Revised methods for Adjoint Calculations

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A common class of shielding problems involves the calculation of biological dose rates from large distributed sources at localised positions. A typical example is that of calculating the dose at points around a transport cask. Sophisticated variance reduction methods must be used in Monte Carlo calculations to sample from the important parts of the source and to propagate particles towards the relatively small detector volumes.

An alternative is to solve the adjoint problem in which the detector acts as a source and the source becomes the detector. In this mode there is a small source and large detector. Since an interpretation of the adjoint flux in a mesh/energy group is the importance of that cell it follows that the best tallies will be obtained in the most important regions without necessarily having to introduce variance reduction.

The principal limitation of this approach is the current availability of adjoint treatments using point energy data. A multigroup treatment is a viable alternative but most data libraries have been derived for deterministic codes and are not particularly suited to Monte Carlo calculations. This paper describes a method in which multigroup libraries specifically for Monte Carlo calculations are derived by sampling from point energy libraries. A derivative of MCBEND [1] has been developed which uses these new data. It also contains internal facilities for transforming a conventional input model into the adjoint form. The task of folding in the adjoint fluxes with the forward sources is performed at the end of the calculation so the user is presented with the required detector dose rate.

INTRODUCTION

Historically, the use of Monte Carlo methods for radiation transport calculations was limited by the availability of computer resources; routine calculations were often carried out using less accurate, deterministic methods. The advent of abundant, cheap computing power now makes it possible to consider Monte Carlo codes for everyday calculations. However, the development history of major codes such as MCBEND [1] means that they are often over qualified for simple tasks where expertise in the use of sophisticated Monte Carlo methods is not available. Essentially, there is a need for software that uses the modelling power of the Monte Carlo method but retains the simplicity of the old deterministic methods.

MULTIGROUP DATA

Monte Carlo codes generally use a continuous energy scale (or a hyperfine group structure) to represent the variations of cross section data. This gives far better accuracy than can be achieved by averaging the cross-sections over a relatively small number of groups. However, there are some advantages to the use of multigroup data - particularly in the solution of problems in adjoint mode.

Use of multigroup data is supported by MCBEND but only in a minor role. It can read multigroup libraries that were originally developed for deterministic codes - primarily to allow comparisons to be made between different methods using common data. The form of the data is not ideal for use in Monte Carlo calculations: for example, it uses truncated Legendre polynomials to represent the angular variation of cross sections. These are approximate fits and the pre-processing needed before they can be sampled in a stochastic calculation introduces further inaccuracies. This paper describes the production and use of alternative multigroup libraries that are designed specifically for Monte Carlo use.

SOURCE OF MULTIGROUP DATA

In principal, multigroup data libraries could be built by processing evaluated nuclear data files. However, this requires experience in using a sophisticated suite of processing codes and access to the large files of raw data. The results would need further processing to adapt them to the format proposed below for use in Monte Carlo applications.

An alternative approach has therefore been used: multigroup libraries are generated by sampling from the point energy libraries used in MCBEND. A program to do this has relatively simple input and has been built using existing collision processing routines extracted from MCBEND. The program allows any group scheme to be specified with a range of weighting options. The number of samples to be taken for each group forms part of

the input. Typically, 100,000 samples are taken per group. This route allows the simple and rapid creation of multigroup libraries appropriate to specific classes of calculation.

WEIGHTING OPTIONS

When point energy data are condensed to multigroup form an assumption must be made about the flux spectra in which the library will be used. For example, if the flux and the cross section in a given group both increase with decreasing energy there will be more events towards the lower end of the group and the average cross section should reflect this. A flux weighted average of the cross section over the range of the group will improve the multigroup representation:

$$\overline{s} = \frac{\int_{E1}^{E2} s\, f dE}{\int_{E1}^{E2} f dE}$$

The flux spectrum will not be known when the multigroup cross sections are generated but selection can be made for a given energy range in an intended application. For example, cross sections intended for use within a reactor core may be weighted with a fission spectrum for neutron energies above 1.0 MeV. The processing program supports the following; the selection is made by a key letter.

U	Unweighted	the spectrum is flat
C	Collision density	emphasises energies where the cross section is highest
F	Fission spectrum	for in-core materials at high neutron energies
L	Lethargy (inverse energy)	for scattered gamma spectra and intermediate energy neutrons
M	Maxwellian.	for thermal energy neutrons.

The choice may be varied throughout the group scheme.

SCATTER DATA

The bulk of a multigroup library is formed from scatter data. In principle, scattering can take place from any group in the scheme to any other group. For a given transfer, the cross section will be a function of the angle of scatter. These data are stored on the library in a scatter table; each row contains:

The total cross section for the group transfer:
The partial cross sections for scattering into each of a number of angular bins.

The angular bins in the library are defined by uniform intervals on a cosine scale from -1 to +1. Adequate accuracy can be achieved in the intended application by using 10 - 20 bins.

If the table contained entries for every potential group-to-group scatter it would be extremely large and would contain many empty rows where a given transfer does not occur. It is therefore confined to rows that contain finite data. A rectangular scatter matrix (each dimension being the number of groups) records the table row number for all transfers with finite cross sections. This is an integer array; two byte integers are sufficient for the purpose so that space is conserved.

PREPARATION FOR MONTE CARLO TRACKING

The multigroup libraries generally contain entries for individual elements - though isotopic data could be stored. It is also possible to sample and record cross sections for specific materials. For practical applications the elemental (or isotopic) library data must be combined with material composition data to generate material data for a particular Monte Carlo execution. Since the library data are all cross sections (rather than fitting coefficients) this is straight forward. For a material containing several elements, the integer scatter matrices are merged and the finite entries re-numbered. Material scatter tables are created within the code from the scatter data tables in the library. They have one row for each finite entry in the material scatter matrix.

Finite entries in the rows of the scatter matrix are combined with corresponding data from the scatter table to generate probabilities for scattering to each secondary group and to derive a non-absorption probability. The angular data in the scatter table (now containing material macroscopic cross sections for scatter to each angular bin) are replaced by the cosine boundaries for a corresponding number of equiprobable angular bins for rapid interrogation during Monte Carlo tracking.

For adjoint mode calculations, the above processing is simply modified to treat the columns of the scatter matrix as rows and the rows as columns. It is possible to derive probability tables for both forward and adjoint mode in a single execution so that, for example, the MIDWAY [2] variance reduction method can be applied in a single step.

IMPLEMENTATION

The multigroup methods described above have been implemented in a simple Monte Carlo code (MCFANG) which is derived from components of the general purpose code MCBEND. The new code is intended primarily for execution in analogue mode but includes an implementation of MIDWAY variance reduction. This method tracks some of the particles in forward mode from the source to a defined surface placed at some position between source and detector. The remainder of the particles are tracked to this surface from the detector in adjoint mode. The surface crossings recorded in these two steps are combined to generate a detector response. This method exploits the facility of the new multigroup scheme whereby forward and adjoint collision processing can readily be implemented in a single execution. The MIDWAY surface may have various shapes. The principal features of MCFANG are as follows.

- Retains the full geometry and source modelling capabilities of MCBEND.
- Uses multigroup data for collision processing.
- Handles neutron, gamma or coupled n,g calculations.
- Executes in forward or adjoint modes – or both.
- Includes simple, robust variance reduction methods:
    - Spatial variation relative to defined lines superimposed on the physical geometry.
    - MIDWAY variance reduction

EXAMPLE APPLICATION

The case considered is a large flask containing radioactive liquor. The biological dose rate is required behind a pair of shielding plates. The latter destroy the radial symmetry of the problem so that the tally volume is relatively small. The geometry is shown schematically in Figure 1

In a conventional Monte Carlo calculation it is necessary to introduce a detailed importance map to encourage the flow of particles to the specific region of the detector. The execution becomes much more efficient in adjoint mode since all particles are generated in the small detector volume and only need to hit the large source volume in order to register a score.

The results of several calculations with various modes and different shapes of midway surface are presented in Table 1

Table 1: Various solutions to the example problem.

Code	Result	Time (min) to 5%	Description/Comment
MCBEND	0.313 ± 4.8%	38	Point energy. Detailed importance map
MCFANG	0.360 ± 5.1%	7.9	Adjoint mode, volume detector
MCFANG	0.3381 ± 2.1%	3.2	MIDWAY rectangle
MCFANG	0.3360 ± 2.1%	3.3	MIDWAY disc
MCFANG	0.3587 ± 2.3%	4.0	MIDWAY cylinder

The multigroup treatment in MCFANG gives results that are in reasonable agreement with the more refined, point energy result generate by MCBEND. The adjoint facility available in MCFANG leads to faster execution without the need for sophisticated variance reduction methods.

SUMMARY

A requirement for a simple, Monte Carlo code has been identified. A multigroup representation of cross section data has a number of advantages for such a code – particularly in the solution of problems in adjoint mode. A form of multigroup data designed specifically for use in Monte Carlo codes has been described. The proposals have been implemented in a prototype code MCFANG, and application to a realistic problem has shown promising results.

REFERENCES

1 Wright, G.A., Shuttleworth, E., Grimstone, M.J. and Bird, A.J. *The status of the general radiation transport code MCBEND.* Nucl. Instr. and Meth. in Phys. Res. B **213**, 162-166 (2004)

2 Serov, I. *Estimation of Detector Responses by Midway Forward and Adjoint Monte Carlo Coupling in Nuclear Systems*. Thesis: Delft University of Technology. December 1996

Figure 1

Schematic representation of the test problem