Nuclear Engineering and Technology 49 (2017) 1095–1099

Contents lists available at ScienceDirect

Nuclear Engineering and Technology

journal homepage: www.elsevier.com/locate/net

Technical Note

Stabilization effect of fission source in coupled Monte Carlo simulations

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A R T I C L E I N F O

Article history:
Received 4 October 2016
Received in revised form
14 February 2017
Accepted 27 February 2017
Available online 11 July 2017

Keywords:
Monte Carlo
Coupled simulation
Fixed-point iteration
Numerical stability
Feedback

A B S T R A C T

A fission source can act as a stabilization element in coupled Monte Carlo simulations. We have observed this while studying numerical instabilities in nonlinear steady-state simulations performed by a Monte Carlo criticality solver that is coupled to a xenon feedback solver via fixed-point iteration. While fixed-point iteration is known to be numerically unstable for some problems, resulting in large spatial oscillations of the neutron flux distribution, we show that it is possible to stabilize it by reducing the number of Monte Carlo criticality cycles simulated within each iteration step. While global convergence is ensured, development of any possible numerical instability is prevented by not allowing the fission source to converge fully within a single iteration step, which is achieved by setting a small number of criticality cycles per iteration step. Moreover, under these conditions, the fission source may converge even faster than in criticality calculations with no feedback, as we demonstrate in our numerical test simulations.

1. Introduction

The Monte Carlo approach has the potential to deliver solutions for complex multiphysics problems in reactor physics, including problems that involve neutronics coupled to thermal hydraulics or other types of feedback. A variety of programs that couple Monte Carlo criticality solvers externally to feedback solvers is available [1,2]. Some Monte Carlo codes have integrated the feedback solvers with the criticality code [3–6]. Recent studies extend the application of coupled Monte Carlo codes to simulate transient scenarios [7]. Despite this progress, many problems still remain unresolved.

One major concern when performing coupled Monte Carlo simulations is numerical stability. Numerical instabilities may arise due to the nonlinearities inherent to coupled neutronics problems. For popular Monte Carlo burnup simulations, several stable coupling schemes have been suggested recently [8,9], and some have also been extended to Monte Carlo burnup calculations with thermal–hydraulic feedback [10]. Nevertheless, more research is needed to ensure numerical stability for other kinds of coupled Monte Carlo simulations.

In this note, we address Monte Carlo solutions to steady-state systems with feedback; these are solutions to nonlinear problems. The solution is commonly obtained iteratively; Monte Carlo solvers provide the neutron flux or power distribution to feedback solvers, while the feedback solvers may provide thermal–hydraulic conditions or other data to Monte Carlo solvers.

Fixed-point iteration [11–14] is a basic numerical way of solving nonlinear problems. The Monte Carlo solver and feedback solvers are executed in a simple iterative manner. At each iteration step, the Monte Carlo solver takes the feedback solver output from the previous step, and the feedback solver uses the latest output from the Monte Carlo solver. The solution is expected to improve with each new step. In the following, the terms “iteration step” and “iteration” relate exclusively to the successive execution of various solvers, while the terms “criticality cycle” and “cycle” relate to the simulation of one neutron generation within a single Monte Carlo criticality simulation.

The nonlinear nature of coupled simulations can introduce numerical instabilities in the simulations, depending on the way the solution is obtained. Dufek and Gudowski [15] argue that numerical instabilities, in the form of large spatial oscillations of the power distribution, may develop in coupled simulations when the neutron flux or power distribution is iterated by the fixed-point method; they suggest obtaining the solution via the stochastic approximation, which combines solutions of all iteration steps. A simplified formulation of this solution is offered by Dufek and Hoogenboom [16]. The efficiency of the stochastic approximation, however,

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http://dx.doi.org/10.1016/j.net.2017.02.008

depends on a number of free parameters that may not be simple to estimate.

Here we show that fixed-point iteration can, in fact, be stable and efficient under specific (yet easily realized) conditions. It is apparent that Dufek and Gudowski [15] assume that the Monte Carlo solution converges at each iteration step, which requires simulating a large number of criticality cycles at each iteration step. When doing so, the simulation may become numerically unstable. Nevertheless, we show that the simulation can be stabilized by reducing the number of criticality cycles simulated at each iteration step. In order to allow the fission source to converge in the long run, we reuse the fission source over the successive iteration steps; i.e., the initial fission source needed by the Monte Carlo solver is taken from the last cycle of the previous iteration step.

We argue that the fixed-point iteration can be stabilized due to certain properties of the fission source. With each criticality cycle, the fission source changes only a little. Therefore, when a relatively small number of criticality cycles is simulated by the Monte Carlo solver at each iteration step, the fission source changes its shape slowly over the successive iteration steps, acting as a stabilization element. As the computed power (or neutron flux) distribution is linked directly to the fission source, the whole simulation can be stabilized this way.

The possibilities of stabilizing the fixed-point iteration are insufficiently explored in the literature. In this work, we identify the fission source as an effective but as yet unused tool for stabilizing the fixed-point iteration. The importance of this scientific contribution lies in its simplicity and the popularity of fixed-point iteration.

2. Materials and Methods

2.1. Solvers

Numerical test simulations are performed with a proprietary nonanalog continuous-energy three-dimensional Monte Carlo code that uses the JEFF-3.1 point-wise neutron cross-section library. The code can run test simulations that are either coupled or noncoupled (i.e., Monte Carlo criticality simulations without feedback).

Our coupled test simulations incorporate feedback from the abundant fission product ^{135}Xe, which has a relatively strong effect on the thermal neutron flux [17,18]. Our xenon feedback solver computes the asymptotic ^{135}Xe concentration distribution that is established in a nuclear reactor after a sufficiently long time under fixed conditions. The solver accounts for the direct and indirect production of ^{135}Xe from ^{235}U, and for the possibility of neutron capture in ^{135}I; however, assuming monoenergetic, thermal conditions, energy dependences are neglected. The feedback solver is used only to change the concentration of ^{135}Xe in various fuel regions of the system modeled by the Monte Carlo criticality solver.

2.2. Numerical test model

The numerical test model comprises a single fuel rod radially centered in a square cell. The fuel is UO_2; the fuel rod is surrounded by cladding and coolant. Table 1 gives the parameters of the system (derived from common specifications of pressurized water reactors).

In order to specify the ^{135}Xe concentration according to the local neutron flux, a spatial mesh is superimposed over the system. The mesh divides the test model axially into 30 equidistant nodes. The neutron flux and xenon concentration distribution are discretized over the mesh; the neutron flux is furthermore normalized with respect to an average linear power of 158.8 W/cm.

Table 1
Fuel pin geometry and material parameters.

Fuel pin length	300 cm
Fuel pellet diameter	0.82 cm
Rod outer diameter	0.95 cm
Pitch	1.26 cm
Fuel	UO_2
Density	10 g/cm^3
Enrichment in ^{235}U	3.10 wt%
Cladding	^{90}Zr
Density	6.5 g/cm^3
Coolant	H_2O
Density	0.70 g/cm^3

We choose to apply reflective boundary conditions on all faces of the system. Under these conditions, the nonlinear solution and the steady-state fission source distribution are axially flat. The fact that we know the solution makes it possible for us to evaluate the error in the computed results without need for a reference simulation.

If void boundary conditions are applied to the axial faces, then the reference steady-state solution will be unknown and cannot be obtained easily. A solution given by a special reference simulation can always be questioned as being affected by possible numerical instability, insufficient statistics, poor source convergence, or the presence of source bias [19–21]. These problems can be overcome here by choosing a system with a known steady-state solution.

The initial fission source at the first iteration step is centered at the first mesh node (a point 5 cm from the boundary) in all tests. The asymptotic ^{135}Xe concentration distribution is set accordingly; i.e., at the first iteration step, ^{135}Xe is present only in the first node. This poor initial guess and asymmetrical arrangement are chosen on purpose to trigger possible numerical instabilities.

The simple numerical model is chosen here purposely for its ability to demonstrate deficiencies in numerical methods. If a numerical method fails in a simulation of a very complex model, the failure can be attributed to the model complexity; the method could still be expected to perform well in simulations of other systems. Nevertheless, when the method fails in a simulation of a simple system, the method should not be expected to perform well in simulations of other, more complex systems. Test simulations of simple models are, therefore, relevant to studies of numerical method deficiencies, such as the possible numerical instability in coupled simulations, as in this study.

2.3. Test cases

We compare five cases of coupled simulations that differ in the number of Monte Carlo criticality cycles simulated at each iteration step (Table 2). In addition, we study one noncoupled test case in which the xenon feedback is neglected. In all other respects, settings for the coupled and noncoupled test cases are the same.

Each criticality cycle simulates 50,000 neutron histories; all criticality cycles are active. The total number of iteration steps in each test case differs depending on the chosen number of cycles per step (Table 2); however, the total number of simulated neutron histories is conserved at 2×10^9.

Table 2
Description of coupled test cases.

Case no.	No. of cycles per step	No. of iteration steps
1	4,000	10
2	1,000	40
3	100	400
4	10	4,000
5	1	40,000

2.4. Test methodology

We choose to analyze the stability of the coupled simulations by studying the spatial distribution of the fission source. When a numerical instability develops in the simulation, the fission source undergoes spatial oscillations over the successive iteration steps. These oscillations can be measured easily.

For the purpose of measuring the error in the fission source, the fission source is discretized over the same mesh as the neutron flux. Since the ideal fission source distribution is axially flat in the test model geometry, the relative error in the fission source can be evaluated as follows:

$$\varepsilon = \frac{\left\|\tilde{\mathbf{f}} - \tilde{\mathbf{f}}^{*}\right\|_1}{2}, \quad (1)$$

where $\mathbf{f}$ is the discretized fission source, $\mathbf{f}^{*}$ is the ideal discretized fission source (a vector with equal elements), and the tilde operator ~ normalizes any vector to its first norm. The factor of 2 in Eq. (1) scales the maximum possible relative error to unity.

If a simulation is repeated with a different seed in the Monte Carlo random number generator, slightly different results will be measured. To deal with these variations in results, we repeat each test case 504 times and average the relative error ε over all repetitions into the mean $\bar{\varepsilon}$ value.

3. Results

To compare test cases with varied numbers of criticality cycles per iteration step, Fig. 1 depicts the mean relative error in the fission source with respect to the total number of simulated neutron histories (i.e., histories combined over iteration steps and all criticality cycles within each step).

The relative error in the initial fission source (placed close to a boundary) is nearly unity in all test cases. As the total number of simulated neutron histories grows, the fission source converges and the error decreases until only the statistical error or an error caused by the numerical instability remains in the fission source.

The error in the fission source cannot decrease below the error caused by the statistical noise that is always present in the fission source, irrespective of the number of simulated cycles or step. The statistical noise in the fission source is of the order $O(1/\sqrt{m})$, where m is the number of neutrons simulated per cycle; therefore, the error in the fission source cannot decay below the limit of the order $O(1/\sqrt{m})$.

The test case with no feedback (the noncoupled case) takes a total of about 4×10^7 neutron histories to achieve fission source convergence (Fig. 1). The relative error in the converged fission source caused by random noise amounts to about 0.022.

Large spatial oscillations in the fission source can be observed in the coupled test cases with 4,000 and 1,000 cycles per iteration step (Fig. 2). Owing to these oscillations, the mean relative error remains larger than in all other test cases (Fig. 1). When the number of cycles per iteration step is this large, the fission source can fully converge at each iteration step; however, it converges to conditions that are far from steady state.

Interestingly, the fission source in the coupled test simulations with one or 10 cycles per step converges not only in a stable manner with no sign of spatial oscillations (Fig. 3), but also considerably faster than the fission source in the noncoupled simulations (Fig. 1). Convergence of the fission source in these coupled test cases bears strong resemblance to that in the noncoupled test case.

While the fission source in the coupled test case with 100 cycles per step converges, its mean error decays in a zigzag pattern during the first several iteration steps (Fig. 1). This suggests that slight spatial oscillations appear in the fission source during the several first steps. Nevertheless, after reaching the converged state, the error in the fission source remains similar to (perhaps even marginally lower than) that in the noncoupled test simulations.

4. Discussion

The presence of strong feedback in the system (i.e., the strong nonlinearity of the problem) is the reason for the possible numerical instabilities of the fixed-point iteration that manifest themselves in the form of strong spatial oscillations of the neutron flux, fission source, and system conditions (e.g., the xenon concentration). We show here that these oscillations can be eliminated when the Monte Carlo fission source is not allowed to converge completely within each iteration step. This can be done simply by

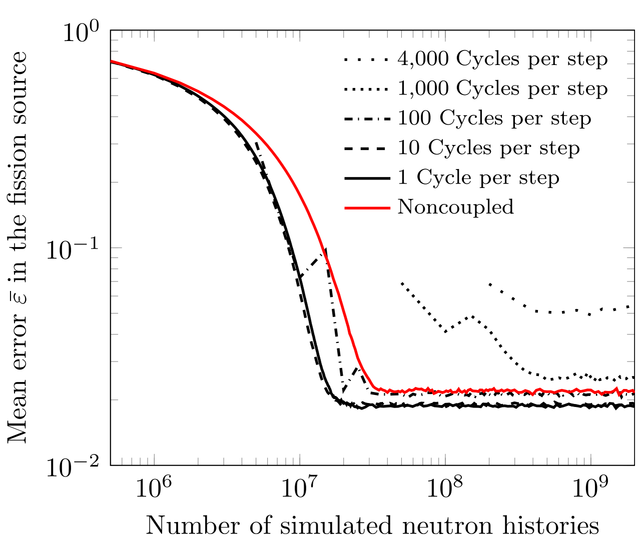

Fig. 1. Mean error in the fission source over the total number of neutron histories simulated by the Monte Carlo solver.

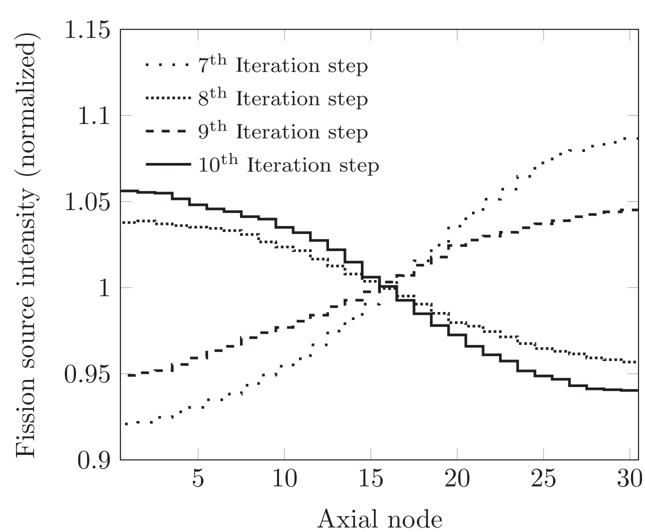

Fig. 2. Fission source distribution at selected iteration steps of a single coupled simulation (with 4,000 criticality cycles per iteration step). To reduce the statistical noise in the depicted fission source, the data are combined over the criticality cycles within the respective iteration steps.

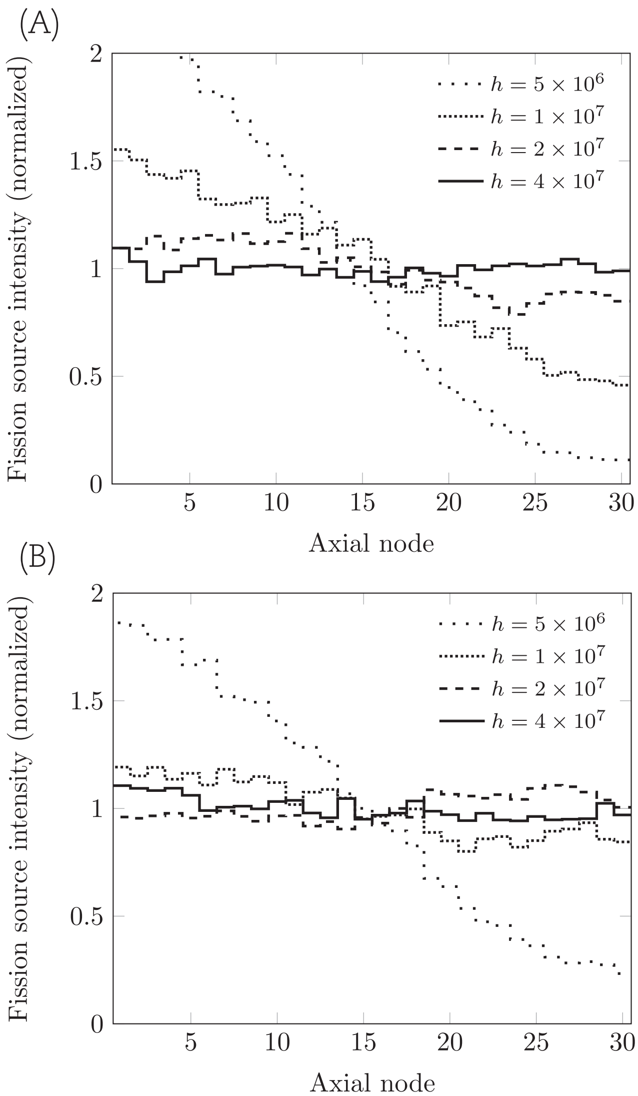

Fig. 3. Fission source distribution depicted at specific points in the simulation when h neutron histories were simulated in total. (A) Single noncoupled test simulation. (B) Single coupled test simulation with 10 cycles per step.

simulating a relatively small number of Monte Carlo criticality cycles within each iteration step.

The small number of criticality cycles per iteration step ensures that the fission source (and the computed neutron flux) does not change significantly within a single iteration step. This way the fission source is not allowed to converge fully to reflect the actual system conditions within each iteration step. This effectively removes the possibility of developing strong spatial oscillations of the neutron flux over successive iteration steps. Global convergence is, however, still reached after a certain number of steps. Our findings are confirmed in a recent study by Gill et al. [22].

When the spatial oscillations of the fission source are prevented by the reduction of the number of cycles per step, the actual convergence rate of the fission source may be even better than that in criticality simulations of the same system with no feedback. This is because deviations from the steady-state fission source are quickly counteracted through the negative feedback when the number of cycles per step is small.

We wish to highlight that in this note we have addressed only the numerical stability of the fixed-point iteration scheme; we have not addressed the efficiency of the coupled simulations. Indeed, Monte Carlo coupling schemes that perform a small number of criticality cycles at each iteration step can be efficient only when the cost of the feedback solver is reasonably small relative to the cost of each iteration step. Similarly, the computing efficiency depends on the way the feedback is implemented in the coupled simulation, and on whether or not the Monte Carlo solver reloads the neutron cross-section libraries at each iteration step.

The condition of a low-cost penalty can be met for analytic and internally coupled feedback solvers such as the xenon feedback solver used in this study. In fact, both MC21 code [4] and SERPENT [5] have a xenon feedback solver, implemented via fixed-point iteration. This note represents a foundation for justifying the numerical stability of simulations coupled via fixed-point iteration under the condition of a reasonably small number of criticality cycles per iteration step.

Our conclusions are based on numerical simulations of a relatively simple model with a single reactivity feedback. Despite its simplicity, the chosen test model incurs the possibility of numerical instabilities. This feature is crucial for the purpose of demonstrating the stabilizing effect of the fission source. Although we may speculate that similar results may be obtained for other more complicated systems, this remains to be confirmed in future studies.

We assume that the numerical instability problems of fixed-point iteration can be observed even if the Monte Carlo solver is substituted for a deterministic solver. While not all fully deterministic coupled codes use fixed-point iteration, those that do could possibly benefit from our conclusions. Nevertheless, deterministic criticality solvers usually converge the fission source at a very fast rate because they may implement effective source convergence acceleration techniques. It may be challenging to tune the number of source iterations made by the deterministic solver so that the source will not converge fully within a single iteration step.

Conflicts of interest

All authors have no conflicts of interest to declare.

Acknowledgments

The simulations were performed on resources provided by the Swedish National Infrastructure for Computing (SNIC) at PDC Center for High Performance Computing at KTH, Royal Institute of Technology.

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