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Reduced order modeling for accelerated Monte Carlo simulations in radiation transport ☆

Indika Udagedara [a], Brian Helenbrook [b,c], Aaron Luttman [d,*], Stephen E. Mitchell [d]

[a] Department of Mathematics, SC388, Clarkson University, P.O. Box 5815, Potsdam, NY 13699-5815, United States
[b] Department of Mathematics, 357 CAMP, Clarkson University, P.O. Box 5725, Potsdam, NY 13699-5725, United States
[c] Department of Mechanical and Aeronautical Engineering, 357 CAMP, Clarkson University, P.O. Box 5725, Potsdam, NY 13699-5725, United States
[d] National Security Technologies LLC, P.O. Box 98521, M/S NLV078, Las Vegas, NV 89030, United States

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ABSTRACT

Large-scale Monte Carlo simulations are the most common computational approach for modeling radiation transport, but, in some applications, the time required for such simulations can make them impractical and the required computational resources can be prohibitive. To increase computational efficiency, there are a wide range of techniques that are designed to reduce the number of so-called particle histories that must simulated to obtain statistically significant results, but it is also possible to use reduced order modeling (ROM) approaches to capture the dynamics of specific transport applications, further reducing the computational requirements for accurate results. This can lead to near real-time approaches for simulating transport for certain classes of problems, and in this work we focus on the application of characterizing radiation spectra measured from weak radiation sources emitting only a small number of particles. The proper orthogonal decomposition (POD) is adapted for use with Monte Carlo simulations to generate reduced order models of terrestrial radiation detection scenarios, and we show that the use of ROMs can result in high fidelity radiation transport simulations computed with many fewer particle histories than are required for standard calculations.

1. Introduction

The Monte Carlo (MC) method is the most widely used technique for solving radiation transport problems, due to its applicability to a wide range of radiation scenarios and its ability to accurately simulate the behavior of ensemble averages of particles [1–3]. The primary drawback of MC is that the accuracy of the results is a function of the number of particles simulated [4], and, in many applications, the number of particles required to generate sufficient precision can be computationally prohibitive [5]. There is a vast literature on techniques for increasing the statistical efficiency of MC calculations–often called "variance reduction" techniques [6–10,5,11,12]–which are generally applicable to all problems and incorporate

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* Corresponding author.
E-mail addresses: udagedig@clarkson.edu (I. Udagedara), helenbrk@clarkson.edu (B. Helenbrook), luttmaab@nv.doe.gov (A. Luttman), mitchese@nv.doe.gov (S.E. Mitchell).

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no knowledge of previous simulations. In this work, a complementary approach is taken, based on reduced order modeling (ROM) [13–19]. ROM is typically used to develop compact representations of a system governed by deterministic partial differential equations. These models are then useful for situations where repeated simulations are needed such as in flow control, design, or optimization, and they incorporate information from detailed simulations of the system under the conditions of interest and thus are specific to a particular class of problems. In this work, we combine ROM techniques with MC simulations of radiation transport to enable fast simulations of problems with only modest changes changes from run to run. There are a myriad of such applications, e.g. performing computational shielding studies for pulsed power X-ray radiography facilities or for modeling neutron transport from controlled fusion reactors, to name just a couple. The novelty of this approach from the reduced order modeling standpoint is that the ROM is still fundamentally based on a MC simulation not a continuum approximation, and the novelty from the radiation transport standpoint is the application of a deterministic approach to ROM paired with stochastic simulations.

The main idea behind developing a ROM to capture radiation transport dynamics for studying radioactive sources is to generate basis functions that can compactly represent the entire energy spectra of the sources. In principle, any approach to generating a basis that can incorporate a priori information about the spectra can be used, but, in this work, we apply the well-known proper orthogonal decomposition (POD). In the literature, there are several examples where POD–or equivalently principal component analysis (PCA)–has been applied to energy spectra, such as [20], where PCA was used to separate iodine and barium from calcium in X-ray spectra, and [21], where soil samples from different geographic origins were classified using PCA of γ spectroscopy data. Although in these examples the PCA was applied to spectral data, to our knowledge, PCA/POD has yet to be used to create a ROM for accelerating Monte Carlo simulations of such data.

Reduced order modeling does not simultaneously solve all radiation transport problems, as there is clearly no single ROM that well represents all particle transport scenarios. Nonetheless, there are many applications for which it is desired to have multiple simulations of the same scene or geometry while varying only a few parameters, such as a radiation source or shielding geometry. In this work we focus on a terrestrial radiation detection scenario, where a ROM is generated from simulations of pure radiation sources, and the resulting model is used for fast simulation of radiation sources composed of mixtures of the pure sources. The basic details of POD are presented in Section 2. Section 3 describes how the training data is generated and the POD is constructed in this application. Section 4 addresses some of the modeling difficulties associated with Monte Carlo simulations of radiation transport problems, and the efficacy of our ROM approach for accelerating Monte Carlo simulations is described in Section 5.

2. Application of the proper orthogonal decomposition

The general idea of the reduced order modeling approach to studying radiation source spectra is to create a compact representation of the normalized photon number distribution, $n(\vec{x}, e)$, where e is the photon energy and $\vec{x}$ is the detector location, such that only a small number of particle histories is needed for an MC simulation to predict the distribution. To do this, a truncated series expansion of the distribution

$$n(\vec{x}, e)_N = \sum_{j=1}^{N} a_j(\vec{x})\varphi_j(e) \tag{1}$$

is used, where $a_j(\vec{x})$ are weighting coefficients and $\{\varphi_1, \ldots, \varphi_N\}$ are the basis functions used to construct the ROM.

There are many possible approaches to constructing the basis functions used in the above expansion. In this work, we use the proper orthogonal decomposition (POD) [22–24] of a set of training data generated by offline Monte Carlo simulations. The specific details of computing the training data are given in Section 3. POD typically uses unsteady data obtained from numerical simulations or experiments to generate an orthogonal set of spatial basis functions that can be used to compactly represent the data. In this work we take the same basic approach, except that the POD modes are not spatial functions but functions of the photon energy, e. Additionally, averages are taken over space in this application, whereas in classical POD the averages are temporal. The goal is to find functions (POD modes) of energy that can represent the normalized photon number distribution (spectra) at different spatial positions as compactly as possible. Mathematically, the dominant POD mode φ_1 is a solution to the optimization problem

$$\varphi_1 = \underset{\tilde{\varphi} \in L^2(\Omega)}{\operatorname{argmax}} \left\langle \left(\int_\Omega \tilde{\varphi}(e) n(\vec{x}, e) de \right)^2 \right\rangle, \tag{2}$$

subject to $\int_\Omega \varphi_1(e)^2 de = 1$, where $\langle \cdot \rangle$ denotes spatial average and Ω is the range of energies over which the radiation is measured. An orthogonal series can be generated where each mode of the series best represents the variations of $n(\vec{x}, e)$ that are not encompassed by the previous modes. In this way, spectra can be represented with as few degrees of freedom as possible.

The actual solution to the POD maximization problem (2) is obtained from the Fredholm integral equation [22]

$$\int_\Omega R(e, e')\varphi(e')de' = \lambda\varphi(e), \tag{3}$$