Application of Acceleration Techniques in MCBEND

Ted SHUTTLEWORTH, Malcolm GRIMSTONE, Steve CHUCAS

AEA Technology, Winfrith Technology Centre, Dorchester, Dorset DT2 8DH, UK

New acceleration methods have been developed for the MCBEND Monte Carlo code. These include alternative techniques for generating importance values and the option to perform adjoint Monte Carlo calculations using continuous energy data. Significant improvements in efficiency have been demonstrated for several practical problems.

KEYWORDS: Monte Carlo method, radiation transport, acceleration, adjoint solution

I.   Introduction

MCBEND[1] is a general geometry, point energy, Monte Carlo code used for radiation transport calculations for neutrons, gamma-rays and electrons. The principal method of variance reduction in MCBEND is the use of splitting and Russian roulette (S/R) under the control of an importance map. As an integral part of the code, an adjoint multigroup diffusion theory calculation may be performed to estimate importances on an orthogonal mesh overlaying the problem space. This method has been available for over 10 years, and it has proved very effective in a wide range of applications; but there are cases, principally those dominated by voids and ducts, in which the limitations of diffusion theory produce inaccurate importance values that lead to inefficiencies in the Monte Carlo calculation. For many of these cases it would also be difficult to obtain an adequate solution of the adjoint problem with deterministic transport theory. Alternative methods of generating importances have therefore been investigated. The paper describes these techniques and gives examples of their use in two practical problems.

Another method of achieving greater efficiency for some problems is to perform the whole Monte Carlo calculation in adjoint mode. If an accurate adjoint function is obtained in this way, the required detector reaction rate can be calculated by integrating the product of the adjoint function and the source function. When using the adjoint technique, it is important that the accurate nuclear data representation should be preserved. MCBEND has therefore been extended to provide the option of performing adjoint Monte Carlo calculations using point energy data. The paper gives an outline of the method and shows two examples of practical applications.

II.   Generation of Importances

1.   Standard Methods

MCBEND includes an inbuilt importance generator[2]. The problem space is overlaid by an orthogonal mesh (XYZ or RθZ) in which the adjoint, multigroup diffusion equation is solved by finite difference methods. Special diffusion constants are used to provide a closer approximation to transport theory. This technique is simple, quick, convenient, robust and applicable to many practical cases. Its principal limitation is its inability to produce efficient importance maps in geometries that are dominated by voids and ducts.

In such cases it is possible to execute a MCBEND multigroup Monte Carlo calculation in adjoint mode to generate an importance map. This preliminary step to the required forward calculation will work where diffusion or deterministic transport methods fail, but it can be quite time consuming. Two new alternatives, which are implemented in the latest release of MCBEND, are described in the following sections.

2.   RECURSIVE Method

Recalling that the adjoint is the expected score made by introducing a particle at a point, it could theoretically be produced by sprinkling the entire problem with test sources and tracking them until they die or score. Scoring samples will make a contribution to the adjoint estimate at their birth site. This is clearly impractical for a large case since the probability of scoring at a detector for a particle born in a remote region is extremely small - particularly in the absence of an importance map.

A refinement of this technique has been implemented in MCBEND. Initially, test samples are generated in a cell of the importance mesh that contains the detector. These have a high probability of scoring and soon generate a reliable value for the adjoint in that particular cell. Test particles are then generated in the cells that are neighbours of the target and tracked. If they cross into the target cell their expected score is known from the value of the adjoint that has already been calculated. The history of these particles is immediately terminated. Particles that cross into unscored cells are allowed a limited number of events before being abandoned. When the immediate neighbours of the target cell have been completed, their adjoint values are estimated from the accumulated scores. Processing then moves to the next layer of cells surrounding those completed, and so on. Eventually, the entire importance map will be determined. In regions of the problem remote from the detector, test samples only have to be tracked as far as their scored neighbours to obtain a score rather than all the way to the detector.

When the importance map is represented in multigroup form, a solution is first obtained for the lowest energy group followed by groups in the order of increasing energy. When tracking test particles in the higher groups, a down scatter

into a scored group terminates the history with a known, expected score.

The method has been assigned the name 'recursive'. The adjoint estimate generated by this method can be very approximate and generally deteriorates with remoteness from the detector. However, the method is an alternative when diffusion methods are inapplicable, and it can form a useful starting point for subsequent improvement.

3. MERGE Method

The adjoint flux in a given space/energy cell may be interpreted as the expected score produced by introducing a particle into that cell. An estimator based on this definition can be used during a forward calculation to score the adjoint. The results may be combined with an initial guess of the importance function to improve the efficiency of the calculation. Consider the particle history illustrated in **Fig. 1**. A particle born at A crosses importance mesh boundaries at B and D and undergoes a collision at C. The final track segment between D and E is in an identified detector. The score may be added into an accumulator for estimating the adjoint in mesh 1 where the particle was born.
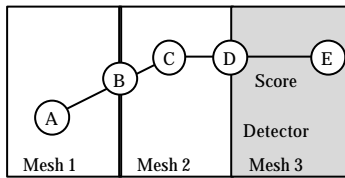

Fig. 1 Particle history in a segment of an importance mesh.

The portion of the particle history BCDE may be considered as that of a particle started at B, so a contribution to the adjoint estimate for mesh 2 may also be made. This logic applies to all the events: the cell into which the particle emerges after an event may be considered as a starting point for the remainder of the history. A contribution to the adjoint estimate may thus be made in every cell of the importance map through which the particle has passed.

At a certain point in the calculation, the results for the adjoint estimator in various space/energy cells of the importance map may be reasonably well scored in some cells but poorly scored or completely unscored in others. A method is required of merging the partially completed adjoint solution with the initial estimate of the importance map to take advantage of the information learned. Trials have shown that simple substitution of the well scored adjoint estimates for the initial estimates of importance in corresponding cells is unsatisfactory. The transition between the retained, initial importance values and the substituted ones can lead to large step changes. The S/R process then becomes inefficient or, in extreme cases, unstable.

A better solution is to scale the initial importances outside the envelope of well scored adjoint estimates so that there is no change in magnitude at the transition. The gradients outside the scored envelope are preserved, as illustrated in **Fig. 2**.

The importance map may be revised several times during the Monte Carlo calculation using this procedure, and the efficiency of the calculations may be optimised by choosing an appropriate frequency for these revisions.
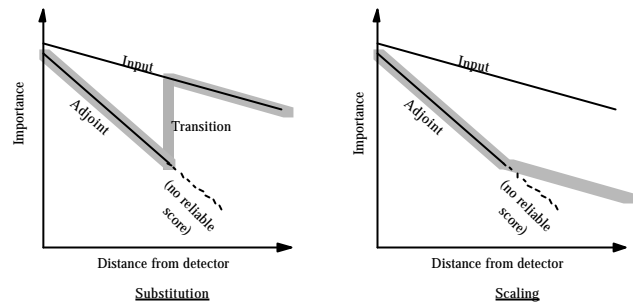

Fig. 2 Methods of merging importance maps.

4. A Ventilation Duct Calculation

This example concerns radiation streaming along a ventilation duct from a cell which holds a source. The cell and duct are illustrated in **Fig. 3**.
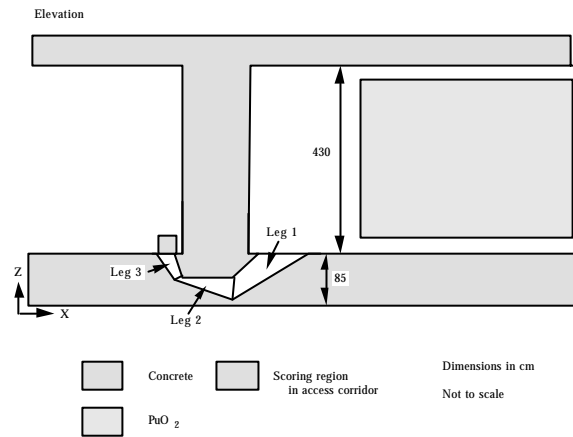

Fig. 3 Ventilation duct

The source is a large tank of PuO_2, and the neutron dose-rate in the access corridor is required. This dose-rate arises mainly from neutrons streaming through the duct. The difficulty in accelerating such a calculation is to persuade the neutrons to navigate the duct efficiently.

Spatial and angular weighting of the MCBEND source was used, as well as importances provided by a multigroup adjoint MCBEND Monte Carlo calculation in a 44x8x13 XYZ splitting mesh in 28 energy groups. However, to reduce the time required to perform the adjoint calculation, the importances were condensed over energy and the y-direction. Consequently, only one energy group was specified for the MERGE option, although variation in the y-direction was catered for.

The results of calculations run for the same length of time using these importances and with the MERGE and RECURSIVE options, as well as in analogue mode (i.e. with no acceleration), are shown in **Table 1**.

The RECURSIVE option in 1 group is only a factor of two less efficient than the calculation accelerated with the MCBEND adjoint. This is creditable since the preliminary calculation required by the RECURSIVE option took less

than 1% of the total execution time, while running the adjoint MCBEND calculation required some 20% - not including the effort required to set up and execute the separate adjoint calculation.

Table 1 Results for ventilation duct

Mode of acceleration	Dose rate in scoring region
Analogue	$0.275 \pm 57.9\%$
MCBEND multigroup adjoint	$0.157 \pm 7.9\%$
RECURSIVE (1 group)	$0.147 \pm 11.2\%$
RECURSIVE (3 groups)	$0.155 \pm 7.6\%$
MERGE from analogue (1 group)	$0.185 \pm 44.1\%$
MERGE from MCBEND adjoint (1 gp)	$0.153 \pm 8.7\%$

Furthermore, using 3 splitting groups with the RECURSIVE method improves the efficiency to a level similar to that of the calculation accelerated with the MCBEND adjoint.

The table shows that, for this problem, the MERGE method did not produce any significant improvements.

5. A Reactor Subcore Calculation

This example is a calculation of reaction-rates in canisters suspended from fuel element support struts beneath the support plate of a Magnox reactor, which is illustrated in **Fig. 4**.
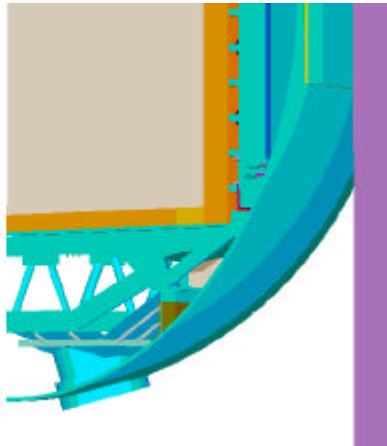

Fig. 4 Lower region of a Magnox reactor

Table 2 shows results for the iron damage response obtained from calculations run for the same length of time. Each is the average over all the scoring regions. The importances from the MCBEND adjoint were obtained in a 17x5x13 RθZ splitting mesh in 15 energy groups spanning 1keV to 15MeV. The MERGE method started from a flat importance map.

This indicates that the MCBEND adjoint, MERGE and RECURSIVE methods improve the efficiency of the calculation by varying amounts. The preliminary calculation required by the RECURSIVE option to determine the importances took 1% of the overall execution time. The effort required to prepare and execute the MCBEND adjoint calculation is substantially greater.

Table 2 Results for reactor subcore

Mode of acceleration	Reaction rate (x10^{13})
Analogue	$3.95 \pm 9.4\%$
MCBEND Adjoint	$3.91 \pm 3.4\%$
MERGE	$3.85 \pm 4.3\%$
RECURSIVE	$3.89 \pm 4.6\%$

Thus both the new options, though not quite as effective as using a MCBEND adjoint calculation to generate importances, give useful increases in efficiency with much less effort. The MERGE option may require trial runs to optimise the number of merges in the calculation, but the RECURSIVE option requires minimal user intervention.

III.   The Use of Adjoint Monte Carlo

1.   Potential Benefits

The previous sections describe methods of generating an approximate adjoint solution to provide an importance function for accelerating a forward Monte Carlo calculation. An alternative approach is to perform the whole Monte Carlo calculation in adjoint mode. A detector reaction rate can then be calculated by integrating the product of the adjoint function and the source function.

One type of problem for which this method is likely to be more efficient is one in which the detector is small compared with the source. In a forward Monte Carlo calculation it may be difficult to ensure that sufficient particle tracks pass through the small detector region: this problem is avoided in an adjoint calculation, since the roles of source and detector are reversed. The adjoint method may also be preferable when it is necessary to calculate the reaction rates of a detector corresponding to a number of different source distributions. This would require a separate forward calculation for each distribution, but it can be achieved with a single adjoint calculation.

When the adjoint technique is used in this way, it is important that it should employ an accurate nuclear data representation, similar to that available for forward calculations. The adjoint calculations reported in the previous section were all multigroup calculations. However, MCBEND has now been extended to provide the option of performing adjoint Monte Carlo calculations using point energy data.

2.   Point Energy Adjoint Method

The adjoint transport equation may be written in the following form:

$$-\boldsymbol{W}\nabla\Phi^*(\mathbf{x},E,\boldsymbol{W}) + \Sigma_t(\mathbf{x},E)\Phi^*(\mathbf{x},E,\boldsymbol{W}) =$$

$$\int \sum_{n,r} \boldsymbol{r}_n(\mathbf{x})\boldsymbol{n}_{nr}(E)\boldsymbol{s}_{nr}(E)P_{nr}(E,\boldsymbol{W}\rightarrow E',\boldsymbol{W})\Phi^*(\mathbf{x},E',\boldsymbol{W})dE'd\boldsymbol{W}$$

$$+ S^*(\mathbf{x},E,\boldsymbol{W})$$

In the integral term, n and r are the nuclide and reaction indices and $\boldsymbol{r}$ is an atomic number density. The adjoint source term S^* is normally equal to the response function for the detector of interest.

A common feature of point energy adjoint Monte Carlo techniques [3][4][5] is the reconstruction of the adjoint equation

so that it looks as similar as possible to the forward equation, thus minimising the changes which have to be made to the Monte Carlo procedure. In MCBEND the restructured equation has the form

$$\mathbf{W}\nabla\Phi^{+}(\mathbf{x},E,\mathbf{W})+\Sigma_{t}(\mathbf{x},E)\Phi^{+}(\mathbf{x},E,\mathbf{W})=$$

$$\int\sum_{n,r}\mathbf{r}_{n}(\mathbf{x})\mathbf{n}_{nr}^{+}(E')\mathbf{s}_{nr}^{+}(E')P_{nr}^{+}(E',\mathbf{W}\rightarrow E,\mathbf{W})\Phi^{+}(\mathbf{x},E',\mathbf{W})dE'd\mathbf{W}$$

$$+S^{+}(\mathbf{x},E,\mathbf{W})$$

where

$$\Phi^{+}(\mathbf{x},E,\mathbf{W})=\Phi^{*}(\mathbf{x},E,-\mathbf{W})/E$$

$$S^{+}(\mathbf{x},E,\mathbf{W})=S^{*}(\mathbf{x},E,-\mathbf{W})/E$$

and (omitting the subscripts for simplicity)

$$\mathbf{s}^{+}(E')=\int\mathbf{s}(E)P(E,\mathbf{W}\rightarrow E',\mathbf{W})(E'/E)dEd\mathbf{W}$$

$$\mathbf{n}^{+}(E')=\frac{\int\mathbf{n}(E)\mathbf{s}(E)P(E,\mathbf{W}\rightarrow E',\mathbf{W})(E'/E)dEd\mathbf{W}}{\mathbf{s}^{+}(E')}$$

$$P^{+}(E',\mathbf{W}\rightarrow E,\mathbf{W})=\frac{\mathbf{n}(E)\mathbf{s}(E)P(E,\mathbf{W}\rightarrow E',\mathbf{W})E'/E}{\mathbf{n}^{+}(E')\mathbf{s}^{+}(E')}$$

The weighting factor $1/E$ improves the efficiency of the adjoint solution. Two other refinements have been applied to the basic method described above. Firstly, the microscopic adjoint partial cross-sections $\mathbf{s}^{+}$ are scaled so that they sum to the true microscopic total cross-section. This is necessary to allow the adjoint transport equation to be solved by a Monte Carlo procedure analogous to the forward case. A compensating factor is applied to the particle weight at each collision. Secondly, the adjoint secondary energy/angle distributions are defined using only the slowly varying part of the cross-section; otherwise these distributions would contain rapid fluctuations due to resonances. Once again, compensation is made through an adjustment of the particle weight.

Different considerations apply to thermal neutrons. A detailed treatment is normally used in forward MCBEND calculations, but for the initial implementation of the adjoint method a simple one-group model has been adopted. This model is also available as an option in forward cases to enable comparisons to be made.

The point energy adjoint method has been implemented as an option within the neutron collision processing module of MCBEND. New input data options and output edits have been provided to assist the user in running adjoint cases. MCBEND's facility for calculating the importances which control variance reduction has been extended to generate importances for an adjoint case by means of a forward diffusion calculation.

Adjoint versions of three MCBEND neutron data libraries (based on UKNDL, JEF-2.2 and ENDF/B-VI) have been produced by applying the transformations described above.

3. A Cavity Streaming Calculation

A mock-up of a PWR radial shield and cavity was constructed in the ASPIS facility at Winfrith in order to validate methods of calculating PWR cavity streaming. The arrangement is illustrated in **Fig. 5**. The source of neutrons is a circular fission plate driven by thermal neutrons from the

NESTOR reactor. Measurements were made using a BF_3 counter at various heights along the centre line of the cavity.
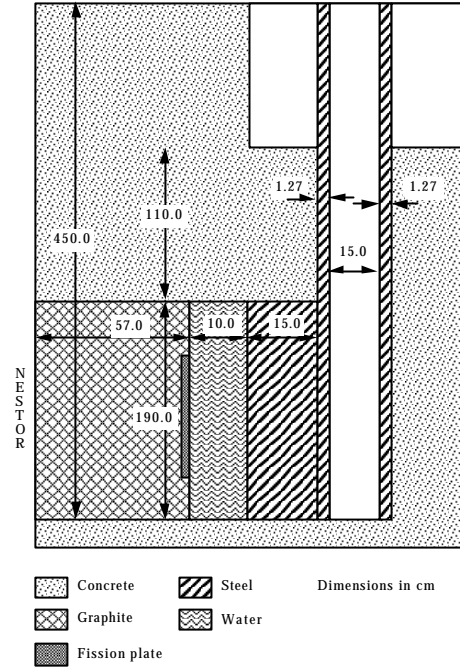
Fig. 5 PWR shield and cavity mock-up

It has been found that very long MCBEND runs are required to calculate detector reaction rates in the upper regions of the cavity. It was therefore of interest to examine whether a calculation in adjoint mode would be more efficient. For this purpose, a position about 1.5m above the level of the centre of the fission plate was chosen, and the BF_3 response at this position was calculated using both forward and adjoint methods with JEF2.2 data. The results are shown in **Table 3**. This includes values of the Figure of Merit (FOM), defined as $1/(\sigma^2 t)$ where σ is the standard deviation and t is the cpu time.

Table 3 BF_3 response in the cavity

	Reaction rate	St Dev %	FOM
Forward calc (1-gp thermal)	1.213E-01	1.3	59
Adjoint calc (1-gp thermal)	1.219E-01	1.0	333
Adjoint/Forward	1.005	1.6	5.6
Forward calc (Full thermal)	1.351E-01	1.3	59
1-gp/Full thermal	0.898	1.8	1.0

There is close agreement between the reaction rates calculated using the forward and adjoint methods (when the one-group thermal treatment is used in both), but the FOM values show that the adjoint method is almost 6 times faster.

A further forward calculation was performed using the full detailed thermal treatment, to assess the accuracy of the one-group treatment. The difference is 10%, which may be larger than would be acceptable for some applications. This indicates the need either to improve the one-group method or to develop the adjoint form of the detailed thermal treatment.

Calculations were also performed for a detector near the top of the cavity, about 3.5m above the level of the centre of the fission plate. At this position it is very difficult to obtain adequate statistical accuracy using forward calculations, but an adjoint calculation was much more efficient, the ratio of the figures of merit being of the order of 1000.

4. A PWR Surveillance Capsule Calculation

The H B Robinson Unit 2 station is a three-loop 665MW(e) Westinghouse PWR owned by the Carolina Power and Light Company and located at Hartsville, South Carolina, USA. An extensive range of measurements was carried out during cycle 9 using special dosimetry introduced into the surveillance position in the downcomer annulus and into the reactor cavity. These measurements provide a means of validating MCBEND for radial shield calculations on PWRs, and a number of comparisons with MCBEND calculations have been carried out in recent years [6].

The use of adjoint calculations for such applications could offer advantages, both because the detectors are small in volume relative to the source over the reactor core and because there is a need to calculate the change in the detector responses due to the changing source distribution during and between cycles.

Some further MCBEND calculations for this system have therefore been carried out using the new point energy adjoint option. They have been compared both with MCBEND calculations in forward mode and with the measurements. ENDF/B-VI data were used. These calculations have been restricted to one position, the surveillance capsule, and to two detectors, the high energy reaction Ni58(n,p) and the low energy reaction Fe58(n,γ).

The measured and calculated results, expressed as end-of-cycle activations, are compared in **Table 4** for Ni58(n,p) and **Table 5** for Fe58(n,γ).

Table 4 Ni58(n,p) activation at surveillance position

	Activation dps/a	St Dev %	C/M
Measurement	2.58E-15	10	
Forward calc	2.508E-15	0.4	0.97
Adjoint calc	2.474E-15	0.4	0.96
Adjoint/Forward	0.986	0.6	

Table 5 Fe58(n,γ) activation at surveillance position

	Activation dps/a	St Dev %	C/M
Measurement	2.06E-14	12	
Forward calc (Full thermal)	1.952E-14	1.8	0.95
Forward calc (1-gp thermal)	1.948E-14	1.7	0.95
Adjoint calc (1-gp thermal)	1.938E-14	1.9	0.94
1-gp/Full thermal	0.998	2.5	
Adjoint/Forward	0.995	2.5	

For Ni58(n,p), the forward and adjoint results agree within 1.4%. This difference, although small, is just over 2 standard deviations and is therefore statistically significant; it is of the order that would be expected for the small uncertainty associated with the representation of the data in the forward and adjoint forms of the MCBEND nuclear data library. The calculated results are lower than the measurement by 3% and 4%. This is well within the uncertainty of 10% on the measurement.

For Fe58(n,γ), the forward and adjoint calculations using the one-group thermal treatment agree within the statistical uncertainties. A further forward calculation was performed to assess the difference between the detailed and one-group thermal treatments, and although the very close agreement is probably fortuitous in view of the statistical uncertainty, the result shows that any error associated with the one-group treatment is unlikely to be greater than 5% in this case. The calculated results are lower than the measurement but the differences are within the uncertainties.

In general the relative efficiency of using forward or adjoint runs depends on the number of detectors and the number of different source distributions which are to be considered. As an example, suppose that there is a requirement to calculate reaction rates for 10 detectors (5 high energy and 5 low energy) arising from 10 different source distributions. On the basis of the running times for the calculations described above, it is estimated that the adjoint method would be about 5 times more efficient.

The techniques described in this paper are also of potential value for BWR calculations [7].

IV. Conclusions

New methods have been developed for accelerating MCBEND Monte Carlo calculations. These have been demonstrated to be effective when applied to some particularly demanding problems.

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