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Original Article

Analysis of inconsistent source sampling in monte carlo weight-window variance reduction methods

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ABSTRACT

The application of Monte Carlo (MC) to large-scale fixed-source problems has recently become possible with new hybrid methods that automate generation of parameters for variance reduction techniques. Two common variance reduction techniques, weight windows and source biasing, have been automated and popularized by the consistent adjoint-driven importance sampling (CADIS) method. This method uses the adjoint solution from an inexpensive deterministic calculation to define a consistent set of weight windows and source particles for a subsequent MC calculation. One of the motivations for source consistency is to avoid the splitting or rouletting of particles at birth, which requires computational resources. However, it is not always possible or desirable to implement such consistency, which results in inconsistent source biasing. This paper develops an original framework that mathematically expresses the coupling of the weight window and source biasing techniques, allowing the authors to explore the impact of inconsistent source sampling on the variance of MC results. A numerical experiment supports this new framework and suggests that certain classes of problems may be relatively insensitive to inconsistent source sampling schemes with moderate levels of splitting and rouletting.

1. Introduction

Many common Monte Carlo (MC) variance reduction techniques rely on weight windows to control the statistical weight of particles during transport in order to minimize the variance of flux or reaction rate tallies in a specified region of phase space (e.g., position, energy, direction). For these techniques, it is well known that the optimal particle weight at each phase location in a problem is given by the objective-driven adjoint flux for that location [1]. Particles with weight outside of a predefined window about the optimal weight are subjected to rouletting or splitting (which adjust the weight in a fair manner) in order to maintain the weight within the weight window. This weight adjustment applies at particle events where the weight changes (e.g., births, collisions) as well as when particles move between regions of phase space with different weight-window parameters.

In early implementations of weight-window variance reduction methods, inconsistencies between the radiation source distribution and the weight window parameters for the simulation resulted in source particles produced with weights that lay outside of the weight window for the corresponding birth state of the particle. Source particles produced with an inconsistent birth weight are immediately subjected to weight adjustment (splitting or roulette), which is widely believed to decrease the overall effectiveness of the weight-window variance reduction scheme.

In 1998, Wagner and Haghighat [2] introduced the consistent adjoint-driven importance sampling (CADIS) method for creating adjoint-based sets of weight-window parameters based off of a deterministic estimate for the adjoint flux. In addition, Wagner and Haghighat showed that the deterministic estimate of the adjoint flux can also be used to define a biased source definition that is consistent with the weight-window parameters. Here, consistent means that source particles from the biased source are born with a weight that lies at the center point of the weight window corresponding to the initial (birth) phase state of the particle. The development of a method for simultaneously creating a consistent source along with the weight-window parameters was a significant advancement and is a major advantage of the CADIS method. The same consistency is also found in the forward-weighted CADIS (FW-CADIS) method used to calculate global MC solutions [3]. However, even with the advancement of the CADIS method, there are some situations where it can be difficult to ensure a completely

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consistent source distribution, and, therefore, the CADIS method cannot be applied as intended.

For example, the biased source produced by CADIS is based on an estimate of the adjoint flux distribution produced from a deterministic solution method – typically the discrete ordinates (S_N) method. As a result, the adjoint flux and the resulting biased source distribution are discretized over space, energy, and direction. In order to reduce the amount of time required to generate weight-window parameters, a relatively coarse discretization may be used to estimate the adjoint flux [3]. Although the discretized biased source produced from CADIS is guaranteed to be consistent with the corresponding weight-window parameters, the CADIS source does not preserve higher-order information about the source distribution, which causes discretization error within the sampled MC source. In practice, many MC codes that use CADIS simply assume that source particles are uniformly distributed within each discretized "bin" of the CADIS source. However, this assumption may still lead to a bias in the results from the MC transport simulation, especially for cases where there is detailed structure in the true source distribution, such as the energy spectrum of a decay source. Any modification of the source distribution to reduce this bias may lead to inconsistencies between the adjusted source and the original weight-window parameters.

In other situations, the radiation source may be "presampled" from a preceding calculation and stored as a census file containing detailed state information about the source particles. This scenario is common when generating secondary radiations during MC transport (e.g., (n,γ) or (γ,n) reactions), exchanging information between MC eigenvalue and fixed-source calculations, or in S_N/MC or MC/MC splice calculations where particles that reach a predefined "trapping surface" are stored for use in a subsequent MC simulation [4]. In these cases, it is straightforward to collapse the particle census into a discretized source representation for use in CADIS. However, replacing the census source by the discretized representation would eliminate valuable information stored in the census, such as the correlations between the position, energy, and direction of each particle, and is not a practical solution for many splice calculations. Therefore, retaining the particle census introduces inconsistent source sampling into the subsequent MC calculation.

In addition, for some types of analyses, it is desirable to generate a single set of weight-window parameters that can be used with a range of similar model configurations, often representing source, geometry, or composition perturbations with respect to a single reference scenario. In these cases, the CADIS method is well suited for determining the weight-window parameters and a consistent source for the reference configuration, but it can become expensive if the weight-window parameters and/or the consistent biased source must be regenerated for every model perturbation. In practice, a single set of weight-window parameters is often used for all of the model perturbations, regardless of whether each source distribution is actually consistent with the weight-window parameters.

Finally, we note that, although the CADIS method has proven to be extremely successful, there are still weight-window variance reduction techniques in use [5,6], and under development, that do not produce a consistent biased source distribution, for a variety of reasons.

For any situation where an inconsistent source distribution may be used with weight-window variance reduction, it is important to have a clear understanding of the effects of weight adjustment via splitting or rouletting immediately after particle birth. Although the conventional wisdom maintains that any weight adjustment at birth will reduce the effectiveness of the weight-window variance reduction, no systematic, formal investigation of this conjecture has ever been performed to our knowledge. Although it appears self-evident that frequently adjusting the initial weight of source particles is counterproductive, it seems reasonable that a small initial weight adjustment for source particles may be acceptable for many applications. However, such a conclusion requires a thorough characterization of the effect of inconsistent source sampling based on the degree of inconsistency.

In this paper, we develop a mathematical framework for quantifying the impact of inconsistent source sampling on the variance of tallied quantities in a MC simulation. The derived relationships are supported with results from numerical experiments and provide a foundation for additional analyses tailored to a variety of specific applications.

2. Expected variance by sample scheme

In this section, we derive the expected variance in estimated response for several different source sampling schemes. Prior to proceeding, it is useful to define notation and significant statistical relationships that will be used throughout the remainder of the paper.

2.1. Notation and basic relationships

In MC transport methods, each history can be viewed as the combination of two separate realizations: the initial (birth) state of the source particle, denoted $\mathbf{x}$, and the response of the history as measured against some predetermined objective, denoted r. In this context, we have assumed that the initial particle state, $\mathbf{x}$, is a vector that includes properties such as the birth energy, position, and direction of the particle, and that the response, r, is a scalar value. Note that these are arbitrary assumptions and may be changed without loss of generality.

To an external observer, ignorant of the inner workings of the MC transport algorithm, it appears that each history produces a realization ($\mathbf{x}$,r) from the joint probability density function (PDF) $p(\mathbf{x},r)$. Based on the properties of joint probability distributions, it follows that the expected value and variance of any function $f(\mathbf{x},r)$ applied to a realization of the joint PDF is given by

$$E[f(\mathbf{x},r)] = \int_{-\infty}^{\infty} \int_{\Gamma} f(\mathbf{x},r)p(\mathbf{x},r)\mathrm{d}\mathbf{x}\mathrm{d}r \tag{1}$$

and

$$\mathrm{Var}[f(\mathbf{x},r)] = E\left[f^2(\mathbf{x},r)\right] - E[f(\mathbf{x},r)]^2, \tag{2}$$

where Γ is the domain for the birth state of the particle.

Note that the joint PDF $p(\mathbf{x},r)$ can be written as the product of conditional and marginal probability distributions, $p(\mathbf{x},r) = p(r|\mathbf{x})\,p(\mathbf{x})$. In this case, the expected value of the function $f(\mathbf{x},r)$ can be expressed as

$$E[f(\mathbf{x},r)] = E_{\mathbf{x}}[E_r[f(\mathbf{x},r)|\mathbf{x}]] = \int_{\Gamma} E_r[f(\mathbf{x},r)|\mathbf{x}]p(\mathbf{x})\mathrm{d}\mathbf{x}, \tag{3}$$

where

$$E_r[f(\mathbf{x},r)|\mathbf{x}] = \int_{-\infty}^{\infty} f(\mathbf{x},r)p(r|\mathbf{x})\mathrm{d}r, \tag{4}$$

and subscripts have been included on the expectation operators to clarify which variable the expectation is taken with respect to. The