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Monte Carlo Midway Forward-Adjoint Coupling with Legendre Polynomials for Borehole Logging Applications

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The Monte Carlo Midway method utilizes the surface integral form of the reciprocity theorem in order to increase computational efficiency. The response of a detector is calculated by integrating the product of the adjoint function and the flux regarding all phase space variables, whereas both functions are stochastically sampled. Formerly, coupling of the two functions has been done by estimating the flux and the adjoint functions in small phase-space segments. In this paper, we investigated the possibility to use Legendre polynomial expansion on a stochastic basis for the surface integral. A formula for the variance of the expansion coefficients is derived. Using a simple mathematical example the systematic error as a function of the number of segments or the Legendre expansion order is investigated. The new algorithm is tested with a borehole logging application, estimating the time-dependent response of a photon detector due to a 14 MeV neutron source. It resulted in a higher accuracy of the forward-adjoint coupling, but the efficiency of the calculation decreased.

KEYWORDS: Monte Carlo, Borehole logging, Legendre Polynomials, Variance Reduction, Adjoint

1. Introduction

The Midway method is a general Monte Carlo variance reduction or efficiency improving technique that calculates a detector response by combining adjoint and forward Monte Carlo scores on a surface between source and detector in order to estimate the surface integral of the adjoint function and the radiation current. [1]

The time dependent Midway method has been proven useful as a variance reduction technique for borehole logging calculations. [2,3]

Estimation of the surface integral previously has been done by segmenting the phase-space into meshes where Monte Carlo adjoint function and radiation currents were calculated and coupled. The efficiency and accuracy of such an approximation depends highly on the structure of this segmentation. Obtaining estimates for each segment will yield a detailed description of the respective function, and increasing the number of segments yields a more accurate estimate of the response. Limit to such an increase of number of meshes, is posed by the decrease of number of samples per each segment, and by –considering the number of dimensions- possible computer memory shortage. The number of given samples for the integral determine the allowed finest segmentation, and this might yield inaccuracies in the response estimate.

In the present paper, a new coupling technique is presented, replacing the segmentation scheme by calculating coefficients of orthogonal basis functions. With this technique, instead of estimates on small phase-space segments, the coefficients describe the corresponding adjoint function or radiation current. Estimation of these coefficients by Monte Carlo for flux and current calculation has been reported before. [4] Monte Carlo estimation of these coefficients has also been used for forward-adjoint coupling with deterministic adjoint calculations.

In course of the next section, we will describe the Midway method with the segmentation technique and we introduce the formulation of the coupling of Monte Carlo scores by orthogonal function expansion coefficients with the corresponding statistical error propagation. The third section contains a numerical example on simple cases, and the application of the method to a borehole logging Monte Carlo calculation. The fourth section will summarize the results.

2. Formulation of the Midway Method

2.1 The Midway Method with Segmentation Technique

Most Monte Carlo particle transport simulations aim to obtain an estimate for a detector response R of the form

$$R = \int_V D(P)\phi(P)\,dP$$

where P stands for the phase-space variables: position, direction, energy and time ($\boldsymbol{r},\boldsymbol{\Omega}, E, t$); $D(P)$ is the detector function describing the detector response, $\phi(P)$ is the flux as a function of all phase space variables. The integral is taken over the whole model domain V. The same response can be calculated using the adjoint function $\phi^+(P)$:.

$$R = \int_V S(P)\phi^+(P)\,dP,$$

where $S(P)$ is the source function. Another alternative form of this response is

$$R = \int_{A_m} \boldsymbol{n}\cdot\boldsymbol{\Omega}\phi(P)\phi^+(P)\,dP, \tag{1}$$

where the integral is taken on a surface enclosing completely either the source or the detector.

This third form of the response according to Equation (1) is used for the Monte Carlo Midway response estimate. Utilization of the Midway response requires bilinear integration, which obviously is a problem for any linear Monte Carlo method. To circumvent this problem we apply two separate (forward and adjoint) calculations that are coupled on the Midway surface A_m. To estimate this integral the scoring domain is subdivided into a number of energy, surface, direction and time meshes (segments), to approximate the Midway response form with a finite summation. First, we obtain a Monte Carlo estimate for the quantity $J(P) = \boldsymbol{n}.\boldsymbol{\Omega}\phi(P)$ in the forward run, then for $\phi^+(P)$ in the adjoint run with a surface crossing flux estimator for every mesh of the phase-space. The estimator reads:

$$R \approx R_m = \sum_j J_j \phi_j^+ \Delta P_j$$

The standard deviation $r(R_m)$of R_m can be propagated from the individual estimated statistical variances of the meshes by

$$r(R_m) = \frac{1}{R_m}\sqrt{\sum_j \{r^2[J_j] + r^2[\phi_j^+]\}\{J_j\phi_j^+\Delta P_j\}^2}$$

The subdivision into meshes of the phase space should be fine enough to give a good estimate of the response R. For a given number of samples, the smaller mesh sizes we have, the less is the probability of obtaining enough scores for a reasonable estimate of J_j and ϕ_j or sometimes to obtain any scores at all. This may introduce a source for statistical error. To illustrate this, two simple two-dimensional functions $f(x,y)$ and $f^+(x,y)$ has been chosen and the integral of their product was set to be estimated by Monte Carlo in a form of

$$I = \int_a^b \int_c^d f(x,y) f^+(x,y)\, dxdy. \qquad (2)$$

Samples were drawn from both $f(x,y)$ and $f^+(x,y)$, the (x,y) space subdivided into small segments, with boundaries a_i and c_j distributed equidistantly. The functions were set to $f(x,y) = x^2/(45y); f^+(x,y) = y/x^2$ on the range of $x \in [1,6]$, $y \in [1,10]$, which yields a value if $I = 1$. From both functions 10^6 samples were drawn. The estimator is given by

$$R \approx \sum_{j=1}^{n} \sum_{i=1}^{n} F_{i,j} F_{i,j}^{+} / \left(|a_{i+1} - a_i| |c_{j+1} - c_j| \right) \qquad i,j = 1,\ldots,n,$$

where $F_{i,j}$ and $F^+_{i,j}$ are integrals of $f(x,y)$ and $f^+(x,y)$ on the respective i^{th} and j^{th} subdivision. These integrals have been calculated analytically and by averaging the Monte Carlo samples falling into the subdivision.

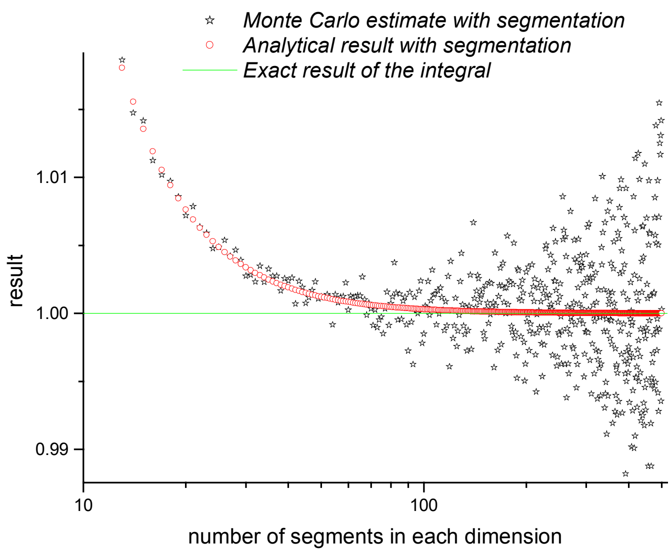

Fig. 1 Monte Carlo evaluation of the integral of the product of two functions with varying number of subdivisions

Figure 1 shows the analytical and Monte Carlo evaluation of the integrals using such an approximation as a function of the number of segments in each x- and y-dimensions. For small number of segments, the estimator is higher than the exact result due to the insufficient number of subdivisions. The Monte Carlo estimate matches reasonably well the analytical solution. For higher number of meshes, the estimator converges to the correct solution. After the number of segments becomes too high for obtaining a good estimate for the integrals on the subdomains, the estimator fluctuates statistically therefore increases the variance of the estimate of R. With no *apriori* knowledge on these functions setting the number segments might yield an inaccurate or an ineffective result.

2.2 The Midway Integration Using Legendre Polynomials

Functions in the $\mathcal{L}_2$ space can be expressed as

$$f(x)=\sum_{i=0}^{\infty} c_i\varphi_i(x),$$

where the $\varphi_i(x)$'s form a full orthogonal basis and the coefficient c_i is expressed as

$$c_i=\int_a^b \varphi_i(x) f(x)\rho(x)dx \Big/ \int_a^b \varphi_i^2(x)\rho(x)dx,$$

having $\rho(x)$ the weight function determining the basis functions and the interval [a,b] on which the orthogonality is fulfilled. The integral of Equation (2) could be alternatively estimated by:

$$I=\int_a^b f(x)f^+(x)dx=\int_a^b\sum_{i=0}^{\infty} c_iP_i(x)f^+(x)dx=\sum_{i=0}^{\infty} c_i\underbrace{\int_{-a}^{b} f^+(x)P_i(x)dx}_{c_i^+}=\sum_{i=0}^{\infty} c_ic_i^+$$

From the position and weight samples x_i and w_i the estimators for the coefficients c_i, read:

$$c_i\approx\frac{1}{N}\sum_{j=1}^{N} w_j\varphi_i(x_j) \Big/ \int_a^b \varphi_i^2(x)\rho(x)dx$$

where N denotes the number of samples. A similar formula can be devised for c_i^+, but the division with the norm of $\varphi_i(x)$ is absent. The series of expansion coefficients is truncated to number L. Each sample is used for each coefficient.

Calculation of an estimate of the relative error in the response is not as straightforward, as for the segmentation technique, as the statistical correlation of the estimates must be taken into account in the error propagation. The calculation of the covariance term is very tedious and computer memory consuming if all cross correlation are to be estimated. Therefore, a simple approximation has been used for the error prediction. For one random variable of the sample, the variance is:

$$\begin{aligned}\mathrm{Var}(R_m)&=\sum_{l=0}^{L}\mathrm{Var}(c_lc_l^+)+2\sum_{l=0}^{L}\sum_{\substack{m=0,\\ m\neq l}}^{L}\mathrm{Cov}(c_lc_l^+,c_mc_m^+)\\ &\le\sum_{l=0}^{L}\mathrm{Var}(c_lc_l^+)+\frac{1}{2}\sum_{l=0}^{L}\sum_{\substack{m=0,\\ m\neq l}}^{L}(c_l^2+c_m^2)(c_l^{+2}+c_m^{+2})-R_m^2\end{aligned}$$

This will lead to an estimator of the relative error:

$$r^2(R_m)\le\frac{\sum_{l=0}^{L}\left(r^2(c_l)+r^2(c_l^+)\right)(c_lc_l^+)^2}{\left(\sum_{l=0}^{L}c_lc_l^+\right)^2}+\frac{L}{2NN^+}\frac{\sum_{l=0}^{L}D^2(c_l^2)\sum_{m=0}^{L}D^2(c_m^{+2})}{\left(\sum_{l=0}^{L}c_lc_l^+\right)^2}$$

The method has been applied to the same set of two-dimensional functions as at section 2.1. For the orthogonal basis functions, Legendre polynomials were used, and the variables in both dimensions were transformed to [-1,1]. The results are shown in Figure 2.

It has been stated [6] that the right choice of the basis functions are essential for getting a good result. Without counting on much apriori knowledge, a fast converging function basis can not be optimally chosen. It should be noted that Legendre polynomials are coping well with discontinuities, and easy to generate in a numerically stable way.

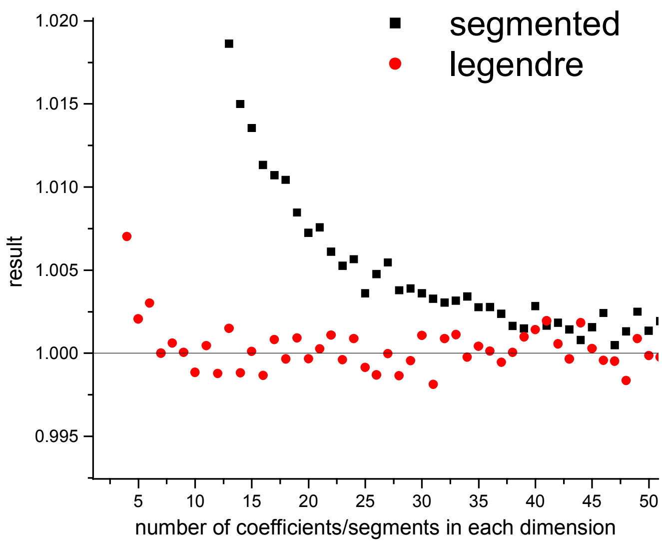

Fig. 2 Comparison of the convergence of coupling with segmentation and using Legendre polynomials

3. Application to a Realistic Borehole Logging Case

3.1 Geometry and Modeling

Applying such a scheme of linear combinations of analytical functions for describing the flux or the current surely does not work in every variable. The energy dependence of the photon flux, for example, could appear as a series of delta functions if coming from inelastic neutron scattering or capture. In spatial variables the second derivative of the flux is not continuous at material boundaries. Moreover, for multiple dimensions, at each surface crossing, contributions to all relevant coefficients should be made, slowing down the calculation significantly. Therefore we chose the angular variable as subject to coupling with Legendre polynomial expansion, and the other variables are discretized by phase-space segmentation. For the cosine of the surface normal, Laguerre polynomials were also used for the sake of comparison of function bases. In this case, the azimuthal angular variation was still handled using Legendre polynomials.

A nuclear borehole logging tool poses a reasonable challenge for variance reduction techniques. [7] Our sample problem models an oil well logging tool with a time-dependent neutron source, and photon detectors.

The model of the borehole-logging environment consists of sandstone (SiO_2) formation, in an 8" borehole with a 7" iron casing, water as the borehole fluid, and salty water filling the pores of the formation (19 % porosity). The tool itself has an outer diameter of $1^{11}/_{16}$", and contains two scintillation detectors (both $1^{3}/_{16}$" in diameter), and a 14 MeV neutron source. The timing of the tool was: burst from 0-50 μs, data collection from 0-1000 μs in 20 time steps.

For the calculations, the MCNP4C2 [5] neutron-photon particle transport code has been used. The Midway calculations were performed using the so-called PTRAC-files of MCNP, that is a logging file of events of particle histories. Because of the lack of continuous-energy adjoint Monte Carlo capability in MCNP, the multigroup MENDEF library was used.

The Midway calculation utilized the so-called black absorber technique [1] that allows calculating either the adjoint function or the flux only in the enclosure half-space bounded by the Midway surface.

3.2 Results

The Midway setup for the segmentation technique consisted of 10x11 spatial bins, 10x11 angular bins, 30 energy groups for neutrons and 12 for photons, and 20 time bins. The spatial and angular distribution of segments was set using empirical knowledge on the flux.

For the Legendre method the same energy, spatial and time segmentation was used. For the Legendre coefficients in azimuthal and polar angles 6 and 4 coefficients were taken, respectively.

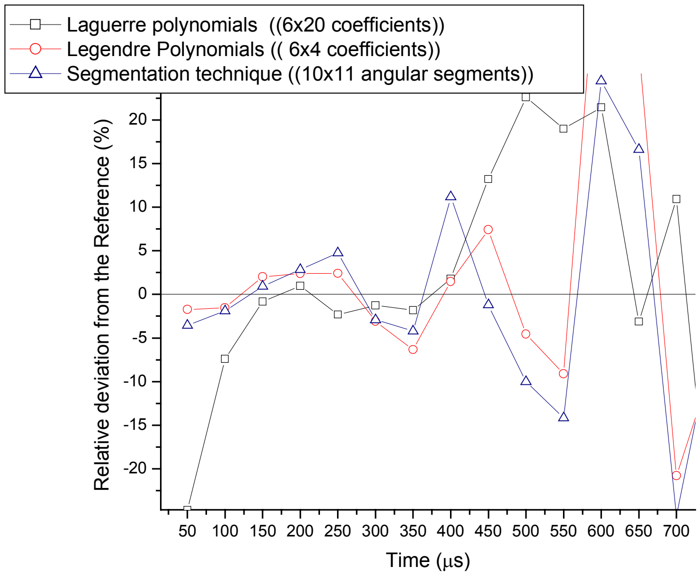

Fig. 3 Coupling Results with Laguerre and Legendre polynomials and with the Segmentation Technique

The results are shown as percentage deviation of results from a reference calculation, that is a forward Monte Carlo run with large number of samples (10^9 particles). Results are given for the "Near" detector, the detector that is closest to the source. The time response is an exponentially decreasing function. The results for more than 700 μs are not reliable from the reference calculation, as the relative error increases above 10 %.

For the segmentation technique, $5x10^6$ and 10^7 neutron particle histories have been used for the adjoint and forward scores, respectively. In case of the Legendre method $5x10^6$ particles were used both for the adjoint and the forward calculations. The graph shows that the accuracy of the Legendre coupling is better until about 600 μs, where the number of scores are too low for a reasonable estimate. The Laguerre polynomials seem to fail to describe effectively the cosine of surface normal, only a high number (20) of coefficients gave reasonable results.

The efficiency of Monte Carlo calculations is often measured by the Figure of Merit (FOM):

$$FOM = T^{-1}r^{-2},$$

where T is the CPU time in minutes, and r is the predicted relative error.

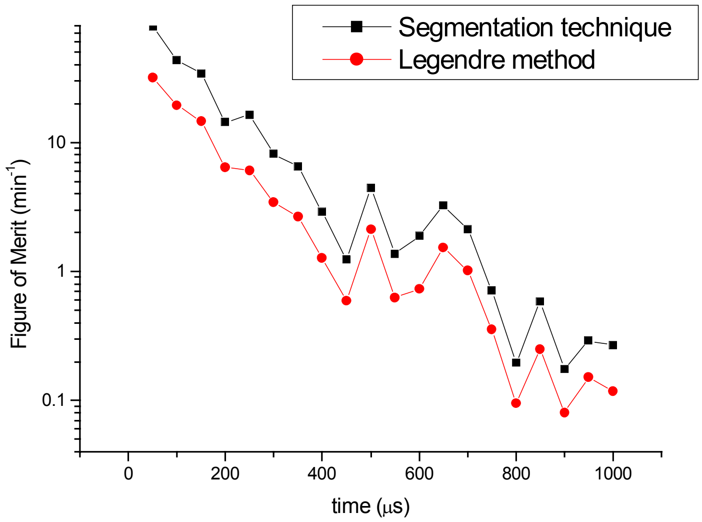

Fig. 4 Figure of Merit for the coupling techniques

Figure 4 shows the efficiency of the calculations with the two methods. Coupling with Legendre polynomials brings an efficiency decrease of a factor 2. As for each score several contributions are generated when using the orthogonal basis functions for the coupling. The Laguerre expansion did not result in an acceptably high enough efficiency.

4. Conclusion and Discussion

Both the simplified numerical example and the borehole logging simulations showed that coupling with Legendre polynomials increases the accuracy of the Midway method without apriori knowledge on the flux and the adjoint function. Application of such a technique is limited by the rapidly decreasing efficiency with the number of coefficients used. The minimum number of coefficients for a given accuracy depends also on the choice of the basis functions.

In general, such coupling seems to be more apt for application at non variance-reduction oriented forward-adjoint coupling.

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