Description of a stable scheme for steady-state coupled Monte Carlo - thermal-hydraulic calculations

Jan Dufek[a,*], J. Eduard Hoogenboom[b]

[a] *Royal Institute of Technology (KTH), Division of Nuclear Reactor Technology AlbaNova University Center, 10691 Stockholm, Sweden*
[b] *Delft Nuclear Consultancy, IJsselzoom 2, 2902 LB Capelle aan den IJssel, The Netherlands*

Abstract

Here, we provide a detailed description of a numerically stable and efficient coupling scheme for steady-state Monte Carlo neutronic calculations with thermal-hydraulic feedback. While we have previously derived and published the stochastic approximation based method for coupling the Monte Carlo criticality and thermal-hydraulic calculations, its possible implementation has not been described in a step-by-step manner. As the simple description of the coupling scheme was repeatedly requested from us, we have decided to make it available via this note.

Keywords: Monte Carlo calculations, thermal-hydraulic feedback, coupling scheme

1. Introduction

The application of the Monte Carlo method is no longer limited to simple criticality calculations; the advances in the computer technology allow its application in more complex problems now. In this work, we focus on steady-state Monte Carlo neutronic calculations with the thermal-hydraulic feedback. The outcome of such calculations gives the steady-state core conditions (the spatial distribution of neutron flux, power, temperature, coolant density, etc.) in a nuclear reactor running at a fixed power.

*Corresponding author.
Email address: jandufek@kth.se (Jan Dufek)

The coupled criticality and thermal-hydraulic equations represent a non-linear problem that should be addressed by a numerically stable method. We have previously derived and published the stochastic approximation based method for coupling the Monte Carlo criticality and thermal-hydraulic calculations (Dufek and Gudowski, 2006). In its basic form the steady-state solution is obtained via a relaxation procedure governed by the Robbins-Monro algorithm that is guaranteed to converge (Robbins and Monro, 1951).

While the stochastic approximation based coupling scheme has been available, we could often see attempts at coupling the Monte Carlo criticality and thermal-hydraulic solvers via a simple fixed-point method that may diverge, depending on the system properties. Partly, we ascribe this to the fact a simple step-by-step description of the coupling scheme was not provided by Dufek and Gudowski (2006). We wish to redeem it by this note that contains the detail descriptions.

The paper is organised as follows. Sec. 2 states simple forms of the governing equations. Sec. 3 briefly describes the stochastic approximation method for computing the steady-state solution, as derived by Dufek and Gudowski (2006). Sec. 4 contains the step-by-step description of the stochastic approximation based coupling scheme. Sec. 5 gives a discussion on the coupling scheme.

2. Governing equations

Geometry and material properties of a nuclear reactor core can be fully described by the nuclide field $\mathbf{N}(\mathbf{r})$, where the elements of $\mathbf{N}(\mathbf{r})$ denote concentrations of various nuclides at position $\mathbf{r}$. Next, let $T(\mathbf{r})$ describe the temperature field in the whole core.

The fundamental-mode neutron flux $\phi(\mathbf{r}, \mathbf{\Omega}, E)$ is then determined by the nuclide and temperature fields and the boundary conditions via the criticality (eigenvalue) neutron transport equation

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

where $L\phi$ represents the migration and loss of neutrons from $(\mathbf{r}, \mathbf{\Omega}, E)$, and $F\phi$ accounts for neutron production in $(\mathbf{r}, \mathbf{\Omega}, E)$ due to fission. Let the solution to Eq. (1) be represented by a function $\phi_B(\mathbf{N}, T)$,

$$\phi = \phi_B(\mathbf{N}, T). \tag{2}$$

We shall further address the variable nuclide field in the coolant (moderator) simply as $\mathbf{N}(\mathbf{r})$, as the nuclide field in other locations is fixed in the considered problem. In the following text, the Monte Carlo solution of Eq. (1) is denoted as $\hat{\phi}_B\big(\mathbf{N}, T, s\big)$ where s is the number of simulated neutron histories.

The temperature and coolant (moderator) nuclide fields, $T(\mathbf{r})$ and $\mathbf{N}(\mathbf{r})$, are determined by thermal-hydraulic equations that ensure that the coolant mass, energy and momentum are conserved in the whole reactor at any time. For given coolant mass flow and inlet pressure boundary conditions, $T(\mathbf{r})$ and $\mathbf{N}_(\mathbf{r})$ are determined by the power distribution (or the neutron flux field $\phi(\mathbf{r}, \mathbf{\Omega}, E)$). Therefore, let $T_\phi(\phi)$ and $\mathbf{N}_\phi(\phi)$ represent the solution to the thermal-hydraulic equations,

$$T(\mathbf{r}) = T_\phi(\phi), \tag{3}$$

$$\mathbf{N}(\mathbf{r}) = \mathbf{N}_\phi(\phi). \tag{4}$$

Substituting T and $\mathbf{N}$ from Eqs. (3) and (4) into Eq. (2) gives

$$\phi = \phi_B\big(\mathbf{N}_\phi(\phi), T_\phi(\phi)\big), \tag{5}$$

which shows that the steady-state neutron flux is determined by the temperature and coolant nuclide fields that are themselves determined by the neutron flux. Eq. (5) is thus a non-linear equation that can be written in a simpler form

$$\phi = G(\phi) \tag{6}$$

where G represents the right-hand side of Eq. (5) as a function of ϕ.

3. The stochastic approximation

We assume that the fundamental neutron flux is computed by a Monte Carlo solver; therefore, G in Eq. (6) must be approximated by a stochastic function

$\hat{G}$ that contains a noise term ε,

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

This changes Eq. (6) into

$$\phi = \hat{G}(\phi), \tag{7}$$

which is the non-linear stochastic root-finding problem. The noise term ε depends on the number of random evaluations, s, of G as

$$\varepsilon \sim \frac{1}{\sqrt{s}}.$$

In the context of Monte Carlo criticality calculations, s represents the number of simulated neutron histories. In the following text, $G(\phi)$ evaluated by a Monte Carlo simulation of s neutron histories is denoted as $\hat{G}_s(\phi)$.

Dufek and Gudowski (2006) showed that Eq. (7) can be efficiently solved via the stochastic approximation based iteration

$$\phi^{(n)} = \phi^{(n-1)} - \alpha_n d(\phi^{(n-1)} - \hat{G}_{s_n}(\phi^{(n-1)})), \quad n = 1, 2, \ldots \tag{8}$$

where $d \in (0, 1]$ is a fixed scalar, α_n is the step-size in the n^{th} step, s_n is the number of neutron histories simulated in the n^{th} step, and $\phi^{(0)}$ is an initial guess of the neutron flux. Unless the initial guess is known to a certain accuracy, we advice to set $d = 1$ to achieve the best efficiency; then Eq. (8) can be rewritten into a common relaxation form

$$\phi^{(n)} = (1 - \alpha_n)\phi^{(n-1)} + \alpha_n \hat{G}_{s_n}(\phi^{(n-1)}). \tag{9}$$

There are several options as to how α_n and s_n can be selected at the n^{th} step. One possibility is to fix s_n at all steps, $s_n = s = \text{const.}$, and choose the step-size according to the Robbins-Monro algorithm (Robbins and Monro, 1951) as

$$\alpha_n = \frac{1}{n}. \tag{10}$$

When α_n is computed by Eq. (10) then Eq. (9) is equivalent to

$$\phi^{(n)} = \frac{1}{n} \sum_{i=1}^{n} \hat{G}_s(\phi^{(i-1)}), \tag{11}$$

as derived by Dufek and Gudowski (2006). The statistical error in the relaxed flux $\phi^{(n)}$ is reduced with each new iteration step thanks to combining the solutions from all previous steps.

Dufek and Gudowski (2006) explained that it is reasonable to let s_n grow over the iterations steps. This is motivated by the fact that the initial guess $\phi^{(0)}$ might contain large errors, and so the initial temperature and coolant nuclide fields that would be computed according to $\phi^{(0)}$ would be erroneous as well. It would be a waste of the computational time to compute $\phi^{(1)}$ using a large sample-size to a great statistical precision when we knew the accuracy of the solution would be still poor due to the large errors in temperature and coolant nuclide field. A possible way to solve this problem would be to keep s_n relatively small (and fixed) over all iteration steps as we know the statistical precision of the relaxed solution improves with each step; however, the frequent re-starts of the Monte Carlo solver would decrease the efficiency of the calculation since a large part of the computing time would be wasted on loading the neutron cross-section libraries, simulating the inactive cycles, and other procedures that must be performed after launching the Monte Carlo solver.

Therefore, Dufek and Gudowski (2006) suggested a system of two equations to calculate unique values of α_n and s_n at each step. The first equation

$$\alpha_n = \frac{s_n}{\sum_{i=1}^{n} s_i} \tag{12}$$

practically demands that the weight of a certain step in the relaxed solution is equal to the relative computing cost of the step, which is motivated by the idea of the Robbins-Monro algorithm. The second equation

$$\alpha_n \propto \frac{1}{\sqrt{\sum_{i=1}^{n} s_i}} \tag{13}$$

demands that α_n decreases in the same rate as the statistical error in standard Monte Carlo calculations. Eqs. (12) and (13) give the quadratic equation

$$s_n^2 - s_1 s_n - s_1 \sum_{i=1}^{n-1} s_i = 0, \tag{14}$$

that has a positive root

$$s_n = \frac{s_1 + \sqrt{s_1^2 + 4s_1 \sum_{i=1}^{n-1} s_i}}{2}. \tag{15}$$

The initial sample-size s_1 must be guessed. Knowing s_n, the value of α_n can be computed by Eq. (12).

Dufek and Gudowski (2006) address the above way of varying α_n and s_n as the "optimal" procedure. They have suggested yet another, "adaptive", procedure that controls α_n and s_n according to the actual stability of the iteration; however, we wish not to include this procedure here to keep this note as simple as possible.

4. Description of the coupling scheme

Algorithm 1 describes the coupling scheme where the sample-size and step-size are varied according to the "optimal" procedure derived by Dufek and Gudowski (2006). Note that the neutron flux and temperature fields are written as vectors in Algorithm 1. These vectors represent spatial distributions of the respective variables, computed using a spatial mesh superimposed over the whole system. Thus, for instance the first element in $\vec{\phi}^{(0)}$ gives the neutron flux integrated over the first spatial zone. The coolant nuclide field is represented by a unique vector at each spatial zone.

The coupling scheme described by Algorithm 1 relaxes the neutron flux distribution since we used the neutron flux in derivations in Sections 2 and 3; however, the relaxation may equally well be applied to the power distribution instead. As the power distribution is the common input to the thermal-hydraulic solvers it is convenient to let the Monte Carlo code calculate directly the power distribution instead of the neutron flux.

Algorithm 1 Description of the MC-TH coupling scheme with the variable sample-size and step-size.

1: **input:** P, s_1, $\vec{\phi}^{(0)}$
2: $S_0 \leftarrow 0$
3: **for** $n \leftarrow 1, 2, \ldots$ **do**
4: $\quad s_n \leftarrow (s_1 + \sqrt{s_1^2 + 4 s_1 S_{n-1}})/2$
5: $\quad S_n \leftarrow S_{n-1} + s_n$
6: $\quad \alpha_n \leftarrow s_n / S_n$
7: $\quad \vec{T}^{(n)} \leftarrow \vec{T}_\phi(\vec{\phi}^{(n-1)})$
8: $\quad \vec{\mathbf{N}}^{(n)} \leftarrow \vec{\mathbf{N}}_\phi(\vec{\phi}^{(n-1)})$
9: $\quad \vec{G}_n \leftarrow \hat{\phi}_B\big(\vec{\mathbf{N}}^{(n)}, \vec{T}^{(n)}, s_n\big)$
10: $\quad$ normalise flux $\vec{G}_n$ to achieve power P
11: $\quad \vec{\phi}^{(n)} \leftarrow (1 - \alpha_n)\vec{\phi}^{(n-1)} + \alpha_n \vec{G}_n$
12: **end for**

Below, we provide comments to specific lines in Algorithm 1:

Line #1: The initial values and input variables are set at this line. The value of P represents the required total power of the reactor. The initial sample-size value, s_1, must be guessed; we provide some recommendations of suitable values in Sec. 5. The initial neutron flux (or power) distribution $\vec{\phi}^{(0)}$ may be set uniform if a better estimate is not available; $\vec{\phi}^{(0)}$ must be normalised so that the corresponding total power equals P.

Line #2: The variable S_n denotes the total size of samples combined over the first n simulated iteration steps, $S_n = \sum_{i=1}^{n} s_i$. When $\vec{\phi}^{(0)}$ is guessed then it is reasonable to set S_0 at zero, as depicted in Algorithm 1. In that case, $\vec{\phi}^{(0)}$ will not be reflected in the relaxed flux (power) solution, and $\vec{\phi}^{(0)}$ will be used only to set up the initial temperature and coolant nuclide fields. When $\vec{\phi}^{(0)}$ is a very good approximation of the steady-state flux (power) distribution then S_0 should represent the sample-size that a Monte Carlo calculation would need to calculate $\vec{\phi}^{(0)}$ to the same precision. When

$S_0 > 0$ then $\vec{\phi}^{(0)}$ is reflected in the final relaxed flux (power) solution.

Line #3: The stopping criterion for the iteration is not covered here; it may be set up e.g. by monitoring the convergence of the relaxed solution, see (Dufek and Gudowski, 2006).

Line #4: Monte Carlo criticality codes usually require to specify the neutron batch size, b, and the number of active cycles, c, to be simulated. Knowing the total number of neutron histories s_n, the user can for instance fix the batch size b for all steps, and compute the number of cycles, $c = s_n/b$. Note that when this line is altered to

$$s_n \leftarrow \text{const.}$$

(i.e., the sample-size is fixed over all steps) and $S_0 = 0$ then the step-size is generated according to the Robbins-Monro algorithm at line #6.

Line #7: Here, the temperature field is computed according to the flux (or power) distribution $\vec{\phi}^{(n-1)}$.

Line #8: While $\vec{\mathbf{N}}^{(n)}$ formally denotes the coolant nuclide field, the thermal-hydraulic calculation may provide directly the coolant density distribution.

Line #9: The Monte Carlo code evaluates the neutron flux (or power) distribution via simulating s_n neutron histories here. The computed distribution is saved in vector $\vec{G}_n$.

Line #10: The neutron flux (or power) distribution $\vec{G}_n$ must be normalised to conform to the total power P.

Line #11: The relaxation is applied to the flux (power) distribution here.

5. Discussion

As for the choice of the initial sample-size s_1, we recommend to choose such a value that the active cycles of the first Monte Carlo criticality calculation would

take only a very small fraction (around one or few %) of the total acceptable computational time allocated to the whole calculation. Moreover, s_1 should not be too large because the increase in the sample-size, $s_n - s_{n-1}$, approaches $s_1/2$ over the iteration steps, as follows from Eq. (14); a large value of s_1 would result in a rapid growth of simulated cycles over the iteration steps.

An open question is the selection of the initial fission source and the number of inactive cycles to be simulated at each Monte Carlo criticality calculation. At the first iteration step, we suggest to set up the fission source distribution same as the one of $\vec{\phi}^{(0)}$ (only scaled appropriately). For each of the following iteration steps it appears reasonable to use the fission source distribution converged in the previous step.

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