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 four 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 BNFL.

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 welcomed and actively sought such that a balanced programme is defined, and one 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 MONK8B, issued in December 2001. MONK8B was a relatively minor upgrade to the major new version MONK8A, the latter release bringing the major enhancement of combining the previously separate criticality and reactor physics variants of the code. Since the completion of MONK8B, development of the package has continued aimed at the next major version, in line with the forward programme assembled as outlined above.

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 exist 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. The neutron collision processing comprises a continuous energy and angle treatment of the neutron/nucleus interactions.

The DICE module has served the MONK code well for many years (and is also used in the ANSWERS general transport code MCBEND[1)]) and has proven itself to be reliable and robust in practical industry application. However, as part of a wide programme of regeneration and renewal, a replacement module (internal name BINGO) has been under development. The aims of BINGO have been threefold:

- to further improve the underlying physical realism available in MONK for both criticality and reactor physics applications;
- to develop and document a modern package in keeping with modern software language capabilities;
- to provide a major development programme that would facilitate the development of key skills in the younger generation.

The major physical realism benefits realised to date include: finer cross-section representation for key

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nuclides; 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.

The BINGO module in MONK is now undergoing field testing in readiness for its formal release. Further details can be found in a companion paper presented at this conference.[2)]

2.2 Geometry Modelling

2.2.1 Fractal Geometry

The MONK geometry modelling package comprises two complementary components: Fractal Geometry, employing conventional 'ray tracing' algorithms through defined geometrical bodies, and Hole Geometry, 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. A further development has now been implemented however, that of the Window Part.

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.

As an example of the additional capability provided, the new Window Part has proven itself to be helpful in simplifying models of transport flasks and storage containers subject to internal local variations due to potential damage caused by impact.

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.

Over the years, additional hole types have been added to MONK in response to particular industrial needs and this will continue as new requirements emerge. A recent development has been a new hole type to model Pebble Bed Modular Reactor (PBMR) type fuel. This is a complex problem, given the quasi-random nature of the fuel distribution but is one well matched to the Woodcock algorithm. This method has enabled MONK to be used to validate deterministic methods of PBMR fuel design and burnup.

Another development has been to add a so-called User Hole to the set of available options. Rather than provide a particular generic geometry type, the User Hole provides a means by which a MONK user can effectively provide a geometrical definition of a new hole type. The input is in terms of simple mathematical functions - the output is a custom-build geometrical option for your particular need. Example applications to date include multiple interlocking spiral ducts (See Figure 1), innovative fuel element grid designs and irregular waste packing configurations.

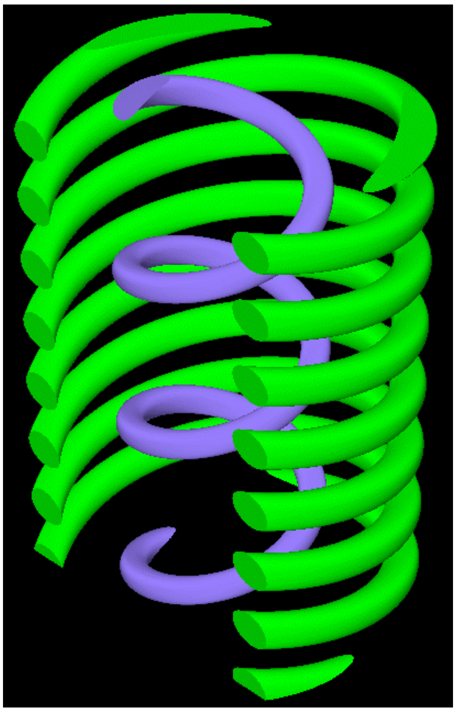

Fig.1 Example of the new hole option to produce concentric coiled ventilation ducts

2.3 Source Convergence

MONK uses its indigenous Superhistory Powering method for managing the convergence of the fission source. This has stood the test of time well and has proven its reliability and robustness in a number of difficult applications.

There is current renewed interest in source convergence issues with an OECD Expert Group[3)] being established to investigate and compare methods, their strengths and limitations.

MONK has been used as part of this exercise and in parallel, further developments are in progress for the code. The main new MONK developments so far have been initiated with two objectives in mind:

- to introduce automation into the selection of the number of discounted neutron generations at the start of calculation (i.e. where the source is transformed from the initial estimate to a fit-for-purpose approximation of the real distribution);
- to introduce additional monitoring and

reporting so that should source convergence issues be suspected, the user is alerted in an easy to understand manner.

The results to date have been encouraging, with the outcomes scheduled for the next release of MONK.

2.4 Nuclear Data

Part of the philosophy of the MONK package has been to provide the user community with choices. The underlying nuclear data used by the code is ultimately the determinant of the accuracy that is achieved. The representation of the data for use within the code and the associated nuclear collision models clearly also impact the accuracy to a significant extent (and this is being enhanced via the BINGO development described above), but the basic sources of nuclear data ultimately drive the accuracy.

In recognition of this, it has been the policy for some time to provide alternative nuclear data libraries from established sources, so that inter-comparisons can be readily performed. These inter-comparisons can be used to provide additional confidence in certain application areas or can be used to investigate uncertainties due to nuclear data. By keeping the underlying energy structure and collision processing system identical (the DICE module and library as described above), the inter-comparison available with MONK is a true test of underlying data library differences.

The MONK code is currently issued with four continuous energy/angle libraries, based on the following original sources: UKNDL, JEF2.2, ENDF/B-VI and JENDL3.2. The libraries have matching contents, currently containing over 160 isotopes.

To facilitate inter-comparisons, the MONK input for material compositions has been made independent of the library used. Hence, 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. Whilst improvements to the efficiency of the methods coupled with the seemingly never-ending computer hardware enhancements enable us to calculate ever more precisely, the real concern remains accuracy, and to test accuracy requires validation.

MONK has a well-developed and evolving 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 (ICSBEP[4)]) 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.

Requests for additions the MONK validation database are received from the user community and this drives the prioritisation of the database expansion. In addition, an annually-updated summary document is produced bringing together the extant validation results and drawing broad conclusions with regard to accuracy for particular application types.

2.6 Supporting Tools

Whilst the Monte Carlo code itself is clearly the front line calculation component of the MONK package, additional tools are also routinely used. These tools cover geometry model visualisation and verification (VISAGE and VISTA) and calculation parameter control and job submission (LaunchPad).

VISAGE and VISTA are mature codes in their own right and development has continued to meet additional customer requirements. The most recent developments have been focussed on improved three-dimensional images via enhanced shading algorithms, new transparent filter options and the ability to overlay a display of source regions. An example of a VISTA image is shown below.

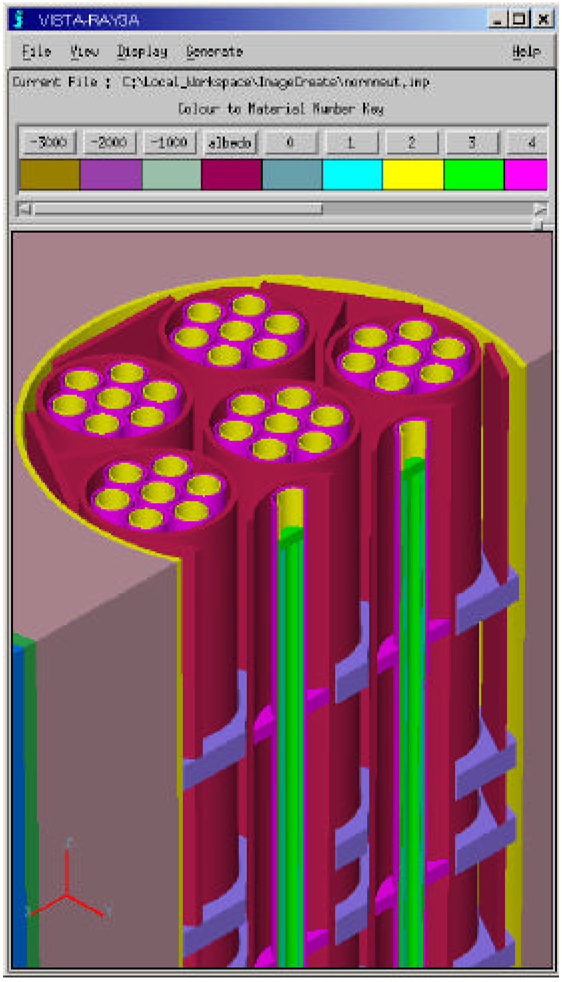

Fig.2 Example of a VISTA image of a transport flask

LaunchPad is a relatively new addition to the MONK package and provides a convenient tool to check, visualise and edit an input file, select major options (e.g. nuclear data library) and launch and monitor the progress of sets of MONK calculations. Further development of the LaunchPad concept is now planned.

Another new development, CODEMORE, has been produced to optimise the use of MONK on a network of computers. This development has been particularly helpful for scoping calculations, where tens of thousands of calculations have been performed by making best use of a large network, taking due note of the power of the individual nodes of the network and their loading, and bringing together the results in a convenient form.

2.7 Customer Services

The ANSWERS Software Service has now been in existence for almost 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.

Recent changes to the service have included:

- Increased use of the internet for distribution of software and documentation, including the development of a password-protected customer area;
- Adoption of a commercial standard software licensing system, for increased flexibility and ease of use;
- Adoption of a commercial help-desk system, to enhance the tracking and reporting of customer enquiries, and to make available to help-desk staff customer and code-specific historical data to improve the delivery of the service at the point of delivery;
- Extension of the standard system platforms supported to cover PC Windows and Linux, in addition to various Unix workstations.

The business world continues to change at a rapid rate and by maintaining close relationships with its customers, the ANSWERS Software Service will continue to strive 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 BNFL both contribute requirements. Serco Assurance's requirements are derived from discussions with its customers, coupled with foresight regarding emerging generic needs or issues. BNFL's input is focussed 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.

A recent change to the formulation of the programme has been the setting up of a system of Long-Term Technical Requirements (LTTRs). A review of recent activities led to the conclusion that by the very nature of current application needs, the MONK development programme would tend to have a relatively short-term focus. The system of LTTRs was set up to encourage members of the partner organisations to propose and champion longer-term ideas concerning the direction of development. Each LTTR may be an individual development (but by definition, one that would take significant resources to achieve) or just a particular desired outcome, that may take one or more complementary developments to reach. The champion of each LTTR is then responsible for overseeing the item as it progresses, inputting requirements as appropriate and ensuring that the desired outcome is obtained. Although a relatively new process, the LTTR system has already produced a broader focus to the overall development programme and led to more widely supported generic development themes.

3.2 Development Plans

Section 2 of this paper described both recent and on-going developments for MONK and the development of the code package over the next four years is envisaged to include further work on some of those items already discussed:

- Completion of the BINGO module and its validation, followed by its release to customers as part of a new version of the MONK package (MONK9);
- Further evolution of the geometry modelling capabilities, to reflect the changing industry needs (e.g. new fuel designs, waste optimisation);
- Finalisation of the source convergence developments into a fit-for-purpose algorithm, backed up by clear supporting guidance;
- Additional nuclear data libraries, in response to developments in that area. For example, a MONK library incorporating some JEFF3 evaluations has already been produced for testing purposes;
- Extensions to the validation database;
- Improvements to the established supporting tools and the development of new tools;
- Further extension and refinement to the ANSWERS Software Service itself.

In addition, new items have been outlined and work has commenced in certain areas.

A new supporting utility ModelBuilder is in production. ModelBuilder is a fully interactive MONK model construction tool, with real time visualisation and checking. The new tool will not only be used to construct new models, but advantage will be taken of the MONK input structure to facilitate the use and re-use of the large investment in existing models. An example of the ModelBuilder prototype user image is shown below:

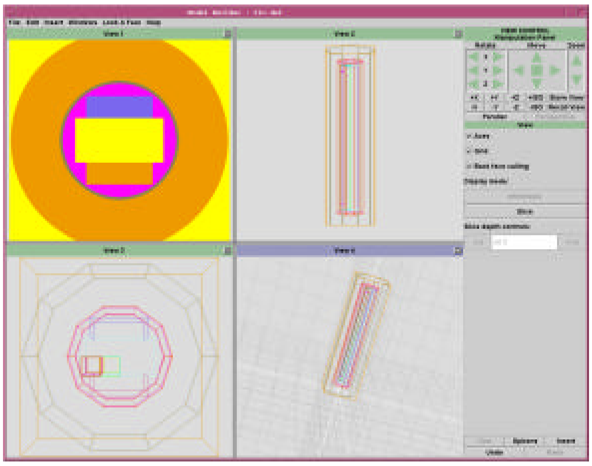

Fig.3 Example of a prototype ModelBuilder screen

Another development that has recently commenced is the Integrated Scoping Tool. As mentioned earlier, the use of MONK for system scoping purposes on a network of computers has recently been facilitated by the use of the package CODEMORE. For use of the code on a single machine, large-scale scoping studies can be overly time-consuming. Prototype developments have already commenced aimed at integrating a deterministic flux solution algorithm from the WIMS[5)] code with the MONK geometry package, thereby providing a 'single model-multiple solution method' capability. This will provide the user of MONK with the option of a rapid deterministic tool for scoping and survey purposes, but one that retains the same geometry description used by the definitive Monte Carlo calculation.

Uncertainty analysis remains an important consideration for criticality assessment and sensitivity methods have a potentially important role to play. MONK8B contains an option that enables the code to calculate the 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). Further extension of this option is envisaged, by inclusion of a geometrical sensitivity option (similar to that used in MCBEND) and by the development of an uncertainty module, which would automatically combine sensitivities and cross-section uncertainties to yield total k-effective uncertainties.

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). For MONK, we have also made available other libraries, both to represent the interests of other customers and to provide the useful cross-check capability described above.

As developments in nuclear data are progressed, it is the intention that MONK will provide new capabilities as and when appropriate. The JEFF project continues to move forward and a provisional version of the JEFF3 library is being assessed within the collaborating countries. MONK is being used as part of this activity. Libraries for MONK to evaluate for criticality purposes the major changes to this (and other) libraries will continue to be produced as part of our development activities. However, it is recognised that, due to the potential safety case update implications, major changes to something as fundamental as the standard MONK nuclear data library should appear only at relatively infrequent intervals, unless major errors or limitations are uncovered. 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, outlining recent and on-going developments and envisaged directions for the future. MONK continues to be focussed on meeting the current and future needs of its customers and the programme is assembled from such stakeholder input. In addition, we look forward to new requirements emerging over the coming years that do not yet feature in the envisaged programme, and it is intended that sufficient flexibility will be retained in the planning and implementation processes such that these items can be agreed and accommodated as appropriate.

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