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# 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 presents 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 (JFNK) methods, that tend to become expensive and inaccurate in presence of Monte Carlo statistical errors in the residual. The proposed approach is presented and demonstrated for a simple 2D PWR case study.*

## I. INTRODUCTION

Multiphysics modeling of fission reactors represents a field of growing interest in the nuclear community (e.g., see [1, 2]). Coupled neutronics–thermal/hydraulics reactor simulations have been usually performed employing deterministic codes. Recently, the adoption of continuous energy Monte Carlo codes for the neutronics solution of multiphysics problems has been the subject of several research activities (e.g., see [3, 4, 5]).

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

This work presents a new approach to stabilize and accelerate the convergence of steady-state coupled Monte Carlo–Thermal/hydraulics simulations adopting then Newton method and Monte Carlo perturbation theory. The method is demonstrated in a simplified PWR multiphysics simulation.

## II. THE COUPLED NEUTRONICS–T/H NON-LINEAR 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:

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

where $k_{\text{eff}}$ is the fundamental eigenvalue, $\mathbf{L}$ , $\mathbf{S}$ and $\mathbf{F}$ are the loss, scattering and fission production operators, and $\boldsymbol{\phi}$ represents the neutron flux, solution of the eigenvalue problem.

The second equation is here represented as a generic non-linear equation in which the T/H solution $T$ depends on the fission source distribution $\boldsymbol{\varphi}$ :

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

In the considered cases, $T$ represents material temperature and density distributions, and the main feedback of $T$ on the neutronics solution is driven by the Doppler effect and the moderator expansion effect. The generic coupling terms can be introduced in Eq. (1) by allowing the $\mathbf{L}$ , $\mathbf{S}$ and $\mathbf{F}$ operators be dependent on the generic T/H solution $T$.

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

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

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

Equation 4 depends on $T$ only. Replacing $T$ with Eq. (2),

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

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.

Equation 5 can be written as:

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

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

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:

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

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

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

## III. MONTE CARLO/CFD COUPLING: FIXED POINT ITERATION

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

One of the easiest and most common way to solve the non-linear problem $\boldsymbol{\varphi} = \mathbf{G}(\boldsymbol{\varphi})$ consists in the adoption of the operator splitting approach along with the fixed point iteration method. This approach consists in solving iteratively the neutronics and the thermal/hysraulics code, adopting as input to each simulation, the output of the previous run. This way, at each coupled iteration $n$ we solve:

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

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

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, adopting as input the previous value $\boldsymbol{\varphi}^{(n)}$. Defining the residuals of each iteration $n$ as:

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

we can rewrite Eq. (11) as:

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

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

To test this method of solution, the coupled Serpent/OpenFOAM simulation of a PWR core from [6] is presented. The CFD solution is obtained with a coarse-mesh/porous-media approach, in which power densities and coolant temperature are homogenized over a scale of several centimeters. The case study is presented in Fig. 1.

Instabilities in the convergence of the fixed point iteration commonly arise when dealing with coupled neutronics–thermal/hydraulics problems in e.g., Light Water Reactors (LWRs). In Fig. 2, the radial power distribution and coolant density distribution in the PWR case study are presented for coupled iterations #37 and #38. In this case, when an unbalance arise in the power distribution e.g., due to the randomness of the Monte Carlo sampling, the fuel temperature and coolant density at the next T/H solution will follow the unbalance in the power. Due to the strong negative Doppler and moderator feedback, the following Monte Carlo solution will result in an opposite power unbalance (see Fig. 2). These oscillations will be damped or amplified according to the peculiarities of

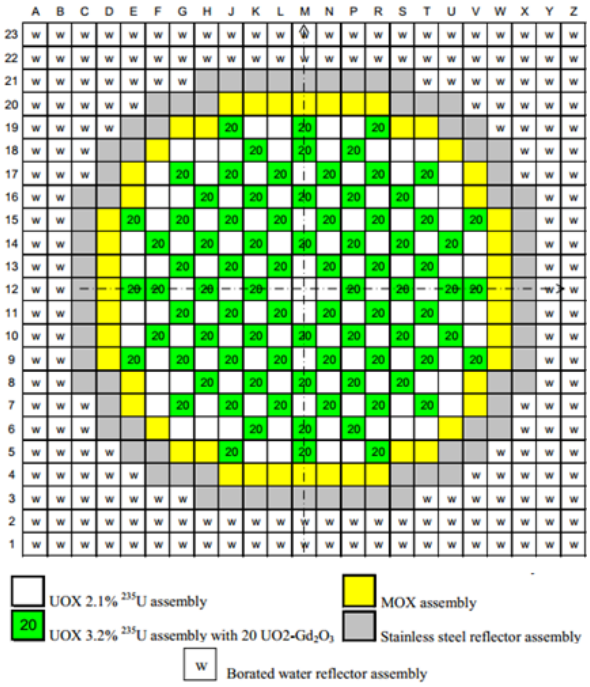


Fig. 1. Geometry of the considered PWR case study.

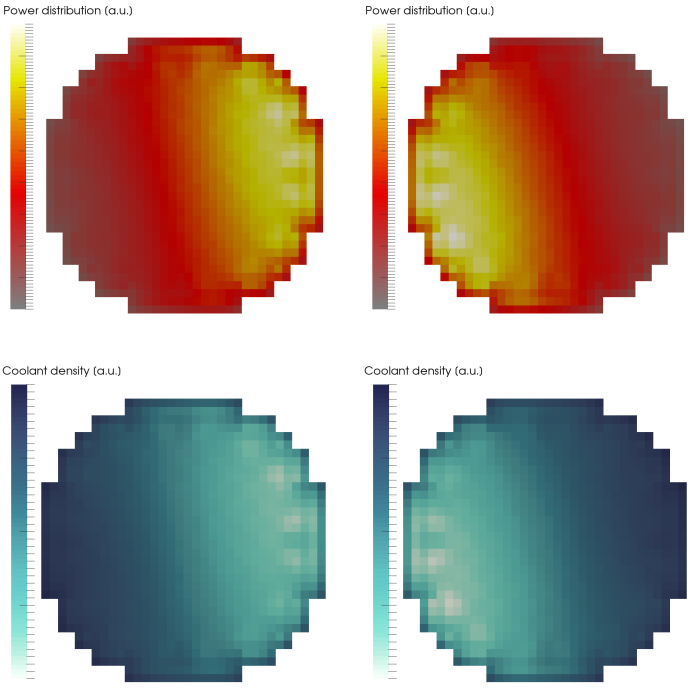


Fig. 2. Radial power distribution (top) and coolant density distribution (bottom) for coupled iterations #37 (left) and #38 (right).

the system (dimensions, power level, magnitude of the T/H feedback on neutronics, etc.).

The condition for the stability of the fixed point iteration

$\boldsymbol{\varphi}^{(n+1)} = \mathbf{G}(\boldsymbol{\varphi}^{(n)})$ can be expressed as:

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

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

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

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

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

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

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

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:

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

The optimal under-relaxation factor $\alpha$ can be obtained as [7]:

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

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

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

## IV. THE NEWTON METHOD

One of the classical way to stabilize and accelerate the convergence of a non-linear problem is the adoption of the Newton method. At each Newton iteration, the update of the variable $\boldsymbol{\varphi}$ is obtained by solving the following linear system:

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

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

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

For this reason, Newton methods adopting an approximated Jacobian gained popularity in the last decades. One of the most popular approach consists in the family of Jacobian-free Newton–Krylov (JFNK) methods [9]. These methods do not require the formation of the full $\mathbf{J_G}$. At each Newton iteration, the systems of Eq. (19) is solved approximately adopting the Krylov subspace method for the Jacobian. Rather than calculating the full $\mathbf{J_G}$, JFNK approaches only require the calculation of a Jacobian-vector product, through the evaluation of the non-linear function $\mathbf{G}$. For example, an approximation of the Jacobian-product $\mathbf{J_G}\left(\boldsymbol{\varphi}^{(n)}\right)\mathbf{e_i}$ can be obtained as [9]:

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

where $\epsilon$ 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 $\mathbf{G}\left(\boldsymbol{\varphi}^{(n)}\right)$ [10]. When dealing with Monte Carlo solvers for the neutronics problem, the evaluation of $\mathbf{G}\left(\boldsymbol{\varphi}^{(n)}\right)$ in Eq. (20) is replaced by $\hat{\mathbf{G}}\left(\boldsymbol{\varphi}^{(n)}\right) = \mathbf{G}\left(\boldsymbol{\varphi}^{(n)}\right) + \varepsilon$. The noise term $\varepsilon$ practically prevents the adoption of small perturbations for the evaluation of Jacobian-vector products. [10] 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 benefit of the adoption of JFNK method.

In the present work, we propose an innovative approach to the Newton method with Monte Carlo. 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.

## V. JACOBIAN APPROXIMATION VIA MONTE CARLO PERTURBATION THEORY

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

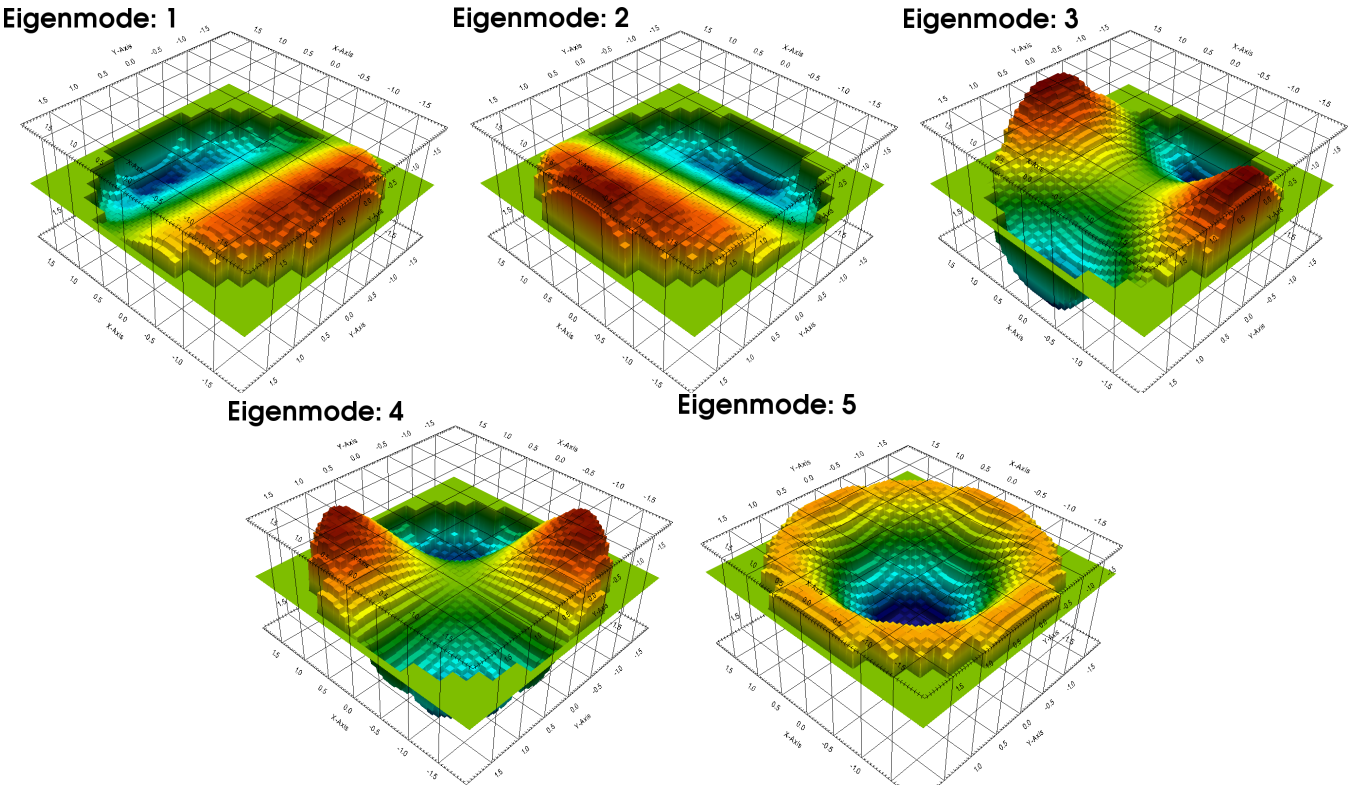


Fig. 3. First few higher forward eigenmodes for the 2D PWR case study depicted with height deformation.

chain rule as:

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

The first term of Eq. (21) is the Jacobian of the function $\mathbf{\Phi}(T)$, 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 $(\mathbf{S_1}, \mathbf{S_2} \cdots \mathbf{S_k})$. 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 $(\boldsymbol{\theta_1}, \boldsymbol{\theta_2} \cdots \boldsymbol{\theta_k})$.

The Iterated Fission Matrix (IFM) method [11] has been adopted to accurately calculate eigentriplets of the discretized $l^{th}$ iterated fission kernel ${}^{(l)}\mathbf{F}$:

$$(k_n)^l \cdot \mathbf{S_n} = {}^{(l)}\mathbf{F} \cdot \mathbf{S_n} \qquad \text{and} \qquad (k_n)^l \cdot \mathbf{S_n^\dagger} = {}^{(l)}\mathbf{F}^T \cdot \mathbf{S_n^\dagger}$$

The first few higher forward eigenmodes for the PWR case study obtained via the IFM method are presented in Fig. 3. While 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 positive.

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

$$\begin{bmatrix} — & \mathbf{S_0^\dagger} & — \\ — & \mathbf{S_1^\dagger} & — \\ & \vdots & \\ — & \mathbf{S_n^\dagger} & — \end{bmatrix} \begin{bmatrix} | & | & & | \\ \mathbf{S_0} & \mathbf{S_1} & \cdots & \mathbf{S_n} \\ | & | & & | \end{bmatrix} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix} \tag{22}$$

the effect of perturbations on the fundamental fission source distribution can be obtained as [12]:

$$\frac{d\mathbf{S_0}}{dT} = \sum_{i=0}^{\infty} \mathbf{S_i} \cdot \frac{\mathbf{S_i^{\dagger T}} \frac{d\,{}^{(l)}\mathbf{F}}{dT} \mathbf{S_0}}{(k_0)^l - (k_i)^l} \tag{23}$$

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 [13].

Assuming for simplicity that relative changes in the fission source distribution are very similar to relative changes in

the fission power distribution, $(\mathbf{S_1}, \mathbf{S_2} \cdots \mathbf{S_k})$ form a reduced basis for the calculation of derivatives $\frac{d\mathbf{\Phi}}{dT}$, to approximate the Jacobian $\mathbf{J_\Theta}$.

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 $\frac{d\mathbf{\Theta}}{d\boldsymbol{\varphi}}$ can be efficiently calculated via numerical differentiation, as in the JFNK approaches:

$$\boldsymbol{\theta_i} = \frac{d\mathbf{\Theta}}{d\boldsymbol{\varphi}_{\mathbf{S_i}}} = \frac{\mathbf{\Theta}(\boldsymbol{\varphi} + \epsilon \cdot \mathbf{S_i}) - \mathbf{\Theta}(\boldsymbol{\varphi})}{\epsilon} \tag{24}$$

$\boldsymbol{\theta_i}$ is a numerical estimate for the Jacobian-vector product $\mathbf{J_\Theta S_i}$. It represents the derivative of the function $\mathbf{\Theta}(\boldsymbol{\varphi})$ 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 $\widetilde{\mathbf{J_G}}$, the projection of the Jacobian-vector products onto the two reduced sets of basis $(\mathbf{S_1}, \mathbf{S_2} \cdots \mathbf{S_k})$ and $(\boldsymbol{\theta_1}, \boldsymbol{\theta_2} \cdots \boldsymbol{\theta_k})$.

## VI. RESULTS FOR A SIMPLIFIED PWR CASE STUDY

To test the new approach, Newtwon 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 (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 adopting 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 $(\boldsymbol{\theta_1}, \boldsymbol{\theta_2} \cdots \boldsymbol{\theta_k})$ for the projection of thermal/hydraulics problem (only considering the coolant density distribution, in this example) are produced adopting Eq. (24) considering numerical differentiation from the first 50 eigenmodes $(\mathbf{S_1}, \mathbf{S_2} \cdots \mathbf{S_k}$, see Fig. 3).

The first few basis functions $\boldsymbol{\theta_1} = \frac{d\mathbf{\Theta}}{d\boldsymbol{\varphi}_{\mathbf{S_1}}}$, $\boldsymbol{\theta_2} = \frac{d\mathbf{\Theta}}{d\boldsymbol{\varphi}_{\mathbf{S_2}}}$, $\boldsymbol{\theta_3} = \frac{d\mathbf{\Theta}}{d\boldsymbol{\varphi}_{\mathbf{S_3}}}$, and $\boldsymbol{\theta_5} = \frac{d\mathbf{\Theta}}{d\boldsymbol{\varphi}_{\mathbf{S_5}}}$, are presented in

Due to the procedure adopted to calculate the Jacobian $\mathbf{J_\Theta}$, the out-of-diagonal elements of this matrix are small, and have been discarded in the present case study, for the sake of simplicity. Moreover, the diagonal elements are equal to 1 by construction.

The Jacobian matrix $\mathbf{J_\Phi}$ is obtained via perturbation theory, as described above, and is projected on the selected eigenmodes. In Fig. 5, the fission source distribution changes due to perturbations in the coolant density distribution along the directions $\boldsymbol{\theta_1}$ , $\boldsymbol{\theta_2}$ , $\boldsymbol{\theta_3}$ , and $\boldsymbol{\theta_5}$ of Fig. 4 are presented.

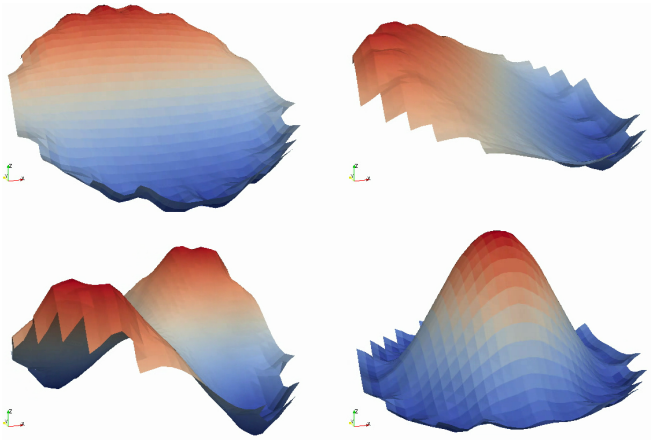

Fig. 4. Basis functions for the projection of the coolant density. $\boldsymbol{\theta_1}$ (top left), $\boldsymbol{\theta_2}$ (top right), $\boldsymbol{\theta_3}$ (bottom left), and $\boldsymbol{\theta_5}$ (bottom right). For better clarity, the 2D basis functions are presented with height deformation.

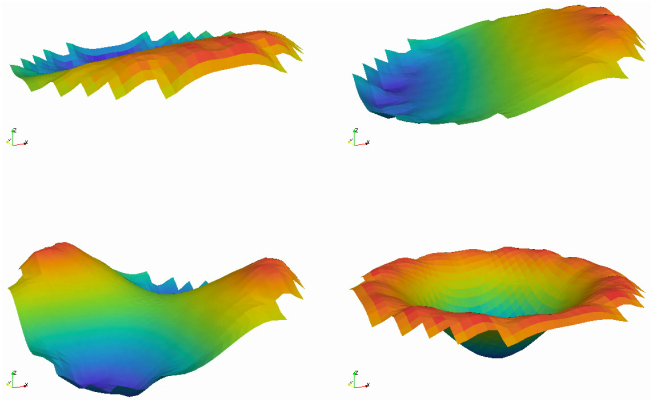

Fig. 5. Selected projections of $\mathbf{J_\Phi}$. $\frac{d\mathbf{\Phi}}{d\boldsymbol{\theta_1}}$ (top left), $\frac{d\mathbf{\Phi}}{d\boldsymbol{\theta_2}}$ (top right), $\frac{d\mathbf{\Phi}}{d\boldsymbol{\theta_3}}$ (bottom left), and $\frac{d\mathbf{\Phi}}{d\boldsymbol{\theta_5}}$ (bottom right). For better clarity, the 2D projections are presented with height deformation.

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

Adopting the Newton method with the approximated Jacobian obtained applying the chain rule to $\mathbf{J_\Phi}$ and $\mathbf{J_\Theta}$ ensures the stabilization of the coupled iterations, and leads to the convergence of the multi-physics simulation within approximately 3 iterations.[1] The normalized fission power distribution and coolant density distribution are presented in Fig. 6.

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 the arising of

[1] A detailed discussion on the advantages of the adoption of approximate Jacobians can be found in [9]

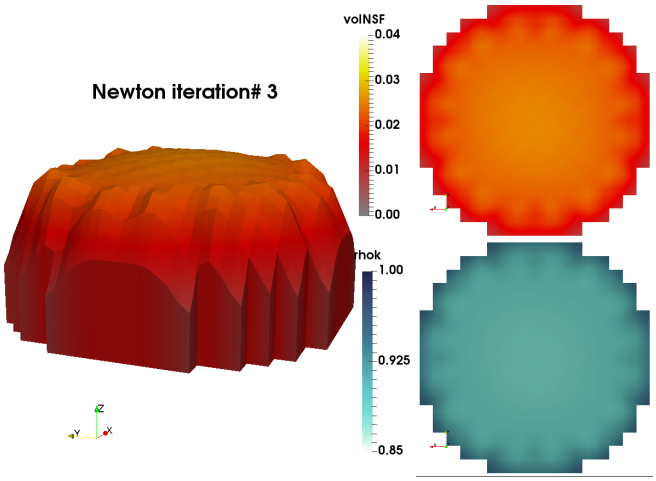


Fig. 6. Radial power distribution (top) and coolant density distribution (bottom) for Newton iteration #3. For better clarity, on the left, the 2D fission source distribution is presented with height deformation.

instabilities along the directions of the first two degenerate eigenmodes. It is expected that a more complete consideration of the thermal/hydraulics feedback, including 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.

## VII. CONCLUSIONS

The standard operator splitting approach in coupled neutronics-thermal/hydraulics problems might result in unstable or slowly converging results. Jacobian-free Newton–Krylov (JFNK) methods proved very useful in many fields of computational engineering. Nonetheless, the adoption of Monte Carlo transport for the neutronic solution of the problem challenges the adoption of JFNK methods due to the difficulties arising from numerical differentiations in presence of statistical errors. This paper presents the adoption of Monte Carlo Perturbation Theory to approximate the Jacobian matrix of the coupled neutronics-thermal/hydraulics problem. The Jacobian matrix is projected along few directions obtained from the eigenvalue decomposition of the fission matrix of the problem, and it is adopted to solve the coupled problem via the Newton method.

The proposed approach has been 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.

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