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THE MONTE CARLO MIDWAY METHOD WITH MULTIPLE MIDWAY SURFACES

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ABSTRACT

The midway Monte Carlo method for estimating a detector response is based on a theorem that expresses that a detector response can also be obtained from an integral over a surface dividing the source and the detector region, with the integrant containing both the particle flux and the adjoint function. The midway method thus combines a forward and an adjoint Monte Carlo calculation resulting in much better calculational efficiency than in a regular Monte Carlo calculation. The theory of midway Monte Carlo is extended to use multiple midway surfaces. This opens the possibilities of further efficiency gains. Using the so called black absorber variant it is possible to calculate efficiently the detector response for systems in which the geometry or material composition between two midway surfaces changes arbitrarily. The method is illustrated with a numerical example showing a gain in efficiency by a factor of 28 compared to a standard Monte Carlo solution.

1. INTRODUCTION

Despite modern variance reduction methods a regular (forward) Monte Carlo calculation with neutrons or photons starting at the source and arriving at the detector to score the required detector response may be rather inefficient if the detector is small and/or at a relatively large distance from the source. For small detectors adjoint Monte Carlo may help but it will not improve the situation if the source is also small. Small should be understood here as small in the phase space, i.e. either in geometry or in sensitive energy range or even sensitive direction range or a combination of these conditions.

The midway Monte Carlo method (Serov, 1999) developed at the Interfaculty Reactor Institute of the Delft University of Technology combines a forward and an adjoint calculation by scoring the forward neutron or photon current at a basically arbitrary surface somewhere between source and detector, as well as the flux of adjoint particles coming from the detector at the same surface. According to a generally valid theorem the detector response can also be obtained as the integral over the midway surface as well as over all directions and energies of the product of the particle current and the adjoint function. For general applicability of the midway method it was built into the MCNP4C code (Briesmeister, 2000) using as much as possible of the tally options already available in MCNP. This requires modification of a limited number of subroutines of MCNP. The next section will demonstrate the basic theory behind the midway method. An extensive account of the midway method is given by Serov (1999).

The theory of the midway method has been extended to include more than one intermediate or midway surface. This provides even much better possibilities for reducing the variance in the detector response or improving the efficiency of the calculation. Intuitively this can be understood as in each part of the midway calculation the transport of particles concentrates on restricted areas of the total system geometry: a forward calculation transporting particles from the physical source to the first midway surface, an adjoint calculation transporting particles from the detector to the second midway surface and a forward or adjoint calculation transporting particles from one midway surface to the other. As the transport probability of particles will feature a more or less exponential behaviour with distance it is more efficient if the transport can be split up in independent parts, while the calculation time will roughly increase only linearly with the number of subdivisions.

A special feature of the midway method is the possibility to restrict the geometry in specific parts of the total calculation to the space enclosed by a midway surface. As this can be considered as filling up the rest of the geometry with a black absorber, this feature is called the black absorber technique. In the case of two midway surfaces it can be proven that the exact detector response is still obtained correctly if the black absorber technique is applied either to the forward calculation starting at the physical source or to the adjoint calculation starting at the detector. For the transport between the midway surfaces the complete geometry must be taken into account. However, it is then possible to calculate very efficiently detector responses for systems with varying composition between the midway surfaces as only the transport part from one midway surface to the other need to be redone for every change in composition.

The next section will review the theory of midway Monte Carlo, including the black absorber technique, and describe the extensions necessary for multiple midway surfaces. In section 3 a numerical illustration of the process will be given with the possible gain in efficiency.

2. THEORY OF MIDWAY MONTE CARLO

2.1 Forward and adjoint Monte Carlo

To derive the basic theorem for the midway method we consider the neutron or photon transport in a (finite or infinite) volume V with a neutron source S and a neutron detector D which are spacially separated (see Fig. 1). The neutron flux $y(P)=y(\boldsymbol{r}, E, W)$ as a function of space $\boldsymbol{r}$, energy E and direction W is determined by the Boltzmann transport equation, which reads in operator form

$$W \cdot \nabla y + \mathbf{B} y = S \tag{1}$$

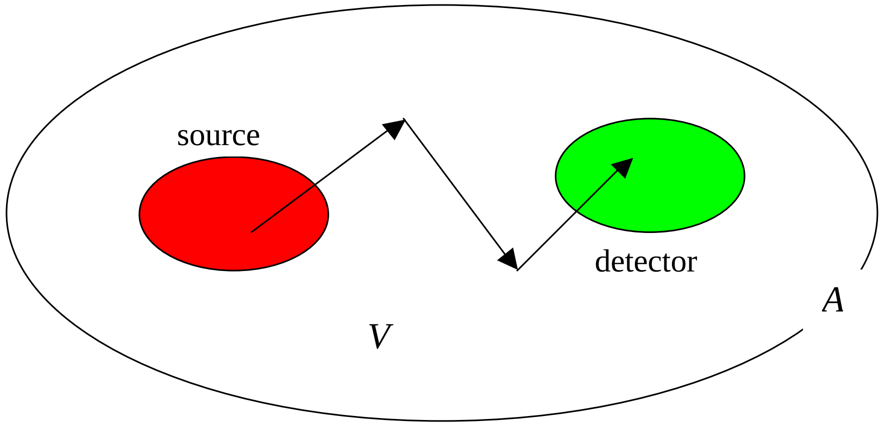

Fig. 1 Forward Monte Carlo calculation.

with **B** the Boltzmann operator, excluding the streaming term. Apropriate boundary conditions are assumed at the outer boundary A of volume V. If $D(P)$ is the detector response function the total detector response is given by

$$R = \int D(P) y\,(P) dP \tag{2}$$

In adjoint Monte Carlo the following equation for the adjoint function y^* is solved

$$-W \cdot \nabla y^* + \mathbf{B}^* y^* = D \tag{3}$$

with **B*** the adjoint Boltzmann operator. Now the detector response R can also be calculated as

$$R = \int S(P) y^* dP \tag{4}$$

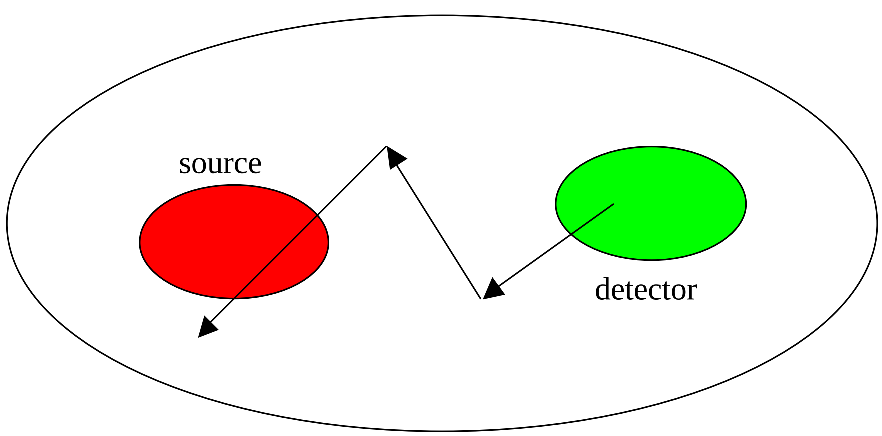

Fig. 2 Adjoint Monte Carlo calculation.

The Monte Carlo interpretation of the adjoint equation implies that “adjoint” particles are tracked starting at the physical detector and score when they interact in or pass through the physical source (see Fig. 2). An adjoint Monte Carlo calculation will in general be more efficient than a regular (forward) calculation if the detector has a small volume in the phase space compared to the source.

2.2 Midway Monte Carlo

The midway Monte Carlo method is a combination of a forward and an adjoint Monte Carlo calculation. It is based on a general theorem which can be derived as follows. Consider the geometry of Fig. 3 where a domain V_m that fully encompasses the detector volume and excludes the source volume but is arbitrary otherwise. If we subtract Eq.(1) multiplied by y^* from Eq.(3) multiplied by y and integrate the result over the volume V_m and over all energies and directions, we have after application of Gauss' divergence theorem

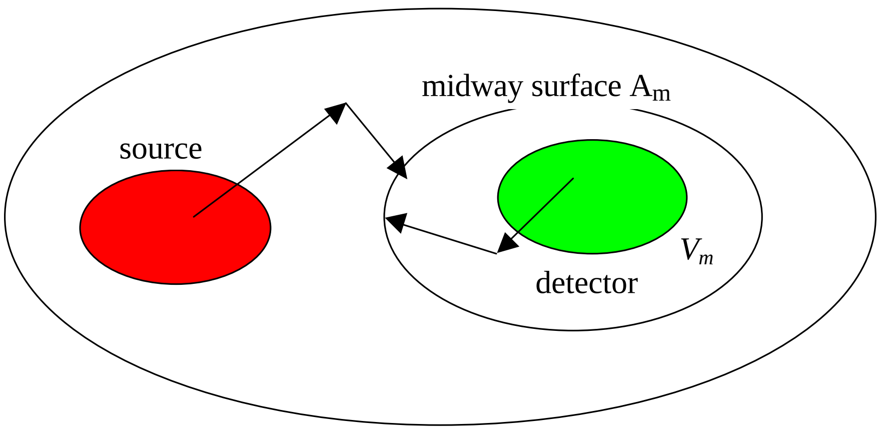

Fig. 3 Midway Monte Carlo calculation.

$$R = \int_{V_m} D(P)y\,(P)dP = -\int_{A_m} \mathbf{n}\cdot W\quad y\,(P)y^*(P)dP \qquad (5)$$

This means in Monte Carlo terms that we have to estimate in a forward calculation the particle current $J(P)=\mathbf{n}.Wy(P)$ at the surface A_m, estimate the flux of adjoint particles y^*(P) from an adjoint calculation starting at the physical detector and integrate the product over the surface A_m, energy and direction. As it will not be possible in this way to get estimates of both quantities at exactly the same position, energy and direction, a numerical integration will be necessary using a discretisation of the phase space variables. If we subdivide the surface in segments, and also energy in groups and direction in intervals for a polar and azimuthal angle and denote an elementary interval in the phase space by ΔP_i we can write

$$R = -\sum_i (\mathbf{n}\cdot W\quad y\,)_i\,.y_i^*\,DP_i \qquad (6)$$

In a Monte Carlo run the particle current $J(P)\Delta P_i = \mathbf{n}.W y(P)\Delta P_i$ through a surface area is estimated by the average statistical weight of particles crossing that surface area with energy and direction within the limits set by the phase space interval i. If $w_n^{(i)}$ is the weight of particle n crossing the surface within ΔP_i we have

$$J_i = \frac{1}{N_f} \sum_{n=1}^{N_f} \frac{w_n^{(i)}}{\Delta P_i} \tag{7}$$

with N_f the total number of histories started at the source in the forward calculation. Likewise the flux of adjoint particles is obtained from

$$y_i^* = \frac{1}{N_a} \sum_{n=1}^{N_a} \frac{w_n^{*(i)}}{|m_i| \Delta P_i} \tag{8}$$

with N_a the total number of histories started at the detector in the adjoint calculation and m_i the cosine of the angle between the particle direction and the normal to the surface.

The relative error $r[X]$ in these quantities can be obtained from (Lux and Koblinger, 1991)

$$r^2[J_i] = \frac{\sum_{n=1}^{N_f} (w_n^{(i)})^2}{(\sum_{n=1}^{N_f} w_n^{(i)})^2} - \frac{1}{N_f} \tag{9}$$

and analogously for the adjoint particle flux. Then the relative error in the detector response R is obtained from

$$r[R] = \frac{1}{R} \sqrt{\sum_i \{r^2[J_i] + r^2[y_i^*]\}\{J_i y_i^* \Delta P_i\}^2} \tag{10}$$

Midway Monte Carlo is especially efficient when both the source and detector volumes are small in the phase space. As in both the forward and the adjoint calculation scoring is at a relatively large surface and not in the small volume of the detector or the source, the smallness of the detector and source volumes do not play a direct role as in the normal forward or adjoint calculation, respectively. Moreover, the distance to be covered by particles from source to detector is split up in two parts: from the source to the midway surface and from the detector to the midway surface. As the probability for survival when covering a certain distance by neutrons or photons is roughly exponentially decreasing with distance, splitting up the transport in two independent parts will be benificial for the efficiency of the calculation as the calculation time will roughly increase linearly with the number of separate parts to be covered by the particles.

The midway Monte Carlo theory can be applied to neutron transport problems, photon transport and coupled neutron-photon transport (Serov, 1999). Legrady (2001) showed the extension to time-dependent problems.

2.3 Using two midway surfaces

The extension of the midway theory to be discussed here is the use of more than one midway plane. As the transport problem is split up further in parts, this promises better efficiency of the overall calculation. In calculating the integrant in the right part of Eq.(5) we can consider the estimation of the particle current $\boldsymbol{n}.W\psi(P)$ or in discrete form $(\boldsymbol{n}.W\psi)_i$ at the midway surface as a separate source-detector problem, which can be handled on its own by the midway method.

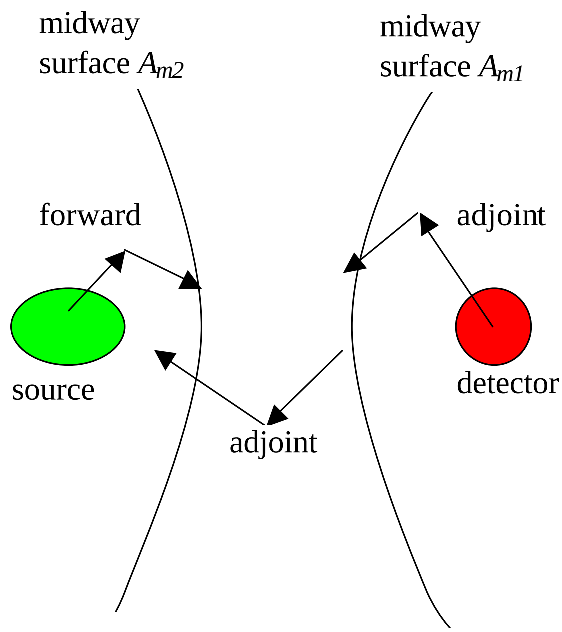

Fig. 4 Midway Monte Carlo calculation with two midway surfaces

To illustrate this further consider the geometry of the source-detector problem of Fig. 4 with the detector response calculated by the midway method using the midway plane A_{m1}. The midway volume V_m is in this case the half space to the right of this midway plane. To estimate the particle current in phase space element i at midplane A_{m1}, we can perform a separate midway problem using a second midway plane A_{m2}. This implies a forward calculation starting a the physical source and scoring at the second midway surface and an adjoint calculation starting at phase space interval i at the first midway surface and scoring at the second midway interval. If we denote the flux of adjoint particles starting at interval i at the first midway surface by $\psi^*(P|i)$, we have

$$(\mathbf{n}.W\ y\ )_{\mathbf{i}} = -\int_{A_{m2}} \mathbf{n}\cdot W \quad y\ (P) y^{*}(P\,|\,i)dP \qquad (11)$$

Using also a discretisation at the second midway surface we get for the original detector response

$$R = \sum_i \sum_j (\mathbf{n}\cdot W \quad y\ )_j\, y^{*}_{j}(|\,i) y^{*}_{i} D P_i D P_j \qquad (12)$$

with y_j*(|*i*) the flux of adjoint particles at phase space interval *j* at the second midway plane due to a surface detector at phase space interval *i* at the first midway surface. As the number of phase space intervals at a midway surface may be very large, it seems that calculating y_j*(|*i*) for all intervals *i* at the first midway surface may be very time consuming. However, these quantities need not to be obtained with small statistical error for every separated value of *i* and *j*. Using a very limited number of histories for each starting interval *i* will be sufficient as the final result is a summation over a very large number of terms, reducing the statistical error. It may even be sufficient to use only one history per starting interval i.

The calculational burden is further reduced when we take into account that from the adjoint equation starting at the physical detector there will be only a limited number of phase space intervals i at the first midway surface for which the estimate of y_i* will be non-zero. In practise we first perform the forward calculation starting at the physical source and save the scores $(\boldsymbol{n}.Wy)_j$ at the second midway surface nearest to the source. Next, we perform the adjoint calculation starting at the physical detector and save separately the scores y_i* at the first midway surface nearest to the detector. Finally we have to do the adjoint calculations starting at intervals at the first midway surface and scoring at the second midway surface. To this end we read in the scores y_i* and start only histories in interval *i* at the first midway surface if the estimate y_i* is non-zero. The number of histories to be started can be chosen dependent on the total number of intervals *i* for which y_i* is non-zero. Then the total number of histories can be made comparable to the total number of histories in the forward calculation and in the adjoint calculation starting at the physical detector. In this way a limited number of histories is spent to the third part of the double midway calculation.

The error in the detector response can be obtained analogously to Eq.(10) as

$$s\,[R] = \sqrt{\sum_i \sum_j \{r^2[J_j] + r^2[y^{*}_{j}(|\,i)] + r^2[y^{*}_{i}]\}\{J_j y^{*}_{j}(|\,i) y^{*}_{i} \Delta P_i \Delta P_j\}^2} \qquad (13)$$

2.4 The black absorber technique

Serov (1999) has shown that in the adjoint part of a midway calculation the geometry can be restricted to the midway volume enclosing the detector (or alternatively restricting the forward calculation to the space outside the midway volume) without any approximation. This means that a particle history can be terminated when it crosses the midway surface in either the adjoint or the forward calculation. Application of this technique to the double midway method leads to a possibility of obtaining the detector response for various systems that differ only in geometry or material composition in a limited part.

If we look again at the geometry of Fig. 4. We apply the black absorber technique to the adjoint calculation starting at the physical detector. This means that we have to consider only the geometry at the right of the first midway surface. As the estimation of $(\boldsymbol{n}.Wy)_i$ at the first midway surface is done with an independent second midway calculation, we can also apply the black absorber technique to the forward part of that calculation, which means that we have only to consider the space to the left of the second midway surface. In the third part, the adjoint calculation from the first midway surface to the second, we have to take into account the full geometry, i.e. particles passing the second midway surface must still be followed as they may be scattered back, recross this surface again and by further scattering may cross the surface once more contributing again to the score. Also particles crossing the first midway surface to the right in Fig. 4 may be scattered back and can still contribute to a score at the second midway surface.

If we need to know the detector response for a system in which the geometry or the material composition between the two midway surfaces is perturbed, we only need to repeat the transport part from the first to the second midway plane, as the forward calculation starting at the source and the adjoint calculation starting at the physical detector are unchanged because of the black absorber technique in both calculations. Note that there is no restriction to the perturbation between the two midway surfaces, so it is not limited to first-order perturbations.

We intend to apply this technique for a fast and efficient calculation of the detector response in a borehole logging problem for oil exploration where the geometry of the logging tool is fixed but calculations need to be done for various compositions of the formation around the borehole.

3. NUMERICAL ILLUSTRATION

To demonstrate the multiple midway technique and to assess the gain in efficiency that can be obtained we implemented the midway method with two midway surfaces in a special program using two energy groups and the infinite geometry of Fig. 5 for simplicity. However, all essential ingredients are present in the problem.

The neutron source in this problem is a sphere with 3 cm radius, emitting isotropically neutrons in the first energy group. The detector is also a sphere with 3 cm radius with its center 12 cm apart from the source center, detecting neutrons only in the second energy group with a cross section S_d=0.2 cm^{-1}. The material composition is uniform over the whole system, including the source and detector regions. The cross sections are given in Table 1.

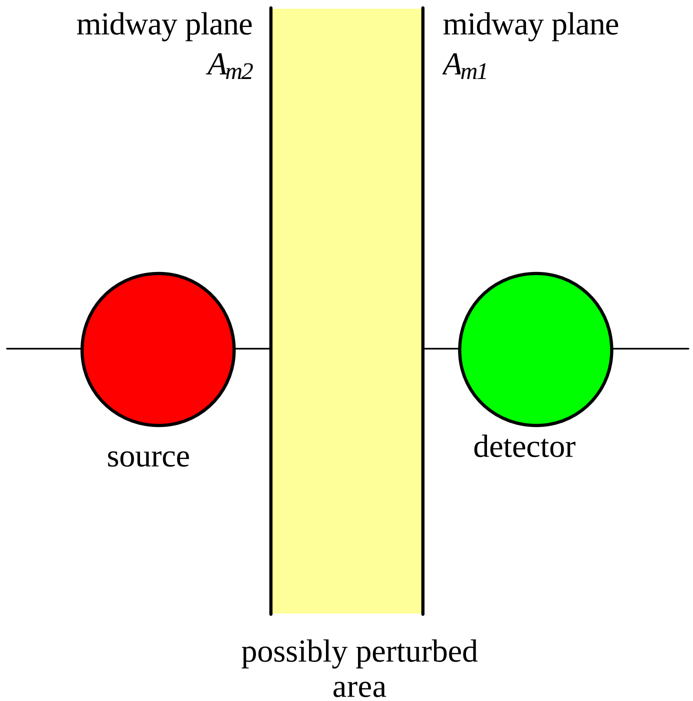

Fig. 5 Geometry of sample problem with two midway planes

Table 1 Two-group cross sections (cm^{-1}) used in the sample problem.

group	*1*	*2*
S_t	0.5	1.0
S_s	0.4	0.7
$S_{1\rightarrow 2}$	0.3	

To check the programme the forward and the direct adjoint calculation of the detector response were also done with the MCNP4C code using a specially prepared two-group cross section library. This showed good agreement. The results of the forward and adjoint calculation are shown in Table 2, together with the figure of merit (*FOM*) as a measure of the calculational efficiency defined by

$$FOM = \frac{1}{r^2 T} \qquad (14)$$

with r the relative statistical error and T the CPU-time for the calculation. For both the forward and the adjoint problem 10^7 histories were generated. Except for a Russian roulette technique with parameters uniform over the geometry and energy groups, no variance reduction techniques were applied. For comparison with further results all values of *FOM* in Table 2 relate to calculations with the special program. The computer time used by MCNP4C for the same number of histories is much larger because of the overhead due to the many options available in this general purpose code. Although the forward and adjoint problems are symmetric in geometry, they are not in energy. Therefore the efficiencies are not exactly equal.

Table 2 Results from the forward and adjoint calculation

	forward	*adjoint*	*single midway*	*double midway*
R	$1.86\ 10^{-4}$	$1.84\ 10^{-4}$	$1.80\ 10^{-4}$	$1.76\ 10^{-4}$
r (%)	1.2	1.4	2.2	0.41
T (s)	62.2	39.6	6.27+4.28	4.28+6.05+8.69
FOM (s^{-1})	112	129	196	3127

In the special programme also the standard midway method was programmed and the result is shown in Table 2. A plane at 7 cm from the source center was taken as the midway surface. For the discretisation 60 concentric rings were defined at the midway surface, each of 1 cm width and subdivided in 20 equal azimuthal parts. For the direction 10 intervals of equal width for positive values of the cosine of the polar angle were used and 20 equidistant intervals for the azimuthal angle of the direction vector. Together with the two energy groups this makes up 480,000 intervals or bins. In both the forward and the adjoint part of the midway calculation 10^6 histories were used. As can be expected the midway method is more efficient than the forward or adjoint calculation, in this case by a factor of about 1.7. The gain would be higher if the source and detector volumes were smaller or further apart.

Table 2 also shows the results of the midway method with two midway planes at 5 and 7 cm from the source center. First an adjoint run was done starting at the physical detector and scoring at the first midway surface. This run was done with the black absorber technique considering only the geometry at the right of the first midway surface. For this calculation 10^6 histories were used and the scores saved in a file for later use. Next a forward run was done starting at the neutron source and scoring at the second midway plane. Here alse 10^6 histories were used and the black absorber technique applied, which means only dealing with the geometry to the left of the second midway surface. These scores were also saved in a file. Finally an adjoint run was done starting at the first midway surfaces. The scores from the adjoint calculation, scoring at this midway surface, were read in. It turned out that there were only 25,255 bins with non-zero scores. Therefore, for each non-zero bin 100 histories were started, leading to about 2.5 10^6 histories for the transport from the first to the second midway plane. The scores in this calculation at the second midway plane were multiplied by the score value from the first adjoint calculation at the starting bin. To obtain the requested detector response these scores are multiplied by the score from the forward calculation for the respective bin at the second midway plane and added up, multiplied by the total bin width at the first and second midway plane, according to Eq.(12). For this calculation the whole geometry has to be taken into account. From the *FOM*-value for this midway calculation with two midway planes it is clear that this provides a big gain in efficiency by another factor of about 16, resulting in a gain factor of 28 over the normal forward calculation.

Finally Table 3 shows the results for the system with the material density between the two midway planes being 1/10th of the original density. The double midway method shows for this situation a comparable gain in efficiency as for the unperturbed case. When running this problem as a perturbation of the double midway method above, i.e. only the transport between the two midway planes repeated, we save the computing time of the forward and adjoint calculations starting from the source and the detector, respectively, which increase the efficiency gain by another factor of 2.

Table 3 Comparison of results for the perturbed system

	forward	*single midway*	*double midway*	*double midway as perturbation*
R	$4.51\ 10^{-4}$	$4.47\ 10^{-4}$	$4.40\ 10^{-4}$	$4.40\ 10^{-4}$
r (%)	2.4	4.28	0.26	0.26
T (s)	6.58	6.67+4.28	4.28+6.46+10.94	10.83
FOM (s^{-1})	264	408	6820	13,700

4. DISCUSSION

The numerical illustration of the application of the Monte Carlo midway method with two midway surfaces demonstrates the high gain in efficiency that can be obtained with this method compared to a normal forward Monte Carlo calculation. The midway method is especially applicable in situation where both the source and the detector are small (in the phase space) and/or they are separated by a large number of mean free path.

The illustration given here is only an example of the possibilities of using multiple midway surfaces. Instead of treating the first term in the integrant of the right hand side of Eq.(5) with a midway calculation, it is of course also possible to do this for the second term in the integral. Even more interesting is treating both terms from Eq.(5) with the midway method, leading to three midway surfaces. In this case the multiple midway method can be combined with the correlated coupling method of Ueki (2001) with particles starting at the middle of the three midway surfaces in the same position and energy but with opposite directions.

In the standard forward calculation of the illustrative example no specific variance reduction methods other than Russian Roulette have been applied. It is therefore possible to improve the figure of merit for this calculation by introducing variance reduction methods like importance sampling. However, for a fair comparison with the results of the midway methods, here also such variance reduction should be applied. In all parts of the midway calculations standard variance reduction methods like Russian roulette and splitting, path length stretching, source biasing and importance sampling can still be applied as in a normal forward calculation, except that one should realise that for calculating an importance function for importance sampling in one or more parts of the multiple midway method the aim of such a partial calculation (the "detector function") is not the response of the physical detector, but the current at a midway surface.

The midway method is not necessarily restricted to the multigroup approximation. Forward parts of the calculation can simply be done in continuous energy mode without restriction. To do the adjoint parts of the calculation in continuous energy requires this option in the basic Monte Carlo code used for the calculations. In MCNP the adjoint option is available for the multigroup treatment but not for continuous energy processing. However, for neutron transport the theory and practise is known already for a long time (Hoogenboom, 1981) and relatively easy to introduce in a general purpose Monte Carlo code like MCNP (Hoogenboom, 1999). For photon transport and coupled neutron-photon transport this requires more modifications, but the possibilities to deal with discrete photon energies are known (Hoogenboom, 2000; 2001). In the midway method with continuous energy mode it is still necessary to define energy groups for which scoring is done at the midway planes.

It was shown before (Serov, 1999) that the single midway method can be implemented in a general purpose Monte Carlo code like MCNP by modification of a limited number of subroutines. The multiple midway method requires some further extensions, especially for starting histories at a midway surface for bins that have a non-zero score in a previous part of a midway calculation.

5. CONCLUSIONS

We can conclude that the multiple midway Monte Carlo methods offers high gains in efficiency for large classes of source-detector problems. It has great flexibility in chosing the position and form of the midway surfaces, which can be tailored to deal with complex deep penetration problems or with difficult streaming problems with bended ducts. The flexibility in choices opens the way for interesting extensions and combinations with other advanced Monte Carlo techniques.

NOMENCLATURE

$\boldsymbol{n}$	normal vector
$\boldsymbol{r}$	space coordinate
r	relative error
m	cosine of angle between direction and normal
s	standard deviation
A	area
B	Boltzmann operator, excluding streaming term
D	detector response function
E	energy
J	particle current
P	phase space coordinate
R	detector response
S	source function
V	volume
Y	particle flux

S macroscopic cross section
W direction

Subscripts

d detector
i phase space interval number at first midway surface
j phase space interval number at second midway surface
m midway

Superscripts

* adjoint function or operator

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