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Sub-step methodology for coupled Monte Carlo depletion and thermal hydraulic codes

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ABSTRACT

The governing procedure in coupled Monte Carlo (MC) codes relies on discretization of the simulation time into time steps. Typically, the MC transport solution at discrete points will generate reaction rates, which in most codes are assumed to be constant within the time step. This assumption can trigger numerical instabilities or result in a loss of accuracy, which, in turn, would require reducing the time steps size. This paper focuses on reducing the time discretization error without requiring additional MC transport solutions and hence with no major computational overhead. The sub-step method presented here accounts for the reaction rate variation due to the variation in nuclide densities and thermal hydraulic (TH) conditions. This is achieved by performing additional depletion and TH calculations within the analyzed time step. The method was implemented in BGCore code and subsequently used to analyze a series of test cases. The results indicate that computational speedup of up to a factor of 10 may be achieved over the existing coupling schemes.

1. Introduction

Many Monte Carlo (MC) coupled computer codes have been developed and are widely used to perform reactor designs and fuel cycle analyses (Bomboni et al., 2010). Coupled codes, such as SERPENT (Leppänen et al., 2015), BGCore (Fridman et al., 2008) and MCNPX (Fensin et al., 2006) are just a small subset of such codes, in which the MC transport solution is linked to a deterministic point depletion solver. There is an ongoing effort to expand the use of such MC based codes to full core analysis (Leppänen et al., 2014). Therefore, there is a need to introduce additional feedback that will account for variation in thermal–hydraulic (TH) conditions in the coupled calculation routine.

The coupling schemes implemented by the various codes typically rely on explicit methods to couple between MC transport solution and burnup with TH calculations. The explicit nature of these coupling schemes relates to the time integration. Recently however, a major deficiency in such explicit coupling methods was reported (Dufek et al., 2013a and Kotlyar and Shwageraus, 2013). Non-physical behavior of the results in a form of oscillations in various local parameters, such as the neutron flux distribution was observed and studied. The mentioned studies showed that large systems (e.g. 3D fuel assemblies or cores) may exhibit such unphysical behavior. Previous results also indicated that the trigger for such numerical instabilities could relate, for example, to slightly asymmetrical flux distribution which may be caused by poor spatial convergence of MC statistics. However, the asymmetry in flux distribution could also be due to an asymmetric distribution of burnup or TH parameters such as coolant density, which is often the case in realistic core conditions. These studies concluded that the issues were linked to the use of explicit coupling methods during time integration. In other words, reducing the length of the time-step to sufficiently small value would be required to eliminate the instability issues.

Therefore, new coupling methods have been developed first for MC-burnup applications (Dufek et al., 2013b) and implemented in Serpent and BGCore. Then, more comprehensive fully coupled MC-burnup-TH schemes (Kotlyar and Shwageraus, 2014) were proposed and implemented in BGCore. The stability issues were resolved through the use of alternative methods such as the Stochastic-Implicit-Euler (SIE) and Stochastic-Implicit-Mid-point (SIMP) methods. 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.

Recent studies (Kotlyar and Shwageraus, 2016) indicated that the efficiency of the SIE may be quite poor. More specifically, in order to obtain accurate results, the time discretization steps are

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required to be extremely small, which increases the overall calculation time. Although, the same study indicated that the SIMP method considerably improves the accuracy of the results, the computational efficiency is still relatively low. The SIE method, for example, relies on the end-of-step (EOS) reaction rates to calculate the EOS nuclide densities, similarly to the explicit methods that rely on the beginning-of-step (BOS) reaction rates. The reason for superior performance of the SIMP method is that the middle-of-step (MOS) reaction rates are assumed to be timestep representative, which is certainly a better approximation than using fixed BOS or EOS reaction rates. However, none of these assumptions are suitable for many practical problems with rapid change of neutron energy spectrum such as Gadolinium depletion.

One of the options to improve the original SIE methods was to include a sub-step approach. Previous studies (Kotlyar and Shwageraus, 2016) introduced the sub-step methodology for coupled MC depletion solution and fixed TH conditions. The method was implemented in BGCore and used a log-linear correlation between the nuclide densities and reaction rates to better account for the variation in reaction rates within the time step. The method required only additional depletion calculations to be carried out but no additional transport calculations. This method was implemented in BGCore code, which was subsequently used to analyze a number of test cases for a typical PWR fuel assembly. The results systematically showed that the method outperforms the original SIE and SIMP methods in accuracy and computational efficiency.

The current research seeks to extend the previously proposed sub-step method by accounting for the variation in TH properties within the analyzed time step. The variation in TH conditions will in turn lead to variation in reaction rates as well. Therefore, the first stage of this research was to develop reasonably accurate correlations between the reaction rates and nuclide densities as well as TH conditions. These correlations that link fuel temperatures (or any other TH conditions) and nuclide densities are constructed on the fly. Each iteration within the analyzed timestep adds an extra data point, from which the reaction rates calculated from the MC transport are linked to a unique fuel temperature and nuclide density set. The sub-step sequence within each time step starts at BOS, for which the reaction rates are known. Depletion with BOS reaction rates allows to obtain the end of sub-step nuclide densities. Then, the new reaction rates are updated from the constructed correlations by substituting the updated nuclide densities. These updated reaction rates are used to calculate the new TH conditions, which are then used to update the reaction rates according to the correlations. This procedure is subsequently performed for the following sub-steps within the calculated time step. This is a coupled routine since reaction rates are continuously updated, however the scheme requires no additional MC solutions. This method was implemented in BGCore and was used to perform various 3D test cases. The results indicate that this method allows to achieve accurate results with considerably larger time steps than required with other coupling methods considered and compared in this study (e.g. explicit, SIE and SIMP).

2. BGCore description

The proposed coupled sub-step method was programmed into BGCore system. BGCore is a system of codes in which Monte-Carlo code MCNP4C (Briesmeister, 2000) is coupled with fuel depletion and thermal–hydraulic (TH) modules. 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-thermal hydraulic coupling methodology

Coupled burnup-TH analyses are used to account for the strong relation between the various neutronic and thermal hydraulic parameters. The nuclide densities, **N**, and TH properties, **T**, depend on each other and also on the energy and space distribution of neutron flux, ϕ. However, calculation of ϕ requires a prior knowledge of **N** and **T**. Practicality, the solution of such time-dependent non-linear problem is obtained by discretizing the simulated time period into time steps. Within a time step, the parameters of interest, such as nuclide densities are computed by assuming that other parameters, such as reaction rates remain constant during the time step. Generally, this assumption may lead to a loss of accuracy when the time steps are not sufficiently small.

The non-linear problem mentioned above can be described by three coupled equations. The first is the neutron transport eigenvalue equation that provides reaction rates, denoted here as $\mathcal{M}$. In this work, the neutron transport operator will be denoted by φ. The MCNP4C code is used here to obtain the reaction rates $\mathcal{M} = \varphi(\mathbf{N}, \mathbf{T})$ for a known mixture of nuclides **N** and TH conditions **T**. The second is the heat balance equation that computes the temperature distribution from which also the coolant and/or moderator densities can be derived. The operator for solving the heat conduction and convection problem, which requires the reaction rates as an input, is denoted here as $\Upsilon(\mathcal{M})$. The last is the burnup equation that determines the change in nuclide densities during time t, as described in Eq. (1).

In order to progress in time, a set of first order Bateman equations (Bateman, 1932) have to be solved. This solution is known as matrix exponential (Eq. (1)).

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

where, $\mathbf{N} = [n_1 \cdots n_n]$ is unique for a certain time point and n_j is the atomic density of nuclide j. The operator $\mathcal{M}$ in Eq. (1) represents the transmutation matrix that includes removal terms on its diagonal and production rates on the off-diagonal locations as explained in Eq. (2):

$$\begin{aligned} M_{j,j} &= -\lambda_j - \sigma_j\phi \\ M_{j,k\neq j} &= \lambda_{k\to j} + \sigma_{k\to j}\phi \end{aligned} \tag{2}$$

where λ_j and σ_j are the decay constant and energy averaged absorption cross section of nuclide j respectively, $\lambda_{k\to j}$ and $\sigma_{k\to j}$ are the decay constant and the average cross section of nuclide k which leads to j respectively. And ϕ is the 1-group neutron flux.

As mentioned earlier, in fuel cycle calculations, the irradiation time is divided into sub-steps. At each time step, the transport, depletion and TH problems are solved separately 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 beginning-of-step explicit method used 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 proposed SUB-STEP algorithm is presented in Section 3.4. The different numerical schemes presented in these sections describe the coupling procedure to solve the coupled problem for a single time-step with time step length $\Delta t = t_1 - t_0$. In addition, $\mathbf{N}_i$, $\mathbf{T}_i$ and $\mathcal{M}_i$ are the nuclide density vector, TH conditions and transmutation matrix at t_i respectively.