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Progress toward Monte Carlo–thermal hydraulic coupling using low-order nonlinear diffusion acceleration methods

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ABSTRACT

A new approach for coupled Monte Carlo (MC) and thermal hydraulics (TH) simulations is proposed using low-order nonlinear diffusion acceleration methods. This approach uses new features such as coarse mesh finite difference diffusion (CMFD), multipole representation for fuel temperature feedback on microscopic cross sections, and support vector machine learning algorithms (SVM) for iterations between CMFD and TH equations. The multipole representation method showed small differences of about 0.3% root mean square (RMS) error in converged assembly source distribution compared to a conventional MC simulation with ACE data at the same temperature. This is within two standard deviations of the real uncertainty. Eigenvalue differences were on the order of 10 pcm. Support vector machine regression was performed on-the-fly during MC simulations. Regression results of macroscopic cross sections parametrized by coolant density and fuel temperature were successful and eliminated the need of partial derivative tables generated from lattice codes. All of these new tools were integrated together to perform MC–CMFD–TH–SVM iterations. Results showed that inner iterations between CMFD–TH–SVM are needed to obtain a stable solution.

1. Introduction

One of the many goals in reactor analysis is to predict accurate spatial power distributions. Currently, the industry standard is to perform simulations using nodal diffusion methods accelerated by nonlinear diffusion acceleration (NDA) methods such as coarse mesh finite difference (CMFD). These nodal methods rely on homogenized multigroup diffusion parameters (cross sections, discontinuity factors, etc.) generated from separate lattice calculations. During homogenization, all detailed information is lost and can only be recovered using reconstruction methods at the end of simulation. Thus, refinement in space and energy is not possible to achieve a more accurate solution. Nodal methods are commonly coupled to low-order thermal hydraulic (TH) methods to treat reactivity feedback through fuel temperature (Doppler), coolant density, etc. Commonly, a full nodal solution is generated, thermal hydraulic fields such as fuel temperature and coolant density are calculated, cross section interpolation is performed and the process repeats. This paper addresses coupling fuel temperature and coolant density fields to a higher order *continuous-energy* Monte Carlo solution.

Monte Carlo methods are attractive for reactor analysis because multigroup cross section generation is not required. These methods use point-wise in energy cross section data. In addition, geometry can be explicitly modeled using constructive solid geometry. This class of methods can provide accurate pin-wise power distributions because tallies can be scored on any size mesh given that enough neutron histories are simulated. Because individual neutrons are simulated to obtain results, these methods are notoriously slow. Also, the stochastic process of sampling probability distributions requires that statistical uncertainty be accumulated and reported. Monte Carlo methods are different in the fact that after a converged source is obtained, tallies for spatial power distributions are then collected.

In this paper, progress toward a different approach is investigated where thermal hydraulic fields are converged during the source convergence stage of Monte Carlo through a low-order CMFD operator. A new on-the-fly Doppler broadening technique called windowed multipole representation is used for fuel temperature feedback (Forget et al., 2014; Josey et al., 2014). Different acceleration methods are explored using machine learning techniques to determine how CMFD parameters depend on TH parameters.

For the analyses presented in this work, the OpenMC Monte Carlo code is used (Romano and Forget, 2013). Section 2 provides a background of how Monte Carlo methods are used for analyzing reactors. Section 3 discusses CMFD and its implementation into

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OpenMC. The thermal hydraulic model incorporated into the Monte Carlo code is presented in Section 4, and the coupling between neutronic and thermal hydraulic fields is described in Section 5. Finally, simulations performed and results are discussed in Sections 6 and 7, respectively.

2. Monte Carlo simulations for reactor analysis

Monte Carlo methods for reactor analysis are commonly referred to as eigenvalue or criticality simulations. These methods differ from fixed source analyses because the neutron source is unknown and depends on the whole system. Thus, eigenvalue simulations are separated into two parts: (1) inactive source iterations to converge the spatial distribution of the fission source, and (2) active source iterations where tallies are accumulated.

During inactive fission source generations, an initially assumed source is iterated on until it is converged analogous to power iteration. Neutrons are born from source sites contained in a finite source bank and simulated until they escape the domain or are absorbed. As these neutrons are simulated they can cause fission where a new site will be stored in the next source bank. The number of inactive fission source generations is determined by the user and convergence is commonly assessed with Shannon entropy (Brown, 2006). This diagnostic produces a scalar value for the spatial distribution of the fission source. Once it is stationary about some mean, the source is determined to be converged. The number of neutrons stored in the source bank can also be controlled by the user and is referred to as number of neutron histories per generation. Because we may tally CMFD quantities during inactive fission source generations, each generation will also be a tally batch. Thus, inactive fission source generations are the same as inactive batches.

Once a source is converged, tally means and variances are accumulated. To reduce bias, the source bank is updated at the end of each fission source generation. Because source sites used in a generation are directly dependent on fission sites from the previous generation, generations are highly correlated. This tends to produce inaccurate estimates of variances and confidence intervals (Brissenden and Garlick, 1986; Ueki, 2010). Kelly et.al. have shown that to reduce this inaccuracy, users can run multiple fission source generations in a tally batch (Kelly et al., 2012). All of these choices that users can make affects the behavior of MC tally and source convergence. The terminology presented in this section will be referred to throughout this paper.

3. CMFD diffusion acceleration

Coarse mesh finite difference diffusion methods were developed decades ago and are now commonly used to accelerate fission source convergence in nodal simulations (Smith, 1983). This nonlinear iteration strategy has been proven to reduce both computational time and storage when used to accelerate nodal methods. Recently, CMFD has been applied to eigenvalue Monte Carlo simulations to accelerate fission source convergence (Lee et al., 2012). When CMFD acceleration takes place, tallies need to be present during inactive batches. The most important equation that needs to be satisfied by MC tallies, to within stochastic uncertainty, is the *neutron balance equation*. This equation is written for a uniform Cartesian CMFD mesh with dimensions $(\Delta_l^u, \Delta_m^v, \Delta_n^w)$ as

$$\sum_{u\in(x,y,z)} \left\langle \bar{J}^{u,g}_{l+1/2,m,n}\Delta_m^v\Delta_n^w \right\rangle - \left\langle \bar{J}^{u,g}_{l-1/2,m,n}\Delta_m^v\Delta_n^w \right\rangle + \left\langle \overline{\overline{\Sigma}}^{g}_{t_{l,m,n}} \overline{\overline{\phi}}^{g}_{l,m,n}\Delta_l^u\Delta_m^v\Delta_n^w \right\rangle = \sum_{h=1}^{G} \left\langle \overline{\overline{\nu_s\Sigma}}^{h\to g}_{s_{l,m,n}} \overline{\overline{\phi}}^{h}_{l,m,n}\Delta_l^u\Delta_m^v\Delta_n^w \right\rangle + \frac{1}{k}\sum_{h=1}^{G} \left\langle \overline{\overline{\nu_f\Sigma}}^{h\to g}_{f_{l,m,n}} \overline{\overline{\phi}}^{h}_{l,m,n}\Delta_l^u\Delta_m^v\Delta_n^w \right\rangle. \quad (1)$$

The parameters in brackets $\langle\cdot\rangle$ in Eq. (1) are quantities that can be tallied in MC. Each tally is described below:

- $\left\langle \bar{J}^{u,g}_{l\pm1/2,m,n}\Delta_m^v\Delta_n^w \right\rangle$ — surface area-integrated net current over surface at $(l\pm1/2, m, n)$ with surface normal in direction u in energy group g. By dividing this quantity by the transverse area, $\Delta_m^v\Delta_n^w$, the surface area averaged net current can be computed.
- $\left\langle \overline{\overline{\Sigma}}^{g}_{t_{l,m,n}} \overline{\overline{\phi}}^{g}_{l,m,n}\Delta_l^u\Delta_m^v\Delta_n^w \right\rangle$ — volume-integrated total reaction rate over energy group g.
- $\left\langle \overline{\overline{\nu_s\Sigma}}^{h\to g}_{s_{l,m,n}} \overline{\overline{\phi}}^{h}_{l,m,n}\Delta_l^u\Delta_m^v\Delta_n^w \right\rangle$ — volume-integrated scattering production rate of neutrons that begins with energy in group h and exits reaction in group g. This reaction rate also includes the energy transfer of reactions (except fission) that produce multiple neutrons such as (n,2n); hence, the need for ν_s to represent neutron multiplicity.
- k — core multiplication factor.
- $\left\langle \overline{\overline{\nu_f\Sigma}}^{h\to g}_{f_{l,m,n}} \overline{\overline{\phi}}^{h}_{l,m,n}\Delta_l^u\Delta_m^v\Delta_n^w \right\rangle$ — volume-integrated fission production rate of neutrons that begins with energy in group h and exits in group g.

MC tallies will satisfy this equation to within stochastic uncertainty as tally batches are accumulated. CMFD parameters can be calculated from this equation and a better fission source can be obtained. An outline of CMFD accelerated MC is presented in Fig. 1. After each batch of neutrons, CMFD feedback may be applied before simulating the next batch of neutrons. The details of each part of CMFD are detailed in the following subsections.

3.1. Calculation of macroscopic cross sections and diffusion coefficients

Results from MC tallies are used to compute macroscopic cross sections (XS) and diffusion coefficients (DC) that are needed to solve the multigroup diffusion equation. In Eq. (1), macroscopic cross sections are already detailed out for each reaction rate. Macroscopic total, scattering production and fission production are obtained respectively with:

$$\overline{\overline{\Sigma}}^{g}_{t_{l,m,n}} = \frac{\left\langle \overline{\overline{\Sigma}}^{g}_{t_{l,m,n}} \overline{\overline{\phi}}^{g}_{l,m,n}\Delta_l^u\Delta_m^v\Delta_n^w \right\rangle}{\left\langle \overline{\overline{\phi}}^{g}_{l,m,n}\Delta_l^u\Delta_m^v\Delta_n^w \right\rangle}, \quad (2)$$

$$\overline{\overline{\nu_s\Sigma}}^{h\to g}_{s_{l,m,n}} = \frac{\left\langle \overline{\overline{\nu_s\Sigma}}^{h\to g}_{s_{l,m,n}} \overline{\overline{\phi}}^{h}_{l,m,n}\Delta_l^u\Delta_m^v\Delta_n^w \right\rangle}{\left\langle \overline{\overline{\phi}}^{h}_{l,m,n}\Delta_l^u\Delta_m^v\Delta_n^w \right\rangle} \quad (3)$$

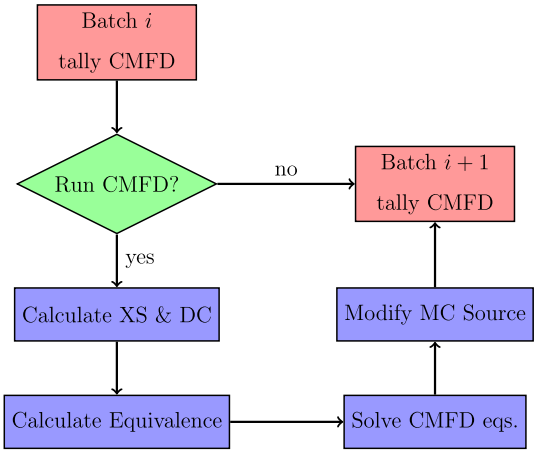

Fig. 1. Flow chart of CMFD execution between tally batches.

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