Nuclear Engineering and Technology 49 (2017) 1181–1188

Contents lists available at ScienceDirect

Nuclear Engineering and Technology

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

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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ARTICLE INFO

*Article history:*
Received 30 May 2017
Received in revised form
26 July 2017
Accepted 7 August 2017
Available online 12 August 2017

*Keywords:*
Jacobian
M&C2017
Monte Carlo
Multiphysics
Newton
Perturbation Theory

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 $k_{\mathrm{eff}}$ is the fundamental eigenvalue, **L**, **S** and **F** are the loss, scattering and fission production operators, and $\phi$ 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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http://dx.doi.org/10.1016/j.net.2017.08.005

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 $\varphi_j$ of the vector input $\boldsymbol{\varphi}$:

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

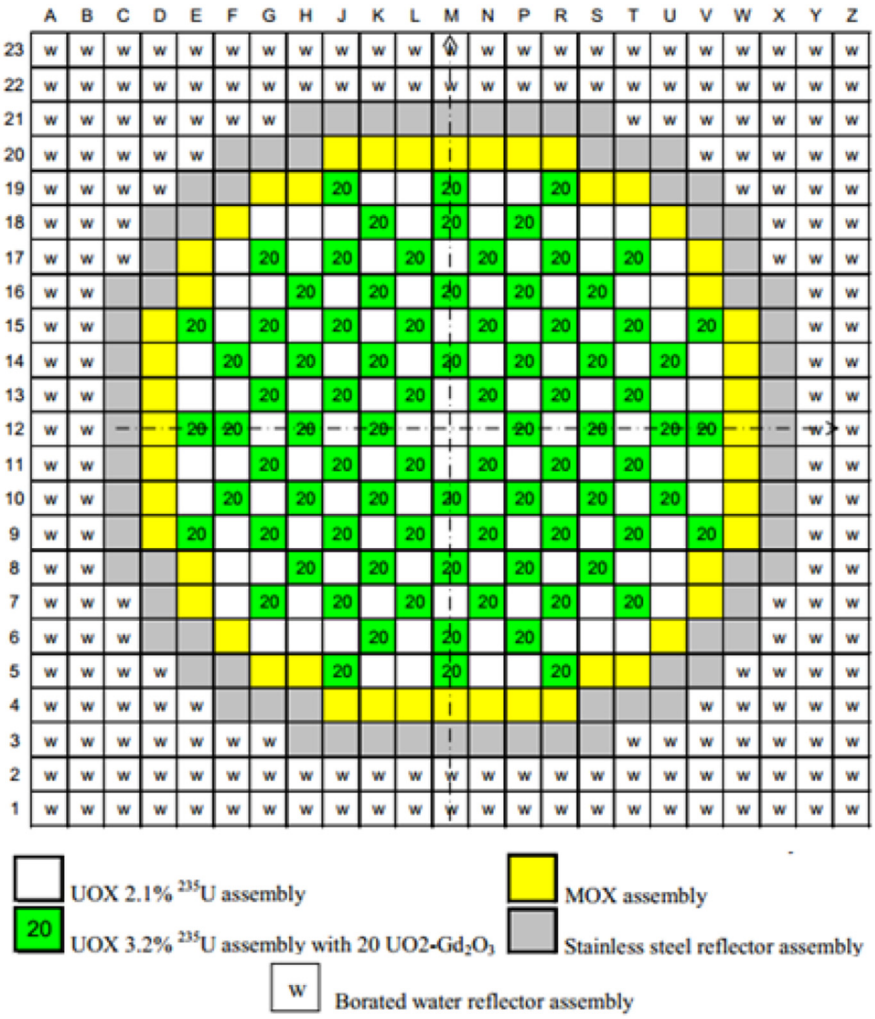


**Fig. 1.** Geometry of the considered PWR case study.

Thus, if the power distribution $\boldsymbol{\varphi}$ is scored in $N$ different volumes, $\mathbf{J_G}$ is an $N \times N$ matrix.

Typically, the presence of strong negative power feedback ensures that most diagonal elements of $\mathbf{J_G}$ are negative, and the eigenvalues $\lambda_1$, $\lambda_2$, $\lambda_3$,… are negative, which ensures the stability of the reactor.

To overcome the problem of numerical instabilities in the fixed-point iteration, under-relaxation is commonly employed to enforce the convergence of the coupled simulation. This is obtained by multiplying the residuals $\mathbf{r}^{(n)}$ by a scalar $\alpha$ with $0 < \alpha < 1$ before the update of one of the coupled variables:

$$\left(\boldsymbol{\varphi}^{(n+1)} - \boldsymbol{\varphi}^{(n)}\right) = -\alpha \cdot \mathbf{r}^{(n)} \tag{17}$$

In Fig. 4, the fission power distribution in selected points is represented for the first few under-relaxed iterations, when assuming $\alpha = 0.65$. Iteration #0 in the under-relaxed simulation has been selected as iteration #38 from the previous unstable case, highlighting how the selection of a suitable $\alpha$ parameter is effectively able to dump severe numerical oscillations.

The optimal under-relaxation factor $\alpha$ can be obtained as [9]:

$$\alpha = \frac{2}{2 + \rho(\mathbf{J_G})} \tag{18}$$

Unfortunately, the spectral radius $\rho(\mathbf{J_G})$ is not known when dealing with a generic multiphysics problem with a fixed-point iteration. Thus, $\alpha$ is usually selected by the user based on its experience.

Dufek and Gudowski [10] proposed an optimal iterative procedure adopting decreasing under-relaxation factor and an increasing neutron population for the Monte Carlo simulation. Unfortunately, any approach based on under-relaxed fixed-point iteration, features a very slow convergence rate (i.e., requires a large number of coupled iterations). Even in the case of variable population size, this might lead to large computational requirements, especially if the thermal/hydraulic solution is obtained via expensive CFD calculations.

## 4. The Newton method

One of the classical methods of stabilizing and accelerating the convergence of a nonlinear problem is the Newton method. At each Newton iteration, $\boldsymbol{\varphi}^{(n+1)}$ is obtained by solving the following linear system:

$$\mathbf{J}_\mathbf{G}^{(n)}\left(\boldsymbol{\varphi}^{(n+1)} - \boldsymbol{\varphi}^{(n)}\right) = -\mathbf{r}^{(n)} \tag{19}$$

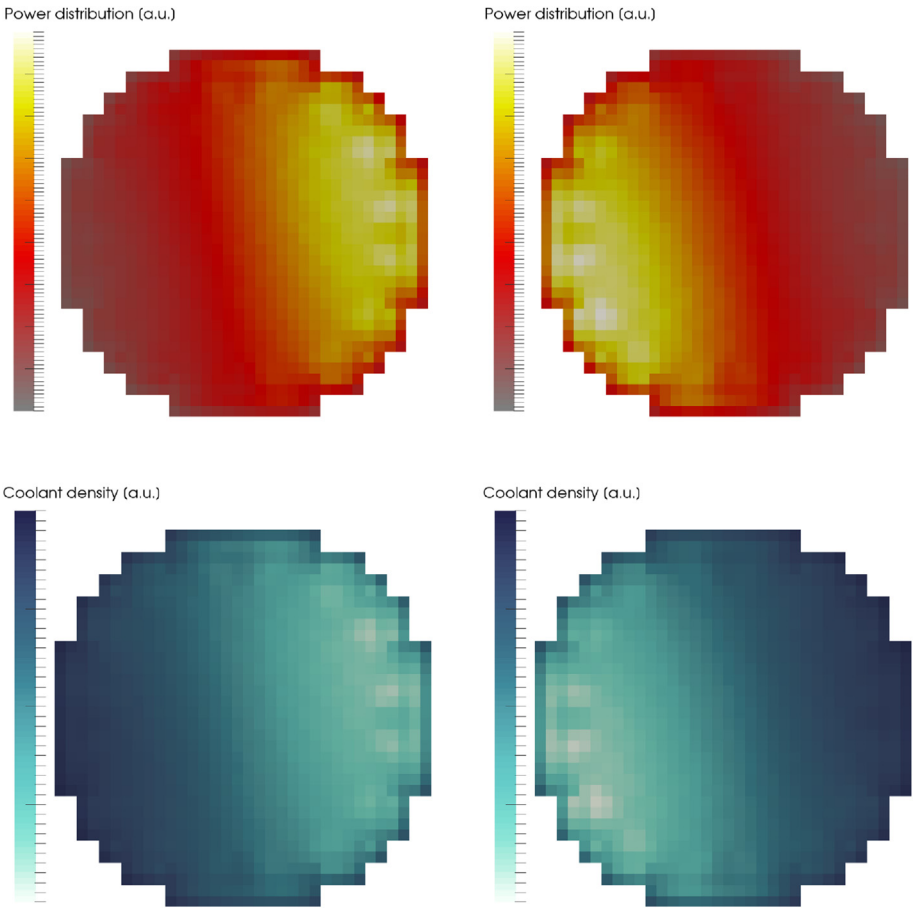


**Fig. 2.** Radial power distribution (top) and coolant density distribution (bottom) for coupled iterations #37 (left) and #38 (right).

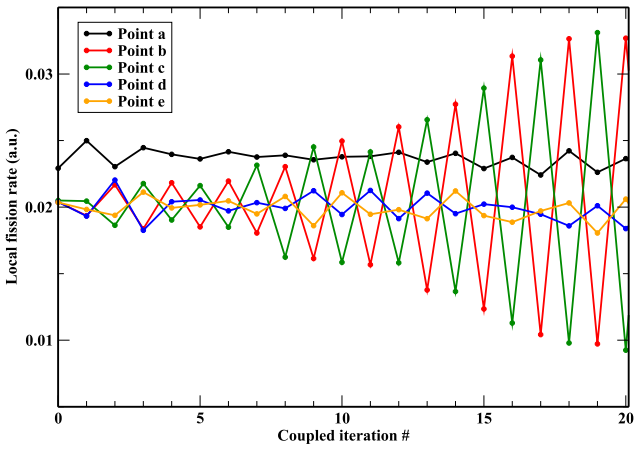


**Fig. 3.** Instabilities in the power distribution at four points in the 2D case study (numerical instabilities in the coupled Picard iterations).

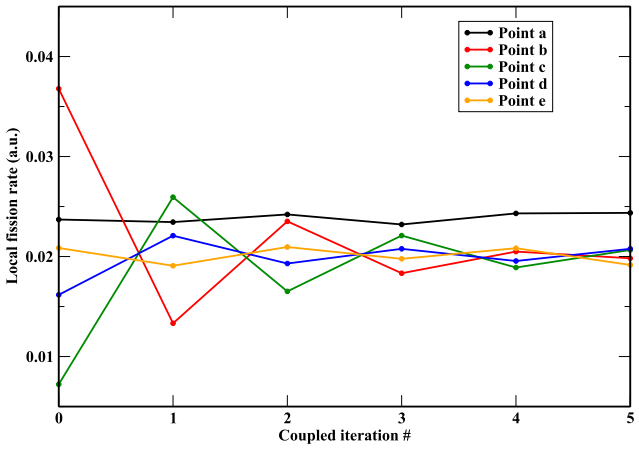


**Fig. 4.** Effect of the under-relaxation in the 2D case study (effect of under-relaxation on the coupled Picard iterations).

where $\mathbf{r}^{(n)}$ are the residuals obtained at the $n^{th}$ iteration as $[\boldsymbol{\varphi}^{(n)}-\mathbf{G}(\boldsymbol{\varphi}^{(n)})]$, and $\mathbf{J}_{\mathbf{G}}^{(n)}$ is the Jacobian matrix of $\mathbf{G}$ evaluated in $\boldsymbol{\varphi}^{(n)}$.

The Newton method can lead to quadratic convergence in most multiphysics problems that are of interest in the field of computational physics. Unfortunately, its use as described by Eq. (19) is impractical in common applications, due to the difficulty of obtaining the full Jacobian $\mathbf{J}_{\mathbf{G}}$ in large multiphysics problems.

For this reason, Newton methods adopting an approximated Jacobian have gained popularity in the last few decades. One of the most popular approaches is the family of Jacobian-free Newton–Krylov (JFNK) methods [11]. These methods do not require the compilation of the full $\mathbf{J}_{\mathbf{G}}$. At each Newton iteration, the system in Eq. (19) is solved by approximately applying the Krylov subspace method for the Jacobian. Rather than calculating the full $\mathbf{J}_{\mathbf{G}}$, JFNK approaches only require the calculation of a Jacobian-vector product, through the evaluation of the nonlinear function $\mathbf{G}$. For example, an approximation of the Jacobian-product $\mathbf{J}_{\mathbf{G}}(\boldsymbol{\varphi}^{(n)})\,\mathbf{e}_{\mathbf{i}}$ can be obtained as [11]:

$$\mathbf{J_G}\left(\boldsymbol{\varphi}^{(n)}\right)\mathbf{e_i} \simeq \frac{\left[\mathbf{G}\left(\boldsymbol{\varphi}^{(n)} + \boldsymbol{\varepsilon}\cdot\mathbf{e_i}\right) - \mathbf{G}\left(\boldsymbol{\varphi}^{(n)}\right)\right]}{\boldsymbol{\varepsilon}} \tag{20}$$

where $\varepsilon$ represents a small perturbation.

At each Newton iteration, Jacobian-vector products are evaluated for each direction $\mathbf{e_i}$ of the selected Krylov subspace.

JFNK methods have been successfully applied as Newton iteration wrappers around fixed-point iteration solvers in many computational physics fields. Unfortunately, their adoption in combination with Monte Carlo calculations of the residuals $\mathbf{r}^{(n)}$ poses some difficulties related to the stochastic behavior of the approach used to evaluate $\mathbf{G}(\boldsymbol{\varphi}^{(n)})$ [12]. When dealing with Monte Carlo solvers for the neutronics problem, the evaluation of $\mathbf{G}(\boldsymbol{\varphi}^{(n)})$ in Eq. (20) is replaced by $\widehat{\mathbf{G}}(\boldsymbol{\varphi}^{(n)}) = \mathbf{G}(\boldsymbol{\varphi}^{(n)}) + \varepsilon$. The noise term $\varepsilon$ practically prevents the adoption of small perturbations for the evaluation of Jacobian-vector products. Willert et al. [12] studied specific techniques to try to circumvent this problem. Nonetheless, these techniques lead to severe limitations on the number of Krylov directions, possibly jeopardizing the benefits of the adoption of JFNK methods.

This work proposes an innovative approach to the Newton method using Monte Carlo methods. The new method benefits from recent developments in the field of Monte Carlo perturbation theory, to obtain a cheap and accurate approximation of $\mathbf{J_G}$ at each Newton iteration.

## 5. Jacobian approximation via Monte Carlo perturbation theory

Recalling that the function $\boldsymbol{\varphi} = \mathbf{G}(\boldsymbol{\varphi})$ is equivalent to $\boldsymbol{\varphi} = \boldsymbol{\Phi}[\boldsymbol{\Theta}(\boldsymbol{\varphi})]$, the Jacobian matrix $\mathbf{J_G}$ can be obtained via the chain rule as:

$$\mathbf{J_G} = \mathbf{J_\Phi}\mathbf{J_\Theta} = \begin{bmatrix} \frac{d\Phi_1}{d\theta_1} & \frac{d\Phi_1}{d\theta_2} & \cdots & \frac{d\Phi_1}{d\theta_N} \\ \frac{d\Phi_2}{d\theta_1} & \frac{d\Phi_2}{d\theta_2} & \cdots & \frac{d\Phi_2}{d\theta_N} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{d\Phi_N}{d\theta_1} & \frac{d\Phi_N}{d\theta_2} & \cdots & \frac{d\Phi_N}{d\theta_N} \end{bmatrix} \begin{bmatrix} \frac{d\Theta_1}{d\varphi_1} & \frac{d\Theta_1}{d\varphi_2} & \cdots & \frac{d\Theta_1}{d\varphi_N} \\ \frac{d\Theta_2}{d\varphi_1} & \frac{d\Theta_2}{d\varphi_2} & \cdots & \frac{d\Theta_2}{d\varphi_N} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{d\Theta_N}{d\varphi_1} & \frac{d\Theta_N}{d\varphi_2} & \cdots & \frac{d\Theta_N}{d\varphi_N} \end{bmatrix} \tag{21}$$

The first term of Eq. (21) is the Jacobian of the function $\boldsymbol{\Phi}(T)$, and represents the change in the power distribution due to a change in the thermal-hydraulics fields. In the present work, it will be approximated via Monte Carlo perturbation theory, along a set of directions ($\mathbf{S_1}$,$\mathbf{S_2}$, …,$\mathbf{S_k}$). The second term ($\mathbf{J_\Theta}$) represents a change in the CFD thermal-hydraulics solution, due to a change in the power distribution. $\mathbf{J_\Theta}$-vector products can be obtained via numerical differentiation onto a set of directions ($\boldsymbol{\theta}_1$, $\boldsymbol{\theta}_2$, …, $\boldsymbol{\theta_k}$).

The Iterated Fission Matrix (IFM) method [13] is used to accurately calculate eigentriplets of the discretized $l^{th}$ iterated fission kernel $\mathbf{F}(l)$:

$$(k_n)^l \cdot \mathbf{S_n} = {}^{(l)}\mathbf{F}\cdot\mathbf{S_n} \tag{22}$$

$$(k_n)^l \cdot \mathbf{S_n^\dagger} = {}^{(l)}\mathbf{F}^T\cdot\mathbf{S_n^\dagger} \tag{23}$$

The first few higher forward eigenmodes for the PWR case study obtained via the IFM method are presented in Fig. 5. Although complex eigenvalues in the Fission Matrix method might arise due to statistical errors, the present approach only adopts the first few eigentriplets, in which case, the eigenvalues are always real.

Provided that the forward and adjoint eigenmodes respect the bi-orthogonality condition:

$$\begin{bmatrix} \mathbf{S_0^\dagger} \\ \mathbf{S_1^\dagger} \\ \vdots \\ \mathbf{S_n^\dagger} \end{bmatrix} \begin{bmatrix} \mathbf{S_0} & \mathbf{S_1} & \cdots & \mathbf{S_n} \end{bmatrix} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix} \tag{24}$$

the effect of perturbations on the fundamental fission source distribution can be obtained as [14]:

$$\frac{d\mathbf{S_0}}{dT} = \sum_{i=0}^{\infty} \mathbf{S_i}\cdot\frac{\mathbf{S_i^{\dagger T}}\frac{d^{(l)}\mathbf{F}}{dT}\mathbf{S_0}}{(k_0)^l - (k_i)^l} \tag{25}$$

where $\frac{d\mathbf{S_0}}{dT}$ represents the derivatives of the fundamental fission source distributions $\mathbf{S_0}$ with respect to the thermal/hydraulics distributions $T$; $\frac{d^{(l)}\mathbf{F}}{dT}$ is the effect of the perturbation in $T$ on the fission kernel ${}^{(l)}\mathbf{F}$; $\mathbf{S_i}$, $\mathbf{S_i^\dagger}$ and $(k_i)^l$ form the $i^{th}$ eigentriplet of the discretized $l^{th}$ iterated eigenproblem. In the present approach, the effect of perturbations on the iterated fission kernel can be estimated via Monte Carlo perturbation theory [15].

Assuming for simplicity that relative changes in the fission source distribution are very similar to relative changes in the fission power distribution, ($\mathbf{S_1}$,$\mathbf{S_2}$⋯$\mathbf{S_k}$) form a reduced basis for the calculation of derivatives $\frac{d\boldsymbol{\Phi}}{dT}$, to approximate the Jacobian $\mathbf{J_\Phi}$.

Due to the fact that the thermal-hydraulic solution is obtained via deterministic solutions (i.e., the CFD solution is not affected by stochastic noise $\varepsilon$), the derivatives $\frac{d\boldsymbol{\Theta}}{d\boldsymbol{\varphi}}$ can be efficiently calculated via numerical differentiation, as in the JFNK approaches:

$$\boldsymbol{\theta_i} = \frac{d\boldsymbol{\Theta}}{d\boldsymbol{\varphi}_{\mathbf{S_i}}} = \frac{\boldsymbol{\Theta}(\boldsymbol{\varphi} + \varepsilon\cdot\mathbf{S_i}) - \boldsymbol{\Theta}(\boldsymbol{\varphi})}{\varepsilon} \tag{26}$$

$\boldsymbol{\theta_i}$ is a numerical estimate for the Jacobian-vector product $\mathbf{J_\Theta}\mathbf{S_i}$. It represents the derivative of the function $\boldsymbol{\Theta}(\boldsymbol{\varphi})$ with respect to a change in the fission power distribution $\boldsymbol{\varphi}$ along the direction $\mathbf{S_i}$.

This way, the Jacobian matrix $\mathbf{J_G}$ can be approximated at each Newton iteration by calculating $\mathbf{J_G}$, the projection of the Jacobian-vector products onto the two reduced sets of basis ($\mathbf{S_1}$, $\mathbf{S_2}$, …,$\mathbf{S_k}$) and ($\boldsymbol{\theta}_1$, $\boldsymbol{\theta}_2$, …,$\boldsymbol{\theta_k}$).

The following algorithm summarizes the main steps of the proposed approach:

Select an appropriate spatial discretization for the coupled problem and the number of directions $k$ for the projection of the Jacobian matrix:

(1) Guess an initial value for the thermal/hydraulic variables $T^{(0)}$
(2) Solve the first Serpent Monte Carlo iteration while scoring the power distribution $\boldsymbol{\varphi}^{(0)} = \boldsymbol{\Phi}(T^{(0)})$ and fission matrix estimates
(3) Solve the IFM eigenvalue problem for the first $k$ eigentriplets via Arnoldi iterations
(4) Solve the thermal/hydraulic problem in OpenFOAM: $T^{(1)} = \boldsymbol{\Theta}(\boldsymbol{\varphi}^{(0)})$
(5) **For** each Newton iteration $n = 1, 2, 3, \ldots$
(6) **For** each forward eigenmode $i = 1, 2, 3, \ldots, k$
(7) Calculate $\boldsymbol{\theta_i} = \frac{d\boldsymbol{\Theta}}{d\boldsymbol{\varphi}_{\mathbf{S_i}}}$ in OpenFOAM via direct perturbation
(8) Solve the Monte Carlo criticality source calculation scoring the fission power distribution $\boldsymbol{\varphi}^{(n)} = \boldsymbol{\Phi}(T^{(n)})$ and GPT estimates for $\frac{d\boldsymbol{\Phi}}{d\boldsymbol{\theta}_i}$ ($i = 1,2,3, \ldots, k$)

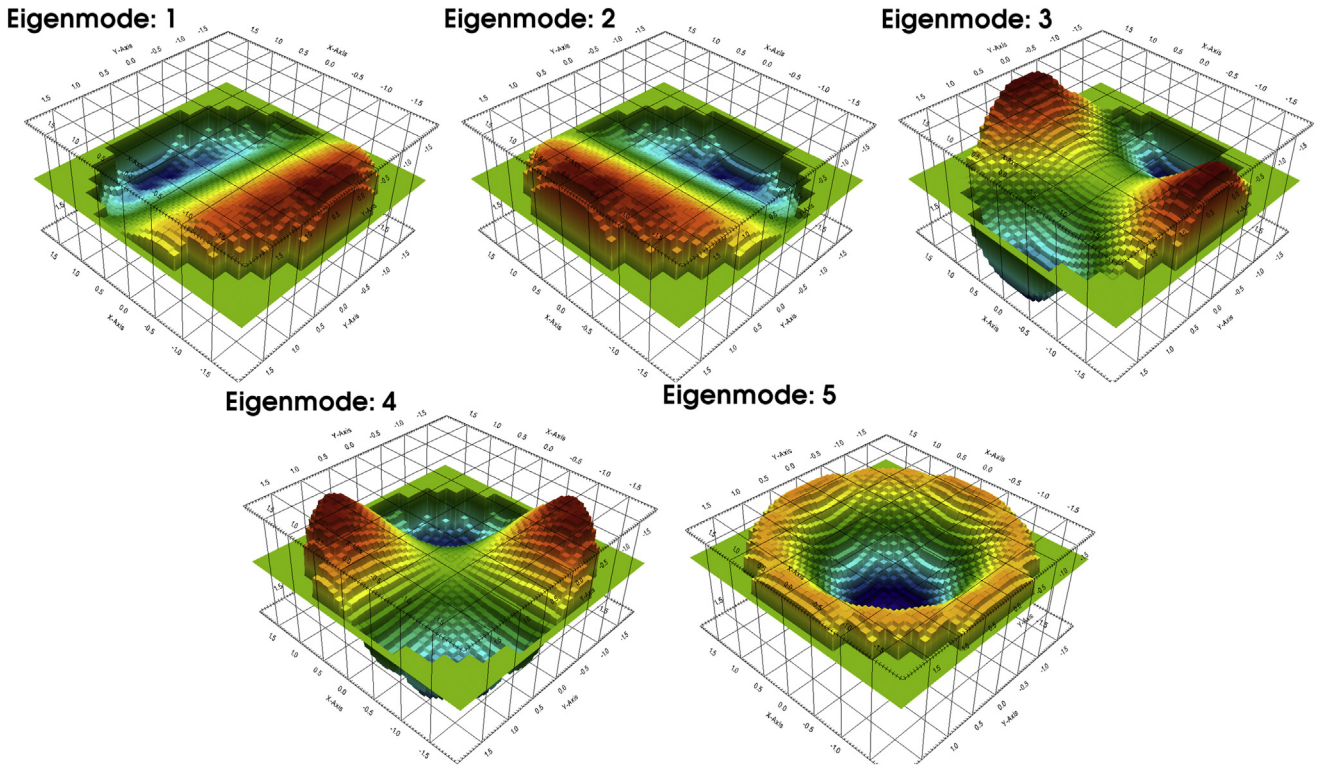


**Fig. 5.** First few higher forward eigenmodes for the 2D PWR case study depicted with height deformation.

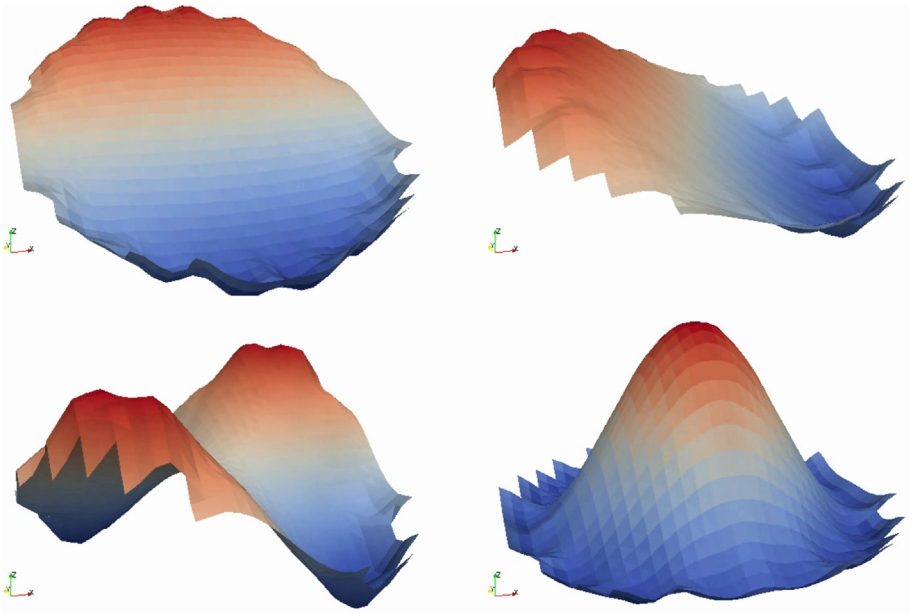

**Fig. 6.** Basis functions for the projection of the coolant density. $\theta_1$ (top left), $\theta_2$ (top right), $\theta_3$ (bottom left), and $\theta_5$ (bottom right). For better clarity, the 2D basis functions are presented with height deformation.

(9) Reconstruct and invert the $k \times k$ Jacobian matrix $\mathbf{J_G} = \mathbf{J_\Phi J_\Theta}$ adopting the Lapack libraries implementation
(10) Calculate the residuals $\mathbf{r}^{(n)}$ in the power distribution and solve Eq. (19) to update the power distribution $\boldsymbol{\varphi}^{(n+1)}$
(11) Solve the thermal/hydraulic problem in OpenFOAM: $T^{(n+1)} = \boldsymbol{\Theta}(\boldsymbol{\varphi}^{(n)})$

## 6. Results for a simplified PWR case study

To test the new approach, Newton iterations adopting the Jacobian approximations described above were performed on the PWR case study with an axial averaging of the thermal-hydraulics solution. This reduces the dimensionality of $T$ to a 2D problem

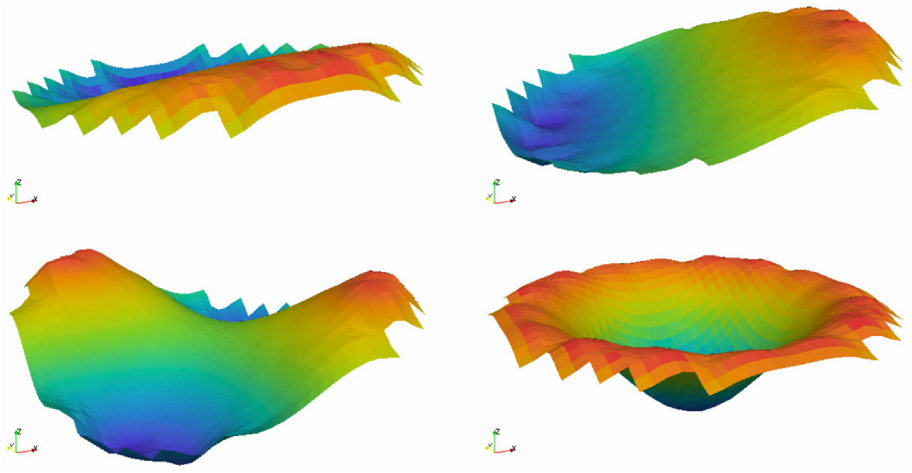

**Fig. 7.** Selected projections of $\mathbf{J}_{\Phi}$. $\frac{d\Phi}{d\theta_1}$ (top left), $\frac{d\Phi}{d\theta_2}$ (top right), $\frac{d\Phi}{d\theta_3}$ (bottom left), and $\frac{d\Phi}{d\theta_5}$ (bottom right). For better clarity, the 2D projections are presented with height deformation.

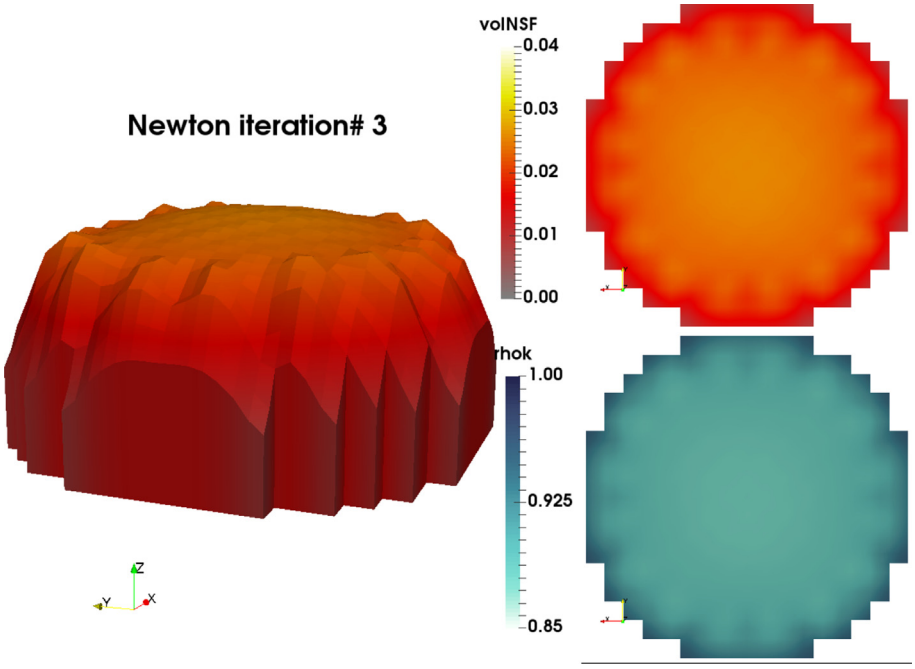


**Fig. 8.** Radial power distribution (top) and coolant density distribution (bottom) for Newton iteration #3. For better clarity, on the left, the 2D fission source distribution is presented with height deformation.

(the Monte Carlo calculations with Serpent were performed in the 3D full core geometry). To further simplify the coupled iterations, only the coolant density feedback on neutronics was considered in the present study.

When using the fixed-point iteration method, this case rapidly diverges (see Fig. 2) due to the strong negative feedback and the very large dominance ratio.

Following the procedure described in the previous section, the basis functions ($\boldsymbol{\theta}_1$, $\boldsymbol{\theta}_2$, …,$\boldsymbol{\theta}_k$) for the projection of the thermal-hydraulics problem (only considering the coolant density distribution, in this example) are produced as in Eq. (26), considering numerical differentiation from the first 50 eigenmodes ($\mathbf{S}_1, \mathbf{S}_2, \cdots \mathbf{S}_k$, see Fig. 5).

The first five basis functions, $\boldsymbol{\theta}_1 = \frac{d\boldsymbol{\Theta}}{d\varphi_{\mathbf{S}_1}}$, $\boldsymbol{\theta}_2 = \frac{d\boldsymbol{\Theta}}{d\varphi_{\mathbf{S}_2}}$, $\boldsymbol{\theta}_3 = \frac{d\boldsymbol{\Theta}}{d\varphi_{\mathbf{S}_3}}$, and $\boldsymbol{\theta}_5 = \frac{d\boldsymbol{\Theta}}{d\varphi_{\mathbf{S}_5}}$, are presented in Fig. 6.

Due to the procedure applied for calculating the Jacobian $\mathbf{J}_{\boldsymbol{\Theta}}$, the out-of-diagonal elements of this matrix are small, thus, for simplicity, they have been discarded in this case study. Moreover, the diagonal elements are equal to 1 by construction.

The Jacobian matrix $\mathbf{J}_{\boldsymbol{\Phi}}$ is obtained via perturbation theory, as described above, and is projected on the selected eigenmodes. Fig. 7 shows the changes in the fission source distribution due to perturbations in the coolant density distribution along the directions $\boldsymbol{\theta}_1$, $\boldsymbol{\theta}_2$, $\boldsymbol{\theta}_3$, and $\boldsymbol{\theta}_5$ (Fig. 6).

It is worth noting that the effects of the feedback on the power distribution act mainly in the opposite direction of the perturbation, as expected.

Adopting the Newton method with the approximated Jacobian obtained by applying the chain rule to $\mathbf{J}_{\boldsymbol{\Phi}}$ and $\mathbf{J}_{\boldsymbol{\Theta}}$ ensures the stabilization of the coupled iterations, and leads to the convergence of the multiphysics simulation within approximately three iterations.[1]

[1] A detailed discussion on the advantages of the adoption of approximate Jacobians can be found in the literature [11].

The normalized fission power distribution and coolant density distribution are presented in Fig. 8.

The availability of an approximated Jacobian allows the analysis of the system stability by estimating the spectral radius of $\mathbf{J_G}$. In the selected case study, the value of $\rho(\mathbf{J_G})$ resulted to be approximately 1.08, confirming that instabilities arise along the directions of the first two degenerate eigenmodes. It is expected that a more complete consideration of the thermal-hydraulics feedback, including the doppler effect, and the adoption of full 3D cases will lead to larger spectral radii and stronger instabilities when the operator splitting approach is employed.

## 7. Conclusions

The standard operator splitting approach in coupled neutronics/thermal-hydraulics problems can result in unstable or slowly converging calculations. JFNK methods proved very useful in many fields of computational engineering. Nonetheless, the use of Monte Carlo transport for the solution of the neutronic problem challenges the applicability of JFNK methods due to the difficulties arising from numerical differentiations in presence of statistical errors. This paper proposes to use Monte Carlo perturbation theory to approximate the Jacobian matrix of the coupled neutronics/thermal-hydraulics problem. In such approach, the Jacobian matrix is projected along few directions obtained from the eigenvalue decomposition of the fission matrix of the problem, and this projection is used to solve the coupled problem via the Newton method. This approach is expressly envisaged for systems with very high dominance ratio that are, at the same time, more prone to numerical instabilities and more easily described by eigenmode decomposition.

The proposed approach was successfully tested in a 2D PWR problem, only considering the coolant density feedback on neutronics, and showing an effective stabilization and convergence acceleration of the coupled problem.

The computational requirements for the proposed methods in full core realistic cases are not expected to increase significantly, thanks to the efficiencies of the Monte Carlo perturbation estimators. Moreover, it is expected that the number of eigentriplets required for the projection of the Jacobian matrix will be at most in the order of hundreds, also in 3D cases, thus limiting the memory demand of the implementation. Nonetheless detailed tests will be required to assess the efficiency of the proposed approach.

## Acknowledgments

The authors thank Prof. Adrien Bidaud (Grenoble Institute of Technology, Grenoble) for stimulating discussions that lead to some of the developments at the basis of this work, and the reviewers for their careful assessment of the manuscript and the useful suggestions that improved its quality.

## Conflicts of interest

The authors declare that there is no conflict of interest.

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