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Unbiased estimators of coincidence and correlation in non-analogous Monte Carlo particle transport

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ABSTRACT

The conventional non-analogous Monte Carlo methods are optimized to preserve the mean value of the distributions. Therefore, they are not suited to non-Boltzmann problems such as the estimation of coincidences or correlations. This paper presents a general method called history splitting for the non-analogous estimation of such quantities. The basic principle of the method is that a non-analogous particle history can be interpreted as a collection of analogous histories with different weights according to the probability of their realization. Calculations with a simple Monte Carlo program for a pulse-height-type estimator prove that the method is feasible and provides unbiased estimation. Different variance reduction techniques have been tried with the method and Russian roulette turned out to be ineffective in high multiplicity systems. An alternative history control method is applied instead. Simulation results of an auto-correlation (Rossi-α) measurement show that even the reconstruction of the higher moments is possible with the history splitting method, which makes the simulation of neutron noise measurements feasible.

1. Introduction

During the investigation of particle transport with Monte Carlo methods one often faces tasks which need the estimation of the coincidence of events or correlations between events. A coincidence is when separate events (e.g. detection) occur during a given time period. Examples for such problems are the additive peaks in detectors or the dead-time effect. The correlation measures the deviation from independency of certain events and its estimation involves higher moments. The general definition of correlation is the following:

$$\rho(\xi,\eta) = \frac{\sigma_{\xi\eta}}{\sigma_{\xi}\sigma_{\eta}} \tag{1}$$

where ξ and η are random variables, ρ denotes the correlation, while σ is the (co) variance. In the case of particle transport problems the random variables refer to the contribution in a certain detector in a given time interval. The different noise measurement techniques (e.g. Feynman-α, Rossi-α, etc.) use different ways to quantify correlations, but all involve the variance or other higher moments. The problem becomes a transport problem when several detection events can originate from the same source event either due to a non-stopping detection event (e.g. scattering), a multiple source event (e.g. spontaneous fission for neutrons, multiple γ-line emission for γ-particles), or because the particle is transported in a multiplicative medium between the source and the detection (e.g. fissile material for neutrons or pair production for photons).

Such problems are often referred to as non-Boltzmann estimators as they depend on the collective effects of particles not described in the Boltzmann transport equation. The conventional non-analogous Monte Carlo methods are optimized to preserve the mean value of the distributions and therefore not suited for non-Boltzmann problems. The different variance reduction techniques applied by them introduce artificial coincidences by splitting particle trajectories and biases the higher moments by weighting of the events. Analogous Monte Carlo simulations avoid these problems but the computer time needed to arrive at acceptable statistics in full-scale problems may be overwhelming.

This problem has already been addressed by Booth (1992, 1994) with the motivation of using variance reduction techniques for the photon pulse height tally (total energy deposition in a detector). The pulse height tally falls into the category of non-Boltzmann estimators because it collects the energy deposition from several collisions of a single particle. Furthermore, photons may undergo pair production or double fluorescence, which result in multiplication. Booth suggests three possible approaches. The *deconvolution* approach applies single particle variance reduction methods to

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each particle of a collection and then analyzes (deconvolutes) how the distribution of the collection of particles is modified and weights the tallies appropriately. The *supertrack* approach applies variance reduction to collections of tracks (supertracks) and requires redefinition of standard Monte Carlo terms. For example, the individual particle tracks would no longer carry any weight; the variance reduction is applied to the supertracks, and thus the weights are associated with the supertracks. The *corrected single particle* approach is perhaps the most difficult. In this approach, the tracks are first treated as single particles with the traditional single particle weights, and then the collective effects are introduced by estimating the difference between transporting the particles as a collection and transporting the particles individually.

The deconvolution approach based on Booth's method was implemented in MCNP5 (Booth, 2004; Sood et al., 2004) and MCNPX (Hendricks and McKinney, 2004; Pelowitz, 2011). A similar method was introduced in MCBEND (Shuttleworth, 2000) for splitting and Russian roulette, also for the photon pulse height tally. In the medical imaging and simulation application GATE based on GEANT4, a method has been implemented to make the geometrical importance sampling technique compatible with the pulse height tally for single photon emission computed tomography (SPECT) simulations (Beenhouwer et al., 2004). More recently, Williams and Tickner (Williams and Tickner, 2012) published a simplified algorithm for the implementation of this approach with the purpose to simulate γ-γ coincidences in detectors.

The above methods are all focused on the photon pulse height tally, which is a problem containing low or no multiplicity and involves only coincidences of events. However, the investigation of neutron fluctuations requires the simulation of sub-critical systems where a single source neutron can generate a large number of secondary neutrons through fission and the correlation of detection events needs to be investigated. The importance of this problem is emphasized by the fact that considerable efforts were made to create fully analogous versions of general neutron transport Monte Carlo codes in order to simulate noise measurements (Ficaro and Wehe, 1994; Valentine and Mihalczo, 1996; Mori et al., 2001) or neutron multiplicity counting systems which are applied in nuclear safeguards (Abhold and Baker, 2002; Looman et al., 2009; Pozzi et al., 2012).

The applicability of non-analogous Monte Carlo methods for the simulation of neutron noise measurements was investigated by Yamamoto (2011). The investigation was performed for a one-speed neutron model in an infinite homogeneous medium. A limited number (typically 2 or 3) of implicit capture and Russian roulette events are allowed in the non-analogous simulation. The author proves that from this limited model the α parameter of the system can be obtained correctly, although other parameters are biased. According to the above categorization by Booth, this approach may fall into the *corrected single particle* category, since the non-analogous transport is done in the conventional way and the result is obtained by corrections from a theoretical model. Therefore, this approach needs a theoretical model and its applicability for the simulation of real systems has not proven yet.

A completely different approach for the Monte Carlo simulation of neutron noise measurements based on the frequency domain Monte Carlo developed by Yamamoto (2013, 2014) is also worth mentioning here. In this approach, the Fourier-transformed Boltzmann transport equation is solved with a special Monte Carlo technique applying complex valued weights. This method can provide direct estimation of quantities used for the frequency domain analysis of reactor noise, i.e. the auto or cross power spectral density (APSD or CPSD). This method does not fit into the above categories but it would also need the development of completely new tool for the simulation of real systems.

This paper presents a general method, which is similar in its philosophy to the deconvolution approach and therefore easy to integrate into the conventional Monte Carlo program flow. Furthermore, besides demonstrating its applicability to pulse height estimation, we show problems arising in systems with higher multiplicity (e.g. neutron simulation in a source driven subcritical assembly). Methods are presented for the simulation of such systems and it is also demonstrated that, contrary to the other similar methods mentioned above, the history splitting method is applicable for the estimation of correlation between events of higher moments. Earlier stages of this work were published in conference publications (Szieberth and Kloosterman, 2003, 2004, 2010).

2. Theory of non-Boltzmann estimators in Monte Carlo particle transport calculations

2.1. Analogous Monte Carlo simulation

In analogous Monte Carlo particle transport – similarly to real systems – particles start from a source event at $t = 0$, spend some time with transport in the media (transport time) while a detection event occurs. In case of simulation of coincidence events from the same source event, the time and the detector contribution of each event has to be registered. The detector response of a given source event (i), which resulted in n_i detection events with d_i^j detector contributions at time t_i^j in a given time interval $[t_0, t_0 + T]$ can be described by the following integral:

$$r_i(t_0) = \int_{t_0}^{t_0+T} \sum_j^{n_i} d_i^j \delta(t - t_i^j) dt \tag{2}$$

which, in case of $t_0 = 0$ and $T = \infty$, gives the total detector response for a single source event, and (2) simplifies to[1]:

$$r_i = \sum_j^{n_i} d_i^j. \tag{3}$$

r_i can be considered as a sample from random variable $\mathbf{r}$, which is described by a probability density function $f_\mathbf{r}$:

$$\mathcal{P}(\mathbf{r} < x) = \int_0^x f_\mathbf{r}(\hat{x}) d\hat{x}. \tag{4}$$

A Monte Carlo estimation of the mean detector response $\bar{\mathbf{r}}$ (e.g. average deposited energy) can be obtained by averaging a large number of simulated source events (N):

$$\bar{\mathbf{r}} = \langle \mathbf{r} \rangle = \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} r_i. \tag{5}$$

One can see that the problem simplifies to the determination of the expected value of the contribution from a single source event. In fact, $\bar{\mathbf{r}}$ is a classical Boltzmann quantity which, can be expressed in the form of the following integral:

$$\bar{\mathbf{r}} = \int D(\vec{r}, E, \vec{\Omega}) \Psi(\vec{r}, E, \vec{\Omega}) d\vec{r} dE d\vec{\Omega} \tag{6}$$

where D is the so-called detector or pay-off function, Ψ is the (incoming) collision density, $\vec{r}, E$ and $\vec{\Omega}$ are the phase-space variables and the integration is done for the complete phase-space. Such quantities can be efficiently estimated by collision or track length type estimators, which gain contribution from each collision or particle track in the phase-space volume selected by the pay-off function. See details in Lux and Koblinger (1991). Therefore, the fully analogous event-type estimator in (5) is not used for the esti-

[1] In the forthcoming, time dependence of the r_i is denoted only when it has significance.