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# ADVANCES IN THE MONTE CARLO CODE MCBEND

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### ABSTRACT

Since ICRS8, MCBEND has undergone development on several fronts to increase the productivity of the user. These range from fundamental methods development to improving the high level of user-friendliness of the code.

For many situations where detectors are small relative to the size of the radiation source, or where variations of the source distribution are present in the same system, the adjoint method is more efficient than the usual forward mode of calculation. Multigroup adjoint capabilities are commonplace but these bring with them the inherent problems of cross-section averaging and approximate representation of the angular distribution of scatter. MCBEND now has the capability to perform adjoint neutron calculations using point energy data. The method adopted for the adjoint solution is to cast the adjoint transport equation into a form resembling the forward equation but containing transformed definitions of the cross-sections and the secondary energy and angular distributions. With the new method, significant gains in efficiency can be achieved over calculations in forward mode without any loss of accuracy.

Monte Carlo is increasingly becoming the preferred method of solving radiation transport problems. However, there is still a need for shield assessors to perform scoping calculations using quicker but approximate methods before switching to a more rigorous method for design substantiation. For neutron calculations, MCBEND now includes a dual diffusion/Monte Carlo capability, so the inefficiency of using two separate codes with separate input data constructs is removed. In order to provide this capability, the module used by MCBEND to derive values of importance by performing an adjoint diffusion calculation has been modified so that it runs in forward mode for neutron cases, thus allowing scoping calculations to be performed using the MCBEND model of the system. The switch between diffusion and Monte Carlo methods requires minimal user effort, so a series of scoping calculations can be easily followed by a definitive Monte Carlo calculation.

The user-friendliness of the code has been enhanced by the production of two Graphical User Interfaces for processing results and providing diagnostic information.

Firstly, VISTA-GRAPH interrogates the code's dump file and extracts the results of the calculation. The user can choose the type of result, manipulate the values by specifying an appropriate function, and tabulate selected results in any desired order for incorporation into a spreadsheet or report. A basic plotting facility is also available.

Secondly, VISTA-TRACK lets the user see the random walk of the Monte Carlo particles. It processes a file written by MCBEND which contains details of the sequence of events undergone by particles which have reached a scoring region, and superimposes the paths of such particles onto a view of the MCBEND model.

This paper briefly covers the capabilities of MCBEND, then goes on to describe the development and application of the point energy adjoint capability, the scoping tool, and VISTA-GRAPH and VISTA-TRACK.

# I. INTRODUCTION

MCBEND<sup>1</sup> is a general geometry, point energy Monte Carlo code used for deep penetration problems in shielding and radiation transport, and is one of the ANSWERS suite of codes for Reactor Physics, Shielding and Criticality. It may be used for neutron, gamma-ray, electron/positron and coupled calculations. The neutron data are presented in 8220 groups and are derived from the UK Nuclear Data Library, JEF-2.2 and ENDF/B-VI compilations. This fine group treatment has explicit representation of the energy/angle laws. The gamma-ray data are described in a continuous energy scheme and are based upon the UKNDL compilations. Coupled (n, ) calculations are performed by running the neutron calculation and writing details of the neutron collisions to a dump file<sup>2</sup>. This is then combined with a gamma-ray production library to produce the source for the gamma-ray calculation. Multi-group data are also available for neutron, gamma-ray or coupled calculations.

The model is built using the techniques of combinatorial geometry with the system being specified as a series of Parts which are then assembled into the complete model, the Parts allowing easy specification of lattices and nested structures<sup>3</sup>. The source specification is very flexible, with freely orientated source bodies, inbuilt spectra, and powerful weighting algorithms. The code's variance reduction techniques are based on splitting and Russian roulette with energy dependent importances specified in a separate orthogonal mesh and being provided by an adjoint diffusion calculation which is performed as an integral part of the MCBEND run<sup>4</sup>, the module performing this function being known as MAGIC. Extra techniques designed for the acceleration of streaming calculations are also available<sup>4</sup>.

Several quantities may be scored in a MCBEND calculation. The basic tally is of volume-averaged flux or response, but facilities exist to score sensitivity, angular fluxes and currents, heat or charge deposition and pulse height distribution. A simple point estimator is also available.

Clear and informative input data and documentation are an integral part of the MCBEND package. For the user guide a simple input syntax, based upon a flow diagram format, has been in successful use for many years. The guide permits a quick and easy assimilation of the input requirements and gives detailed notes to clarify specific items. The user guide is supported by an expanding range of introductory texts and applications guides. Diagnostic information and geometry display of the MCBEND model are provided by the VISTA suite of graphics packages<sup>3</sup>.

Since ICRS8, MCBEND has undergone development on several fronts ranging from fundamental methods development to improving the image and user-friendliness of the code, in all cases with the aim of increasing the code's speed of calculation and its ease of use, but above all enhancing the productivity of the user.

The following sections describe the development of a capability for performing adjoint calculations for neutrons using point energy cross-section data; the use of diffusion theory to provide a rapid scoping capability within MCBEND; and two Graphical User Interfaces (GUI's) for the manipulation of the code's results and for the display of paths taken by the Monte Carlo particles through the system.

# II. POINT ENERGY ADJOINT CALCULATIONS

The benefits of performing adjoint, rather than forward, calculations for some systems are well known. In a system with a distributed source and a small detector, a forward calculation may have difficulty in obtaining a statistically accurate value of the quantity to be scored in a particular region (eg the reaction-rate in a detector) because it is time-consuming to ensure that sufficient particle tracks enter the detector. In an adjoint calculation the roles are reversed with the source becoming a distributed scoring region for the adjoint flux, and the calculation is consequently more efficient. Another application for which it can be more efficient to use the adjoint solution is the calculation of the values of a particular score produced by a number of different source distributions in the same system, eg the effect of changing power profiles in a reactor core on the response of a dosimetry capsule<sup>5</sup>. A single Monte Carlo calculation can be used to provide an adjoint solution which can be folded with each of the source distributions to give all the required values.

Adjoint calculations have been available in MCBEND for many years, but only using multigroup cross-sections. Modern applications require greater accuracy than is possible with such data, and MCBEND now has the capability for performing adjoint calculations with point energy data for neutrons.

# A. Theory

The adjoint transport equation may be written in the following form (with the spatial, angular and energy subscripts x, and E omitted for brevity):

$$- \cdot \cdot + \cdot = S^{\dagger} + \frac{1}{2} - \cdot \cdot (E) P_{r,n}(\mu, E - E) + (- \cdot E) d dE$$

In the integral term, r and n are reaction and nuclide indices,  $\mu = \dots$ , and the macroscopic cross-section is the product of the number density *N*, the microscopic cross-section and the number of secondary particles per event .

A common feature of point energy adjoint Monte Carlo techniques<sup>6,7,8</sup> 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

$$\cdot * + \cdot * = S^* + \frac{1}{2} * \cdot \cdot E P^*_{r,n}(E) P^*_{r,n}(\mu, E) * (\cdot, E) d dE$$

where (omitting subscripts)

$${}^{*}(x, , E) = \frac{1}{E} {}^{\dagger}(x, - , E) \qquad S^{*}(x, , E) = \frac{1}{E} S^{\dagger}(x, - , E)$$
$${}^{*}(E) = (E)P(\mu, E - E)\frac{E}{E} dE \qquad {}^{*}(E) = \frac{(E) (E)P(\mu, E - E)\frac{E}{E} dE}{{}^{*}(E)}$$
$$P^{*}(\mu, E - E) = \frac{(E) (E)P(\mu, E - E)\frac{E}{E}}{{}^{*}(E) {}^{*}(E)}$$

The weighting factor of 1/E improves the efficiency of the adjoint solution by producing better behaved secondary energy/angle distributions and by making \* into a more "flux-like" quantity. Two other refinements have been applied to the basic method described above. Firstly, the microscopic adjoint partial cross-sections \* 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, and implies that the frequency of collisions will be approximately the same in forward and adjoint calculations. 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.

#### **B.** Implementation

The transformations described above have been applied to the nuclear data library used by MCBEND. This is a one-off task which provides an "adjoint nuclear data library" for use whenever the point energy adjoint option is requested in MCBEND. The structure of the adjoint library has been made as similar as possible to that of the standard library, so as to minimise the differences between the forward and adjoint collision processing within the code itself. The method is not yet applicable to thermal neutrons, which have a separate collision processing package.

# C. Testing

The accuracy and efficiency of the MCBEND point energy adjoint method have been assessed in a series of tests. The results will be illustrated here by two examples.

The first case is a calculation for a simulated PWR radial shield which was studied in the NESDIP2 experiment conducted at Winfrith<sup>9</sup>. The adjoint method was used to calculate the S32(n,p)P32 reactionrate at the outer face of the simulated pressure vessel. In this calculation, the adjoint source was located at the detector position and its spectrum was derived from the detector cross-section. The reaction-rate was calculated by folding the physical source distribution with the adjoint function produced by MCBEND. This result was checked by calculating the same quantity using a conventional forward MCBEND run. The main features of the comparison are as follows:

	Ratio: Adjoint/Forward
S32(n,p) reaction-rate	0.984 (=0.012)
Figure of Merit $(1/2t)$	1.33
Collisions per second	0.94

The reaction-rates obtained by the forward and adjoint techniques agree within 2 standard deviations (2). Judged by the figure of merit, the adjoint method is the more efficient, as would be expected since the detector is smaller in volume than the source. The rather small difference in the number of collisions processed per second during the MCBEND runs shows that there is no significant time penalty associated with the adjoint collision processing.

The second illustrative case is a calculation for an experiment in the DIMPLE reactor at Winfrith simulating a rectangular corner section of the core of a PWR together with the radial shield<sup>10</sup>. In this case, the point energy adjoint calculation was compared with a multigroup adjoint calculation using 100 group EURLIB data. The S32(n,p)P32 reaction-rate at the inner surface of the simulated pressure vessel was chosen for this test. The results of the comparison are as follows:

	Ratio: Point/M'group
S32(n,p) reaction-rate	1.091 (=0.010)
Figure of Merit $(1/2t)$	0.70
Collisions per second	0.79

The calculated reaction-rates are significantly different; the result obtained with the point energy data is closer to the value measured in the experiment, giving C/M=0.93 compared with 0.85 for the multigroup result. The multigroup method is slightly faster in terms of the collision processing rate and in its overall figure of merit, but the difference is no longer sufficient to justify its use in place of the more accurate point energy method.

# **III. DIFFUSION CAPABILITY**

Over the last decade or so, Monte Carlo has become the preferred calculational method for many radiation and transport applications. However, there remains a need for more rapid techniques which can be used in shield design, with Monte Carlo being used for a final, definitive calculation. Additionally, the effects of changes in shield configuration can be assessed quickly using less rigorous methods than Monte Carlo. Such scoping calculations have traditionally been performed with diffusion or deterministic transport theory in a limited number of dimensions. Inevitable inefficiency is caused by the use of two separate methods with different input data.

MCBEND has for many years had the capability of using diffusion theory for the determination of values of importance. This capability can now be used in forward mode in order to provide a rapid scoping tool within MCBEND which can be applied with minimal user effort.

# A. MAGIC and the scoping tool

The functionality of MAGIC is fully described elsewhere<sup>4</sup>. It is summarised here to give some background to the evolution and functionality of the scoping tool.

In MCBEND, the variation of importance in space and energy is specified in an orthogonal XYZ or R Z mesh overlaid on the geometry of the system. The material composition occupying each mesh is automatically determined by sampling the materials present in the MCBEND model and smearing them over the mesh. Within this material search, the meshes containing the scoring regions are determined, these being associated with the adjoint source for the diffusion calculation whose spectrum is selected from the response functions specified by the user. The boundary conditions for the diffusion calculation are determined by the presence of black or reflecting regions at the edges of the system. The adjoint diffusion calculation is performed for neutron, gamma-ray or coupled (n, ) analyses as appropriate and the values of importance passed to the Monte Carlo calculation.

MAGIC has now been modified to run in forward mode. During the material search described above, meshes containing source are identified, as are those where scoring is required. The forward calculation is performed and the fluxes folded with the requested response functions. If the scores have been requested within geometric regions rather than in the orthogonal splitting mesh, the results in the latter are mapped onto the former using a volume-weighted average of the scores in the splitting meshes which overlay the scoring region.

All the input data for the scoping tool, ie source specification, geometry, material compositions and mesh spacing, is derived from the traditional MCBEND input data. The switch between Monte Carlo and diffusion theory is achieved by only two keywords, namely DIFFUSION SOLUTION, which means that minimal user effort is required to change between the two methods of calculation.

#### B. Adjusted Diffusion Constants

For decades in the UK, diffusion theory has been successfully tuned to more rigorous methods in order to overcome its deficiencies at deep penetration - such methods being known as Adjusted Diffusion Constants (ADC) methods<sup>11</sup>. In the scoping tool, the data are formulated using ADC method E, which represents the flux in each energy group by the sum of two components. Each of these components may be described by the solution of the general equation giving the flux as a function of distance x from a plane source S for a one-dimensional slab of material:

$$= \frac{SL}{2D} \exp \frac{-x}{L}$$

where L is the diffusion length and D is the diffusion coefficient.

In Method E, the values of D and L are derived by fitting this equation for the two components of each energy group to the results of calculations of the attenuation through one-dimensional slabs of material using the deterministic transport code ANISN<sup>12</sup>. Scatter cross-sections  $_{\rm S}({\rm g}'-{\rm g})$  controlling the transfer between energy groups g' and g are condensed from a 175-group JEF-1 evaluation<sup>13</sup>, and the absorption cross-section for each group is given by the relationship  $_{\rm a} = D/L^2$ . The cross-section data are presented in 33 energy groups ranging from 20MeV to thermal energies for a comprehensive range of nuclides. The scoping tool then solves the multigroup diffusion equation

$$-D(g)^{-2}(g) + a(g)(g) = S(g) + g^{-1} + s(g'-g)(g')$$
  
g'=1

for the system being analysed.

#### C. Limitations

At present, the scoping tool is only available for neutron calculations, but plans exist for its extension to gamma-ray and coupled (n, ) systems.

A fundamental limitation of diffusion theory is its inability to treat radiation streaming in voids. Diffusion theory is based on the assumptions of isotropic flux and absence of strong absorbers and leakage surfaces. In a void, the flux tends to be anisotropic and there are obviously leakage surfaces bounding the void. In MAGIC, and therefore in the scoping tool, regions of void are automatically filled with aluminium with an artificially low density of 0.1g/cm<sup>3</sup>. This is adequate for treating small regions of void, but not for large regions or systems where radiation streaming is important. The inaccuracy of the scoping tool in voids is considered later.

### **D.** Applications

The scoping tool has been tested against Monte Carlo calculations for a number of applications. The first to be described is the determination of the radial variation at core mid-height of the reaction-rate for neutron damage in iron out to the cavity of a schematic PWR (an example used for illustrative purposes in the MCBEND user guide). Azimuthal symmetry led to only an octant of the PWR being modelled, this being overlaid by a 16x30x22 XYZ splitting mesh with importances for the Monte Carlo calculation being targeted on the damage in the reactor pressure vessel (RPV) and provided automatically by MAGIC in 28 energy groups.

The ratio of the results produced by the two methods at various positions is presented overleaf. Through most of the core and shield, the scoping tool gives results which are within 20% of the Monte Carlo calculation, indicating that the scoping tool is performing well. The two sets of results differ somewhat in the cavity region as would be expected since diffusion theory does not treat voids accurately.

Regarding run times, the Monte Carlo results were obtained from a calculation taking some 70,000 seconds where the statistical accuracy on the response results was about 2%, whereas the diffusion case took about 500 seconds, some 140 times quicker. The scoping tool therefore provides a useful means of determining, say the sensitivity of damage to the RPV to variations in power distribution or water density.

Radius	Position	Diffusion/
(cm)		Monte Carlo
52.5	Core	0.98
87.5	Core	1.03
115.0	Core	1.04
162.0	Water	1.02
168.0	Barrel	0.83
172.0	Water	1.08
178.0	Thermal shield	0.89
184.0	Water	1.07
202.0	Middle of RPV	0.94
220.0	Insulation	0.62
230.0	Cavity	0.58

The second example is the axial variation of neutron dose-rate at the surface of a transport flask, specifically a TN12 flask<sup>14</sup>. MAGIC again provided the importances in a 22x36x27 R Z splitting mesh. The axial variation of neutron dose-rate at the edge of the flask wall as determined by the two methods is illustrated below, the scoping tool results being within 20% of the Monte Carlo values. (The plateau indicates the axial extent of the fuel.)



When results in the void surrounding the flask are considered, the scoping tool becomes increasingly pessimistic because diffusion theory cannot account for the geometric attenuation of the radiation outside the flask.

The Monte Carlo calculation was run for 50,000 seconds to produce results with statistical errors of about 10%, whereas the diffusion case ran in about 700 seconds. Given that 10% is an acceptable level of statistical accuracy for the Monte Carlo calculation, the scoping tool runs seventy times quicker than the Monte Carlo calculation.

In summary, the scoping tool provides MCBEND with a rapid calculational method which compares well with Monte Carlo calculations for systems which do not involve radiation streaming, and which is about a hundred times quicker.

### IV. VISTA-GRAPH

VISTA is a suite of utilities which provides diagnostic information about the MCBEND calculation. VISTA-WIRE and VISTA-RAY<sup>3</sup> provide three-dimensional displays of the geometry, using wire-frame and ray-tracing techniques respectively. They have recently been joined by VISTA-GRAPH, which processes the code's output; and VISTA-TRACK, which display the paths taken by the Monte Carlo particles as they move through the system.

The format of the output from MCBEND is fixed: for every energy group and response, the flux or reaction-rate is presented for each scoring region in turn. Often, the user has to "cut and paste" MCBEND results from the output file into a spreadsheet, perhaps fold the results with some function (eg a source normalisation factor), and re-order the values into the required format for presentation (eg the flux spectrum in a given region). This process can be tedious, is prone to error, and requires the user to take responsibility for the QA of the post-processing.

To address these problems, MCBEND now includes a post-processing capability known as the Tabular Output module, whereby the user can select particular results, decide the order in which they are to be presented, and manipulate them using arithmetic functions. The module output tables of results in the required format, and thus reduces the effort required, the possibility of errors, and the QA implications for the user. The module is accompanied by a GUI known as VISTA-GRAPH which interrogates the MCBEND's dump file and extracts the information concerning the results. VISTA-GRAPH uses the Fortran "engine" of the Tabular Output module to allow the user to select, manipulate and tabulate results, and it also includes a plotter for the convenient viewing of the variation of the results in any dimension (including energy and time).

The illustration of the use of VISTA-GRAPH uses the PWR analysis described in section III. On accessing the dump file, information about the calculation is presented which includes details of the run time, number of samples, particle type, and source, scoring and acceleration options. The user is shown which results are present (not shown), and can choose a sub-set of these for further processing, eg by folding them with arithmetic functions. Having defined the subset, the modified results can be plotted. Either axis may be linear or logarithmic, and the plot may be a bar chart or histogram with error bars optionally included. In this example, the plot is of the variation of the flux in energy group 4 in the x direction for splitting meshes y=15 and z=12, as specified in the box titled Range. Any multi-dimensional set of results may be selected, but the plots are only two-dimensional.

After initial examination of the results, they may be written to formatted files for inclusion in proprietary word-processing or spreadsheet packages, much of the effort in transferring results of a calculation to the final report having been alleviated.

# V. VISTA-TRACK

When performing a calculation with MCBEND, the user does not obtain much information regarding how the particles were transported from the source, through the system to the detector(s). Such information is useful for specific applications such as determining the depth of penetration of particles into the formation surrounding an oil-well borehole, and in general to ensure that the important penetration paths through a system are being followed.

MCBEND can now provide what is known as a history log which holds the sequence of events from the source to the detector of particles which score. Relevant parameters of all source, collision and scoring events are held on the log - such as position, energy, weight, time, nuclide and reaction type. The history log is processed by a GUI called VISTA-TRACK (which includes the proprietary graphics package Matlab) so that the paths from source to detector can be displayed in three dimensions. Tracks associated with a specified set of the above parameters can be chosen if required, say to identify which scores were due to particles which had passed through a particular material.

To identify the paths taken through the system more clearly, the display can be superimposed on a twodimensional colour representation of the model which shows the different material regions. The illustration overleaf shows the path taken by gamma-rays from the source (the small region at the bottom of the central window) out into the formation and back to a detector in a logging tool situated at the side of a bore-hole. The subset of particle tracks to be displayed is specified in the left-hand window. On clicking on any track on the display, the parameters of that track are displayed on the screen to allow detailed analysis of the different penetration paths through the system.

By displaying the actual paths taken by the particles in a MCBEND calculation, VISTA-TRACK gives the user the ability to interrogate the details of the Monte Carlo process for diagnostic purposes and present his Monte Carlo calculations in a form suitable for understanding by clients.

# VI. SUMMARY

This paper has presented several recent developments associated with MCBEND. The ability to perform adjoint calculations using point energy neutron cross-sections widens the range of problems which can be efficiently analysed using Monte Carlo, the scoping tool provides a rapid calculational method which can be used in shield design, and VISTA-GRAPH and VISTA-TRACK give the code's users two packages for the graphical display of results and of particle tracks through the system. All these developments follow a policy of increasing productivity by making MCBEND more efficient and more user-friendly.

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