RECENT DEVELOPMENTS TO THE MONTE CARLO CODE MCBEND

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Purpose: *MCBEND is a well established Monte Carlo code from the ANSWERS Software Service in the UK. It is being continually developed to meet the needs of its users. Recent developments to MCBEND are described here. These cover improvements to the underlying physics and data libraries, improvements in calculation efficiency and improvements to the usability of the code.*

Methods and Materials: *Recent developments include a Unified Tally option for scoring, including enhanced methods for scoring by material, extension of point energy adjoint calculations to include detailed thermal treatment, incorporation of a covariance library for detector cross-sections, a number of new "hole" geometries in which Woodcock tracking takes place, including a tetrahedral mesh hole that imports a converted CAD file, a new collision processor and automatic meshing for acceleration of gamma-ray calculations.*

Results: *These developments have resulted in more flexibility in scoring, for example the ability to score by material in regions incorporating Woodcock tracking, potentially more accurate adjoint calculations utilizing thermal detectors, automatic calculation of uncertainty due to detector cross-sections, greater flexibility in geometry modelling, improved collision processing, for example the ability to utilize bound data for thermal neutron transport in graphite and less user input for efficient calculation acceleration.*

Conclusions: *Some recent developments of MCBEND are described and examples of their use given.*

I. INTRODUCTION

MCBEND is a well-established powerful Monte Carlo software tool for general radiation transport analysis for shielding and dosimetry applications. MCBEND is developed within a Nuclear Code Development partnership (NCD) between Serco and Sellafield Ltd and is licensed for use by Serco's ANSWERS Software Service. The MCBEND package comprises not only the Monte Carlo code itself but also nuclear data libraries, user documentation, productivity tools of various kinds and user support services. Supporting geometry model visualisation and verification tools are also available.

The current version is MCBEND version 10A (Ref. 1). MCBEND is being continually developed to meet the needs of its users. The ANSWERS vision is 'to provide easy-to-use software that meets the current and emerging needs of the user community'. In the case of MCBEND this vision focuses on the key areas of accuracy, understanding of uncertainties, efficiency and user-friendliness.

This paper describes some recent and on-going developments to the MCBEND package.

II. RECENT AND ON-GOING DEVELOPMENTS IN MCBEND

The recent and on-going developments cover a range of areas of activity and are presented below under the following headings: Geometry Modelling, Physics Modelling, Scoring Options, Nuclear Data and Acceleration Options.

II.A. Geometry Modelling

The MCBEND geometry modelling and tracking package comprises two components: Fractal Geometry which uses conventional ray tracing through geometrical bodies and Hole Geometry which uses Woodcock tracking. The same geometry modelling package is also available in the ANSWERS criticality code MONK[2].

II.A.1. Fractal Geometry

Fractal Geometry is a well-established system of solid geometry modelling in which the problem geometry is subdivided into zones - defined as the intersections and differences of mathematical bodies. MCBEND has a large selection of body shapes ranging from simple bodies such as cuboids, cylinders and spheres to more complex bodies such as prisms, ellipses and tori. The bodies are assembled into structures called parts, which are self contained with their own local co-ordinate system to simplify the model construction. Parts may be included

within other parts to any depth of nesting and a given part may be included more than once within the geometry. The ability to break down complex models into parts simplifies the preparation and checking of the input data.

II.A.2. Hole Geometry

The Woodcock tracking algorithm in MCBEND is implemented via the Hole Geometry package, and brings significant additional modelling power to the user. Hole geometries can be used to model common replicating arrangements and simple intersecting configurations in a short-cut form.

The Hole Geometry package continues to grow as additional hole types are added in response to industrial needs. Recent developments include: the User Hole to provide the user with a method of specifying the geometrical definition for a new hole type using simple mathematical functions; the Bent-Pins Hole to model the deformation or loss of pins due to dropping or other forces on a fuel element; the Pipes Hole to easily model complex arrangements of pipes and their joints; the Random-Rods Hole to model a random arrangement of cylindrical rods in a container; the Voxel Hole which allows cube-shaped zones (known as voxels) – each with a different material if required - to be easily modelled in MCBEND with significantly reduced internal storage space required compared with the existing XYZmesh Hole.

Another new hole type is the PBMR Hole to model the arrangement of pebbles in a Pebble Bed Modular Reactor and the Grain Hole to model its fuel pebble structure. This is a complex problem, given the quasi-random nature of the fuel distribution but is well matched to the Woodcock algorithm.

A capability has been developed that enables CAD generated tetrahedral mesh geometries to be imported into MCBEND and treated as a hole geometry. Further details of this development are given in a companion paper at this conference[3].

II.B. Physics Modelling

On-going developments to the Physics Modelling in MCBEND include a new collision processor and an extension of the point energy adjoint method to include detailed thermal treatment.

II.B.1. BINGO Collision Processor

MCBEND uses a module named DICE for its neutron collision processing, together with DICE format nuclear data libraries. These libraries contain data derived from various evaluated files (UKNDL, JEF2.2, ENDF/B-VI, JENDL3.2) and the neutron cross-sections are stored on a fixed hyperfine energy grid of 13,193 groups. For gamma-ray collision processing MCBEND uses a module named GAMBLE, together with UKNDL data whilst for charged particle transport a condensed history method is used.

A new collision processing package is currently being implemented in MCBEND named BINGO, together with appropriate nuclear data libraries. Improvements in BINGO include: use of cross sections tabulated at energy points that are specific to each nuclide; improved variable temperature treatment; enhanced thermal scattering modelling including use of bound data for graphite; better representation of correlated energy/angle laws; more detailed representation of the tails of the fission spectrum; and explicit modelling of bremsstrahlung.

These capabilities give MCBEND the tools to model complex systems with a greater degree of realism than with the DICE package.

II.B.2. Detailed Thermal Point Energy Adjoint

A standard MCBEND calculation simulates the movement of particles from the source, taking account of collisions, material boundaries and so on, until the particle is either absorbed or escapes from the model. In the process, tallies may be taken at detector locations to estimate fluxes, responses etc. In an adjoint calculation, neutrons are initiated at a detector, and tallies are taken at the source locations. A fundamental theorem shows that the adjoint flux combined with the source distribution gives the same result that the conventional flux would give when combined with the detector response. An adjoint capability allows solution of certain problems that would be highly inefficient in a forward calculation, including cases with a distributed source and a small detector. Additionally, the adjoint method allows the response from a number of different source distributions to be calculated from a single Monte Carlo adjoint calculation.

The current point energy adjoint employs a single energy group in the thermal range which cannot take account of flux variations at thermal energies. In reality, each neutron has its own value of energy, which changes following a collision. In the one group point energy adjoint, neutrons only scatter to higher energies, there is no possibility of returning to lower energies. The exception to this is if particles start at thermal energies, in which case, following a collision, there is the possibility that a neutron stays in the thermal group, or that it scatters outside the thermal group. If it scatters outside the thermal group, again subsequent scatters can only take the particle to higher energies. There is no concept of the particle having its own value of energy in the thermal group. Thermal energies are important for some detectors, and so the model needed to be extended to cover the entire energy range.

In the detailed thermal point energy adjoint model, neutrons have a specific value for energy throughout the whole energy range. At thermal energies, scattering to both higher and lower energies is possible. Thus there may be many collisions before the neutron escapes to higher energies where only up-scatters occur.

The implementation of the detailed thermal point energy adjoint is an on-going development and is based mainly in the development of adjoint nuclear data libraries. Modifications to MCBEND itself are needed in the collision processor, the source definition, the scoring, the acceleration routines, and for post-processing to allow easy access to the results.

II.C. Scoring Options

Until now scoring options in MCBEND record results in volumes defined either in the geometry of the model or in the model's importance mesh (which is used for variance reduction). These methods of scoring have a number of disadvantages, some of which are listed here:

- The size of some geometry zones may be too large to give adequate resolution for scoring. This leads to the introduction of non-physical boundaries to subdivide zones of interest, which can make the geometry model unnecessarily complicated.
- Correct normalisation of results requires the volumes of the zones. These cannot be determined analytically for zones defined by intersecting bodies and must be derived and input by the user – however use of the accompanying SKETCH code allows the user to determine zones volumes even for complicated shapes.
- The importance mesh is restricted to simple rectangular or cylindrical geometry aligned with the material geometry axis.
- The positions of the importance mesh boundaries are generally governed by variance reduction criteria. Where the cells are small the results scored within them can have poor statistics. Where the cells are large, resolution of flux variation is lost.

II.C.1. Unified Tally Module

A new Unified Tally Module (UT) allows scoring to be carried out in sets of meshes that are independent of the geometry model and importance mesh. The method is based on the principle of *scoring bodies* that may be subdivided to form localised scoring meshes of any required size. Any number of bodies may be defined and may overlap freely.

Each scoring body has a named shape e.g. BOX, ZROD and is located by its origin. The size of each scoring body is determined by shape parameters e.g. length, radius, height, and the bodies can be rotated as required. Each scoring body may be subdivided to allow localised scoring. All scoring bodies and their permitted methods of subdivision allow the code to calculate the volumes of the scoring mesh cells.

As many scoring bodies as required may be defined. The scoring in each body is independent of other bodies so that bodies may overlap. For example, it would be acceptable to superimpose two bodies of identical shape. One could use a fine internal mesh to obtain good resolution of results; the other could use a coarser mesh to obtain better statistics. Alternatively, superimposed bodies could be used for scoring in different group schemes. The Unified Tally module may also be used in conjunction with the existing scoring facilities.

II.C.2. Scoring by Material

Scoring capabilities in the UT module also include *scoring by material*. This divides the scores recorded in a given mesh between the events in individual materials. It is principally intended for scoring results in the components of 'hole' geometries - as hole geometries do not have distinct 'zones' of different materials. Since tracking through such materials does not identify surface crossings it is not possible to use track length estimation; material scoring is therefore confined to collision density estimation. Essentially the material identified at a collision point becomes an additional subscript in the scoring registers. Normalisation of the results requires the volume of each material in each mesh. An option is therefore provided in the code to estimate relevant volumes by Monte Carlo.

II.D. Nuclear Data

II.D.1. IRDF2002 Detector Cross-Section Library

The IRDF2002 dosimetry library has recently been released by the IAEA. The library was formed following a thorough review of existing and new evaluations of dosimetry data. For most reactions the library contains point energy cross-sections as well as cross-sections in the SAND-IIa 640 energy group scheme used for the IRDF90 library. Use of the point energy data allows the possibility of more accurate representation of detector cross-sections for use in applications codes. This is important for threshold reactions in deep penetration problems and for resonance reactions. The IRDF2002 library also contains covariance data for the majority of reactions.

The IRDF2002 data have been processed using NJOY to produce a detector cross-section library and a detector covariance library for use with MCBEND[4]. The cross-sections were processed into an ultrafine 13,230

energy group scheme that is fine enough to account for resonance self shielding of single resonance reactions and also gives a good representation of threshold reactions whilst the covariances were processed into 25 broad groups.

II.D.2. Detector Covariance Library

The uncertainty in the result from a MCBEND calculation includes the uncertainty due to material cross-sections and the uncertainty due to detector cross-sections. These uncertainties are calculated by combining the sensitivity of the result to the cross-section with the uncertainty on the cross-section. These cross-section uncertainties are expressed in the form of covariances and stored in covariance libraries. MCBEND has had a material covariance library for some years and now a detector covariance library has been produced using IRDF2002 covariance data as described above.

Sensitivities to material and detector cross-sections are calculated during the calculation and these are then folded with covariance matrices read from the MCBEND material covariance library and the MCBEND detector covariance library. The sensitivities to material cross-sections are calculated using a differential method and those to detector cross-sections are simply the fractional contributions to the reaction-rate from each energy group. This facility is very useful and allows the analyst to calculate uncertainties with a minimum of additional work, thus making uncertainty analysis more accessible.

II.E. Acceleration Options

MCBEND has efficient and robust built-in acceleration (variance reduction) techniques which enable even novice users to perform efficient calculations. The principal method of variance reduction in MCBEND is the use of splitting and Russian roulette (S/R) under the control of a space/energy importance map. As an integral part of the code, an adjoint multigroup diffusion theory calculation may be performed to estimate importances in an orthogonal (XYZ or RθZ) mesh, known as a splitting mesh, that overlays the problem space. As the splitting mesh is completely separate from the geometry model, the problem geometry does not have to be complicated by dividing material regions into cells for acceleration purposes. This method has been available for nearly 20 years, and it has proved very effective in a wide range of applications.

II.E.1. Automatic Meshing for Acceleration

In MCBEND version 10A a facility for automatically positioning the splitting meshes has been implemented for neutron calculations. In a recent development this has now been extended to gamma-ray calculations. For gamma-rays the automatic importance mesh option chooses the positions of mesh boundaries based on the diffusion lengths in the highest importance energy group. The user has to specify basic information such as the target response, a reference (target) point and the principal attenuation direction(s). An additional feature that has been implemented into the automatic importance mesh is the ability to allow the user to confine the meshing to the real part of the geometry by entering appropriate limits. The undesirable presence of extensive voids can therefore be overcome. However, since the aim of automatic meshing is to minimise user intervention, such limits are automatically defined if none are entered by the user.

III. EXAMPLES

In this section an example utilizing recent developments of MCBEND is given.

III.A. Whole Body Modelling using the VOXEL hole and Scoring by Materials

A Whole Body test case has been set up in MCBEND using the Voxel hole. The voxel size used was 0.4cm x 0.4cm x 0.4cm, and the model contained 128 x 128 voxels in the x, y plane and 243 slices in the z plane. 56 different organs/tissues were represented in the model. The resulting model is shown using Visual Workshop[5] in Figure 1. A significant reduction in space (by about 90%) was observed compared to the space required for an XYZmesh hole. This means that much larger and more complex models can be run with MCBEND than was previously possible. In addition the run times using the Voxel hole were approximately 15-20% faster than the same calculation using the XYZmesh hole.

To calculate individual organ doses using the current scoring options in MCBEND required a scoring mesh of the same size and orientation as the voxels to be overlaid on the XYZmesh. Summation of all voxel scores belonging to an organ of interest was necessary. This is very cumbersome because knowledge of the position of each individual organ's voxels in 3,981,312 voxels is required

The calculation of individual organ doses has been made significantly easier by the introduction of the option to 'Score by Material' in the new Unified Tally module. Since each individual organ/tissue generally has a unique material index number, scoring in a particular organ only requires the knowledge of the material index number.

IV. CONCLUSIONS

This paper has summarised some recent and on-going developments of the MCBEND package. These cover improvements to the underlying physics and data libraries, improvements in calculation efficiency and improvements to the usability of the code. MCBEND continues to be focused on meeting the current and future needs of its customers.

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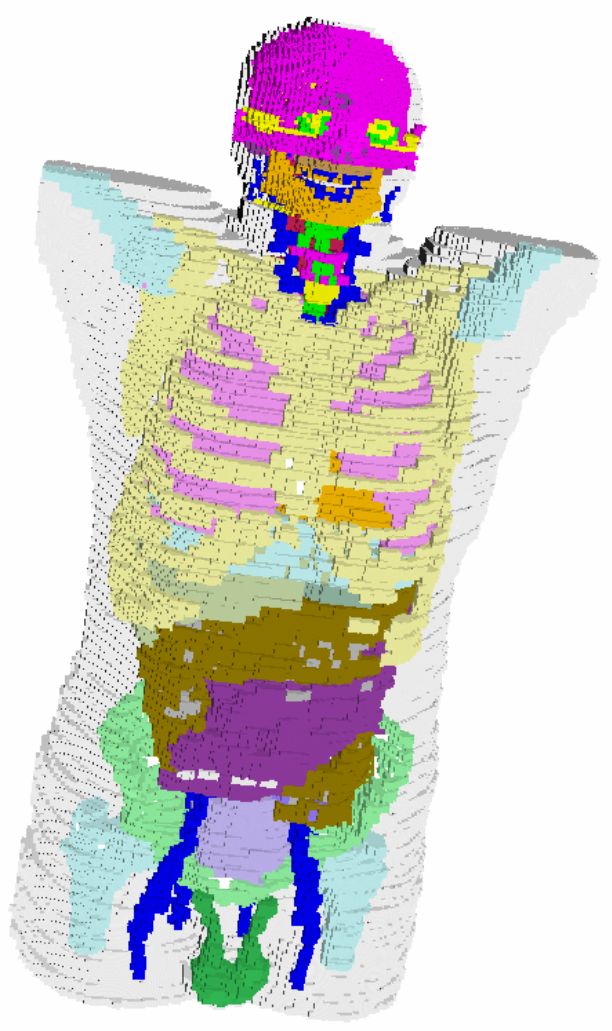

Fig. 1. Visual Workshop image of Whole Body test case using Voxel Hole