The Current Status and Future Plans for the Monte Carlo Codes MONK and MCBEND

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Abstract

MONK and MCBEND are software tools used for criticality/reactor physics and shielding/dosimetry/general radiation transport applications respectively. The codes are developed by a collaboration comprising AEA Technology and BNFL, and AEA Technology's ANSWERS Software Service supplies them to customers throughout the world on a commercial basis. In keeping with this commercial nature it is vital that the codes' development programmes evolve to meet the diverse expectations of the current and potential customer base. This involves striving to maintain an acceptable balance in the development of the various components that comprise a modern software package. This paper summarises the current status of MONK and MCBEND by indicating how the task of trying to achieve this difficult balance has been addressed in the recent past and is being addressed for the future.

1. The Challenge of Commercial Software Development

MONK and MCBEND are commercial software products, a unique attribute in a market place where large-scale government support and free access is the norm. Why is this so and how can the codes survive? The reason why is easy to address. For some time, the civil nuclear industry in the traditional UK home of the codes has operated in an entirely commercial manner. Development of software is no exception. Hence for the ANSWERS codes to remain in existence they had to become commercial codes. As to how the codes have survived and indeed grown in this environment for more than a decade is perhaps less obvious.

Planning the development of MONK and MCBEND involves maintaining a difficult balancing act between many different aspects of a commercial service. We are required to:

- Develop methods to provide solutions to emerging customer problems;
- Enhance the product image to facilitate use for existing customers and attract new customers;
- Produce nuclear data libraries to meet local needs and specific requirements;
- Provide supporting productivity tools taking advantage of the capabilities of modern computing facilities;
- Enhance documentation and validation (and the means of accessing both);
- Commit to the provision of a wide range of support services to maximise customer productivity (e.g. help-desk, consultancy, training).

For each of the above items, the individual ANSWERS customers may have widely varying requirements and priorities. The development of the ANSWERS products therefore seeks to achieve a balance, to try and meet as many of the customers' expectations as possible, within the constraints of available resources. Whether this balance is achieved or not is ultimately up to the individual customers to decide. This papers sets out our recent efforts and future plans aimed at ensuring their continued custom.

2. Background

MONK is primarily used for the solution of nuclear criticality safety and reactor physics problems. Major features such as hyper-fine energy nuclear data libraries, continuous energy collision modelling, superhistory powering and hole geometry modelling provide real application benefits to code users in terms of increased accuracy, efficiency, confidence and flexibility. MCBEND is a general-purpose radiation transport package that can calculate neutron, gamma-ray and electron transport in sub-critical systems; coupling of the different radiation types is also possible and powerful variance reduction techniques allow for wide ranging code application. With an extensive track record of use in support of nuclear operations across the whole fuel cycle, both codes provide sophisticated modelling capabilities in easy-to-use packages. Both codes are developed within a partnership between AEA Technology and BNFL.

3. Status of MONK and MCBEND

The production of MONK8 and the recent versions of MCBEND have brought into general use a number of facilities to extend the accuracy and efficiency of reactor physics, criticality and shielding analyses.

3.1 Geometry

MONK and MCBEND share a common geometry modelling package comprising two major components:

- A geometry body-based system built around hierarchically structured collections of bodies of general orientation. The collections of bodies can have simple relationships (e.g. nested or arrays) or complete freedom of overlap. Particle tracking is performed using conventional ray tracing techniques.
- A system of ‘hole’ geometry options that provides detailed structure and repeating configurations within the body-based system. The particle tracking in this option is performed using Woodcock tracking, which allows for a considerable increase in modelling capability and efficiency.

In combination, these options provide almost unlimited modelling capability, yet retain the simplicity of concept of the originators. Major extensions to both options have taken place in the recent past to meet emerging customer needs.

3.2 Nuclear Data

The recent past has also seen a major development of the nuclear data options available with MONK and MCBEND, particularly for neutron applications. Traditional use of UK nuclear data library-based compilations has declined in preference for more modern evaluations such as JEF2.2 [1]. In addition, other options have been provided to meet the broader international usage of the codes. A summary of the neutron options available is as follows:

- UK nuclear data library-based hyperfine energy group library (8,220 groups) using a continuous energy/angle slowing down treatment;
- JEF2.2-based hyperfine energy group library (13,193 groups) using a continuous energy/angle slowing down treatment;

- This has been followed by ENDF/B-VI-based and JENDL3-based libraries with the same characteristics as the JEF2.2-based library;
- UK-based and JEF2.2-based WIMS multigroup libraries (69 or 172 groups).

3.3 MCBEND Acceleration

For many years, MCBEND has contained an integral adjoint multigroup diffusion capability that can be used to calculate importances on an orthogonal mesh overlaying the problem space. These are used to control particle splitting/Russian roulette and weighted source sampling. In many diverse applications, this method has proved very effective in accelerating radiation transport calculations. However, there are cases, principally those dominated by voids and ducts, in which the limitations of a deterministic approach leads to inefficiencies in the Monte Carlo calculation. Alternative ways of generating importances have therefore been developed based on Monte Carlo methods [2]:

- Importance values can theoretically be estimated by sprinkling the entire problem with test sources and tracking them, with scoring samples contributing to the adjoint estimate at their birth site. Although impractical for large cases, a refinement of this technique has been implemented in MCBEND and has been assigned the name ‘recursive’.
- 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.

3.4 Major New Development

<u>Point Energy Adjoint</u>

An alternative approach to some problems is to perform a Monte Carlo calculation in adjoint mode. For example, detector reaction rates can be calculated by integrating the product of the adjoint function and the source function. To-date, the adjoint capability in MCBEND has been solely a multigroup one. However, MCBEND has now been extended to provide the option of performing adjoint calculations using point energy data [2].

<u>Reactor Burnup</u>

The MONK code now includes a microscopic burn-up capability which enables the code to treat whole core burn-up in small reactors. In a reactor core the material compositions change continuously with time during burnup. Monte Carlo calculations are used to calculate the flux at a given time point and this flux is used to determine the reaction rates of the materials in the problem. These reaction rates are then used to calculate the new material compositions by solving the depletion equations.

<u>Sensitivity Options</u>

The ability to calculate the sensitivity of scored fluxes and responses to changes in cross-sections has long been a feature of MCBEND. It has been used to good effect for application uncertainty analysis and to guide data improvement studies. Three recent developments have extended the range of sensitivity calculations:

- The original first order MCBEND sensitivity approximation has been extended to cover second order terms.
- A sensitivity option has been added to MONK to enable the sensitivity of k-effective to changes in cross-sections to be determined.

- A geometry sensitivity option in available in MCBEND to calculate the flux and response sensitivity to source and model geometry changes [3].

3.5 Ease of Use

To enable our customers to make best use of the power available from the combination of Monte Carlo techniques and high performance computers, new options have been developed to aid input specification and output analysis:

- Input data parameters are available to facilitate the setting up of calculations. The use of algebraic expressions as input data is possible. Automatic calculation sequences can be specified;
- MONK and MCBEND share a common nuclide and materials database, so that standard mixtures can be easily specified. This database can be augmented by user additions and provides a link between the various nuclear data libraries used with the codes;
- Output from MONK and MCBEND can be requested in standard and customisable formats, to provide direct links with other software packages such as spreadsheets.

3.6 Productivity Tools

A range of supporting productivity tools [4] continue to be developed for use with MONK and MCBEND as follows:

- VISAGE provides detailed interactive viewing of 2D slices of a geometry model, using the tracking routines of MONK/MCBEND;
- VISTA-RAY provides detailed interactive viewing of 3D images of a geometry model, again using MONK/MCBEND tracking;
- VISTA-WIRE gives rapid interactive viewing of a wire-frame representation of a model;
- VISTA-MOVIE can be used to show animated sequences of 3D model images;
- VISTA-GRAPH enables interactive presentation of calculated results;
- VISTA-TRACK displays Monte Carlo particle trajectories;
- LAUNCHPAD is an easy to use interface for preparing calculations.

3.7 Code Structure and Infrastructure

In addition to development of the codes, data libraries and supporting tools, several changes to the code structure and infrastructure have been made:

- The codes are assembled from a collection of independent functional and service modules, for optimum developer convenience;
- For the FORTRAN code components, extensive use is made of FORTRAN90 constructs, to provide significant structural simplifications;
- Embedded commentary and PDL (Programme Definition Language) is used to ‘self document’ the source code;
- Validation programmes continue on various fronts. The MONK programme now makes substantial use of ICSBEP [5] data;
- Commercial packages are used to prepare the software to ease customer installation;
- A modern commercial package is being used to service and monitor help-desk enquiries, to help provide the level of support expected in a commercial environment. Dedicated staff deal with enquiries from customers, with working hours scheduled to match the international nature of the business;
- The internet is being used not only to promote products but also, in a protected area, to provide an on-line information resource for customers;

- A range of computer platforms continue to be supported, the most popular being Sun/Solaris and PC/Windows;
- In addition to hardcopy, all user documentation is now provided as Adobe Acrobat™ PDFs.

4. On-going and Future Plans

The previous section indicated the breadth of activity undertaken in the recent past for MONK and MCBEND in order to try and provide the essential balance required for successful commercial software development. However, development of both MONK and MCBEND is a continuing process and a summary of current major developments is given below.

<u>Automatic Importance Mesh Generation</u>
The in-built importance value generation option of MCBEND has proved very successful over the last decade or more but the requirement still exists for the code user to select the orthogonal mesh that overlays the problem geometry. For some systems, this is not a difficult requirement but for others some automatic assistance would be of value. The latest MCBEND acceleration development is seeking to provide this assistance.

<u>Unified Source Capability</u>
A replacement unified source specification capability is being developed for MONK and MCBEND aimed at rationalising the existing options and providing more widely applicable implementations of variance reduction options such as source weighting. Additional user convenient features such as source contribution analysis will also be provided.

<u>The BINGO Project</u>
The module DICE is the collision processing engine within MONK and MCBEND; DICE assesses the outcome of particle interactions with nuclides. DICE is one of the longest-standing modules of MONK and MCBEND and despite its excellent service over many years, has been a candidate for replacement for some time. A new nuclear data library and collision processing package (BINGO) is therefore being developed for MONK and MCBEND aimed at making even better use of the available ENDF-6 format data (as used in JEFF, ENDF/B-VI and JENDL3). BINGO will exploit improvements in hardware, software and programming languages and incorporate new/extended physics modelling. In addition, the following technical developments will be implemented: fine-point cross-sections with interpolation; better unresolved resonance representations; delayed neutron treatment; enhanced thermal scattering; improved temperature capability; coupled and fully integrated $n/\gamma/e^{\pm}$ physics.

5. Conclusion

This paper has reviewed the current status of the uniquely commercial Monte Carlo codes MONK and MCBEND. Recent developments have been highlighted and on-going programmes outlined, all aimed firmly at meeting the diverse current and future needs of our customers. By focussing on issues as identified by our customers around the world and developing the products accordingly, we continue to strive to maintain the codes' leading edge position and develop the staff required to achieve this.

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