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Original Article

A new approach to the stabilization and convergence acceleration in coupled Monte Carlo–CFD calculations: The Newton method via Monte Carlo perturbation theory

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ABSTRACT

This paper proposes the adoption of Monte Carlo perturbation theory to approximate the Jacobian matrix of coupled neutronics/thermal-hydraulics problems. The projected Jacobian is obtained from the eigenvalue decomposition of the fission matrix, and it is adopted to solve the coupled problem via the Newton method. This avoids numerical differentiations commonly adopted in Jacobian-free Newton–Krylov methods that tend to become expensive and inaccurate in the presence of Monte Carlo statistical errors in the residual. The proposed approach is presented and preliminarily demonstrated for a simple two-dimensional pressurized water reactor case study.

1. Introduction

Multiphysics modeling of fission reactors represents a field of growing interest in the nuclear community [1,2]. Although coupled neutronics/thermal-hydraulics reactor simulations usually employ deterministic codes, more recently, several studies have proposed the adoption of continuous energy Monte Carlo codes for the neutronics solution of multiphysics problems [3–5].

The use of Monte Carlo in coupled simulations is motivated by the desire to obtain more accurate results and more flexible implementations, with respect to legacy deterministic codes. On the other hand, stochastic neutron transport usually involves higher computational requirements when compared to deterministic approaches, and poses barriers to the adoption of common techniques for the solution of nonlinear problems.

This work presents a new approach to stabilize and accelerate the convergence of steady-state coupled Monte Carlo/thermal-hydraulics simulations, by combining the Newton method and Monte Carlo perturbation theory. The method is demonstrated in a simplified pressurized water reactor (PWR) multiphysics simulation.

2. The coupled neutronics/thermal-hydraulics nonlinear problem

For the purpose of the present work, it is useful to describe the coupled neutronics/thermal-hydraulics problem as a system of two equations. The first equation represents the generic neutron transport eigenvalue problem:

$$[\mathbf{L}-\mathbf{S}]\boldsymbol{\varphi}=\frac{1}{k_{eff}}\mathbf{F}\boldsymbol{\varphi} \tag{1}$$

where k_{eff} is the fundamental eigenvalue, **L**, **S** and **F** are the loss, scattering and fission production operators, and ϕ represents the neutron flux solution of the eigenvalue problem.

The second equation is represented here as a generic nonlinear equation in which the thermal-hydraulics (TH) solution T depends on the fission source distribution $\boldsymbol{\varphi}$:

$$T=\boldsymbol{\Theta}(\boldsymbol{\varphi}) \tag{2}$$

In the considered cases, T represents the material temperature and density distributions, and the main feedback of T on the neutronics solution is driven by the Doppler effect and moderator expansion effect. The generic coupling terms can be introduced in

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Eq. (1) by allowing the **L**, **S** and **F** operators to be dependent on the generic TH solution *T*.

$$[\mathbf{L}(T) - \mathbf{S}(T)]\boldsymbol{\varphi} = \frac{1}{k_{\text{eff}}}\mathbf{F}(T)\boldsymbol{\varphi} \tag{3}$$

For simplicity, it is assumed that the fission power distribution $\boldsymbol{\varphi}$ is the only term of Eq. (3) required for solving the coupled problem. Thus, the neutronics equation can be simplified to:

$$\boldsymbol{\varphi} = \boldsymbol{\Phi}(T) \tag{4}$$

Eq. (4) depends on *T* only. Replacing *T* with Eq. (2):

$$\boldsymbol{\varphi} = \boldsymbol{\Phi}[\boldsymbol{\Theta}(\boldsymbol{\varphi})] \tag{5}$$

it is shown that the fission power distribution $\boldsymbol{\varphi}$ depends on the material temperatures and densities (*T*), which depend on the power distribution itself.

Eq. (5) can be written as

$$\boldsymbol{\varphi} = \mathbf{G}(\boldsymbol{\varphi}) \tag{6}$$

so that the coupled neutronics/thermal-hydraulics problem reduces to finding $\boldsymbol{\varphi}$, the solution to **G**.

In practical applications of multiphysics reactor analysis, the power distribution $\boldsymbol{\varphi}$ is scored or discretized into *N* volumes within the reactor core. In this case, $\boldsymbol{\varphi}$ is a vector of *N* components:

$$\boldsymbol{\varphi} = (\varphi_1, \varphi_2 \ldots \varphi_N) \tag{7}$$

and $\mathbf{G}(\boldsymbol{\varphi})$ is a function $\mathbf{G} : \mathbb{R}^N \rightarrow \mathbb{R}^N$:

$$\mathbf{G}(\boldsymbol{\varphi}) = (G_1, G_2 \ldots G_N) \tag{8}$$

3. Monte Carlo/CFD coupling: fixed-point iteration

In the present work, the solution to the nonlinear equation $T = \boldsymbol{\Theta}(\boldsymbol{\varphi})$ is obtained via CFD, adopting the multiphysics C++ toolkit OpenFOAM [6]. The fission power distribution $\boldsymbol{\varphi} = \boldsymbol{\Phi}(T)$ is obtained via the Monte Carlo code Serpent [7].

One of the most common methods of solving the nonlinear problem $\boldsymbol{\varphi} = \mathbf{G}(\boldsymbol{\varphi})$ is to apply the operator splitting approach along with the fixed-point iteration method. This approach iterates between the neutronics and the thermal-hydraulics codes, using the output of the previous run as the input to each simulation. At each coupled iteration *n* the following equations are solved:

$$T^{(n+1)} = \boldsymbol{\Theta}\left(\boldsymbol{\varphi}^{(n)}\right) \tag{9}$$

$$\boldsymbol{\varphi}^{(n+1)} = \boldsymbol{\Phi}\left(T^{(n+1)}\right) \tag{10}$$

or:

$$\boldsymbol{\varphi}^{(n+1)} = \mathbf{G}\left(\boldsymbol{\varphi}^{(n)}\right) \tag{11}$$

That is, at each iteration, the new value for the fission power distribution $\boldsymbol{\varphi}^{(n+1)}$ is the output obtained from the coupled simulation, using the previous value of $\boldsymbol{\varphi}^{(n)}$ as the input. The residual of any iteration *n* can be defined as:

$$\mathbf{r}^{(n)} = \boldsymbol{\varphi}^{(n)} - \mathbf{G}\left(\boldsymbol{\varphi}^{(n)}\right) \tag{12}$$

therefore, using Eq. (11):

$$\left(\boldsymbol{\varphi}^{(n+1)} - \boldsymbol{\varphi}^{(n)}\right) = -\mathbf{r}^{(n)} \tag{13}$$

The fixed-point iteration method is very simple and does not require major modifications to the code used to solve the neutronics and thermal-hydraulics problems. Unfortunately, this approach is prone to numerical instabilities and a low speed of convergence.

A coupled Serpent/OpenFOAM simulation of a PWR core [8] is used in order to test the fixed-point iteration method. The CFD solution is obtained with a coarse-mesh/porous-media approach, in which power densities and the coolant temperature are homogenized over a scale of several centimeters. Fig. 1 illustrates the case study.

Instabilities in the convergence of the fixed-point iteration commonly arise when dealing with coupled neutronics/thermal-hydraulics calculations, for example, in light water reactors. Fig. 2 shows the radial power distribution and coolant density distribution in the PWR case study, for two consecutive iterations. In this case, an unbalance arises in the power distribution, most likely due to the randomness of the Monte Carlo sampling. An unbalance in the fuel temperature and coolant density follows in the next TH calculation. Due to the strong negative Doppler and moderator feedbacks, the following Monte Carlo solution results in the opposite power unbalance (see Fig. 2).

Fig. 3 shows the onset of numerical oscillations in the fission rate distribution during the first 20 iterations, at five different points in the two-dimensional (2D) PWR test case. With reference to the geometry description in Fig. 1, the selected points are:

- Point **a**: central assembly (12, M);
- Point **b**: left reactor side (12, G);
- Point **c**: right reactor side (12, T);
- Point **d**: upper reactor side (17, M);
- Point **e**: lower reactor side (7, M).

In the initial iteration, the power distribution is uniform in the radial points (Points **b**–**e**) and slightly higher in the central point (Point **a**). After the first few iterations, Fig. 3 shows linearly growing oscillation amplitudes up to a saturation point due to nonlinearity effects. These oscillations will be damped or amplified according to the peculiarities of the system (dimensions, power level, magnitude of the TH feedback on neutronics, etc.).

As a first order approximation, if the initial iteration is close to the fixed-point solution, the condition for the stability of the fixed-point iteration $\boldsymbol{\varphi}^{(n+1)} = \mathbf{G}(\boldsymbol{\varphi}^{(n)})$ can be expressed as:

$$\rho(\mathbf{J_G}) < 1 \tag{14}$$

where $\rho(\mathbf{J_G})$ is the spectral radius of the Jacobian matrix J_G of **G**:

$$\rho(\mathbf{J_G}) = max\{|\lambda_1|, |\lambda_2| \ldots |\lambda_N|\} \tag{15}$$

and $\{|\lambda_1|, |\lambda_2| \ldots |\lambda_N|\}$ are the eigenvalues of $\mathbf{J_G}$.

The $J_{G_{ij}}$ element of the Jacobian matrix $\mathbf{J_G}$ is the derivative of the i^{th} value G_i of the vector function **G**, with respect to the j^{th} value φ_j of the vector input $\boldsymbol{\varphi}$:

$$\mathbf{J_G} = \begin{bmatrix} \frac{dG_1}{d\varphi_1} & \frac{dG_1}{d\varphi_2} & \cdots & \frac{dG_1}{d\varphi_N} \\ \frac{dG_2}{d\varphi_1} & \frac{dG_2}{d\varphi_2} & \cdots & \frac{dG_2}{d\varphi_N} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{dG_N}{d\varphi_1} & \frac{dG_N}{d\varphi_2} & \cdots & \frac{dG_N}{d\varphi_N} \end{bmatrix} \tag{16}$$