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Technical note

Derivation of a stable coupling scheme for Monte Carlo burnup calculations with the thermal–hydraulic feedback

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ABSTRACT

Numerically stable Monte Carlo burnup calculations of nuclear fuel cycles are now possible with the previously derived Stochastic Implicit Euler method based coupling scheme. In this paper, we show that this scheme can be easily extended to include the thermal–hydraulic feedback during the Monte Carlo burnup simulations, while preserving its unconditional stability property. At each time step, the implicit solution (for the end-of-step neutron flux, fuel nuclide densities and thermal–hydraulic conditions) is calculated iteratively by the stochastic approximation; the fuel nuclide densities and thermal–hydraulic conditions are iterated simultaneously. This coupling scheme is derived as stable in theory; i.e., its stability is not conditioned by the choice of time steps.

1. Introduction

The purpose of this paper is to further develop methods allowing for realistic and accurate Monte Carlo burnup calculations of fuel cycles of critical reactors. A variety of Monte Carlo burnup codes, linking various Monte Carlo neutron transport codes to depletion codes or built-in procedures, is available at present, e.g. MCB2 (Cetnar et al., 2000), MOCUP (Moore et al., 1995), MONTEBURNS2 (Poston and Trellue, 1999), ALEPH (Haeck et al., 2006), MCNPX2.6 (Fensin et al., 2010), SERPENT (Leppänen, 2012), and many others.

The accuracy of the Monte Carlo fuel cycle calculations (the difference between the computed and correct data) is affected by a number of factors, such as the statistical precision of the calculation, errors in nuclear data libraries, approximations made to the reactor core model, and also the numerical stability of the calculation. The inadequate numerical stability of the coupling schemes in the existing Monte Carlo burnup codes has been identified as an important problem (Dufek and Hoogenboom, 2009; Dufek et al., 2013b); the instability is driven by a strong neutronic feedback from the nuclide field. While a stable coupling scheme was recently derived based on the new Stochastic Implicit Euler (SIE) method (Dufek et al., 2013a), the scheme assumed fixed thermal–hydraulic conditions during the whole fuel cycle calculation. Yet, especially in boiling water reactors (BWRs) the coolant (moderator) density distribution does change during the fuel cycle, and the changes should be simulated. Since the coolant represents a strong reactivity feedback in these reactors, adjusting the coolant density distribution over the time steps during Monte Carlo burnup calculations may cause numerical instability even when a stable coupling scheme is applied on the fuel depletion process.

In this paper, we eliminate the assumption of the fixed thermal–hydraulic conditions that are commonly applied to reactor core models in Monte Carlo burnup calculations. The thermal–hydraulic feedback is realised here by extending the previously derived Stochastic Implicit Euler (SIE) based coupling scheme for Monte Carlo burnup calculations. The extended coupling scheme iterates the end-of-step neutron flux, fuel nuclide densities and thermal–hydraulic conditions simultaneously during an inner iteration at each time step. The unconditional stability property of this coupling scheme is preserved.

The paper is organised as follows. Section 2 states the governing equations for neutron transport criticality, fuel depletion, thermal–hydraulic conditions and additional constrains. In Section 3 we derive the Stochastic Implicit Euler (SIE) method based coupling scheme for Monte Carlo burnup calculations with the thermal–hydraulic feedback, and suggest the possible algorithms of implementing the method in Monte Carlo burnup codes. Section 4 summarises our conclusions.

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2. Governing equations

The geometry and material properties of a nuclear reactor can be described by $\mathbf{N}_F(\mathbf{r})$ – the nuclide field in fuel and other static materials, $\mathbf{N}_R(\mathbf{r})$ – the nuclide field in locations of control rods, $\mathbf{N}_C(\mathbf{r})$ – the nuclide field in coolant (moderator), and the temperature field $T(\mathbf{r})$. The elements of the nuclide field vectors denote concentrations of various nuclides at the position $\mathbf{r}$. The fundamental-mode neutron flux $\phi(\mathbf{r},\Omega,E)$ is then determined by these nuclide fields and the boundary conditions.

The nuclide field $\mathbf{N}_F(\mathbf{r})$ changes during the reactor operation due to the depletion process driven by the neutron flux $\phi(\mathbf{r},\Omega,E)$. Due to its dependence on$\mathbf{N}_F(\mathbf{r})$, the fundamental-mode neutron flux changes during the reactor operation as well. Consequently, the changes in the neutron flux are reflected into the changes in$\mathbf{N}_C(\mathbf{r})$. The purpose of fuel cycle calculations is to determine the changes in the nuclide fields and $\phi(\mathbf{s}) \equiv \phi(\mathbf{r},\Omega,E,t)$ during the whole fuel cycle.

The above problem can be described by a system of coupled equations: the burnup (ODE) equation that describes the time change of the nuclide field, the criticality (eigenvalue) neutron transport equation that gives the fundamental-mode neutron flux in the core, and thermal–hydraulic equations that describe the coolant (moderator) mass density distribution.

The fuel burnup equation (Bell and Glasstone, 1970),

$$\frac{\mathrm{d}\mathbf{N}_F(\mathbf{r},t)}{\mathrm{d}t} = \mathbb{M}(\phi,T)\mathbf{N}_F(\mathbf{r},t), \tag{1}$$

is an ordinary differential equation where

$$\mathbb{M}(\phi) = \int_0^\infty \phi(\mathbf{r},E,t)\mathbb{X}(T)\mathrm{d}E + \mathbb{D},$$

where $\mathbb{X}$ is a cross-section and fission yield matrix, $\mathbb{D}$ is a decay matrix, and $T(\mathbf{r},t)$ is the temperature at $\mathbf{r}$ in time t. Eq. (1) has a formal solution (Bell and Glasstone, 1970)

$$\mathbf{N}_F(\mathbf{r},t) = \mathbf{N}_{F,0}(\mathbf{r})\exp[\mathbb{M}(\phi,T)(t-t_0)], \tag{2}$$

where $\mathbf{N}_{F,0}(\mathbf{r})$ is the fuel nuclide field at time t_0. We wish to stress that $\mathbb{M}(\phi)$ is determined by the neutron energy spectrum; thus, all references to Eq. (2) in this paper assume the reaction rates were determined by ϕ.

The neutron flux $\phi(\mathbf{r},E,t)$ is approximated at time t by the fundamental-mode eigenfunction of the criticality equation

$$B(\mathbf{N})\phi(\mathbf{s}) \equiv \left[L(\mathbf{N}) - \frac{1}{k}F(\mathbf{N})\right]\phi(\mathbf{s}) = 0, \tag{3}$$

where $\mathbf{N}$ describes the nuclide field in the whole reactor

$$\mathbf{N}(\mathbf{r}) = \begin{cases} \mathbf{N}_F(\mathbf{r}) & \text{for } \mathbf{r} \text{ in fuel} \\ \mathbf{N}_C(\mathbf{r}) & \text{for } \mathbf{r} \text{ in coolant} \end{cases}, \tag{4}$$

$L(\mathbf{N})\phi(\mathbf{s})$ represents the migration and loss of neutrons from $\mathbf{s}$, and $F(\mathbf{N})\phi(\mathbf{s})$ accounts for neutron production in $\mathbf{s}$ due to fission.

The coolant (moderator) nuclide field $\mathbf{N}_C(\mathbf{r})$ is given by thermal–hydraulic equations that ensure that the coolant mass, energy and momentum are conserved in the whole reactor at any time. The thermal–hydraulic equations are to be completed with boundary conditions for the coolant mass flow rate, inlet coolant temperature and inlet pressure. In the following text, the nuclide field vector $\mathbf{N}_C(\mathbf{r})$ (determining the coolant density) is given by the function $\mathbf{C}(\phi(\mathbf{s}))$ as the solution to the thermal–hydraulic equations:

$$\mathbf{N}_C(\mathbf{r},t) = \mathbf{C}(\phi(\mathbf{s})). \tag{5}$$

Since the core conditions are required to be steady-state at all time steps of the fuel cycle calculations, it is necessary to prevent even the natural xenon oscillations that could develop in the calculations with short time steps of few hours. This can be achieved by forcing the concentration of ^{135}Xe to its saturated level; i.e., a level that is naturally established for $t \to \infty$ (with the neutron flux and fission rate fixed). The saturated concentration of ^{135}Xe is reached practically after several days; thus, this additional constrain to the above system of equations is not necessary when the time steps are larger than several days. The saturated xenon concentration can be derived directly from the burnup equation.

In the following text, the fundamental-mode flux $\phi(\mathbf{s})$ that satisfies Eq. (3) with the operator B is denoted as ϕ_B. In Section 3.2, $\phi_{B(\mathbf{N}_F,\mathbf{N}_C)}$ specifically denotes the fundamental-mode neutron flux computed by a Monte Carlo criticality code in a reactor with the nuclide fields $\mathbf{N}_F$ and $\mathbf{N}_C$, and $\phi_{B(\mathbf{N})}$ denotes the fundamental-mode neutron flux computed by a Monte Carlo criticality code in a reactor with the combined nuclide field $\mathbf{N}$.

3. The SIE method for MC burnup calculations with TH feedback

3.1. Derivation of the method

The Stochastic Implicit Euler method was derived for Monte Carlo burnup calculations of nuclear fuel cycles by Dufek et al., 2013a. Here, we extend the method derivation so that the thermal–hydraulic feedback is reflected.

The implicit Euler method is the simplest method that satisfies the unconditional stability property (Hoffman, 2001). In the context of burnup calculations with thermal–hydraulic feedback, the implicit Euler method uses the end-of-step neutron flux to deplete the fuel over the whole time step and to calculate the thermal–hydraulic conditions.

In the following text, we derive an efficient way of calculating the end-of-step neutron flux. Let $\mathbf{N}_{F,i}$, $\mathbf{N}_{C,i}$ and ϕ_i denote the nuclide field in fuel and coolant (moderator) and neutron flux at the end of i^{th} time step, respectively. When $\mathbf{N}_{F,i-1}$ is depleted with the end-of-step flux ϕ_i over the ith time step then $\mathbf{N}_{F,i}$ equals

$$\mathbf{N}_{F,i} = \mathbf{N}_{F,i-1}\exp[\mathbb{M}(\phi_i,T)(t_i - t_{i-1})]. \tag{6}$$

Similarly, the coolant (moderator) nuclide field is given at the end of the ith time step as

$$\mathbf{N}_{C,i}(\mathbf{r},t) = \mathbf{C}(\phi_i), \tag{7}$$

while ϕ_i is given by

$$\phi_i = \phi_{B(\mathbf{N}_{F,i},\mathbf{N}_{C,i})}. \tag{8}$$

Substituting $N_{F,i}$ from Eq. (6) and $\mathbf{N}_{C,i}$ from Eq. (7) into Eq. (8) forms a non-linear equation for ϕ_i,

$$\phi_i = \phi_{B\left(\mathbf{N}_{F,i-1}\exp[\mathbb{M}(\phi_i,T)(t_i-t_{i-1})],\mathbf{C}(\phi_i)\right)}. \tag{9}$$

For sake of simplicity, let G denote the right-hand side of Eq. (9) as a function of ϕ_i. Then Eq. (9) reduces into a simple form

$$\phi_i = G(\phi_i). \tag{10}$$

In case of Monte Carlo calculation, G is approximated by a stochastic function G that contains an additional noise term ε,

$$\widehat{G} = G + \varepsilon.$$

This changes Eq. (10) into

$$\phi_i = \widehat{G}(\phi_i), \tag{11}$$

which is the non-linear stochastic root-finding problem (Dufek and Gudowski, 2006).

A similar non-linear equation can be formed for N_i when ϕ_i from Eq. (8) is substituted into Eqs. (6) and (7), which gives

$$\mathbf{N}_i = \begin{cases} \mathbf{N}_{\mathrm{F},i-1} \exp[\mathbb{M}(\phi_{B(\mathbf{N}_i)}, T)(\Delta t)] & \text{for } \mathbf{r} \text{ in fuel} \\ \mathbf{C}(\phi_{B(\mathbf{N}_i)}) & \text{for } \mathbf{r} \text{ in coolant} \end{cases}, \tag{12}$$

which can be again reduced into a simple form

$$\mathbf{N}_i = H(\mathbf{N}_i), \tag{13}$$

where H denotes the right-hand side of Eq. (12) as a function of $\mathbf{N}_i$.

Dufek and Gudowski (2006) showed that Eq. (11) can be efficiently solved via the stochastic approximation based iteration

$$\phi_i^{(n+1)} = \phi_i^{(n)} - \alpha_n d(\phi_i^{(n)} - \widehat{G}(\phi_i^{(n)})), \tag{14}$$

where d is positive and smaller than 1, and the step-size α_n is given by the Robbins-Monro algorithm

$$\alpha_n = \frac{1}{n}. \tag{15}$$

Robbins and Monro (1951) proved that the stochastic approximation converges when the step-size follows Eq. (15).

Unless the initial guess is known to a certain accuracy, we advice to set $d = 1$ to achieve the best efficiency; then Eq. (14) can be re-written into a common relaxation form

$$\phi_i^{(n+1)} = (1 - \alpha_n)\phi_i^{(n)} + \alpha_n \widehat{G}(\phi_i^{(n)}). \tag{16}$$

The same iterative approach can be applied to solving the stochastic version of Eq. (13),

$$\mathbf{N}_i = \widehat{H}(\mathbf{N}_i), \tag{17}$$

as it is demonstrated in Section 3.2.

We would like to point out that Eq. (16) is equivalent to

$$\phi_i^{(n+1)} = \frac{1}{n}\sum_{j=1}^{n} \widehat{G}(\phi_i^{(j)}), \tag{18}$$

when the Robbins-Monro algorithm is used to generate the reduced step-size, see (Dufek and Gudowski, 2006). According to Eq. (18), all Monte Carlo criticality calculations are reflected in the final solution with equal statistical weight $1/n$, which ensures a good efficiency of this iteration. The statistical errors in the iterated flux are reduced with each new iteration step.

3.2. Implementation of the method

Here, we describe the basic implementations of the coupling scheme that was derived in Section 3.1. Either the neutron flux or the nuclide field is relaxed during the inner iteration (relaxation) at each time step; therefore, two basic implementations are possible. Algorithm 1 describes the scheme with relaxation of the neutron flux, while Algorithm 2 describes the scheme with relaxation of the nuclide field.

Note that while the inner iteration in Algorithm 2 is based on relaxing the fuel and coolant nuclide fields, the neutron flux is combined over all inner iteration steps at line #2 as well. This operation does not relax the neutron flux; in fact, this operation is not necessary for the calculation at all since its outcome is not used. The only purpose of this operation is to provide the neutron flux as one of the results that is often requested from Monte Carlo burnup calculations.

The number of inner iteration steps, c, is fixed in Algorithms 1 and 2; however, the inner iteration can in principle continue until a specific convergence criterion is satisfied.

Algorithm 1. The Stochastic Implicit Euler method with relaxation of the neutron flux

1: **input:** $\mathbf{N}_{\mathrm{F},0}$, $\mathbf{N}_{\mathrm{C},0}$
2: $\phi_0 \leftarrow \phi_{B(\mathbf{N}_{\mathrm{F},0},\mathbf{N}_{\mathrm{C},0})}$
3: **for** $i \leftarrow 0,1,\ldots$ **do**
4: $\quad \mathbf{N}_{\mathrm{F},i+1}^{(0)} \leftarrow \mathbf{N}_{\mathrm{F},i} \exp[\mathbb{M}(\phi_i)\Delta t]$
5: $\quad \mathbf{N}_{\mathrm{C},i+1^{(0)}} \leftarrow \mathbf{C}(\phi_i)$
6: $\quad$ **for** $n \leftarrow 1,2,\ldots,c$ **do**
7: $\quad\quad \phi_{i+1}^{(n)} \leftarrow \phi_{B(\mathbf{N}_{\mathrm{F},i+1}^{(n-1)},\mathbf{N}_{\mathrm{C},i+1}^{(n-1)})}$
8: $\quad\quad \bar{\phi}_{i+1}^{(n)} \leftarrow \sum_{j=1}^{n} \phi_{i+1}^{(j)}/n$
9: $\quad\quad \mathbf{N}_{\mathrm{F},i+1}^{(n)} \leftarrow \mathbf{N}_{\mathrm{F},i} \exp[\mathbb{M}(\bar{\phi}_{i+1}^{(n)})\Delta t]$
10: $\quad\quad \mathbf{N}_{\mathrm{C}}, i+1^{(n)} \leftarrow \mathbf{C}(\bar{\phi}_{i+1}^{(n)})$
11: $\quad$ **end for**
12: $\quad \mathbf{N}_{\mathrm{F},i+1} \leftarrow \mathbf{N}_{\mathrm{F},i+1}{}^{(c)}$
13: $\quad \mathbf{N}_{\mathrm{C},i+1} \leftarrow \mathbf{N}_{\mathrm{C},i+1}{}^{(c)}$
14: $\quad \phi_{i+1} \leftarrow \bar{\phi}_{i+1}^{(c)}$
15: **end for**

Algorithm 2. The Stochastic Implicit Euler method with relaxation of the nuclide field

1: **input:** $\mathbf{N}_{\mathrm{F},0}$,$\mathbf{N}_{\mathrm{C},0}$
2: $\phi_0 \leftarrow \phi_{B(\mathbf{N}_{\mathrm{F},0},\mathbf{N}_{\mathrm{C},0})}$
3: **for** $i \leftarrow 0,1,\ldots,$**do**
4: $\quad \bar{\mathbf{N}}_{\mathrm{F},i+1}^{(0)} \leftarrow \mathbf{N}_{\mathrm{F},i} \exp[\mathbb{M}(\phi_i)\Delta t]$
5: $\quad \bar{\mathbf{N}}_{\mathrm{c},i+1}^{(0)} \leftarrow \mathbf{C}(\phi_i)$
6: $\quad$ **for** $n \leftarrow 1,2,\ldots,c$ **do**
7: $\quad\quad \phi_{i+1}^{(n)} \leftarrow \phi_{B\left(\bar{\mathbf{N}}_{\mathrm{F},i+1}^{(n-1)},\bar{\mathbf{N}}_{\mathrm{C},i+1}^{(n-1)}\right)}$
8: $\quad\quad \mathbf{N}_{\mathrm{F},i+1}^{(n)} \bar{\mathbf{N}}_{\mathrm{F},\mathbf{i}} \exp[\mathbb{M}(\phi_{\mathbf{i+1}}^{(\mathbf{n})})\Delta \mathbf{t}]$
9: $\quad\quad \mathbf{N}_{\mathrm{C},i+1}^{(n)} \leftarrow \mathbf{C}(\phi_{i+1}^{(n)})$
10: $\quad\quad \bar{\mathbf{N}}_{\mathrm{F},i+1}^{(n)} \leftarrow \sum_{j=1}^{n} \mathbf{N}_{\mathrm{F},i+1}^{(j)}/n$
11: $\quad\quad \bar{\mathbf{N}}_{\mathrm{C},i+1}^{(n)} \leftarrow \sum_{j=1}^{n} \mathbf{N}_{\mathrm{C},i+1}^{(j)}/n$
12: $\quad$ **end for**
13: $\quad \mathbf{N}_{\mathrm{F},i+1} \leftarrow \bar{\mathbf{N}}_{\mathrm{F},i+1}^{(c)}$
14: $\quad \mathbf{N}_{\mathrm{C},i+1} \leftarrow \bar{\mathbf{N}}_{\mathrm{C},i+1}^{(c)}$
15: $\quad \phi_{i+1} \leftarrow \sum_{j=1}^{c} \phi_{i+1}^{(j)}/c$
16: **end for**

4. Conclusions

We have described the way the thermal–hydraulic feedback can be implemented into the stable Monte Carlo burnup coupling scheme based on the Stochastic Implicit Euler method, allowing more realistic simulations of nuclear fuel cycles where the thermal–hydraulic conditions have significant effect on the actual fuel depletion. The extended coupling scheme was derived as stable, allowing stable burnup calculations even with large time steps. Yet, as the implicit Euler method is a first-order method, the error of this scheme is proportional to the time step length; therefore, we advise to set the time steps as short as possible in order to simulate accurately the spatial and spectral changes in the neutron flux.

We have suggested two possible implementations of the extended SIE method: Algorithm 1 relaxes the neutron flux in the inner iteration, while Algorithm 2 relaxes the nuclide field. By relaxing the neutron flux the relaxation is automatically applied on the nuclide field through the burnup and thermal–hydraulic equations; similarly, by relaxing the nuclide field the relaxation is applied on the neutron flux through the criticality equation.

The description of Algorithms 1 and 2 is schematic; while they make use of Eq. (18), they could equally well relax the neutron flux or the nuclide density using Eqs. (14) and (15). Algorithm 1 can be implemented easily as the calculation of the relaxed neutron flux and one-group cross sections can simply combine samples over the inner iteration steps. Algorithms 2 may be less suitable for Monte Carlo calculations since the fuel is depleted with a neutron flux that may suffer from large statistical errors (as the flux is computed in a single inner iteration step).

The purpose of this paper was to derive a stable coupling scheme for Monte Carlo burnup calculations with the thermal–hydraulic feedback. Specific optimisations of this scheme were not addressed in this paper.

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