CURRENT STATUS AND FUTURE DIRECTION OF THE MONK SOFTWARE PACKAGE

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This paper provides a view of the MONK criticality software package in terms of recent and current developments and future plans aimed at meeting the short and long-term needs of the code user community.

KEYWORDS: MONK, Codes, Software Development, Validation

1. Introduction

This paper describes the main recent and on-going developments to the MONK package and outlines the proposed development programme for the next five years. This programme comprises a mixture of the continuation and further evolution of some current activities, a selection of well-understood new activities and more general broad directions to be filled out by specific activities as we move forward.

The Monte Carlo code MONK is a well-established criticality tool with a proven track record of application covering the whole of the nuclear fuel cycle. The development of MONK is performed and managed within NCD (Nuclear Codes Development), a collaborative arrangement between Serco Assurance (as part of its ANSWERS Software Service) and British Nuclear Group Sellafield Ltd (BNGSL).

The MONK package comprises not only the Monte Carlo code itself but also nuclear data libraries, validation data, documentation, geometry model visualisation tools, productivity tools of various kinds and user support services. In identifying the development direction for the package, input is obtained not only from the two collaborating partners but also from others customers of the ANSWERS Software Service. Indeed such input is actively sought such that a programme is defined that meets industry application needs. The development programme also seeks to maintain a balance between short-term and longer-term requirements and small and larger developments. An example of how this is managed is the system of Long-Term Technical Requirements that has been established by NCD to ensure more substantial and longer-term developments are sufficiently well represented in the programme.

The current production version of MONK is version 9A, issued in September 2006. MONK version 9A was a major upgrade to the MONK code, incorporating the new BINGO continuous energy nuclear data library and collision processing package.

2. Recent and On-going Developments

The recent and current developments cover a range of areas of activity and are presented below under the following seven headings: Physics Modelling, Geometry Modelling, Source Convergence, Nuclear Data, Validation, Supporting Tools and Customer Services.

2.1 Physics Modelling

For many years, MONK has used a module called DICE for its nuclear collision processing, together with DICE format nuclear data libraries. These libraries derive their data from various sources (UKNDL, JEF2.2, ENDF/B-VI, JENDL3.2) and store the nuclide cross-sections on a fixed hyperfine energy grid of 13,193 groups. This collision package is also available in the ANSWERS general transport code MCBEND1.

The new collision processing package in MONK is called BINGO2, and together with its nuclear data library provides cross sections tabulated at optimal energy points for each nuclide; improved variable temperature treatment; enhanced thermal scattering modelling; better representation of ENDF correlated energy/angle laws; and more detailed representation of the off-peak parts of the fission spectrum. In practice each nuclide has its own data file, and the data is stored in the most efficient manner to best represent the energy dependency of the cross-sections for that nuclide.

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

In addition, there was a need to update the collision processing package in line with modern programming techniques, and the development of the BINGO package has enabled us to do this.

2.2 Geometry Modelling

2.2.1 Fractal Geometry

The MONK geometry modelling package comprises two complementary components: Fractal Geometry (FG), employing conventional 'ray tracing' algorithms through defined geometrical bodies, and Hole Geometry (HG), using the powerful and versatile Woodcock Tracking.

MONK has a particularly rich set of ray tracing options, with a large selection of body shapes and a number of combination options linked to application requirements. New developments available in version 9A include: the Window Part, the Overlap Part, enhanced rotation options, and relative body origins.

A MONK geometry model is constructed as a geometry hierarchy, with small components being combined to form larger items, and these larger items being themselves combined, and so on. At present, the hierarchical relationship demands that the outer shape of a combined set of items itself matches one of the MONK body shapes. For the Window Part this restriction is removed, providing yet more flexibility of construction for the MONK modeller.

The Overlap Part provides the freedom of a combinatorial geometry input, but the order of input defines the hierarchy and thus a degree of input checking.

The rotation options allow bodies to be rotated about their centre, their body origin, or some arbitrary point in space – for example the centre of a transport flask when modelling the fins on its surface.

The relative body origins allow sections of the model within a part to be linked, so that moving one of the bodies will move all the components related to it, saving the effort of recalculating all the origins.

2.2.2 Hole Geometry

The Woodcock tracking algorithm in MONK is a powerful adjunct to the conventional body modelling provided by Fractal Geometry. Implemented via the Hole Geometry package, Woodcock tracking brings significant additional modelling power to the user, as well as providing convenient short-cuts to common modelling situations.

The Hole Geometry package continues to grow as additional hole types are added in response to industrial needs. Recent developments have been new hole types to model both the arrangement of pebbles in a Pebble Bed Modular Reactor (PBMR) and 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. This method has enabled MONK to be used to validate deterministic methods of PBMR fuel design and burnup.

Other 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 model easily complex arrangements of pipes and their joints; the Random-Rods Hole to model the arrangement of cylindrical rods in a container – this is now being used to verify modelling assumptions made prior to the availability of this option (see Figure 1 and Table 1). Table 1 shows the results from modelling a system of rods in four different ways: explicitly using an FG CLUSTER PART; using the new RANDROD hole; using the typical smeared model. For this system, the results show good agreement between the explicit model and the RANDROD hole, whereas the smeared model shows a significant difference. The run times are also significant, with the RANDROD hole running in half the time of the explicit model and requiring much less user effort to set up.

A capability has been developed that enables CAD generated tetrahedral mesh geometries to be imported into MONK and treated as a hole geometry. Comparison of such models with explicitly modelled input has so far shown excellent agreement.

A further development has been the ability to use named holes and named materials in holes rather than the old numbering scheme. This is the same as is available in the Fractal Geometry package and now enables users to specify all their geometry using named components, thus simplifying data banking of sections or all of a model.

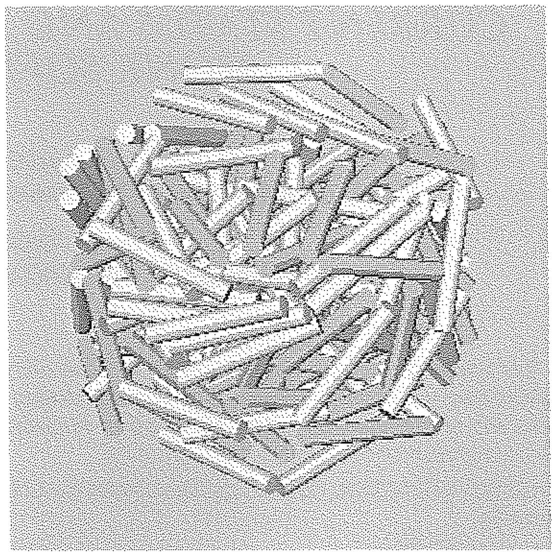

Fig. 1 VISTA image of the new Random Rods hole

Table 1 Results using the Random Rods hole

MONK Model	K-effective	s	CPU (s)
CLUSTER PART	0.8407	0.0010	10266
RANDROD HOLE	0.8401	0.0010	4949
SMEARED Model	1.4380	0.0010	148

2.3 Source Convergence

MONK employs its own Superhistory Powering method for managing the convergence of the fission source, forcing samples through a number of fissions before considering its use in a subsequent stage. This has proved its reliability and robustness in a number of difficult applications, but still requires the user to estimate the number of settling stages (discarded generations) prior to starting the calculation.

There is now in version 9A of MONK an Automatic Settling option that monitors the progress of the calculation and determines when the source has converged. Tests on a number of poorly converging systems3 have proved encouraging.

2.4 Nuclear Data

The development of the BINGO nuclear data library provides a significant benefit to the user in terms of increased accuracy of the results. This is due to the better representation of the data stored in the BINGO library. At present we only have a library based on JEF2.2 evaluated data, but there are plans to produce separate BINGO libraries based on JEFF3.1 and ENDF/B-VII data in the near future.

MONK will continue to be able to access the DICE nuclear data libraries, and those issued with MONK version 9A are based on the UKNDL, JEF2.2, ENDF/B-VI and JENDL3.2 evaluated data. These libraries have matching contents and contain over 160 isotopes.

To simplify the user input for all these libraries the input for material compositions has been made independent of the library used – a database maps the users material compositions onto the selected library, thus a simple menu selection from the MONK LaunchPad user environment (see Section 2.6) will enable the same calculation to be run with a different nuclear data library.

2.5 Validation

Validation remains an issue at the heart of criticality code usage. Comparison with experimental results is the only method of checking that new methods and new nuclear data libraries can accurately model complex geometrical structures comprising a range of materials.

MONK already has a well-developed validation database that supports its use in practical applications. Many hundreds of experimental configuration descriptions have been taken from the handbook of the International Criticality Safety Benchmark Evaluation Project (ICSBEP4) and quality-assured MONK models produced. These models are then computed using the range of nuclear data libraries currently available and the results reported via extensions to the MONK User Manual.

This validation database has new evaluations added to it annually, with requests from the user community being used to determine what experiments to study. In addition we have in place a programme to validate the BINGO library at elevated temperatures.

2.6 Supporting Tools

The Monte Carlo code itself is clearly the main component of the MONK package, however additional tools are provided and routinely used. These tools cover geometry model visualisation and verification (VISAGE, VISTA and Visual Workshop) and calculation parameter control and job submission (LaunchPad and CODEMORE).

VISAGE and VISTA have been used for many years to display MONK model geometries, and while support will continue, we are no longer actively developing these products. All development effort is now targeted at Visual Workshop (the current working title), which combines the functionality of all the above tools into a single package. Thus Visual Workshop provides real-time interactive model generation and intuitive manipulation in both 2D and 3D using the same tracking package that is used in MONK – hence the user sees what MONK will track through. The user interface has been made simple to use and this intuitive interface makes it easy for the first time user, as well as the expert, to generate and manipulate the images. Zooming, rotating, ghosting and other image controls are achieved with great simplicity through simple mouse movement and can be learned in minutes. This is a major enhancement over the VISTA method of typing in model coordinates.

The package also includes the LaunchPad job submission capability, and a Case Viewer, the latter to enable a user to view or edit all the input and output files associated with a project.

The development of a CAD tetrahedral-mesh input capability for MONK has resulted in the need for the graphics package to render the model MONK will be tracking through. Hence Visual Workshop will include the capability to display such input data.

An example of a Visual Workshop image is given in Figure 2. This image shows a transport flask with the external structure 'ghosted' so the inside of the flask can be seen, and two cutaways to show more clearly the elements within the flask. This is generated in real-time using the tracking routines built into MONK and can be easily manipulated by the user to view the detail of the model.

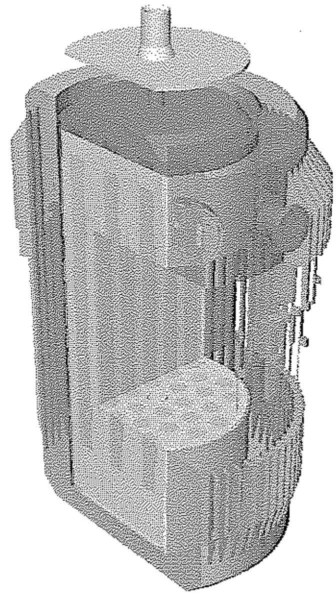

Fig.2 Example image of a transport flask

The CODEMORE package has been produced to automatically distribute a parameterised suite of calculations across a network of computers. This development has been useful for scoping calculations, where many thousands of calculations have been performed by making best use of a large network, with the power of the individual nodes and their loading being used to control job execution.

2.7 Customer Services

The ANSWERS Software Service has now been in existence for over twenty years, with the service starting in 1984 and MONK being incorporated in 1987. During that time, the service has continued to evolve and develop to meet the expectations of its customers as their needs have changed and new requirements emerge.

The service includes:

- The use of the internet for the distribution of software and documentation, including the development of a password-protected customer area;
- A commercial standard software licensing system, for increased flexibility and ease of use;
- A commercial help-desk system, to enhance the tracking and reporting of customer enquiries, and to make available customer and code-specific historical data to help-desk staff to improve the delivery of the service at the point of delivery;
- Support for PC Windows, Linux, and various Unix workstations, 64-bit machines and grid computing systems.

The business world and nuclear community continues to change at a rapid rate, and the ANSWERS Software Service recognises that it will need to maintain close contacts with all concerned to provide codes and services that match the needs and expectations of industry.

3. Future Plans

3.1 Formulation of the Development Programme

The development programme for MONK is formed from a number of inputs. As collaborators in the development, Serco Assurance and BNGSL both contribute requirements. The development requirements are also derived from dis-

cussions with its customers, both via the hotline or at the annual ANSWERS Seminar held in the UK. These inputs are coupled with foresight regarding emerging generic needs or issues. BNGSL's input is focused on meeting the present and future needs of its myriad industrial activities, both in the UK and elsewhere. From these inputs, a programme is discussed, reviewed, agreed and then implemented. In addition, some flexibility is retained in the programme to cope with urgent issues that need to be accommodated.

The Long-Term Technical Requirements (LTTRs). were set up to encourage members of the partner organisations to propose and champion longer-term ideas concerning the direction of development. This was to ensure that large developments or significant outcomes were not neglected because they could not be developed quickly. Examples of projects that originated in the LTTRs include CODEMORE, Visual Workshop and the Grid Computing developments.

3.2 Development Plans

The development of MONK is based upon a short term development plan and a five-year development plan. Included in these plans are:

- *The integration of a Monte-Carlo based perturbation code (MAX5) to simplify the study of small or large changes to the system;*
- *The integration of a Method of Characteristics solution (CACTUS-3D6) for MONK;*
- *Further evolution of the Fractal Geometry modelling capabilities, to reflect the changing industry needs (e.g. new fuel designs, waste optimisation);*
- *Additional Hole Geometries to support emerging problems or to verify modelling assumptions;*
- *Extensions to the validation database, including elevated temperature validation;*
- *Additional BINGO nuclear data libraries based on alternative evaluations;*
- *Extensions to the input processor for MONK to enable greater input control through parameters, looping, formulae, if...endif, and embedded files;*
- *On-going improvements to the established supporting tools and the development of new tools, in particular improved graphical representation of geometry models and output, improved input capability, enhanced use of grid/networked computer systems and enhanced geometry input from CAD files;*
- *On-going study of genetic algorithms and grid-computing methods for goal-seeking with MONK;*
- *Further extension and refinement to the ANSWERS Software Service itself.*

Uncertainty analysis remains an important consideration for criticality assessment and sensitivity methods have a potentially important role to play. MONK contains an option that enables the code to calculate the first-order sensitivity of k-effective to uncertainties in cross-section values. These uncertainties can be for particular energy ranges, specific reactions, for specific nuclides in one or more materials. Material density sensitivities can be obtained by considering the whole energy range for each reaction and nuclide in a material. This option has already been used to good effect to investigate the sensitivity of calculated MONK result to uncertainties in the cross-sections of relatively unusual nuclides (i.e. ones not commonly featured in significant quantities in validation experiments).

The MAX capability will extend this sensitivity capability by using Monte-Carlo methods to calculate the change in k-effective for perturbations to any quantity within the MONK model.

Nuclear data will also remain at the forefront of the development programme. Within the UK, JEF2.2 has been adopted by a number of organisations as a 'standard' source of data for many applications (including criticality). However as developments in nuclear data are progressed, it is the intention that MONK will provide new capabilities as and when appropriate. The JEFF3 library is being assessed within the collaborating countries and MONK is being used as part of this activity. Libraries will be made available for MONK to evaluate the effect of these new evaluations. However, it is recognised that potential safety case update implications will determine major changes to something as fundamental as the standard MONK nuclear data library. Hence decisions on the adoption of additional standard libraries will be taken in consultation with those stakeholders most affected.

4. Conclusion

This paper has summarised the current status of the MONK code, recent and on-going developments, and planned developments for the future. MONK continues to be focused on meeting the current and future needs of its customers, and the programme is assembled from such stakeholder input. In addition, we look for new requirements emerging over the coming years that do not yet feature in the programme, and it is intended that sufficient flexibility will be retained in the planning and implementation processes that new items can be agreed and accommodated as appropriate.

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