDR at the location of each mesh tally element or at each point where SDDR is calculated.

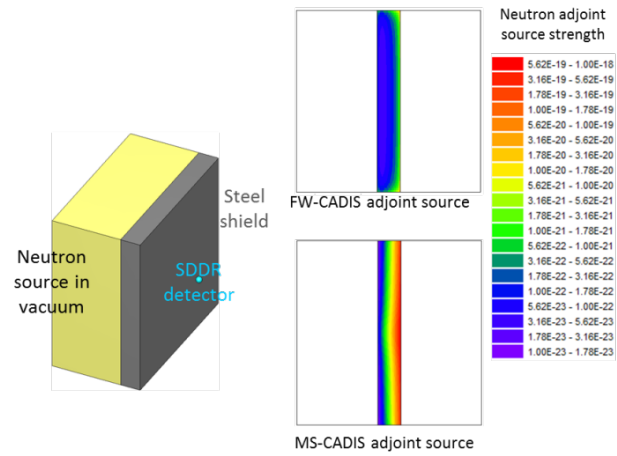

Fig. 1. FW-CADIS and MS-CADIS adjoint sources.

UNCERTAINTY PROPAGATION

A method that uses a single deterministic photon adjoint calculation has been developed to estimate the lower bound of the SDDR uncertainty resulting from uncertainties in the photon source. This method [12] cannot be used directly in R2S calculations without propagating the uncertainties in the neutron fluxes into the activation calculations. However, using quantities generated during the implementation of the MS-CADIS method, an extension of this method can be derived to calculate the SDDR uncertainties resulting from stochastic uncertainties in the neutron fluxes.

In the R2S computational system, the total SDDR uncertainty is expressed as

$$\sigma_{SDDR}^2 = \sigma_n^2 + \sigma_p^2. \tag{7}$$

The standard deviation σ_p, which reflects the stochastic uncertainty of the MC photon transport simulation, can be calculated during the MC photon transport calculation. However, the SDDR uncertainty due to the neutron MC calculation σ_n cannot be easily calculated. If the neutron fluxes are calculated using a mesh tally, the total SDDR uncertainty due to the uncertainty in the neutron MC calculation can be expressed as

$$\sigma_n^2 = \sum_{ijkg} \left(\frac{\partial SDDR}{\partial \phi_{n_{ijkg}}}\right)^2 \sigma_{ijkg}^2 + 2\sum_{ijkg \neq l} \left(\frac{\partial SDDR}{\partial \phi_{n_{ijkg}}}\right)\left(\frac{\partial SDDR}{\partial \phi_{n_l}}\right) \rho_{ijkg,l}\sigma_{ijkg}\sigma_l, \tag{8}$$

where $\rho_{ijkg,l}$ is the correlation coefficient expressing how correlated/uncorrelated/anticorrelated fluxes at the space-

energy elements $ijkg$ and l are. Space-energy elements farther away from each other are most likely uncorrelated ($\rho_{ijkg,l} = 0$), but it is unlikely that any pair of elements have any degree of anticorrelatation ($\rho_{ijkg,l} < 0$) [12]. A lower bound σ_n can be found by ignoring the correlation between the space-energy elements of the source (assuming each space-energy element is independent):

$$\sigma_n^2 = \sum_{ijkg} \left(\frac{\partial SDDR}{\partial \phi_{n_{ijkg}}} \right)^2 \sigma_{ijkg}^2. \tag{9}$$

The first equality in Eq. (3) can be approximately expressed in a discretized form as

$$SDDR = \sum_{ijkg} \phi_{n_{ijkg}} q_{n\,ijkg}^{+}, \tag{10}$$

where the MS-CADIS adjoint neutron source $q_{n\,ijkg}^{+}$ represents the SDDR due to the neutron flux at space-energy element $ijkg$. By differentiating this discretized form, Eq. (9) can be expressed as

$$\sigma_n^2 = \sum_{ijkg} \left(q_{n\,ijkg}^{+} \right)^2 \sigma_{ijkg}^2. \tag{11}$$

Because of the ignored terms in Eq. (8), this uncertainty estimate is a lower bound. Future work should explore the degree to which the neutron flux space-energy elements are correlated.

DISCUSSION

The MS-CADIS method has been proposed to speed up MC neutron transport simulations of SDDR calculations. The MS-CADIS adjoint neutron source represents the SDDR resulting from decay of the radioisotopes created through irradiation by a unit neutron flux at a certain phase-space location. The MS-CADIS adjoint neutron flux represents the contribution of neutrons produced at a certain phase-space location relative to the final. Therefore this adjoint neutron flux is well suited to speed up SDDR MC neutron calculations using the CADIS method. The MS-CADIS adjoint neutron source can also be used to determine SDDR uncertainties due to uncertainties in the neutron fluxes of the neutron MC calculation.

A companion paper will demonstrate application of the MS-CADIS method in problems related to fusion energy systems design analysis and will compare the efficiency and reliability of the MS-CADIS method to methods that are currently used in SDDR calculations of fusion energy systems.

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