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Stochastic semi-implicit substep method for coupled depletion Monte-Carlo codes

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ABSTRACT

Coupled Monte Carlo burnup codes aim to evaluate the time evolution of different parameters, such as nuclide densities, for accurate modeling of the different reactor designs and associated fuel cycles. Recently a major deficiency in numerical stability of existing Monte Carlo coupling schemes was identified. Alternative, stable coupling schemes were derived, implemented and verified. These methods are iterative and rely on either the end- or middle-of-step (MOS) reaction rates to evaluate the end-of-step (EOS) nuclide densities. Here, we demonstrate that applying the EOS methods for realistic problems may lead to highly inaccurate results. Considerable improvement can be made by adopting MOS method but the accuracy may still be insufficient. The solution proposed in this work relies on the substep method that allows reducing the time discretization errors. The proposed and tested substep method also assumes that the reaction rates are linear functions of the logarithm of the nuclide densities. The method was implemented in BGCore code and subsequently used to perform a series of test case calculations. The results demonstrate that better accuracy and hence efficiency can be achieved with negligible additional computational burden.

1. Introduction

Monte Carlo (MC) neutron transport codes are increasingly widely used as a standard calculation tool in reactor analysis. In order to evaluate fuel isotopic changes as a function of time, MC transport code must be linked to a deterministic point depletion solver. Up to day, many MC-burnup coupling programs have been developed and shown to produce accurate results, for example as shown in Bomboni et al. (2010). Among such coupled codes are SERPENT (Leppänen et al., 2015), BGCore (Fridman et al., 2008), MCNPX (Fensin et al., 2006) and many others. There is currently an on-going trend to use these codes for full core analysis (Damian and Brun, 2015).

One of the important aspects, which differ among the various codes, is the coupling scheme used to integrate MC with burnup calculations. In recent studies, a major deficiency of the current coupling schemes was reported by Dufek and Hoogenboom (2009), Dufek et al. (2013a), and Kotlyar and Shwageraus (2013). Their research has shown that applying existing explicit methods for coupled MC calculations may result in oscillatory behavior of local and integral parameters. This stimulated the need to adopt new, numerically stable, methods to be used in MC coupled codes. In response to this need, new coupling methods have been developed first for MC-burnup applications (Dufek et al., 2013b) and eventually followed by the more comprehensive fully coupled MC-burnup-thermal hydraulic (TH) schemes (Kotlyar and Shwageraus, 2014). The methods were implemented in the BGCore code and were shown to produce numerically stable results. The numerical stability issues were resolved through the use of alternative methods denoted as the SIE and SIMP. The methods solve the depletion and TH problems simultaneously and iteratively. Each iteration updates either the end-of-step (SIE) or middle-of-step (SIMP) flux, which is weighted with variable under-relaxation factor and combined with the values obtained in previous iterations. These methods were shown to solve the stability issue. The comparison of the various methods (i.e. SIE, SIMP and explicit) in terms of accuracy is reported here.

The SIE method, as will be shown later, may be inaccurate since it relies on the end-of-step (EOS) parameters, such as reaction rates, to calculate the EOS nuclide densities. In realistic problems, with rapid change of spectrum for example, this EOS approach could lead to a systematic under (or over) prediction of some reaction rates. However, even more alarming is the fact that the iterative approach required to stabilize the solution may deteriorate its accuracy even further. More specifically, as the number of iterations increases, the under or over prediction becomes greater.

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The SIMP method that relies on the middle-of-step quantities is much more accurate than SIE. However, the method also relies on the constant reaction rates (MOS) throughout the analyzed timestep, which is only an approximation to reality. It appears that these errors are a result of not knowing the precise shape of the reaction rates versus time function within the time interval.

Therefore, this work focuses on extending the stochastic implicit Euler methodology with the substep method and will be denoted here as the SUBSTEP. The method uses a log-linear correlation between the nuclide densities and reaction rates to better account for the variation in reaction rates within the timestep. The method requires only additional depletion calculations to be carried out with no additional transport calculations and therefore has negligible additional computational burden.

The method was implemented in BGCore code, which was subsequently used to perform three, 2 and 3-dimensional (2D and 3D), test calculations of typical PWR fuel pin and assembly models. The results systematically show that the proposed method outperforms the original SIE and SIMP methods in accuracy and therefore computational efficiency.

2. BGCore description

The proposed SUBSTEP method was programmed into BGCore system. BGCore is a system of codes developed at Ben-Gurion University, in which Monte-Carlo code MCNP4C (Briesmeister, 2000) is coupled with fuel depletion and decay module. BGCore utilizes multi-group methodology for calculation of one-group transmutation cross-sections (Haeck and Verboomen, 2007; Fridman et al., 2008) which significantly improves the speed of burnup calculations. In addition to the depletion module, BGCore system also includes a built-in thermal–hydraulic (TH) feedbacks module. The modules are executed iteratively so that the coupled system is capable of predicting fuel composition, power, coolant density and temperature distributions in various types of reactor systems (Kotlyar et al., 2011).

3. Burnup coupling methodology

The depletion equations use time dependent fluxes, although still assumed to be constant for each time step, to determine the evolution of nuclide inventories with time. However, nuclide inventories depend on the flux, which by itself requires a prior knowledge of the nuclide inventories. There are several approaches to solve this non-linear problem.

First, the solution requires discretizing the full time scale into time steps, in which the parameters of interest (i.e. reaction rates and nuclide densities) are to be computed. At each time step, the procedure requires solving 2 independent problems. The first is the neutron transport eigenvalue equation that provides reaction rates. In this work, it will be denoted by the operator $\varphi(\mathbf{N})$. MCNP4C code is used here to obtain the reaction rates $\mathbf{X} = \varphi(\mathbf{N})$ for a known mixture of $\mathbf{N}$ different nuclides.

In order to progress in time, the Bateman equations (Bateman, 1932) which have the matrix exponential solution (Eq. (1)) must also be solved.

$$\mathbf{N}(t) = e^{\mathcal{M}\Delta t}\mathbf{N}(0) \tag{1}$$

where, $\mathbf{N} = [n_1 \dots n_n]$ is unique for a certain time point and n_j is the atomic nuclide density of nuclide j. BGCore follows the evolution of $n = 1743$ nuclides for accurate estimation of decay heat and radiotoxicity following shutdown. The operator $\mathcal{M}$ in Eq. (1) represents the transmutation matrix which depends on the reaction rates $\mathbf{X}$. The relation between $\mathcal{M}$ and $\mathbf{X}$ is described in Eq. (2):

$$\mathcal{M}(t) = \Lambda + \mathbf{X}(t) \tag{2}$$

where, Λ is the decay matrix and includes removal terms on its diagonal and production rates on the off-diagonal as explained in Eq. (3):

$$\begin{aligned} \Lambda_{j,j} &= -\lambda_j \\ \Lambda_{j,k\neq j} &= \lambda_{k\to j} \end{aligned} \tag{3}$$

where λ_j is the decay constant of nuclide j and $\lambda_{k\to j}$ is the decay constant from nuclide k to nuclide j. This matrix is pre-generated and remains constant through the entire fuel cycle calculations.

$\mathbf{X}$ is the neutron induced transmutation matrix that is obtained from the transport solution for a pre-determent $\mathbf{N}$ and therefore is unique at each time point. The diagonal elements of this matrix are removal rates following neutron absorption and the off-diagonal elements describe the production from other reactions (e.g. fission, inelastic scattering, etc.) as described in Eq. (4):

$$\begin{aligned} \mathrm{X}_{j,j} &= -\sigma_j\phi \\ \mathrm{X}_{j,k\neq j} &= \sigma_{k\to j}\phi \end{aligned} \tag{4}$$

where, σ_j is the energy average absorption cross section of nuclide j, $\sigma_{k\to j}$ is the average cross section of nuclide k which leads to j and ϕ is the 1-group flux.

As mentioned earlier, in fuel cycle calculations, the irradiation time is divided into time steps. At each timestep, the transport and depletion problems are solved independently (operator splitting approach) and the solutions are iteratively coupled in a designated subroutine. The coupling scheme determines the accuracy and numerical stability of the solution.

Section 3.1 describes the explicit Euler method implemented in many of the existing computational tools used in reactor physics analyses. This is then followed by the SIE and SIMP algorithms introduction in Sections 3.2 and 3.3 respectively. Lastly, the newly proposed SUBSTEP algorithm is presented in Section 3.4 The different numerical schemes in these sections describe the coupling procedure to solve a single timestep depletion $\forall t \in [t_0, t_1]$ with timestep length $\Delta t = t_1 - t_0$. In addition, $\mathbf{N}_i$ and $\mathcal{M}_i$ are the nuclide density vector and transmutation matrix at t_i respectively.

3.1. Explicit Euler method

According to the explicit Euler method, the neutron transport solution is obtained at the beginning-of-step (BOS) for a predetermined fuel inventory. Then, the space and energy dependent microscopic reaction rates are assumed to be constant during the depleted time step. Knowing these reaction rates allows obtaining the concentration at the end-of-step (EOS) in a single calculation step.

1	$\mathcal{M}_0 \leftarrow \varphi(\mathbf{N}_0)$
2	$\mathbf{N}_1 \leftarrow e^{\mathcal{M}_0\Delta t}\mathbf{N}_0$

3.2. Stochastic implicit Euler (SIE) method

SIE (Dufek et al., 2013b) is a recently proposed method that uses EOS values of reaction rates to calculate EOS quantities of interest (i.e. nuclide densities). The solution is obtained by using the so-called stochastic approximation with under-relaxation factor based on the Robbins–Monro algorithm (Robbins and Monro, 1951). The relaxation algorithm could be either applied to the nuclide density field (i.e. SIE/ND) or the flux field (i.e. SIE/FLUX). The mathematical derivation of the methods and their implementation is presented in the original paper and hence will not be repeated here.