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Review

Optimization of multidimensional cross-section tables for few-group core calculations

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ABSTRACT

Multigroup diffusion codes for three dimensional LWR core analysis use as input data pre-generated homogenized few group cross sections and discontinuity factors for certain combinations of state variables, such as temperatures or densities.

The simplest way of compiling those data are tabulated libraries, where a grid covering the domain of state variables is defined and the homogenized cross sections are computed at the grid points. Then, during the core calculation, an interpolation algorithm is used to compute the cross sections from the table values. Since interpolation errors depend on the distance between the grid points, a determined refinement of the mesh is required to reach a target accuracy, which could lead to large data storage volume and a large number of lattice transport calculations.

In this paper, a simple and effective procedure to optimize the distribution of grid points for tabulated libraries is presented. Optimality is considered in the sense of building a non-uniform point distribution with the minimum number of grid points for each state variable satisfying a given target accuracy in k-effective.

The procedure consists of determining the sensitivity coefficients of k-effective to cross sections using perturbation theory; and estimating the interpolation errors committed with different mesh steps for each state variable. These results allow evaluating the influence of interpolation errors of each cross section on k-effective for any combination of state variables, and estimating the optimal distance between grid points.

Contents

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1. Introduction

Diffusion codes are the most extended option for three dimensional LWR core analyses. In order to obtain realistic solutions of the neutron diffusion equation, the required spatially homogenized and energy collapsed nuclear data should be representative of the actual local and spectral conditions of each region in the core. Those data are to be generated by a lattice transport code and its adequacy strongly influences the accuracy of the reactor core calculation, constituting an important aspect of the work in developing advanced neutronics methodologies.

One of the approaches proposed to develop the so called Next Generation Methods (NGM) for core design and analysis consists of embedding the node homogenization in the global core calculation (Ivanov et al., 2008; Zhang, 2008). The common key idea of NGM is that cross sections are computed on-the-fly, getting rid of pre-generated tables for a homogenized node. However, those combined methodologies are computationally too expensive, especially during coupled thermal-hydraulics/neutron-kinetics transient simulations, and further investigations should be conducted.

As a consequence, the more practical two-step approach is still extensively used nowadays: first, pre-generated homogenized few group cross sections for certain combinations of state variables are produced and compiled in data libraries; second, the global core calculation is performed using those libraries as input data. Basically, two types of data libraries can be found: multidimensional tables and parameterized libraries. Both of them have advantages and disadvantages, as explained in (Zimin and Semenov, 2005) and (Bokov, 2009), and their construction can have a large impact in the core neutronics simulations, as shown in (Ferroukhi et al., 2009) on PWR main steam line break transient analyses.

Parameterized libraries include more or less complex models of the cross sections dependencies on the state variables. Construction of accurate models can require long polynomials and may result in a loss of accuracy for certain parameter ranges, what constitute the main drawbacks of this type of libraries. However, parameterized libraries have important advantages, such us the significantly reduced size with respect to multidimensional tables or its additional flexibility to include corrections for spectral effects.

Multidimensional tabulated libraries are the most straightforward form of cross section compilation. A mesh covering the range of state variables must be defined and the cross sections are computed at the mesh points. Then, during the core calculation, an interpolation algorithm is used to compute the cross sections at any state from the values at the mesh points. The main advantage of this method is that cross section dependencies do not need to be approximated by functional forms, eliminating the effort of finding accurate polynomials. However, the main drawbacks are that tables can consider only relatively few state variables to keep the practicality of the library; and they would require a considerable number of mesh points in order to make negligible the uncertainties due to interpolation, which would result in relatively large data storage and in a high number of lattice transport calculations. In other words, the closer the mesh points are in a tabulated library, the higher the accuracy of the interpolation, but that goes against the practicality of the library. Consequently, there is a need of building an optimal mesh point distribution, which will depend on the required level of accuracy.

At present, both approaches are used inside core simulators. To list a few, CORETRAN (Eisenhart et al., 2000) usually employ parameterized libraries; while others like SIMULATE (Grandi, 2005), CRONOS (Lautard et al., 1990) or DYN3D (Grundmann et al., 2005) are prepared to use tabulated libraries for their calculations. This indicates that both methodologies are appropriate, in principle, for data libraries storage.

A method to build optimized meshes for parameterized libraries generation was presented by (Zimin and Semenov, 2005). Instead of using a regular Cartesian mesh for the cross section calculations, an algorithm based on quasi-random sequences of Sobol was used to adjust cross section dependencies to polynomial expressions via stepwise regression. An important ingredient in this work was the inclusion of the idea of optimality in terms of the error committed for each cross section evaluation which was "arbitrarily" set to 0.05%.

This paper suggests a method to optimize tabulated libraries. Optimality is considered in the sense of building a regular but non-uniform grid point distribution with the minimum number of points for each state variable satisfying a user given target accuracy in the computed k-effective.

In our case, where a table library is being constructed, a structured Cartesian mesh where the grid points are constrained to fall along grid lines that are parallel to the axis is preferred since interpolation algorithms are very simple compared to interpolation with other types of meshes, which would require a search of neighboring grid points to be used in the computation of each interpolated output value although could turn out to be more effective (Botes and Bokov, 2011). The procedure consists of determining the sensitivity coefficients of k-effective with respect to the cross sections. Adjoint flux calculation has been implemented in the multigroup diffusion code COBAYA3 (Herrero, 2012). The adjoint sensitivities allow evaluating the influence of interpolation errors of each cross section on k-effective for any combination of state variables; and estimating the optimal distance between grid points.

Basic methodology is explained in Section 2. In Section 3, the method is applied to construct an optimal mesh for PWR tables depending on coolant and fuel temperature, coolant density and boron concentration. Also the influence of some variables such as the fuel assembly type and burnup considered or the number of energy groups are analyzed. The code COBAYA3 is used to perform two dimensional fuel assembly diffusion calculations in order to check the accuracy of the generated tables. Finally, in Section 4 the main conclusions are summarized.

2. Methodology

2.1. Statement of the problem

When using tabulated libraries, one source of error in the employed cross sections comes from the interpolation procedure of the values from the mesh points. Interpolation errors can be reduced by refining the mesh, but at the cost of increasing time needed for lattice transport calculations and increasing the library storage size; or by increasing the interpolation polynomial complexity which also affects storage size and reconstruction time.

In reality, cross sections are not equally sensitive to changes of the different state variables all over the entire domain; and parameters of interest, such as k-effective, are not equally sensitive to changes of the different cross sections. Consequently, the mesh should be refined only when necessary, taking into consideration the physical behavior.

Let us consider D state variables, and define a D-dimensional Cartesian mesh over the state variables domain. Focusing on one variable ρ (that could be identified for example with the moderator density) defined in the interval $I := [a, b]$ and choosing a mesh $\{\rho_i\}_{i=1}^{N+1}, \rho_i \in [a, b]$ not necessarily uniform, where the macroscopic cross section values Σ are computed via $N + 1$ branch lattice calculations $\{\Sigma_i\}_{i=1}^{N+1}, \Sigma_i := \Sigma(\rho_i)$; one can approximate the cross section value at any point of the interval I by a polynomial $P(\rho)$ of order less than or equal to N: