

THE STATUS OF THE GENERAL RADIATION TRANSPORT CODE MCBEND

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Abstract

MCBEND is an established Monte Carlo code in the fields of shielding, dosimetry and general radiation transport. The code is licensed and actively supported in use by the ANSWERS Software Service of Serco Assurance. The development of the code is continuing within a partnership between Serco Assurance and BNFL and this paper reviews the current status of the code and describes some recent developments.

KEYWORDS : Monte Carlo method, radiation transport, acceleration

Introduction

MCBEND is an established Monte Carlo code in the fields of shielding, dosimetry and general radiation transport. It can calculate neutron, gamma-ray and electron transport ; coupling of the different radiation types is also possible. The code is the result of over 30 years' development. The aim of the on-going development programme continues to be the delivery of accurate, robust and fit for purpose techniques into the hands of the user. User support and easy to understand input data and documentation are designed to make the techniques easily accessible, even to the novice.

The next section of the paper briefly describes the currently released version (9E) of the code, highlighting some particularly useful features. The following section describes developments which will be in the next released version of the code, concentrating on point energy adjoint and automatic splitting mesh generation, together with some examples of their application.

Standard Features of MCBEND

Geometry

MCBEND utilises the flexible Fractal Geometry package [1], in which bodies are used to define regions of space. For complicated shapes Hole Geometry, which utilises Woodcock tracking, is available. Thus a system may be modelled in MCBEND to whatever degree of accuracy is required.

Collision Processing and Nuclear Data

For neutron calculations, the cross-sections are held in 13,193 ultrafine energy groups. Secondary angular distributions are represented using 32 equi-probable bins and secondary energy distributions, where required, are also represented using 32 equi-probable bins. Subgroup treatment is utilised in the unresolved resonance region of U238 and Pu239. In this way the transport of individual particles is treated accurately. Nuclear data libraries based on UKNDL, JEF2.2, ENDF/B-VI and JENDL3.2 data are currently available. Detailed treatment of thermal neutron transport is included using $S(\alpha,\beta)$ data or free gas treatment as appropriate.

For gamma-ray calculations, cross-sections are held at 400 energy points and angular distributions of scatter are held in 32 equi-probable bins. For electron and positron calculations the condensed history method is used.

Source Representation

MCBEND includes facilities to model a variety of sources, with various geometries and built-in energy spectra. This flexible package allows any source to be represented accurately. Facilities to model reactor sources for RPV and other dosimetry are also included [2].

Variance Reduction

Efficient and robust variance reduction is a key requirement of a Monte Carlo calculation. The standard method utilised by MCBEND is splitting/Russian roulette in space and energy together with source weighting. Both methods rely on a set of space/energy dependent importances. The ability to employ appropriate importances is vital and a suitable choice cannot in general be made *a priori* by the user.

In MCBEND the importances are calculated using adjoint diffusion theory. The library of diffusion coefficients has been carefully adjusted so that the solution approaches that which a transport calculation would

provide. For the purposes of variance reduction, this approach is sufficiently accurate. The importances are calculated in an orthogonal mesh ("splitting mesh") which overlays the problem geometry. The user simply has to define the mesh, the target response function and its location - the code does the rest. This facility, available since 1990 [3], has taken a lot of the difficulty out of efficient, robust variance reduction. Additional techniques, such as forced flight and revision of importances [4], are also available for difficult radiation streaming problems.

Scoring

The standard techniques in MCBEND for scoring are by track length or collision density in regions. Fluxes and responses may be scored. A response library, based largely on the IRDF95 dosimetry file, is included with the code. Responses are scored as the calculation progresses rather than folding group averaged detector cross-sections with group fluxes at the end of the calculation.

Sensitivity of fluxes and responses to material cross-sections can be scored. Both first and second order sensitivities are available [5]. These may be used to calculate uncertainties in the result due to data uncertainties or due to uncertainties or perturbations of physical parameters such as density, porosity, etc. A geometrical sensitivity option also exists, which allows the effect of geometrical uncertainties or perturbations to be determined [6].

Accurate prediction of detector response in terms of energy deposition requires the code to simulate the physical processes occurring in the detector. In MCBEND the raw energy deposition spectrum (pulse height distribution) is accurately recorded, even in the presence of events such as pair production and variance reduction which cause a number of fragments from the same sample to score [7].

Recent Developments

Recent developments to MCBEND, which will be included in the next full release of the code include : automatic splitting mesh generation, point energy adjoint for neutrons, calculation of uncertainty in the results due to material cross-section uncertainties, a unified source facility [5], improved temperature treatment, extended scoring of sensitivity to geometry perturbations and Fractal Geometry and Hole Geometry improvements. The point energy adjoint facility and automatic splitting mesh generation are described below, together with examples of their application

Point Energy Adjoint Calculations

The point energy adjoint facility in MCBEND has been described in detail previously [4] : a synopsis and example of its application will be given here.

An alternative approach to the normal forward calculation 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 than a forward calculation 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. MCBEND has now been extended to provide the option of performing adjoint Monte Carlo calculations using point energy data. The adjoint transport equation is reconstructed 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. Adjoint versions of nuclear data libraries are required and are available for UKNDL, JEF2.2 and ENDF/B-VI data.

For thermal neutron transport 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.

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 source of neutrons is a circular fission plate driven by thermal neutrons from the NESTOR reactor. Measurements were made using a BF₃ counter at various heights along the centre line of the cavity.

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 1 and show that there is close agreement between the reaction rates calculated using the forward and adjoint methods but the Figure of Merit (FOM) values show that the adjoint method is almost 6 times faster.

Automatic Splitting Mesh Generation

As described in the previous section, the standard variance reduction techniques in MCBEND are splitting/Russian roulette and source weighting using importances which are calculated using adjoint diffusion theory in a user-defined splitting mesh which overlays the problem geometry. In this process the main burden on the user is the definition of the splitting mesh boundaries. Whilst this is not particularly onerous compared with setting the importances, automatic splitting mesh generation would make variance reduction even more straightforward and would be a useful addition to the code.

In MCBEND, splitting /Russian roulette occurs when a particle's importance differs by more than a factor of two from the space/energy importance of the splitting mesh (in space or energy) which it is entering. Binary splitting is always employed. Thus the ideal attenuation factor across a single splitting mesh is a factor of two. This is also a factor which allows an appropriately accurate solution of the adjoint diffusion equations to be achieved.

The mesh spacing which gives a factor of two attenuation clearly varies with particle energy as well as with material. Thus one could construct a splitting mesh by working out the smallest spacing for any neutron energy in any of the materials in the problem and use this to set an ultrafine mesh covering the whole problem. However, the size of this mesh is restricted by the memory available to solve the adjoint diffusion equations and, possibly, by the time available for this purpose. Thus using an ultrafine mesh is not practical.

Generally the splitting mesh at low energies needs to be fine near a thermal detector but can be coarser further away from the detector. At high energies a coarser mesh is appropriate. Thus one solution to the memory problem would be to use different meshes at different energies, thus allowing an accurate solution of the adjoint diffusion equations and providing a suitable importance map at all energies, whilst keeping the memory requirement reasonable.

In MCBEND a facility for automatically setting the splitting mesh intervals has been implemented, based on the above approach. The user specifies the number of meshes in each direction, the target response, a reference (target) point and the principal attenuation direction(s) ; MCBEND uses this information to set a splitting mesh for each energy group and evaluates the importance map. The sets of boundaries form a composite mesh, to which the importances are mapped. Tracking then uses the composite mesh to determine when splitting/Russian roulette in space and energy are required.

A further enhancement allows the code to choose the number of meshes in each direction, thus reducing user input still further. This is as far as automation of variance reduction could possibly go : the user specifies the reference point, target response and attenuation direction(s) and the code does the rest.

The two requirements of any variance reduction technique are that it should be robust and efficient. The answers must agree with the analogue case and should be obtained relatively quickly. Thus the technique has been tested on a number of problems, two of which are described below. For each problem, cases were run in analogue mode, with a user-defined splitting mesh and with the number and placement of the splitting mesh boundaries chosen by MCBEND.

- Winfrith Iron Benchmark This problem involves a fission source and a mild steel shield made of a series of plates. The required response is the $\text{Rh103}(n,n')\text{Rh103m}$ reaction-rate after 62cm of steel. Results are shown in Table 2.
- Neutron Source Container This case involves a Cf252 source located in a cylindrical container. The container includes lead of thickness 2cm and boric acid/paraffin wax of thickness 42cm. The required response is the neutron dose-rate outside the container. Results are shown in Table 3.

The results from these two cases show that

- Splitting/Russian roulette as implemented in MCBEND is robust and, as expected, much more efficient than analogue calculations - factors of between 50 to 100 in these cases. Cases with greater attenuation would show even more benefit.
- Automatic splitting mesh generation is also robust and efficient : the automatic choice of splitting meshes still produces accurate results and does not reduce the efficiency significantly. Indeed, in some cases the efficiency is improved.

Conclusions

The status of the Monte Carlo code MCBEND has been given briefly. Recent developments, including point energy adjoint for neutrons and automatic splitting mesh generation have been described and examples of their application given.

References

1. N.R.Smith, E.Shuttleworth, S.J.Carter and M.Evans "Geometry Modelling and Visualisation for the Monte Carlo Code MCBEND" Proc. 8th International Conference on Radiation Shielding, 1994
2. G.A.Wright, E.Shuttleworth, P.Cowan, I.,J, Curl and C-G.Mattsson "MCBEND - A Fluence Modeling Tool" Proc 10th International Symposium on Reactor Dosimetry, 1999
3. P.C.Miller, G.A.Wright, S.W.Power and C.Boyle "The Use of an Inbuilt Importance Generator for Acceleration of the Monte Carlo Code MCBEND", Proc. International Conference on the Physics of Reactors : Operation Design and Computation, 1990
4. E.Shuttleworth, M.J.Grimstone and S.J.Chucas "Application of Acceleration Techniques in MCBEND" Proc 9th International Conference on Radiation Shielding, 1999
5. N.R.Smith, E.Shuttleworth, M.J.Grimstone, J.L.Hutton, M.J.Armishaw, A.J.Bird, N.J.France and S.M.Connolly "The Current Status and Future Plans for the Monte Carlo Codes MONK and MCBEND" Proc. Monte Carlo 2000 Conference
6. E.Shuttleworth "The Geometrical Sensitivity Option in MCBEND" Proc. Monte Carlo 2000 Conference
7. E.Shuttleworth "The Pulse Height Tally Distribution in MCBEND" Proc 9th International Conference on Radiation Shielding, 1999

Table 1 PWR Mockup : BF₃ 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

Table 2 Iron Benchmark : Rh103(n,n')Rh103m Reaction -Rate after 62cm of steel.

	Analogue	User-Defined Mesh	Automatic Mesh
Rh103(n,n')Rh103m rr	1.01E-05	1.02E-05	9.86E-06
Standard deviation	8.8%	1.8%	2.2%
Cpu time	22579 sec	5312 sec	4064 sec
FOM = 1/($\sigma^2 t$)	5.72E-07	5.81E-05	5.08E-05
Result/Analogue	-	1.01	0.98
Standard deviation	-	0.09	0.09
FOM/Analogue	-	102	89

Table 3 Dose-Rate Outside a Neutron Source Container

	Analogue	User-Defined Mesh	Automatic Mesh
Dose-Rate	1.84E+02	1.95E+02	1.92E+02
Standard deviation	10.0 %	2.6 %	2.8 %
Cpu time	14151 sec	3625 sec	1244 sec
FOM = 1/($\sigma^2 t$)	7.07E-07	4.08E-05	1.03E-04
Result/Analogue	-	1.06	1.04
Standard Deviation	-	0.11	0.11
FOM/Analogue	-	58	145