Use of a Hybrid Monte Carlo Technique for Power Shape Calculations

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Abstract

There are many modelling situations in nuclear power reactors where a full three-dimensional solution of the transport equation would be of benefit. For example, in UK gas reactors there are significant three-dimensional effects associated with axial gaps in the fuel element, which cause significant perturbations to the flux and hence power. Other reactors also exhibit 3D effects, for example grids, partially inserted control rods and axial reflectors. To date these effects have been evaluated by approximate synthesis methods. There is a further requirement to accurately predict the effect of perturbations to parameters such as temperature and material density, an area where conventional Monte Carlo methods can be inefficient. Recent work has led to the development of an accurate and efficient 3D method, based on a hybrid Monte Carlo approach, to model the three-dimensional situations and provide accurate estimates of perturbed states. This paper outlines the approaches used for this method and demonstrates its application to practical situations.

1. Background

The WIMS [1] code suite has been established as a world-standard reactor physics package for more than thirty years. During that time, WIMS has been successfully applied to solve practical problems associated with a wide range of commercial power reactors and experimental and test facilities. The latest version of the code is WIMS8, which provides established calculation routes for LWR, heavy water moderated and gas cooled reactors. A range of solution methods exists, including diffusion theory, discrete ordinates, collision probabilities, characteristics and Monte Carlo.

WIMS also has an option that allows users to employ a hybrid Monte Carlo method to solve three-dimensional problems. This option has efficiency gains over conventional Monte Carlo approaches and accuracy benefits when compared with traditional reactor physics deterministic methods. This paper summarises the hybrid method and provides examples of its application to solve practical problems.

2. The Hybrid Monte Carlo Method MAX

2.1 Overview

MAX is a module of the WIMS reactor physics suite that solves the multigroup neutron transport equations by a hybrid deterministic/Monte Carlo method based on exact perturbation theory. The calculation consists of a series of perturbations from a simple homogeneous geometry, each one being an incremental approach to the three-dimensional final model. The simple model is calculated (deterministically) using one of the other WIMS modules. This is then augmented by a series of Monte Carlo calculations for the perturbed flux and eigenvalue,

as each perturbation to the simple model is performed. Thus the final perturbed flux solution is obtained from a hybrid of the deterministic and Monte Carlo fluxes.

2.2 Outline of MAX Theory

Using operator notation, the time independent Boltzmann Equation can be written as:

$$(\tilde{\mathrm{T}} - \tilde{\mathrm{S}} - l\,\tilde{\mathrm{F}})\, f = 0$$

where the transport, scatter and fission yield operators are defined as:

$$\tilde{T}\, f(r, E, \Omega) = \Omega \cdot \nabla f(r, E, \Omega) + \Sigma_{\mathrm{T}}(r, E) f(r, E, \Omega)$$

$$\tilde{S}\, f(r, E, \Omega) = \int \Sigma_S(r, \mathrm{E}' \to \mathrm{E}, \Omega' \to \Omega) f(\mathrm{r}, \mathrm{E}', \Omega')\mathrm{dE}'\,\mathrm{d}\Omega'$$

$$\tilde{\mathrm{F}}\,\phi(\mathrm{r}, \mathrm{E}, \Omega) = \chi(\mathrm{E}) \int \nu\Sigma_{\mathrm{f}}(\mathrm{r}, \mathrm{E}')\phi(\mathrm{r}, \mathrm{E}', \Omega')\mathrm{dE}'\,\mathrm{d}\Omega'$$

Now consider the unperturbed problem and let suffix 0 denote the operators and solution:

$$\left(\tilde{\mathrm{T}}_0 - \tilde{\mathrm{S}}_0 - \lambda_0 \tilde{\mathrm{F}}_0\right)\phi_0 = 0$$

Now let this problem be perturbed with operators perturbed by the change in the cross sections between the problems as follows:

$$\tilde{T} = \tilde{T}_0 + \Delta\tilde{\mathrm{T}}, \qquad \tilde{\mathrm{S}} = \tilde{\mathrm{S}}_0 + \Delta\tilde{S}, \qquad \tilde{\mathrm{F}} = \tilde{F}_0 + \Delta\tilde{F}$$

The angular flux and eigenvalue will change due to the change in the operators:

$$f = f_0 + \Delta f, \qquad l = l_0 + \Delta l$$

and hence we have, for the change in the angular flux:

$$(\tilde{\mathrm{T}} - \tilde{\mathrm{S}} - \lambda\tilde{\mathrm{F}})\ (\phi_0 + \Delta\phi)\ = 0$$

Taking the initial angular flux to the right hand side, expanding the operators and eigenvalue in terms of the initial solution and remembering that the unperturbed problem satisfies the 'suffix 0' equation gives:

$$(\tilde{\mathrm{T}} - \tilde{\mathrm{S}} - \lambda\tilde{\mathrm{F}})\,\Delta\phi = \left(\lambda_0\Delta\tilde{\mathrm{F}} + \Delta\tilde{\mathrm{S}} - \Delta\tilde{\mathrm{T}}\right)\phi_0 + \Delta\lambda\tilde{\mathrm{F}}\phi_0 \qquad \ldots\ldots \text{(Equation 1)}$$

The change in the eigenvalue may be estimated by considering the adjoint equation. Multiplying by the adjoint flux and integrating over all space, angles and energy ranges, expanding the left hand side and re-arranging gives:

$$\int f_0^* \left(\tilde{\mathrm{T}}_0 - \tilde{\mathrm{S}}_0 - l_0\tilde{\mathrm{F}}_0\right)\Delta f\, dV dE d\Omega =$$

$$\int f_0^* \left(l_0\Delta\tilde{F} + \Delta\tilde{\mathrm{S}} - \Delta\tilde{\mathrm{T}}\right)(f_0 + \Delta f)\,\mathrm{dVdEd}\Omega + \Delta l \int f_0^* \tilde{F}\,(f_0 + \Delta f)\,\mathrm{dVdEd}\,\Omega$$

By virtue of the adjoint solution, the left hand side is zero, thereby defining the change in the eigenvalue. Using this, equation (1) can then be written:

$$(\tilde{T}-\tilde{S}-\lambda\tilde{F})\Delta\psi = (\lambda_0\Delta\tilde{F}+\Delta\tilde{S}-\Delta\tilde{T})\psi_0 + \frac{\int \psi_0^* (\Delta\tilde{T}-\Delta\tilde{S}-\lambda_0\Delta\tilde{F})\psi dV dE d\Omega}{\int \psi_0^* \tilde{F}\psi dV dE d\Omega}\tilde{F}\psi_0$$

2.3 Implementation Overview

During the development of the MAX method, several implementation issues were successfully addressed. The following sections discuss some of these issues.

Source Particles

The final equation from the above MAX theoretical section can be thought of as a fixed source equation with the source term defined by the right hand side. The source expression depends on the values of the perturbation operators, which in turn depend on the geometry of the perturbed problem. The source will also depend on the unperturbed flux, which can be any analytic function of space, energy and angle, and the eigenvalue. However, the current implementation of MAX assumes that the unperturbed case is a homogeneous cell with reflective boundary conditions.

The above source term will thus be an analytic function that is continuous in zones which have the same materials, with discontinuities at material boundaries. Also the source will have zones in space and energy where the value is negative as well as zones where it is positive (the operators in the source contain differences between the material cross sections). This approach leads to the concept of a negative weight particle tracking through space as well as the conventional positive weight particles. Both types of particles are tracked in the normal way, but throughout the tracking these particles can annihilate each other.

Sequences of Perturbations

It is possible using the MAX technique to break the complexity of realistic perturbations into several incremental stages. This improves both the efficiency of the calculation and the analysis and hence understanding of the problem. For example (which is discussed below), an AGR (Advanced Gas Reactor, a UK graphite moderated reactor design) lattice cell calculation can be generated from a homogeneous calculation in three or more stages:

- Separate the fuel zone into a 36 pin cluster and introduce voids into the moderator zone;
- Introduce axial variation in the fuel due to the presence of end gaps, aluminium pellets and fuel end caps;
- Introduce burnable poison toroids.

Each of these changes can be represented by a perturbation to the immediate lower level of complexity. In this way, the effect of each perturbation can be assessed separately. In addition, the uncertainties associated with each change can be separately controlled be optimising the Monte Carlo sampling for each perturbation individually.

Treatment of Absorbers

The source term for a perturbation that involves the introduction of a material with high absorption (e.g. gadolinium) can be very significant due to the change in the transport operator. This will lead to a markedly higher weight for neutrons tracked from the perturbation source, due to neutrons being started in all zones of the absorber; in fact, many of these particles have a

negligible probability of escape from the absorber. The MAX implementation avoids this potential inefficiency by tracking source neutrons from a boundary enclosing the absorber.

3. Application of MAX

3.1 Comparison with MONK Calculations

The MAX method has been recently used to calculate reactivity and power profiles for a 3D model of a poisoned AGR fuel element. In particular the method has been applied to AGR problems with axial gaps in the fuel and toroids of burnable poisons. The geometry is an idealised AGR fuel element, with reflective boundaries at the mid-point of the fuel and the mid-point in the gap between fuel elements. Comparison calculations have been performed with MONK [2]. The relative power results from the MAX and MONK calculations are shown in Table 1, with efficiency comparisons given in Table 2.

These results show excellent agreement between MAX and MONK, with the fine power structure results (the two pellets at each end of the element) consistent within two standard deviations in all cases. In terms of efficiency, there is a general increase of at least an order of magnitude for the end of pin locations. For the results in the centre of the fuel, the efficiency gain is smaller due to the better sampling possible from a 'standard' Monte Carlo calculation.

Table 1 – Comparison of MAX and MONK for AGR Relative Power

	Inner Ring (MAX-MONK)		Middle Ring (MAX-MONK)		Outer Ring (MAX-MONK)	
Position	Difference	St Dev	Difference	St Dev	Difference	St Dev
Bottom pellet	-1.21	1.79	0.62	1.10	1.42	1.19
2nd bottom pellet	2.35	1.39	1.83	1.03	1.75	1.04
Mid-element pellet	0.13	0.06	0.15	0.04	0.32	0.05
2nd top pellet	-0.65	1.63	-0.26	1.22	0.65	0.75
Top pellet	0.30	2.34	1.51	1.55	0.66	1.00

Table 2 – Comparison of MAX and MONK Calculation Times for AGR Relative Power

Position	MONK/MAX time ratio	MONK/MAX time ratio	MONK/MAX time ratio
Bottom pellet	13.0	14.2	45.2
2nd bottom pellet	14.0	27.1	59.1
Mid-element pellet	1.8	1.4	2.0
2nd top pellet	12.9	22.4	19.9
Top pellet	21.8	27.2	29.0

3.2 Comparison with Experiment

As part of an on-going monitoring programme, a series of PIE (post irradiation examination) measurements have been carried out to examine the axial variation in power in an AGR fuel element. The measurements considered a range of fuel enrichment from 1.16w/o to 2.5 w/o; the irradiation at which measurements were taken varied from 0 to ~20GWd/Te. These situations have been calculated by WIMS using the MAX method. Table 3 shows the mean differences between experiment (E) and MAX calculations (C) for a range of enrichments and irradiations. In general the agreement with MAX is very good and shows that MAX reproduces the variation with both enrichment and irradiation.

Table 3 – Mean (C-E)/E % for AGR Stage 1 Fuel

	Irradiation (GWd/te)				
Position	0	5	10	15	20
End Fuel Pellets - Mean	0.87	0.65	2.04	1.50	1.01
Standard Deviation	*1.38*	*0.89*	*1.56*	*0.80*	*0.81*
Next-to-end Fuel Pellets - Mean	1.21	0.55	0.28	-0.07	-0.09
Standard Deviation	*1.17*	*0.65*	*1.17*	*0.71*	*0.92*
Overall Mean	0.94				
Standard Deviation	*0.68*				

4. Benefits of MAX Approach

The above sections have outlined the method and application of a hybrid Monte Carlo approach to solving three-dimensional reactor analysis problems. This technique fits into the gap that exists between deterministic methods and full Monte Carlo approaches. The major benefits of this hybrid approach are:

- The method allows for improved geometry modelling capabilities compared with those that are present in conventional deterministic methods. In principle, full Monte Carlo modelling is available for the perturbation calculations, such that geometrical approximations required by lattice codes can be removed.
- The calculation time is much reduced compared with a full Monte Carlo analysis. For the example used here, the improvement in calculation time is of the order of at least a factor of ten in favour of MAX when calculating fine power profiles or poison worth.
- The efficiency of the MAX calculation is related to the sequences of perturbations employed. To date, MAX has started from a homogeneous calculation, with incremental perturbations thereafter to produce the 3D model. It has been shown that the first step in the perturbation sequence (from one-dimensional model to cluster geometry) is the largest source of uncertainty in the calculation. Further work is now in progress aimed at removing this source of uncertainty by enabling the starting process to be a CACTUS model, the main characteristics deterministic solution method in WIMS.

5. Conclusions

Recent work has led to the development of an accurate and efficient 3D method in the WIMS reactor physics code suite, based on a hybrid Monte Carlo approach. This paper has outlined the approaches used for the method and demonstrated its application to practical situations, where agreement with full Monte Carlo calculations and experiment has shown to be good. The major benefits of this approach are improved modelling accuracy compared with deterministic methods and improved efficiency over full Monte Carlo approaches, particularly for the calculation of fine details such as power profiles. Work is now in progress to improve the efficiency of the approach further, which will also lead to an extension in the range of calculations that is possible.

References

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2. N R Smith et al, 'The Current Status and Future Plans for the Monte Carlo Codes MONK and MCBEND', Proceedings of MC 2000 (Lisbon, October 2000)