Hybrid Monte Carlo/Deterministic Methods for Streaming/Beam Problems

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INTRODUCTION

Herein hybrid methods use approximate deterministic calculations to create biasing parameters for Monte Carlo. For source-detector problems, the CADIS[1] method uses the result of an adjoint calculation, $\phi^+(\vec{r},E)$, to generate consistent weight windows $\bar{w}(\vec{r},E)$ and biased source $\hat{q}(\vec{r},E)$ for the Monte Carlo simulation. These parameters are as follows:

$$R = \iint q(\vec{r},E)\,\phi^+(\vec{r},E)\,dE\,dV \tag{1}$$

$$\hat{q}(\vec{r},E) = \frac{1}{R}q(\vec{r},E)\,\phi^+(\vec{r},E) \tag{2}$$

$$\bar{w}(\vec{r},E) = \frac{R}{\phi^+(\vec{r},E)} \tag{3}$$

This approach optimizes the simulation for the calculation of the response that was used as the adjoint source. For optimizing multiple tallies or mesh tallies, an extension called FW-CADIS[2] was developed that uses a forward deterministic calculation to appropriately weight the source term used in the adjoint deterministic calculation. The importance map generated from this method helps to balance the numbers of MC particles so that multiple tallies or global quantities are computed with similar relative uncertainties.

These methods have been automated in SCALE and ADVANTG[3] (for MCNP) and applied to many practical problems. Both of these implementations consider only the space and energy components, and neither considers the particle direction in the weight windows or the biased source. Angular information was intentionally left out during the development of these codes because, even for a coarse S_N mesh and small number of energy groups, the weight window map can require a large amount of computer memory. For deep penetration problems, these methods give considerable increases in Monte Carlo efficiency [figure-of-merit, (FOM)] without considering particle direction in the weight windows or biased source.

For some problems involving long streaming paths or beam sources, the CADIS method using only space and energy information may not increase the Monte Carlo FOMs relative to analog calculations. In some cases, large changes in the computed weight window target values can be seen along a particle trajectory through an almost negligibly attenuating material (e.g., air), where the true physical importance should be no different. This is because in the space/energy approach, the angular importance has been integrated out at each location. In these streaming cases, using an average importance for a particle crossing a region in *any* direction is not representative of the true physical importance of particles traveling in *specific* directions.

The goal of the work described here is to include some directional information into the biasing parameters without storing values for every quadrature direction for every mesh cell and energy group used in the S_N calculation. For example, a problem using a 100×100×100 mesh, 30 energy groups, and an S_8 quadrature would require nearly 2×10^9 values to store. The biased version of volumetric sources would also become very large and negatively impact the speed of source sampling.

DESCRIPTION OF THE ACTUAL WORK

Theory

Van Riper et al.[4] implemented a space/energy/angle weight window in MCNP called AVATAR. They assumed that the angular component of the adjoint flux $\psi^+(\vec{r},E,\hat{\Omega})$ was separable and symmetric about the average adjoint current direction $\hat{n}(\vec{r},E)$ such that

$$\psi^+(\vec{r},E,\hat{\Omega}) \cong \phi^+(\vec{r},E)\,f(\hat{\Omega}\cdot\hat{n}) \tag{4}$$

with the average adjoint current direction defined as

$$\hat{n}(\vec{r},E) = \frac{\vec{J}(\vec{r},E)}{\|\vec{J}(\vec{r},E)\|}\ . \tag{5}$$

The form of the assumed directional component is an exponential probability distribution function

$$f(\mu) = \frac{\lambda}{2\sinh(\lambda)}e^{\lambda\mu} \tag{6}$$

where the parameter $\lambda(\vec{r},E)$ can be found from requiring that the first two angular moments of the above form be identical to that of the P_1 approximation[5], giving

$$\coth\lambda - \frac{1}{\lambda} = \bar{\mu}(\vec{r},E) = \frac{\|\vec{J}(\vec{r},E)\|}{\phi^+(\vec{r},E)}\,. \tag{7}$$

Van Riper et al. expressed λ as a fit to a ratio of polynomials in $\bar{\mu}$.

Implementation

In implementing direction-based CADIS using the above approximation to the angular adjoint flux, adjoint current information must be obtained from the S_N code. The discrete ordinates code Denovo is based on the Krylov subspace acceleration and is used by both the MAVRIC sequence of SCALE and ADVANTG. Denovo was modified to report not only the scalar adjoint fluxes $\phi^+(\vec{r},E)$ but also the adjoint currents in each direction: $J_x(\vec{r},E)$, $J_y(\vec{r},E)$, and $J_z(\vec{r},E)$. These can then be used to determine the average cosine $\bar{\mu}(\vec{r},E)$ and $\lambda(\vec{r},E)$.

The weight window targets are inversely proportional to the approximation of the angular adjoint flux

$$\bar{w}(\vec{r},E,\hat{\Omega}) = \frac{2\pi\, k}{\phi^+(\vec{r},E)\ f(\hat{\Omega}\cdot\hat{n})} \tag{8}$$

where the normalization constant k is determined by how the biased source is defined.

For a small-angle beam source (described by its space/energy distribution, $q(\vec{r},E)$, and its directional distribution, $q(\hat{\Omega}\cdot\hat{d})$ azimuthally symmetric about direction $\hat{d}$), a biased source can be defined as proportional to both the true source distribution and the space/energy component of the adjoint flux

$$\hat{q}(\vec{r},E,\hat{\Omega}) = \frac{1}{c}\left[q(\vec{r},E)\ \frac{1}{2\pi}q(\hat{\Omega}\cdot\hat{d})\right]\ \phi^+(\vec{r},E) \tag{9}$$

where the constant c is determined by normalizing $\hat{q}$ to be a probability distribution function. This leads to weight window targets and a biased source that are modifications of the standard space/energy CADIS values:

$$\hat{q}(\vec{r},E,\hat{\Omega}) \ = \ \hat{q}(\vec{r},E)\ \frac{1}{2\pi}q(\hat{\Omega}\cdot\hat{d}) \tag{10}$$

$$\bar{w}(\vec{r},E,\hat{\Omega}) \ = \ \bar{w}(\vec{r},E)\frac{1}{f(\hat{\Omega}\cdot\hat{n})} \tag{11}$$

For a more general source that is azimuthally symmetric about direction $\hat{d}$, a biased source can be defined as proportional to the true source distribution and the approximation of the angular adjoint flux

$$\hat{q}(\vec{r},E,\hat{\Omega}) \propto q(\vec{r},E,\hat{\Omega})\ \psi^+(\vec{r},E,\hat{\Omega}) \tag{12}$$

This yields a biased source and weight window targets of

$$\hat{q}(\vec{r},E,\hat{\Omega}) = \frac{1}{c}\hat{q}(\vec{r},E)\ q(\hat{\Omega}\cdot\hat{d})f(\hat{\Omega}\cdot\hat{n}) \tag{13}$$

$$\bar{w}(\vec{r},E,\hat{\Omega}) = \bar{w}(\vec{r},E)\frac{2\pi}{f(\hat{\Omega}\cdot\hat{n})} \tag{14}$$

RESULTS

These new implementations of CADIS with direction will be demonstrated on several sample problems and compared with the standard space/energy CADIS. One sample problem represents active interrogation—the calculation of a fission rate in a small amount of fissile material caused by a distant source. A second example estimates the dose rates everywhere outside the thick shielding surrounding a well-collimated beamline. Both of these problems are very difficult for analog Monte Carlo and are not always helped by traditional space/energy CADIS.

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