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Technical note

Time step length versus efficiency of Monte Carlo burnup calculations

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ABSTRACT

We demonstrate that efficiency of Monte Carlo burnup calculations can be largely affected by the selected time step length. This study employs the stochastic implicit Euler based coupling scheme for Monte Carlo burnup calculations that performs a number of inner iteration steps within each time step. In a series of calculations, we vary the time step length and the number of inner iteration steps; the results suggest that Monte Carlo burnup calculations get more efficient as the time step length is reduced. More time steps must be simulated as they get shorter; however, this is more than compensated by the decrease in computing cost per time step needed for achieving a certain accuracy.

1. Introduction

Monte Carlo burnup codes allow to perform fuel cycle analyses of a wide variety of nuclear reactors without the need of tuning the computing procedures and cross section libraries to a specific reactor design. This general advantage over deterministic codes comes at the cost of low maturity/reliability and computing efficiency of existing Monte Carlo burnup codes (Dufek and Hoogenboom, 2009; Dufek et al., 2013b).

Efficiency of Monte Carlo burnup calculations is generally affected by numerous aspects, such as the evaluation procedure of one-group microscopic cross sections that are needed for depletion calculations (Haeck and Verboomen, 2007), or by the choice of free parameters, including the time step length and the number of neutron histories simulated at each time step. The purpose of this note is to study the dependence of efficiency of Monte Carlo burnup calculations on the selected time step length.

The test calculations are based on the stochastic implicit Euler (SIE) based coupling scheme (Dufek et al., 2013a) that performs an inner iteration at each time step. The SIE-based coupling scheme is briefly described in Section 2. The description, results and discussion of numerical tests are given in Section 3. Our conclusions are summarised in Section 4.

2. Description of the SIE-based coupling scheme

First we define the nuclide field $\mathbf{N}(\mathbf{r})$ as a vector whose ith element denotes the atomic concentration of ith nuclide at $\mathbf{r}$; the geometry and material properties of a nuclear reactor are all captured in $\mathbf{N}(\mathbf{r})$. Next, let $\phi(\mathbf{r},\Omega,E)$ be the fundamental-mode neutron flux in the system, defined as the fundamental solution of the criticality (eigenvalue) neutron transport equation

$$[L(\mathbf{N},T)-\frac{1}{k}F(\mathbf{N},T)]\phi(\mathbf{s})=0, \tag{1}$$

where $T(\mathbf{r})$ is the temperature field, $L(\mathbf{N},T)\phi(\mathbf{s})$ represents the migration and loss of neutrons from $\mathbf{s}\equiv(\mathbf{r},\Omega,E)$, and $F(\mathbf{N},T)\phi(\mathbf{s})$ accounts for neutron production in $\mathbf{s}$ due to fission. Thus, ϕ is generally given by $\mathbf{N}(\mathbf{r}),T(\mathbf{r})$ and the boundary conditions. To simplify the notation, we consider the nuclide field in other than fuel regions as well as the temperature field $T(\mathbf{r})$ in the whole system being fixed. In the following text, $\hat{\phi}(\mathbf{N})$ specifically denotes the fundamental-mode neutron flux computed by a Monte Carlo criticality code in a reactor with the fuel nuclide field $\mathbf{N}$.

The fuel nuclide field $\mathbf{N}(\mathbf{r})$ changes during the reactor operation due to the depletion process that can be described by the differential burnup equation (Bell and Glasstone, 1970),

$$\frac{\mathrm{d}\mathbf{N}(\mathbf{r},t)}{\mathrm{d}t}=\mathbb{M}(\phi,T)\mathbf{N}(\mathbf{r},t), \tag{2}$$

where

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

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where $\mathbb{X}$ is a cross-section and fission yield matrix, $\mathbb{D}$ is a decay matrix. When ϕ is fixed then Eq. (2) has a formal solution (Bell and Glasstone, 1970)

$$\mathbf{N}(\mathbf{r},t) = \exp[\mathbb{M}(\phi,T)(t-t_0)]\mathbf{N}_0(\mathbf{r}), \tag{3}$$

where $\mathbf{N}_0(\mathbf{r})$ is the fuel nuclide field at time t_0. The numerical solution of Eq. (2) with a fixed neutron flux can be obtained by various methods (Cetnar, 2006; Pusa and Leppänen, 2010). Note that $\mathbb{M}(\phi)$ is determined by the neutron energy spectrum; thus, all references to Eq. (3) in this paper assume the reaction rates reflect the neutron energy spectrum given by ϕ. The temperature dependence in Eq. (3) is dropped in the following text as the temperature field is fixed.

The stochastic implicit Euler method was derived and described by Dufek et al. (2013a); here, we include only its brief description. As other Monte Carlo burnup schemes, the SIE-based scheme discretises the target time period into a number of time steps, and updates $\mathbf{N}$ and ϕ at each step. In the context of burnup calculations, the implicit Euler method uses the end-of-step neutron flux to deplete the fuel over the whole time step. Since the end-of-step flux and nuclide field are not known, the SIE scheme iterates them via an inner iteration, as described in Algorithms 1 that represents one of two possible implementations of the inner iteration (Dufek et al., 2013a). The number of inner iteration steps in the ith time step is denoted by q_i in Algorithms 1.

Algorithm 1. The SIE coupling scheme with the relaxation applied on the neutron flux.

input: $\mathbf{N}_0, \Delta t$
$\phi_0 \leftarrow \hat{\phi}(\mathbf{N}_0)$
for $i \leftarrow 0, 1, \ldots$ **do**
  $\bar{\mathbf{N}}_{i+1}^{(0)} \leftarrow \exp[\mathbb{M}(\phi_i)\Delta t]\mathbf{N}_i$
  for $n \leftarrow 1, 2, \ldots, q_i$ **do**
    $\phi_{i+1}^{(n)} \leftarrow \hat{\phi}\left(\bar{\mathbf{N}}_{i+1}^{(n-1)}\right)$
    $\bar{\phi}_{i+1}^{(n)} \leftarrow \sum_{j=1}^{n} \phi_{i+1}^{(j)}/n$
    $\bar{\mathbf{N}}_{i+1}^{(n)} \leftarrow \exp[\mathbb{M}(\bar{\phi}_{i+1}^{(n)})\Delta t]\mathbf{N}_i$
  end for
  $\mathbf{N}_{i+1} \leftarrow \bar{\mathbf{N}}_{i+1}^{(q_i)}$
  $\phi_{i+1} \leftarrow \bar{\phi}_{i+1}^{(q_i)}$
end for

3. Numerical tests

3.1. Numerical test model

The numerical test model should have properties allowing a simple evaluation of the error in the test calculations. We therefore prefer to use a simple numerical model where the solution is, at least partly, known. In our previous test calculations (Dufek et al., 2013a,b), we have used a simple fuel pin cell model where the neutron flux and fuel depletion was known to be axially uniform; we use the same test model here. The numerical test model is a square fuel cell with the following properties:

Fuel	UO_2
Cladding material	Zr
Moderator	light water
Radius of fuel pellets	0.41 cm
Outer radius of cladding	0.475 cm
Rod pitch	1.26 cm
Length of the fuel rod	300 cm
U enrichment in ^{235}U	3.1 wt%
Fuel density	10 g/cm^3
Water density	0.7 g/cm^3
Axial profile of water density	flat
Linear power rating	40 kW/m
Boundary conditions (all faces)	reflective

The model is axially divided into eight equidistant spatial zones; the fuel materials in the zones are defined with unique material numbers (their nuclide compositions can vary independently during the burnup calculation). The fuel material in each zone is depleted only using the local neutron flux computed in the actual zone.

The model has no neutron leakage due to reflective boundary conditions applied to all faces. Therefore, the correct steady-state flux, the fuel depletion and thus the total macroscopic cross section must be uniform along the fuel rod at any time. Although we know the total macroscopic cross sections should ideally be equal in all zones, we do not know the correct absolute value. Therefore, a reference solution is still needed, see Section 3.2.

The primary result of Monte Carlo burnup calculations describes how the nuclide field changes over the time steps. As the nuclide field is a vector quantity dependent on position, calculation of its error is not straightforward. Due to unequal importance of various nuclides for neutron transport, the nuclide concentration should be weighted by its one-group cross section. Therefore, we evaluate the error in the nuclide field during the test Monte Carlo burnup calculations via the deviation of the total macroscopic cross section of the fuel material in various zones from the reference solution. For this purpose, we define the standard deviation s_Σ as

$$s_\Sigma^2 = \frac{1}{8}\sum_{c=1}^{8}(\Sigma_c - \Sigma_{\text{ref}})^2, \tag{4}$$

where Σ_c is the total macroscopic cross section of the fuel material in zone c in a specific Monte Carlo burnup calculation at a specific depletion, and Σ_{ref} is the reference total macroscopic cross section corresponding to the same depletion. The reference value is obtained from a special calculation with only a single fuel material, see Section 3.2.

The final relative error, e, is then evaluated as

$$e = \frac{s_\Sigma}{\Sigma_{\text{ref}}} = \frac{\sqrt{\frac{1}{8}\sum_{c=1}^{8}(\Sigma_c - \Sigma_{\text{ref}})^2}}{\Sigma_{\text{ref}}}. \tag{5}$$

The efficiency of the test calculations is evaluated by the figure-of-merit, *FOM*,

$$FOM = \frac{1}{\bar{e}^2 h} \tag{6}$$

where h is the total number of neutron histories simulated during the whole calculation, and $\bar{e}$ is the relative error defined by Eq. (5) averaged over all simulated time steps. We choose to evaluate the computing cost in the figure-of-merit in terms of the total number of simulated neutron histories in Eq. (6) rather than in the computing time in order to eliminate the dependence on CPU speed and efficiency of various parallel-computing schemes for Monte Carlo criticality calculations, and allow a fair comparison of our results with future results obtained on other computers.

In order to evaluate the effect of inactive cycles, we also define FOM^* as