

A Neutronics and Thermal-Hydraulics Coupling Method for Reactor Simulations Based on Monte Carlo Perturbation Theory

Kaiwen Li^{a,b}, Wu Wang^b, Hao Luo^b, Nan An^b, Shanfang Huang^{b,*}, Ding She^a, Kan Wang^b

^aInstitute of Nuclear and New Energy Technology, Tsinghua Univ., Beijing, China, 100084

^bDepartment of Engineering Physics, Tsinghua Univ., Beijing, China, 100084

*Corresponding author: sfhuang@tsinghua.edu.cn

1. Introduction

There are typically two main groups of neutronics and thermal-hydraulics coupling methods that are widely researched over the world, the Picard iteration method [1] and the Newton iteration method [2].

For Monte Carlo particle transport, almost all the studies on the neutronics and thermal-hydraulics coupling are using Picard iteration method, like MCNP 5 and STAR-CD [3], Serpent 2 and SUBCHANFLOW [4], MC21 and CTF [5], RMC/CTF [6,7], etc.

However, Picard iteration is only a method of first-order convergence while the Newton iteration method can be of second-order convergence. Higher order convergence may lead to fewer iteration numbers and thus less time consumption. Therefore, Newton iteration between neutronics and thermal-hydraulics is worthy to be deeply studied.

Newton method has been widely researched on coupling simulations with deterministic methods [8,9,10]. For Monte Carlo methods, representative works includes: Mylonakis et al. [11] implemented a standard JFNK procedure between Monte Carlo particle transport code and the thermal-hydraulics code in 2017. Finite differences were calculated to substitute the matrix-vector product terms required in the GMERS procedure. To accelerate the simulations, Approximate Block Newton method was proposed to reduce the calculation burden; in the same year, Manuele Aufiero et al. [12,13] applied the Generalized Perturbation Theory (GPT) to obtain the sensitivity coefficients between the power distributions and the thermal-hydraulics parameter distributions. Combined with the calculations of the finite differences in the thermal-hydraulics module, the Jacobian matrix of the coupling iteration is completely built, and then directly used in a Newton iteration procedure. Those two implementations of Newton iteration methods can both realize second-order convergence, and the iteration numbers are significantly reduced. However, finite difference calculations are both required, which may account for a lot of time, especially when the target problems are getting larger.

In this work, we have proposed an efficient neutronics and thermal-hydraulics coupling method based on the Monte Carlo perturbation theory. This method is a new implementation of the Newton iteration procedure, and the redundant finite difference calculations in the thermal-hydraulics module are avoided.

2. Coupling Theory and Methods

In this section, the coupling problems are represented with equations, and then Picard iteration and Newton iteration procedures will be introduced with formulas.

2.1 Equations for the Coupling Problems

For the neutronics module, what actually needs to be solved is the Boltzmann neutron transport equation, and its operator form is as follows:

$$(L + R)\phi = \frac{1}{k_{eff}}F\phi \quad (1)$$

where L , R , F are leakage operator, removal operator and fission operator respectively, and ϕ is the neutron flux. The operators are related to their corresponding macro cross-sections, and those macro cross-sections are affected by thermal-hydraulics parameters like the temperature distributions of the fuel and coolant, and the density distribution of the coolant. Therefore, Eq. (1) can be expressed as

$$\Psi(\theta, \phi) = 0 \quad (2)$$

where θ represents the thermal-hydraulics parameters, and Ψ denotes the neutron transport equation.

For the thermal-hydraulics module, the equations to be solved are the mass, momentum, and energy conservation equations. As the heat source term in the energy conservation equation actually comes from heat production of neutron transport, mainly fission reactions, the three conservation equations can be expressed as:

$$\Theta(\theta, P) = 0 \quad (3)$$

where Θ represents the thermal-hydraulics conservation equation and P represents the thermal power distribution. The thermal power distribution is affected by the neutron flux distribution and the macro cross-sections of heat release reactions, like fission reactions. Therefore, Eq. (3) can be represented as:

$$\Theta(\theta, P(\theta, \phi)) = 0 \quad (4)$$

Further, if we rewrite the equations (2)(4) in the form of solutions, namely

$$\phi = \Psi^*(\theta) \quad (5)$$

$$\theta = \Theta^*(\phi) \quad (6)$$

then an iterative relation can be constructed:

$$\phi_{n+1} = \Psi^*(\Theta^*(\phi_n)) \quad (7)$$

Eq. (7) is the representation of the iterative procedure of the neutronics and thermal-hydraulics coupling system.

2.2 Picard iteration and Newton iteration methods

Eq. (7) can be directly used to represent the Picard iteration procedure, and the iteration operator can be written as G in Eq. (8).

$$\phi_{n+1} = \Psi^*(\Theta^*(\phi_n)) = G(\phi_n) \quad (8)$$

There may be vibrations during the Picard iterations, so relaxation is generally required:

$$\phi_{n+1}^* = c\phi_{n+1} + (1-c)\phi_n \quad (9)$$

where c is the relaxation coefficient and ϕ_{n+1}^* is the corrected neutron flux that will be used in the following iterations.

Picard iteration method is first-order convergent, and a more efficient second-order convergent iterative method is to calculate the residual r of Eq. (8) and then solve the residual equation (11) to update ϕ in Eq. (12):

$$r = \Psi^*(\Theta^*(\phi_n)) - \phi_n \quad (10)$$

$$J_G \delta_\phi = -r \quad (11)$$

$$\phi_{n+1} = \phi_n + \delta_\phi \quad (12)$$

where J_G is the Jacobian matrix of the iterative operator G . If the neutron flux ϕ is discretized into N regions, the shape of Jacobian matrix J_G should be $N \times N$. The iterative process constructed by Eq. (10)(11)(12) is a typical Newton iteration method, where the residual equation (11) can be solved with Krylov subspace method or others. With partial derivatives in the Jacobian matrix, a better direction and size of the iterative update δ_ϕ can be calculated, and thus has the potential to achieve second-order convergence.

3. Coupling Method based on Perturbation Theory

In this section, we will introduce our proposed coupling method based on Monte Carlo perturbation theory. We may first give the original iteration processes of Newton method applied in Monte Carlo coupling simulations in Section 3.1, and then introduce the changes and innovations of the proposed method in Section 3.2.

3.1 Newton method in Monte Carlo coupling simulations

A typical and commonly used implementation of the Newton method is Jacobian-free Newton Krylov (JFNK) method. Mylonakis et al. [11] used the standard JFNK method to solve the neutronics and thermal-hydraulics coupling problem, and applied the Arnold method to solve the residual equation (11) on the Krylov subspace $\mathcal{K}\{r, J_G r, J_G^2 r, \dots, J_G^{N-1} r\}$. Since the Jacobian matrix J_G is generally very large, and only Jv form is used in the process, JFNK method only calculates the Jv terms instead of the whole Jacobian matrix to save memory, and thus achieves "Jacobian-free". The Jv terms can be approximated by finite differences:

$$J_G v \approx \frac{G(\phi_n + \epsilon v) - G(\phi_n)}{\epsilon} \quad (13)$$

where ϵ is a carefully selected value. In NITSOL software suite [14], ϵ is recommended to be set as:

$$\epsilon = \frac{\sqrt{\epsilon_{mach}(1 + \|\phi_n\|)}}{\|\nu\|} \quad (14)$$

where ϵ_{mach} is the floating-point calculation precision of the machine.

In the approximation formula (13), an additional neutron transport and thermal-hydraulics calculation (i.e., $G(\phi_n + \epsilon v)$) is required for each v . Therefore, a single JFNK iteration may introduce N times of neutron transport and thermal-hydraulics calculations, the total time consumption may be even larger than Picard iteration even though the iteration numbers are reduced.

Manuele et al. [12,13] implemented the Newton method in a different way: they built the whole Jacobian matrix J_G and then performed the residual equation solving on a subspace constructed by eigenvectors of the iterative fission matrix of the system. The Jacobian matrix J_G can be decomposed as the product of two Jacobian matrices of the neutron transport and thermal-hydraulics module respectively, that is:

$$J_G = J_{\Psi^*} J_{\Theta^*} = \begin{bmatrix} \frac{\partial \phi_1}{\partial \theta_1} & \frac{\partial \phi_1}{\partial \theta_2} & \dots & \frac{\partial \phi_1}{\partial \theta_M} & \frac{\partial \theta_1}{\partial \phi_1} & \frac{\partial \theta_1}{\partial \phi_2} & \dots & \frac{\partial \theta_1}{\partial \phi_N} \\ \frac{\partial \phi_2}{\partial \theta_1} & \frac{\partial \phi_2}{\partial \theta_2} & \dots & \frac{\partial \phi_2}{\partial \theta_M} & \frac{\partial \theta_2}{\partial \phi_1} & \frac{\partial \theta_2}{\partial \phi_2} & \dots & \frac{\partial \theta_2}{\partial \phi_N} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{\partial \phi_N}{\partial \theta_1} & \frac{\partial \phi_N}{\partial \theta_2} & \dots & \frac{\partial \phi_N}{\partial \theta_M} & \frac{\partial \theta_M}{\partial \phi_1} & \frac{\partial \theta_M}{\partial \phi_2} & \dots & \frac{\partial \theta_M}{\partial \phi_N} \end{bmatrix} \quad (15)$$

The Jacobian matrix of the neutron transport J_{Ψ^*} can be directly calculated with the source perturbation algorithm, while the thermal-hydraulics Jacobian matrix J_{Θ^*} still needs to be approximated by finite differences $J_{\Theta^*} v$. The Krylov subspace is no longer used, instead, the subspace built from the eigenvectors of the iterative fission matrix is used to solve the residual equation. The statistical error of the first few eigenvectors can be relatively small, thus reducing the impact of Monte Carlo statistical uncertainty. However, a series of assumptions are made in this method, including that all the heat comes from fission reactions, thus there may be some methodological errors. In addition, this method still requires N times of thermal-hydraulics calculations in each iteration step. Together with the time consumption on the iterative fission matrix, the time cost of one iteration is still too large.

3.2 Coupling Method Based on Perturbation Theory

To tackle the issues of the methods above, we designed a coupling method based on the Monte Carlo perturbation theory and eliminated the $O(N)$ times of extra calculations.

First, we used the differential operator method in Monte Carlo perturbation theory to solve the perturbation coefficients of power distribution to all the thermal-hydraulics parameters, that is, matrix J_{Ψ^*} ; then, instead of solving the thermal-hydraulics Jacobian matrix J_{Θ^*} , an internal iteration of thermal-hydraulics calculation is designed to obtain the distributions of the

corrected thermal-hydraulics parameters. The calculation workflow can be represented by the following equations:

$$\phi_{n,0} = \phi_n = \Psi^*(\theta_n) \quad (16)$$

$$\theta_{n,1} = \Theta^*(\phi_n) \quad (17)$$

$$\phi_{n,1} = \phi_n + J_{\phi_n}(\theta_{n,1} - \theta_{n,0}) \quad (18)$$

$$\dots$$

$$\theta_{n,j+1} = \Theta^*(\phi_{n,j}) \quad (19)$$

$$\phi_{n,j+1} = \phi_{n,j} + J_{\phi_n}(\theta_{n,j+1} - \theta_{n,j}) \quad (20)$$

$$\dots$$

$$\theta_{n+1} = \Theta^*(\phi_{n,k}) \quad (21)$$

where k is the number of internal iterations, J_{ϕ_n} represents Jacobian matrix of neutron transport in the n -th iteration.

The internal iterations (19)(20) are actually calculating the intersection between the N -dimensional plane $\phi = J_{\phi_n}(\theta - \theta_{n,j}) + \phi_{n,j}$ and the thermal-hydraulics equation (6) plus the neutron flux normalization. Practically, the iteration process for the high-dimensional plane intersection is very efficient, a constant number of iterations may converge the solution. This may reduce the number of thermal-hydraulics simulations from $O(N)$ to $O(1)$.

Details of the proposed method will be introduced in the following subsections.

3.2.1 Overall Workflow and Convergence Criteria

The entire workflow of the proposed coupling method is illustrated in Fig. 1. There are two iteration loops in the workflow: the internal loop in the right part of the figure is the intersection calculation mentioned in the last section, and the external loop is the coupling iteration.

The external iteration loop in Fig. 1 is consistent with the Picard iteration process. If the convergence criteria in the internal iteration loop are set as constant true, and the calculation of J_{ϕ} is removed, the whole process is a standard Picard iteration. Therefore, it is easy to upgrade from a Picard iteration to the proposed method - just add the calculation of J_{ϕ} and the internal iteration.

For the internal iteration loop, the “refine the power distribution” step is the calculation represented by Eq. (20), where the neutron transport results of the last iteration $\phi_{n,j}$, Jacobian matrix of neutron transport J_{Ψ^*} , and the difference between the two adjacent thermal-hydraulics simulation results are combined to refine the power distribution (or neutron flux) under current thermal-hydraulics parameters.

The key to the effectiveness of this process is that the intersection of the N -dimensional plane $\phi = J_{\phi_n}(\theta - \theta_{n,j}) + \phi_{n,j}$, the thermal-hydraulics equation (6), and the normalization of the neutron flux can converge in a limited number of iterations. Due to the simplicity of the N -dimensional plane, the fast convergence of the intersection iteration can be reached even with Monte Carlo statistical error.

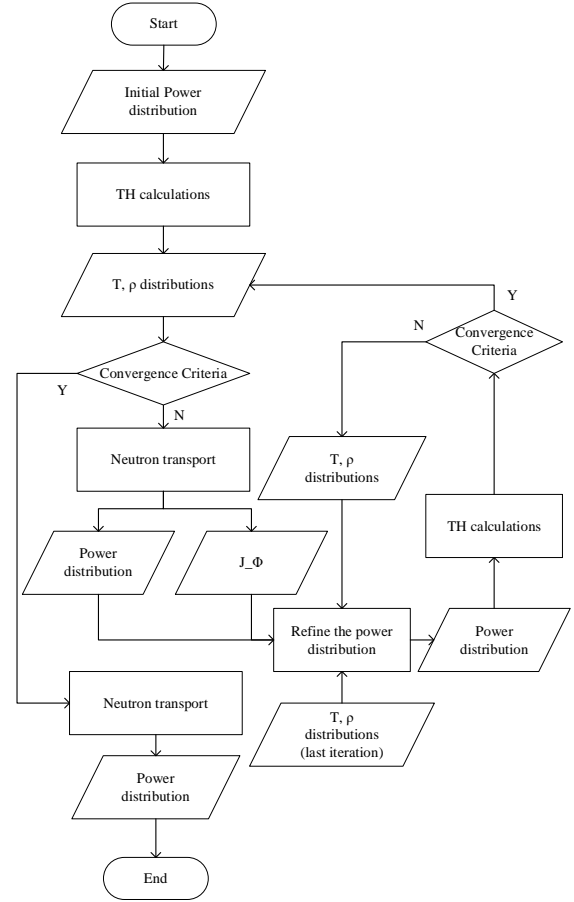


Fig. 1. Workflow of the proposed Newton iterative coupling method based on Monte Carlo perturbation theory.

In terms of the convergence criteria of the internal and external iterations, the convergence criterion of the internal iteration is measured by the L_2 norm of the power distribution change between two adjacent iterations: if

$$\frac{L_2}{\sqrt{N}} = \sqrt{\frac{1}{N} \sum_{i=1}^N \left| \frac{p_{n,i+1} - p_{n,i}}{p_{n,i}} \right|^2} < \epsilon_{internal} \quad (22)$$

stands, then the internal iteration has converged. The $\epsilon_{internal}$ in Eq. (22) can be designed according to the order of the averaged relative deviation of the power distribution. In practice, a fixed number of iterations rather than the judgement can also be used as the criteria to avoid too many iterations. From our experience, the internal loop converges within 3 iterations.

For external iterations, the convergence criteria can also be designed similar to Eq. (22), except that the $\epsilon_{internal}$ is substituted by $\epsilon_{external}$. Moreover, it can be noted that if the first step of the internal iteration already meets the convergence criterion, then there must be:

$$\|J_{\phi_n}(\theta_{n,1} - \theta_{n,0})\|_2 < \epsilon_{internal} \quad (23)$$

There are two possible conditions that may lead to Eq. (23): 1). the thermal-hydraulics parameters θ have already converged; 2). the change of thermal parameters has little effect on the neutron transport module, that is,

J_{ϕ_n} is orthogonal to the change of θ . Both reveals that the external iterations should be terminated. Therefore, the convergence criterion of the external iteration can be:

$$\frac{L_2}{\sqrt{N}} = \sqrt{\frac{1}{N} \sum_{i=1}^N \left| \frac{p_{n,1} - p_n}{p_n} \right|^2} < \epsilon_{internal} \quad (24)$$

Note that $\epsilon_{internal}$ rather than $\epsilon_{external}$ is used, and that may reduce the number of hyper parameters of the proposed method.

The proposed method and the convergence criterion (23) have been proved to be correct and efficient in Section 4. The code changes from Picard iteration are limited and the independence of the two simulation modules are still maintained, which is convenient for maintenance and development in the future.

Apart from the workflow and convergence criteria designs, the core problem of this method is to efficiently solve J_{ϕ_n} , which will be introduced in Section 3.2.2.

3.2.2 Calculation of the neutron transport Jacobian matrix by differential operator method

In this section, we may use power distribution P to replace the neutron flux ϕ in all the equations. As P and ϕ are one-to-one correspondent, this replacement will not affect the correctness of the equations. After that, the equations (5)(6) will be rewritten as:

$$P = \Psi^*(\theta) \quad (25)$$

$$\theta = \Theta^*(P) \quad (26)$$

Then, the elements in the Jacobian matrix J_{Ψ^*} should be changed to $\partial P_i / \partial \theta_j$, which can be regarded as the perturbation coefficients between power and thermal-hydraulics parameters. Therefore, differential operator method can be used to solve those derivatives and build the complete Jacobian matrix J_{Ψ^*} . The differential operator method is briefly described as follows:

The power tally during neutron transport is estimated by the following equation:

$$P = \frac{1}{N} \sum_{i=1}^N \sum_j p_{i,j} f_{i,j} \quad (27)$$

where $p_{i,j}$ is the probability of the j -th track of the i -th neutron, and $f_{i,j}$ is the power estimator. $p_{i,j}$ can be further decomposed as:

$$p_{i,j} = S(\mathbf{R}_0, E_0, \boldsymbol{\Omega}_0) \prod_{m=1}^j r_m \quad (28)$$

where S is the probability that the parent neutron produces the i -th neutron in a specific phase $(\mathbf{R}_0, E_0, \boldsymbol{\Omega}_0)$, and r_m is the probability of the m -th track on condition that the former $m - 1$ tracks have already appeared. r_m can be further decomposed into transport term T_m and collision term C_m :

$$r_m = T_m(\mathbf{R}_{m-1} \rightarrow \mathbf{R}_m, E_{m-1}, \boldsymbol{\Omega}_{m-1}) \cdot C_m(\mathbf{R}_m, E_{m-1} \rightarrow E_m, \boldsymbol{\Omega}_{m-1} \rightarrow \boldsymbol{\Omega}_m) \quad (29)$$

Therefore, the derivatives of power over temperature are:

$$\begin{aligned} \frac{\partial P}{\partial T} &= \frac{1}{N} \sum_{i=1}^N \sum_j \left[\frac{1}{p_{i,j} f_{i,j}} \frac{\partial(p_{i,j} f_{i,j})}{\partial T} \right] p_{i,j} f_{i,j} \\ &= \frac{1}{N} \sum_{i=1}^N \sum_j w_{i,j} p_{i,j} f_{i,j} \end{aligned} \quad (30)$$

Similarly, the derivatives of power over density are:

$$\begin{aligned} \frac{\partial P}{\partial \rho} &= \frac{1}{N} \sum_{i=1}^N \sum_j \left[\frac{1}{p_{i,j} f_{i,j}} \frac{\partial(p_{i,j} f_{i,j})}{\partial \rho} \right] p_{i,j} f_{i,j} \\ &= \frac{1}{N} \sum_{i=1}^N \sum_j w_{i,j} p_{i,j} f_{i,j} \end{aligned} \quad (31)$$

where $w_{i,j}$ is the weight of each track, which can be calculated with Eq. (32) below. Note that the specific values of the terms in Eq. (32) can be different when calculating different perturbation parameters.

$$\begin{aligned} w_{i,j} &= \frac{p'_{i,j}}{p_{i,j}} + \frac{f'_{i,j}}{f_{i,j}} = \frac{S'}{S} + \sum_{m=1}^j \frac{r'_m}{r_m} + \frac{f'_{i,j}}{f_{i,j}} \\ &= \frac{S'}{S} + \frac{T'_m}{T_m} + \frac{C'_m}{C_m} + \frac{f'_{i,j}}{f_{i,j}} \end{aligned} \quad (32)$$

In this way, all the elements in the Jacobian matrix J_{Ψ^*} can be solved. For large-scale models or high-fidelity simulations, the size of the matrix may be large. To handle this, merging adjacent regions to reduce the number of derivatives can be considered to accelerate the calculations.

3.2.3 Implementation in RMC/CTF Coupling System

In recent years, the perturbation and sensitivity calculation capabilities have been continuously improved [15,16,17,18] in RMC [19], which makes it possible to conduct studies on efficient multi-physics coupling methods based on Newton method and perturbation theory. Therefore, we implemented the proposed method above in the coupling system of Monte Carlo neutron transport code RMC and thermal-hydraulics sub-channel code CTF [20]. The implementation has been validated with practical cases in Section 4.

4. Validation of the Proposed Method

In this section, a PWR fuel pin is used to validate the correctness and effectiveness of the proposed method. The length of the fuel pin is 360 cm, and it is evenly split into 10 axial layers to analyze the axial power profile. The radial boundaries of the model are set as reflective, and the axial boundaries are vacuum.

Model parameters and the calculation parameters are listed in Table I. The Newton iteration method based on perturbation theory is compared with the Picard iteration. The Picard iteration method is performed in two modes: without relaxation and with relaxation ($c = 0.5$).

Table 1 Verification model geometry, material and other parameters

Table I: Model parameters and calculation parameters.

parameter	Picard	Newton
No. Axial layer	10	10
No. inactive cycles	100	100
No. active cycles	400	400
No. particles	100,000	100,000
No. internal iterations	-	5

Fig. 2 shows the calculation results of the three methods: Picard iteration without relaxation, Picard iteration with relaxation, and Newton iteration method based on Monte Carlo perturbation theory. All of them iterated from an assumed cosine power distribution (the black lines in the three subfigures) and converged to a curve with peaks tilting to the lower side. Those biases of peaks resulted from the non-uniformity of the moderator's density along the axial direction – the moderation in the lower region was stronger and thus fission reaction rate became higher.

Fig. 3 gives the changes of the L_2 norms over iterations. There are totally 3 types of L_2 norms in Fig. 3: 1). L_2 -final (black lines) is the L_2 norm of the relative differences between the current calculation results and the converged result of Picard iteration method with relaxation;

2). L_2 -relative (red lines) is the L_2 norm of the relative differences between two adjacent external iterations;

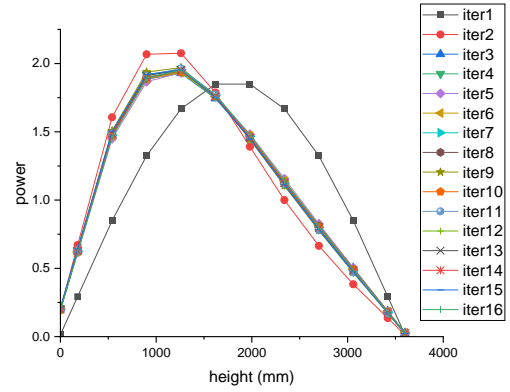
3). L_2 -internal (blue line) is the L_2 norm of the relative differences between the external power distribution and the corresponding first internal power distribution, which is Eq. (24).

As the reference solution is unknown in the practical calculations, red lines rather than black lines should be used to judge convergence. If the convergence criterion is set as $\epsilon = 10^{-4}$, then the required numbers of iterations for the three methods are 7, 6, and 4, respectively, which demonstrates the convergence efficiency of the proposed Newton method based on Monte Carlo perturbation theory.

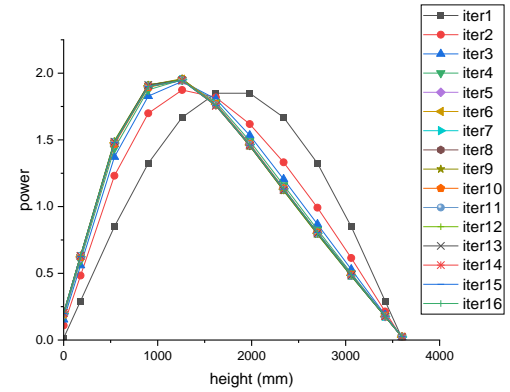
For the stability of the iterations, the oscillation ranges can be seen from the "thickness" of the overlapped curves in Fig. 2. Picard iteration without relaxation has the strongest oscillation, which can also be observed from the large shakes in Fig. 3(a). This instability has been tackled in the Picard iteration with relaxation method in Fig. 2(b) and Fig. 3(b). The Newton method based on the Monte Carlo perturbation theory has no relaxation, but still achieves a similar oscillation suppression phenomenon. From the blue line in Fig. 3(c), we can clearly observe the excellent convergence stability of the proposed method.

Furthermore, the trend of L_2 -internal in Fig. 3(c) is similar to that of L_2 -relative, but the range is wider,

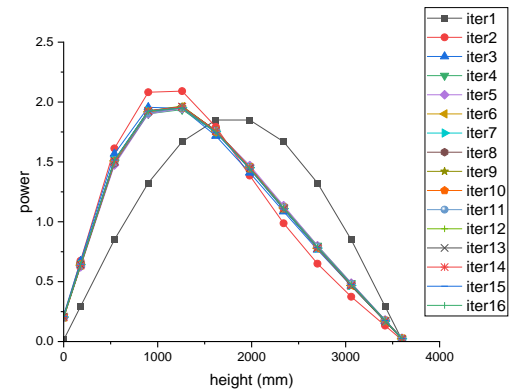
which is more convenient to judge convergence. Therefore, L_2 -internal (Eq. (24)) is a better convergence indicator for the Newton method based on Monte Carlo perturbation theory.



(a)

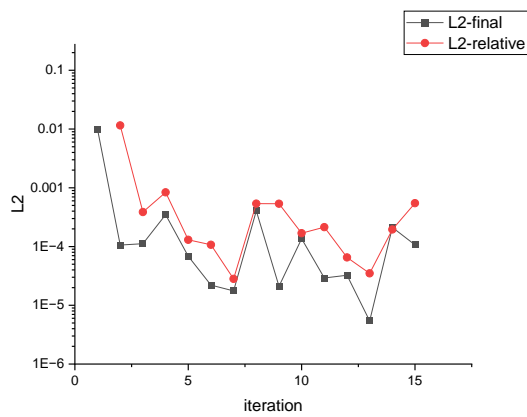


(b)

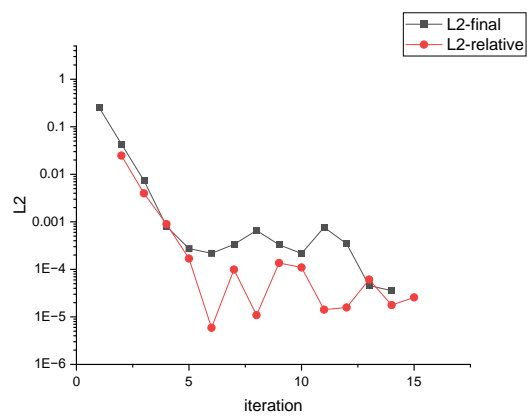


(c)

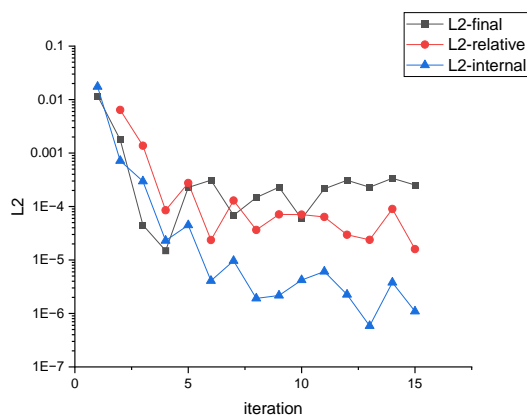
Fig. 2. Axial power profiles over iterations for the three methods: (a) Picard iteration without relaxation; (b) Picard iteration with relaxation; (c) Newton iteration based on Monte Carlo perturbation theory.



(a)



(b)



(c)

Fig. 3. L_2 norms over iterations for the three methods: (a) Picard iteration without relaxation; (b) Picard iteration with relaxation; (c) Newton iteration based on Monte Carlo perturbation theory.

5. Conclusions

This paper proposes a neutronics and thermal-hydraulics coupling method based on the Monte Carlo perturbation theory. We use the differential operator method in Monte Carlo perturbation theory to calculate the neutron transport Jacobian matrix, and then establish an internal iteration loop to refine the distributions of the

power and thermal-hydraulics parameters. This method realizes partial second-order convergence, and at the same time avoids the unbearable extra calculations that may rapidly expand with the problem scale. The proposed method was validated on a practical model and showed higher convergence efficiency and better convergence stability. However, Monte Carlo perturbation may increase the total calculation time, which would be even worse for large and high-fidelity problems. Therefore in the future, this method will be extended to simulations of large-scale problems, and acceleration methods including block merging and diagonal approximation will be studied to further optimize the computational efficiency of this method.

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