

Estimation of Ex-Core Detector Responses by Adjoint Monte Carlo

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Abstract

Ex-core detector responses can be efficiently calculated by combining an adjoint Monte Carlo calculation with the converged source distribution of a forward Monte Carlo calculation. As the fission source distribution from a Monte Carlo calculation is given only as a collection of discrete space positions, the coupling requires a point flux estimator for each collision in the adjoint calculation. To avoid the infinite variance problems of the point flux estimator, a next-event finite-variance point flux estimator has been applied, which is an energy dependent form for heterogeneous media of a finite-variance estimator known from the literature.

To test the effects of this combined adjoint-forward calculation a simple geometry of a homogeneous core with a reflector was adopted with a small detector in the reflector. To demonstrate the potential of the method the continuous-energy adjoint Monte Carlo technique with anisotropic scattering was implemented with energy dependent absorption and fission cross sections and constant scattering cross section. A gain in efficiency over a completely forward calculation of the detector response was obtained, which is strongly dependent on the specific system and especially the size and position of the ex-core detector and the energy range considered. Further improvements are possible. The method works without problems for small detectors, even for a point detector and a small or even zero energy range.

KEYWORDS: *Monte Carlo, ex-core detector, adjoint Monte Carlo, flux at a point, finite variance estimator*

1. Introduction

Estimation of ex-core neutron detector responses by the Monte Carlo method is generally a difficult task as the detectors are relatively small and far away from the core, so that only few neutrons will actually reach the detector and the variance of the estimated response will be large. Nonetheless the Monte Carlo method is often applied to these types of problems as the geometry is strongly heterogeneous and cannot be modeled accurately in a finite-difference flux solver. The problem of ex-core detector estimation by Monte Carlo can be overcome by performing an adjoint Monte Carlo calculation, which effectively starts particles at the detector and scores in the core according to the fission neutron production rate distribution. Using an adjoint calculation avoids the problem of a forward calculation in which one has to score in a relatively small volume of the detector, while now the scoring volume is basically the whole core, or to be more precise, all fuel containing volumes in the core. This procedure would be very effective if the neutron source distribution is known analytically in space, energy and direction. This is,

however, not the case in practice.

It is possible to perform an adjoint Monte Carlo calculation for a multiplying system using successive generations of particles as in a forward criticality calculation [1], but this may also be a heavy task. Another solution is to use the converged source distribution of fission source neutrons from a forward Monte Carlo criticality calculation. Such a calculation will often be done anyway to determine the effective multiplication factor and the source positions for a next generation may be stored in a file on disk. The angular distribution of source neutrons is always assumed to be isotropic and the energy distribution given by the analytical form of the fission spectrum, e.g. the Watt spectrum.

This leaves the spatial source distribution as a collection of discrete space points. To get scores in the adjoint calculation at these discrete special source positions we need to use a point estimator from each collision site in the adjoint calculation. However, as the collision site in the adjoint calculation can be arbitrary close to the forward fission site, the point flux estimator will have an infinite variance due to its $1/d^2$ behavior and the results cannot be trusted. In this paper it will be shown how the adjoint Monte Carlo calculation for estimating the ex-core detector responses can be coupled to the discrete fission source distribution from a forward Monte Carlo calculation using a flux at a point estimator with finite variance, which is known in the literature for a long time.

2. Adjoint Monte Carlo calculation

2.1 Forward integral transport equations

For Monte Carlo calculations the transport equation is most conveniently formulated in integral form. Here we have to distinguish between the neutron flux $\phi(P)$ or the collision density $\psi(P)=\Sigma_t\phi(P)$ with $P=(\mathbf{r},E,\boldsymbol{\Omega})$ a point in the phase space, and the emission density $\chi(P)$. The response of a detector can be written as an integral over the flux or the collision density as follows

$$R = \int \eta_\phi(P)\phi(P)dP = \int \eta_\psi(P)\psi(P)dP \quad (1)$$

with η_ϕ and $\eta_\psi=\eta_\phi/\Sigma_t$ the detector response functions with respect to the flux and collision density, respectively. The integral equation for the collision density contains a source term with the density of first collisions,

$$\psi(P) = S_1(P) + \int K(P' \rightarrow P)\psi(P')dP', \quad (2)$$

with the transport kernel K a combination of first the collision kernel $C(\mathbf{r}',E' \rightarrow E, \boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega})$ kernel and next the transition kernel $T(\mathbf{r}' \rightarrow \mathbf{r}, E, \boldsymbol{\Omega})$. The integral equation for the emission density is given by

$$\chi(P) = S(P) + \int L(P' \rightarrow P)\chi(P')dP' \quad (3)$$

with $S(P)$ the neutron source and the transport kernel L applies first the transition kernel and the collision kernel C thereafter. For a criticality problem the source term S is generated by successively solving Eq. (3) for a next generations of neutrons using a new source term obtained from

$$S(P) = \frac{1}{4\pi} \chi_{fis}(E) \int \int \frac{v\Sigma_f}{\Sigma_t} \psi(\mathbf{r}, E', \boldsymbol{\Omega}') dE' d\Omega' \quad (4)$$

with χ_{fis} the fission spectrum and assuming the fission neutrons to be emitted isotropically.

2.2 Adjoint integral equations

The equation adjoint to Eqs. (3) and (1) is

$$\psi^*(P) = \eta_\psi(P) + \int K(P \rightarrow P') \psi^*(P') dP' \quad (5)$$

and the detector response can be calculated from

$$R = \int S_1(P) \psi^*(P) dP. \quad (6)$$

For more convenient Monte Carlo sampling of the adjoint equation it is useful to apply two transformations to Eq.(5), one for solving $\Sigma_t \psi^*(P)$ instead of $\psi^*(P)$ and one as a biasing function in energy equal to $1/E$. [3] Then we are solving an adjoint equation for the quantity $\xi^*(P) = \Sigma_t \psi^*(P)/E$

$$\xi^*(P) = \frac{\Sigma_t \psi^*(P)}{E} = \eta_\phi(P)/E + \int M^*(P' \rightarrow P) \xi^*(P') dP' \quad (7)$$

with the adjoint transport kernel given by

$$M^*(P' \rightarrow P) = D^*(\mathbf{r}', E' \rightarrow E, \boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega}) T^*(\mathbf{r}' \rightarrow \mathbf{r}, E, \boldsymbol{\Omega}). \quad (8)$$

Here, T^* is the adjoint transition kernel for which sampling is the same as the normal transition kernel T except that the particle moves into the direction $-\boldsymbol{\Omega}$. The adjoint collision kernel D^* can be expressed as

$$D^*(\mathbf{r}, E' \rightarrow E, \boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega}) = \frac{\Sigma_t(\mathbf{r}, E) C(\mathbf{r}, E \rightarrow E', \boldsymbol{\Omega} \rightarrow \boldsymbol{\Omega}') \frac{E'}{E}}{\Sigma^*(\mathbf{r}, E')} \quad (9)$$

with Σ^* the so-called adjoint cross section, defined by [3]

$$\Sigma^*(\mathbf{r}, E') = \int \int \Sigma_t(\mathbf{r}, E) C(\mathbf{r}, E \rightarrow E', \boldsymbol{\Omega} \rightarrow \boldsymbol{\Omega}') \frac{E'}{E} dE d\Omega. \quad (10)$$

If we consider η_ϕ/E in Eq.(7) the adjoint source, $\xi^*(P)$ is the adjoint emission density. Like in the forward case one can also define the adjoint collision density $\zeta^*(P)$, now as follows

$$\zeta^*(P) = \int T^*(\mathbf{r}' \rightarrow \mathbf{r}, E, \boldsymbol{\Omega}) \xi^*(\mathbf{r}') dV' \quad (11)$$

The detector response is now obtained from

$$\begin{aligned} R &= \int S_1(P) \psi^*(P) dP = \int \int T(\mathbf{r}' \rightarrow \mathbf{r}, E, \boldsymbol{\Omega}) S(\mathbf{r}', E, \boldsymbol{\Omega}) dV' \frac{E}{\Sigma_t(\mathbf{r}, E)} \xi^*(P) dP \\ &= \int \frac{ES(P)}{\Sigma_t(P)} \zeta^*(P) dP \end{aligned} \quad (12)$$

which means a scoring function $ES(P)/\Sigma_t$ at each collision of the adjoint particle.

If the source density $S(P)$ was known analytically the adjoint calculation could easily be used to estimate the detector response. However, from the source distribution we know only the energy and directional dependence analytically. The spatial distribution is given as a collection of discrete fission sites from the forward Monte Carlo calculation. Therefore, we have to apply a point flux estimator to estimate the score at a fission site \mathbf{r}_f from a collision site \mathbf{r}_c of the adjoint particle. Such estimators will be discussed in the next section.

2.3 Continuous-energy adjoint Monte Carlo simulation

The above equations for the (transformed) adjoint Monte Carlo calculation include the energy as a continuous variable. Most often adjoint calculations are allowed in multi purpose Monte Carlo codes in multigroup form. However, on basis of the above equations the energy variable in the adjoint equation can be treated as a continuous variable. [1] This implies sampling of the energy after an adjoint scattering from the kernel D^* given by Eq.(9) and applying an analogon of the non-absorption probability equal to Σ^*/Σ_t .

3. Flux at a point estimator

3.1 Energy independent and homogeneous case

The standard estimator for the flux at a point \mathbf{r}_0 for a particle having a collision at \mathbf{r} is

$$F_{est}(\mathbf{r}, \mathbf{r}_0) = p(\boldsymbol{\Omega}_{r_0}) \frac{e^{-\Sigma_t |\mathbf{r}-\mathbf{r}_0|}}{|\mathbf{r}-\mathbf{r}_0|^2} \quad (13)$$

with $p(\boldsymbol{\Omega}_{r_0})$ the probability for scattering from the direction $\boldsymbol{\Omega}$ before the collision into the direction of \mathbf{r}_0 . It is well-known that due to the inverse squared behavior with the distance between the points, this estimator has an infinite variance if the collision site \mathbf{r} can be arbitrarily close to \mathbf{r}_0 . Therefore, we cannot use this estimator in our adjoint problem.

To overcome this problem we used the flux at a point estimator proposed by Kalos many years ago, which has a finite variance [2]. With reference to figure 1, in which \mathbf{r}_c is the last collision site of the adjoint particle and \mathbf{r}_f is the selected fission site from all available fission sites from a forward calculation, a next collision site \mathbf{r} for the adjoint particle is selected from the pdf

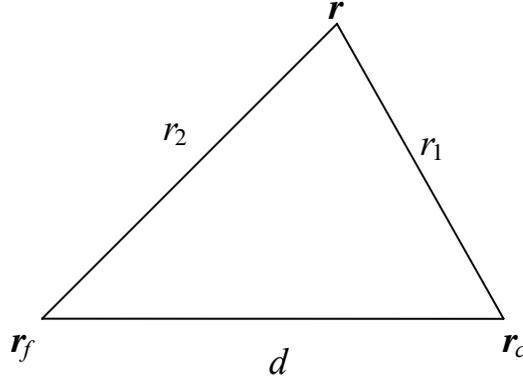
$$\bar{p}(\mathbf{r}) = \frac{1}{4\pi} \frac{1}{2} \left(\frac{\Sigma' e^{-\Sigma' r_1}}{r_1^2} + \frac{\Sigma' e^{-\Sigma' r_2}}{r_2^2} \right). \quad (14)$$

This is in fact an averaged of two pdfs, both selecting a next collision site on basis of normal particle transport, but with an artificial total cross section Σ' and the first one starting at the last adjoint collision site \mathbf{r}_c and the second one starting at the selected fission site \mathbf{r}_f . To arrive at a finite variance Kalos proposed for the artificial cross section

$$\Sigma' = \Sigma_t + \frac{1}{d} \quad (15)$$

with d the distance between \mathbf{r}_c and \mathbf{r}_f . This results in a finite variance as the score becomes

Figure 1: Geometry for selecting an intermediate collision site \mathbf{r} for the finite-variance point flux estimator. [2]



$$\begin{aligned}
 F_{est}(\mathbf{r}_c, \mathbf{r}, \mathbf{r}_f) &= \frac{p(\boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega}_1) \Sigma_t e^{-\Sigma_t r_1 / r_1^2} \Sigma_s}{p(\mathbf{r})} \frac{p(\boldsymbol{\Omega}_1 \rightarrow \boldsymbol{\Omega}_2) \Sigma_t e^{-\Sigma_t r_2}}{\Sigma_t} \frac{1}{r_2^2} \frac{1}{4\pi \Sigma_t} \\
 &= 2p(\mu_1) \frac{\Sigma_t}{\Sigma'} \frac{e^{-\Sigma_t r_1 / r_1^2}}{2 \left(\frac{e^{-\Sigma_t r_1}}{r_1^2} + \frac{e^{-\Sigma_t r_2}}{r_2^2} \right)} \frac{\Sigma_s}{\Sigma_t} \frac{2p(\mu_{12}) e^{-\Sigma_t r_2}}{4\pi} \frac{1}{r_2^2} \frac{1}{4\pi} \\
 &= \frac{8}{(4\pi)^2} p(\mu_1) p(\mu_{12}) \frac{e^{-\Sigma_t r_1} e^{-\Sigma_t r_2}}{r_2^2 e^{-\Sigma_t r_1} + r_1^2 e^{-\Sigma_t r_2}} \frac{\Sigma_s}{\Sigma'}
 \end{aligned} \tag{16}$$

From the scoring function of Eq.(12) only the directional part of the neutron source function has to be taken into account.

As this method gives the once more collided contribution, for (adjoint) source particles we need to add the uncollided contribution, which equals to

$$F_{unc}(\mathbf{r}_0) = \frac{1}{4\pi} \frac{e^{-\Sigma_t |\mathbf{r}_0 - \mathbf{r}_f|}}{|\mathbf{r}_0 - \mathbf{r}_f|^2} \tag{17}$$

for an adjoint particle starting at \mathbf{r}_0 .

3.2 Energy dependent case

The above given flux at a point estimator can be generalized for a heterogeneous system with energy dependence. If the system is heterogeneous, As the selection of the intermediate point \mathbf{r} is closely related to the normal selection of a next collision point the usual procedure for heterogeneous media can be applied, once the starting position \mathbf{r}_c or \mathbf{r}_f have been chosen. In all media that will be crossed the total cross section must be artificially enlarged by an amount $1/d$ according to Eq.(15).

In the energy dependent case the adjoint particle energy will change from its energy E' before the collision at \mathbf{r}_c to a value, say, E_1 along the trajectory r_1 and to E_2 along the trajectory r_2 .

However, these energies will be dependent on the scattering angles, which are not yet known when the intermediate collision point \mathbf{r} is to be selected. Therefore, for the determination of the artificial cross section Σ' the energy is taken equal to the energy before the collision at \mathbf{r}_c . However, when calculating the score for the point flux estimator, the correct energies E_1 and E_2 must be calculated from the scattering angles and the mean free paths z_1 from \mathbf{r}_c to \mathbf{r} and z_2 from \mathbf{r} to \mathbf{r}_f must be evaluated at energy E_1 and E_2 , respectively. From the scoring function in Eq.(12) the energy and directional part $E\chi_{fis}(E)/(4\pi\Sigma_l)$ remains, leading to

$$F_{est}(\mathbf{r}_c, \mathbf{r}, \mathbf{r}_f, E') = \frac{8}{(4\pi)^2} p(\mu_1)p(\mu_2) \frac{e^{-z_1(\mathbf{r}_c, \mathbf{r})} e^{-z_2(\mathbf{r}, \mathbf{r}_f)}}{r_2^2 e^{-z_1(\mathbf{r}_c, \mathbf{r})} + r_1^2 e^{-z_2(\mathbf{r}, \mathbf{r}_f)}} \frac{\Sigma_s}{\Sigma'} E\chi_{fis}(E) \quad (18)$$

If the scattering probabilities are specified in the centre-of-mass system we need to calculate the cosine of the scattering angle μ_C in the centre-of-mass system from the cosine of the scattering angle μ_0 in the laboratory system

$$\mu_C = \frac{\mu_0 \sqrt{A^2 + \mu_0^2 - 1} + \mu_0^2 - 1}{A}. \quad (19)$$

Then the probability of scattering through an angle of cosine μ_C is

$$p(\mu_0) = p(\mu_C) \left| \frac{d\mu_C}{d\mu_0} \right| = p(\mu_C) \frac{(A^2 + 2A\mu_C + 1)^{3/2}}{A^2(A + \mu_C)}. \quad (20)$$

The energy after an adjoint scattering through an angle of cosine μ_C is given by

$$E_{after} = E_{before} \frac{(A+1)^2}{A^2 + 2A\mu_C + 1}. \quad (21)$$

The uncollided contribution becomes

$$F_{unc}(\mathbf{r}_0, E) = \frac{1}{4\pi} \frac{e^{-\Sigma_l |\mathbf{r}_0 - \mathbf{r}_f|}}{|\mathbf{r}_0 - \mathbf{r}_f|^2} E\chi_{fis}(E) \quad (22)$$

4. Numerical example

To demonstrate the theory developed in this paper we wrote a relatively simple Monte Carlo program to handle the forward simulations with successive neutron generations and the adjoint simulation with the finite-variance point flux estimator. The geometry is limited to a homogeneous box form core surrounded by a finite reflector. The detector is also rectangular and is placed in the detector and assumed to have the same material properties as the reflector material. Although adjoint Monte Carlo simulations are mostly done in multigroup form, here a continuous-energy approach was taken in order to demonstrate the potential of the method. For simplicity the absorption and fission scattering cross sections vary inversely proportional with the neutron speed and the scattering cross sections were taken constant with energy. As thermal scattering would complicate the continuous-energy adjoint simulation considerably, in this demonstration thermal neutrons were treated with a one-group model. [3] Both for the core and

the reflector material a scatterer of the same effective mass $A=3$ was assumed to simulate a reasonably thermal system. The dimensions of the core were taken as $20 \times 20 \times 24 \text{ cm}^3$. The dimensions of the reflector $40 \times 40 \times 40 \text{ cm}^3$. The detector dimensions are $0.5 \times 0.5 \times 1 \text{ cm}^3$. The center of the detector is located at $x=12 \text{ cm}$ from the core origin.

First a forward calculation with 50 successive batches (neutron generations) was performed to estimate the effective multiplication factor and to generate the fission source distribution to be used in the adjoint simulation. The fission spectrum was taken as a Maxwell spectrum with temperature $T=1.2985 \text{ MeV}$. From the last batch the detector response was also estimated as the space averaged flux over the detector volume using a collision estimator. The detector response was taken over various energy intervals.

Next, the adjoint calculation was performed as an alternative method to estimate the detector response. As the averaged flux in the detector is estimated, we have

$$\eta_{\phi}(P)/E = \frac{1}{V_{det}} \frac{1}{E} \quad \begin{array}{l} \mathbf{r} \in V_{det} \\ E_{min} < E < E_{max} \end{array} \quad (23)$$

From this adjoint source function according to Eq. (7) we see that the adjoint particles must start uniformly and isotropically in the detector. Their energies are selected from the function $1/E$. This results in a normalization factor of $4\pi \ln(E_{max}/E_{min})$ with E_{min} and E_{max} the energy limits between which the detector response is to be calculated. At each collision site in the adjoint calculation the point flux estimator was applied, selecting at random a fission source position from all available fission sites from the last forward batch. As the forward and adjoint calculations are completely independent, selecting a fission site from the forward calculation is a fair game.

As the point flux estimator uses the selection of an intermediate scattering point, the uncollided contribution to the detector response must be estimated separately for each initial position in the adjoint simulation. This can be done straight-forwardly using the estimator of Eq.(22), as the distance between the starting position in the detector and the randomly selected fission site out of all stored fission sites can never be arbitrarily small. The probability for selecting the right direction is $1/(4\pi)$ in this case.

Table 1 shows the results for the adjoint simulation with 10^7 particle histories. Also the CPU time is given and the figure of merit being equal to

$$FOM = \frac{1}{\sigma_{rel}^2 T} \quad (24)$$

with T the CPU-time and σ_{rel} the relative standard deviation in the detector response estimate.

From the table we can see a fair agreement in the detector response for the forward and adjoint calculation. We also see from the FOM figures that the adjoint calculation is more than 400 times as efficient for the highest energy interval from 1 to 10 MeV. For lower energy ranges the gain is less or absent (for the current implementation; see the discussion in the next section). Note that in neither of the calculations the time for arriving at a converged source in the forward calculation was taken into account in the FOM figures. It is assumed that this calculation has to be done anyway, for instance to obtain the effective multiplication factor.

Table 1: Comparison of results of detector response estimation for various energy intervals by forward and adjoint Monte Carlo.

case	energy range	R ($\text{cm}^{-2}\text{s}^{-1}$)	σ (%)	T (s)	FOM (s^{-1})
forward	1-10 MeV	$2.25 \cdot 10^{-6}$	32	746	0.013
adjoint	1-10 MeV	$3.24 \cdot 10^{-6}$	2.1	417	5.5
forward	0.1-1 MeV	$2.45 \cdot 10^{-5}$	11	746	0.11
adjoint	0.1-1 MeV	$2.02 \cdot 10^{-5}$	1.6	850	4.8
forward	thermal – 0.1 MeV	$4.74 \cdot 10^{-4}$	2.0	746	3.4
adjoint	thermal – 0.1 MeV	$4.56 \cdot 10^{-4}$	2.2	2269	0.91

5. Conclusions and discussion

In this paper the theory has been derived for an adjoint Monte Carlo calculation that is coupled to the forward fission source distribution to estimate the detector response of an (ex-core) detector. From the numerical results one can see that valid results are obtained and that the adjoint route can provide considerable advantageous in computing efficiency.

One should note that the smaller the detector volume is, the worse will be the standard deviation of the detector response estimate in the forward case, while the adjoint case is hardly affected and can be even slightly more efficient as there will be less spread in the start of all histories.

The gain in efficiency for the adjoint calculation will also improve if one needs to estimate the detector response for smaller energy intervals. Especially for energy intervals in the high energy range, which may be important to determine the effective neutron fluence on the core vessel or other construction parts outside the core, the forward estimation will be less efficient as neutrons will be slowed down before they reach the detector at those high energies. One should realize that for every energy interval for which the detector response is to be calculated, a separate adjoint calculation has to be done. Only if the Monte Carlo code used has an option to link a score to the initial energy (interval) at the start of that particle (like the SCX option in MCNP), it is possible to combine the estimation of the detector response for different energy ranges in one run.

As this is a first demonstration, there are several possibilities to further improve the efficiency of the adjoint calculation. In the current example a next-event point flux estimator is applied at every collision site in the adjoint simulation. Especially for particles colliding in the reflector, far away from the core, the expected contribution is small and one may consider to calculate the estimate only with a certain probability, compensating with its inverse value if the estimate is

indeed applied. This may also be applied for adjoint particles with a relatively low energy, at which the fission spectrum appearing in the score is low. This also applies to adjoint particles having a collision in the core. Moreover, the selection of an initial direction for the adjoint particles may be simply biased towards the core with compensation in its weight.

If one considers the implementation of this method into a general purpose Monte Carlo code, one can greatly benefit if a point flux estimator is already present in the code. Then the calculation of the probability for scattering into a certain direction is already available, as well as the calculation of the number of mean free path z between two points. Note, however, that also the number of mean free path z' based on the enlarged total cross section Σ' must be calculated for the estimator of Eq.(18). This needs additional programming. It will be most easy if during tracking between two points the lengths of the tracks in different media are memorized. This will be the case when tracking is done from r_c to r or from r_f to r to select the intermediate scattering point r . As this is done at enlarged cross section Σ' , the number of mean free path z'_1 or z'_2 , respectively, are known. Next the path from r to r_f or from r to r_c , respectively, has to be tracked to determine z'_2 or z'_1 , respectively. In this case also much of the programming for a point detector can be used, including the scattering probability through the appropriate angle. When the partial tracks in different media are known, it is possible to calculate later, when the actual energies along these tracks are determined, the actual number of mean free paths z_1 and z_2 without tracking again through the geometry. Of course, for the final score the standard point flux estimators also have to be adapted to get the estimator from Eq.(18).

When such an implementation in a general purpose Monte Carlo code has been completed, the coupled forward-adjoint method can be tested for more realistic reactor geometries than the small and artificial system taken for the numerical demonstration in Sect. 4.

References

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