The Monte Carlo Thermal-Physics Coupling Method Based on Functional Expansion Tallies

Nan An[1,*], *Yuanhao* Gou[1,**], and *Hao* Luo[1,***] *Zhaoyuan* Liu[1,****] *Kan* Wang[1,†]

[1]Department of Engineering Physics, Tsinghua University Tsinghua Yuan #1, Haidian District, Beijing, China

Abstract. In the Monte Carlo thermal-physical calculations for nuclear reactors, the precise and effective transfer of data between different meshes is a difficult issue of thermal and physical coupling. Converting two separate meshes and transferring the data is an exceptionally difficult and complex task within the conventional nuclear thermal-physics coupling approach. The newly developed Functional Expansion Tallies (FET) method can obtain the continuous distribution of parameters in the solution space.

By applying FET method to nuclear thermal-physics coupling, the no-mesh continuous fission energy distribution can be obtained, which is suitable for more complex meshes. Additionally, the computational memory can be minimized by substituting the data from numerous mesh power distribution data points with the coefficients of the function.

1 Introduction

The Monte Carlo computing method has become more significant in the industry as the computer technology has improved [1].

In the process of nuclear reactor design and analysis, it is necessary to analyze a variety of mutually coupled physical processes in nuclear reactors. Among these processes, the coupling between particle transport and thermal-hydraulics, known as nuclear thermal-physics coupling, plays a vital role in reactor multi-physics analysis. Considering the influence of the time step, studying, evaluating, and advancing state-of-the-art nuclear thermal coupling techniques is of utmost importance for achieving high-fidelity analysis of reactors.

The precise and effective transfer of data between different meshes is a difficult issue of thermal and physical coupling. Converting two separate meshes and transferring the data is an exceptionally difficult and complex task within the conventional nuclear thermal-physics coupling approach.

The newly developed Functional Expansion Tallies (FET) method [2] expands the unknown quantity to a certain order by multiple sets of orthogonal functions and estimates the corresponding expansion coefficients by Monte Carlo simulation or other simulation methods. The continuous distribution of parameters in the solution space can be obtained by the

*e-mail: an19@mails.tsinghua.edu.cn
**e-mail: gouyh20@mails.tsinghua.edu.cn
***e-mail: l-huo19@mails.tsinghua.edu.cn
****e-mail: liuzy7@mail.tsinghua.edu.cn
†e-mail: wangkan@tsinghua.edu.cn

FET method. Therefore, employing the FET method can address the issue of data transfer between different meshes in thermal-physics coupling.

In 2015, Ellis and Gaston [5] used the Moose multi-physical coupling platform, based on Monte Carlo code OpenMC [6] coupled with Cerberus, to calculate two-dimensional PWR fuel assemblies with FET. In 2018, Novak [7] used the Moose platform to perform two-dimensional single-rod coupling calculations with OpenMC, Nek5000 and Buffalo by using FET. And the FET method was also developed in the Monte Carlo program Serpent 2 [8], which was later used to simplify the mesh transformation of Serpent and BISON coupling [9] and reduce the error problem of bin boundary.

The Reactor Monte Carlo code, RMC [3], is an Self-developed developed stochastic simulation code maintained by REAL laboratory of Tsinghua University. After many years of continuous development, RMC has been a general-purpose, reactor-oriented, multi-physics platform with functionalities of criticality analysis, burnup calculation, criticality search, shielding simulation, group constants generation, kinetics calculation, neutronics and thermal-hydraulics simulations, and so on. And it encapsulates several new algorithms [10, 11, 14] we proposed in recent years.

The sub-channel thermal-hydraulic analysis code, SUBCHAN [4], features four partial differential equations and can simulate a single-component two-phase mixture. The code uses the Industrial Formulation 1997 as the water property package which is commonly recommended for industrial use. SUBCHAN is originally designed for the simulation of a Supercritical-Water-Cooled Reactor (SCWR) and applied for the thermal-hydraulic analysis of a Pressurized Water Reactor (PWR) in this work.

In this paper, by employing the FET method in nuclear thermal-physics coupling, it becomes possible to obtain a continuous fission energy distribution without the need for mesh discretization. This approach is particularly advantageous for handling more intricate meshes. Additionally, the computational memory can be minimized by substituting the data from numerous mesh power distribution data points with the coefficients of the function.

Based on the feature of FET in RMC, in section 2, we apply FET method to nuclear thermal-physics coupling. The method for FET thermal-physics coupling is verified and validated in Section 3. Finally comes the conclusions in Section 4.

2 Thermal-Physics Coupling Method Based on Functional Expansion Tallies

This section will introduce the functional expansion tallies-based Monte Carlo thermal-physics coupling method. Firstly, we need to go through the FET method to understand how to how to get no-mesh power distribution in solution space.

2.1 Brief Introduction of FET Method

The Functional Expansion Tallies (FET) method is a method to expand an unknown quantity to a certain order with several orthogonal functions and estimate the corresponding expansion coefficients by Monte Carlo calculation.

The function of the FET method can be any function of any form $F(\xi)$, where $F(\xi)$ is the unknown function to be solved as Eq. (1).

$$F(\xi) = \sum_{n=0}^{\infty} a_n k_n \varphi_n(\xi), \tag{1}$$

In Eq. (1), $\varphi_n(\xi)$ is the orthogonal basis function, it can be Legendre polynomials as Eq. (2) or Zernike polynomials as Eq. (3), (4), and (5).

$$P_{n+1}(\xi) = \frac{(2n+1)\xi P_n(\xi) - nP_{n-1}(\xi)}{n+1}, \tag{2}$$

$$\varphi_c(\xi) = \varphi_{m,n}(r,\theta) = Z_n^m(r,\theta), \tag{3}$$

$$\varphi_c(\xi) = \begin{cases} Z_n^m(r,\theta) = R_n^m(r)\cos(m\theta), & m > 0 \\ Z_n^m(r,\theta) = R_n^m(r)\sin(m\theta), & m < 0 \\ Z_n^m(r,\theta) = R_n^m(r), & m = 0 \end{cases}, \tag{4}$$

$$R_n^m(r) = \sum_{k=0}^{\frac{n-m}{2}} \frac{(-1)^k (n-k)!}{k!(\frac{n+m}{2}-k)!(\frac{n-m}{2}-k)!} r^{n-2k}, \tag{5}$$

Based on track-length estimation, the flux can be calculated by the FET method, and the estimation of a_n is calculated through Eq. (6).

$$\hat{a}_n = V\frac{\sum_{i=1}^{N}\phi(\xi_i)\omega_i\varphi_n(\xi_i)\rho_\varphi(\xi_i)}{\sum_{i=1}^{N}\omega_i} = \sum_{i=1}^{N} T_{l,i}\omega_i\varphi_n(\xi_i)\rho_\varphi(\xi_i), \tag{6}$$

In Eq. (6), $T_{l,i}$ is the length of a track of a particle, $\phi(\xi_i)$ is the flux function, ρ_φ is the weight function of φ_n, ξ_i is the position of particle i.

Different solution parameters can be produced by multiplying flux by the corresponding calculation coefficients based on Eq. (6). For instance, the coefficient of fission power is represented by Eq. (7).

$$H_f = \sum_i (\omega_i T_{l,i}\sigma_{f,i} Q \frac{\rho_\alpha}{m}), \tag{7}$$

In Eq. (7), ω_i is the particle weight, $\sigma_{f,i}$ is the microscopic fission cross-section, m is the cell mass, ρ_α is the atomic density, and Q is the average fission energy of neutrons.

2.2 FET Thermal-Physics Coupling Method

Previous work reported the coupling of RMC and COBRA-TF (CTF) [12] for the analysis of a PWR assembly and a physical reactor with different coupling scheme including the loose-coupling scheme, i.e., the external scheme or the file-based coupling scheme, the internal-coupling scheme, and also the hybrid coupling scheme. Although loose-coupling scheme has certain defects in computational accuracy, efficiency and versatility compared with the internal scheme, its greatest advantage lies in its avoidance of complicated code modifications and the file-based coupling significantly reduces the difficulty of the coupling of the two codes.

In this work, RMC is coupled to SUBCHAN using the new FET coupling framework with an in-house Python script developed for the coupling of a neutronic code and a thermal-hydraulic one, as shown in Fig. 1 and described below.

The coupling input processing is performed using the input parser in RMC Python module where the input is actually a normal RMC physics model with some necessary coupling parameters, especially the convergence criteria.

After the initialization of the RMC and SUBCHAN model, a Picard iteration is performed to converge the N-TH solutions. In the first coupling cycle, a typical radial uniform distribution and axial sinusoidal distribution is predicted and transformed in power tally files,

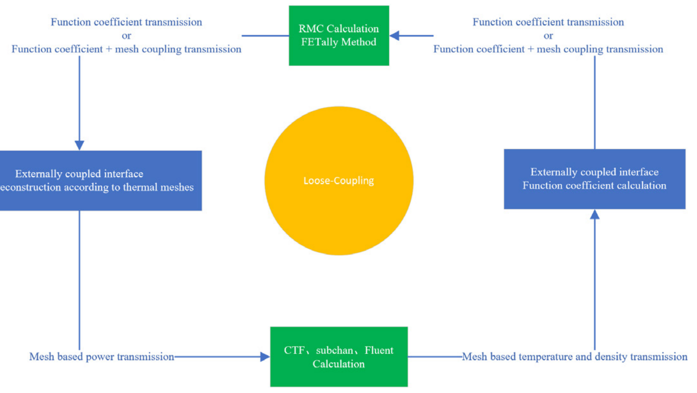

Figure 1. FET nuclear thermal-physics coupling flow chart.

MeshTally.h5 and FETally.h5. The built-in RMC2Subchan.py script will subsequently calculate the absolute line power distributions according to the MC tallied power and output them in a power input file of SUBCHAN, POWERSRC.CPL. The SUBCHAN code then solves the thermal hydraulics equations and outputs the fuel rod volume-averaged temperatures, the subchannel temperatures and densities in a coupling file, SUBCHAN.CPL. These three thermal hydraulic parameters will be collected by another built-in Subchan2RMC.py script and translated to the proper mesh regions. The thermal hydraulics parameters in the mesh file, SUBCHAN.h5, is imported in the following execution of RMC. A problem-dependent 3-D power distribution is tallied from the particle transport calculation and output in the initial power tally files, MeshTally.h5 and FETally.h5, which are the input of next Picard iteration. The Picard iteration in the loose-coupling scheme is repeated until the convergence criteria is achieved.

Applying FET method to nuclear thermal-physics coupling, the no-mesh continuous fission energy distribution can be obtained, which is suitable for more complex meshes. Additionally, the computational memory can be minimized by substituting the data from numerous mesh power distribution data points with the coefficients of the function.

For traditional PWR assembly or full-core cases, FET and mesh-tally method can be combined for coupling data transmission. For a PWR assembly, we can use 17×17 radial meshes and 6th order Legendre FETally for the axial direction method in the active core region.

The FET thermal-physics coupling method will be tested and compared with the traditional mesh-tally method with RMC/SUBCHAN coupling system in Section 3.

3 Verification and Validation for the FET Thermal-Physics Coupling

In this section, the method for the FET thermal-physics coupling will be verified and validated. We tests the thermal-physics coupling method based on FET with RMC/SUBCHAN coupling system using a criticality assembly case and a burn-up full-core case.

3.1 Criticality Calculation of Nuclear Thermal-Physics Coupling of Assembly

The VERA Problem ♯6 is a single Westinghouse 17×17 type PWR fuel assembly at the BOC and HFP conditions, whose material compositions and geometry information can be referred to in the official specifications [13]. There are 264 fuel rods, 24 guide tubes and 1 instrument tube, and 324 coolant subchannels, without burnable poison rods and control rod clusters. All the fuel pins, guide tubes and moderator subchannels are explicitly modeled in RMC and SUBCHAN.

The FET method employs 17×17 radial meshes and 6th order Legendre polynomials for the axial direction in the active core region of 365.76 cm within the RMC and Subchan models. The FET results are then compared with results obtained using different axial meshes. RMC uses neutron ACE cross sections data from ENDF/B-VII.0 evaluation library and the on-the-fly doppler broadening (OTFDB) is utilized to consider the doppler broadening effect from the temperature changes from the thermal-hydraulic feedback. For Monte Carlo (MC) calculations, 100,000 particles are tracked in 50 inactive cycles and 400 active cycles with 25 MPI processes.

The results of FET coupling method including the convergent eigenvalue k-effective, the spatial power distributions of rods (radial and axial) and the calculation time, memory and average standard deviation, are compared with the mesh-tally based RMC/SUBCHAN results.

The radial, axial and spatial power distribution of the assembly results are shown in Fig. 2 and 3.

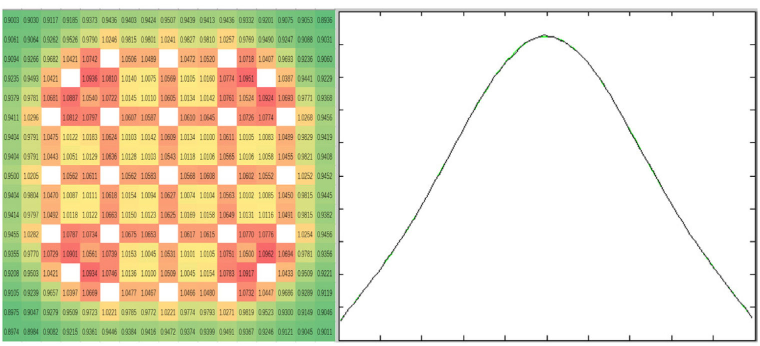

Figure 2. rods radial and axial power distribution of the assembly.

In Fig. 2, the radial rods power distributions obtained from the two methods exhibit complete consistency. The axial assembly power distribution obtained from the FET method is compared with the results obtained using 100 meshes. The green line represents the FET method, while the black line represents the mesh-tally method. These two lines demonstrate good agreement, indicating a high level of agreement between the FET method and the finely mesh-tally method.

Based on Fig. 3, we can observe that the average error between the two methods is 2.20%, with a maximum error of 19.24%. Out of the total 28,900 meshes analyzed, only nine meshes exhibit a result error greater than 5%. Notably, these meshes are located at the corners of the assembly. This analysis provides evidence supporting the consistency of the results and the validity of the FET method.

Moreover, the calculation time, memory and average standard deviation of the two methods are compared. The results are shown in Table 1.

Table 1 clearly demonstrates that the FET coupling method, when compared with the traditional mesh-tally coupling data transmission method, offers partial acceleration and significantly reduces the memory footprint required for data transmission.

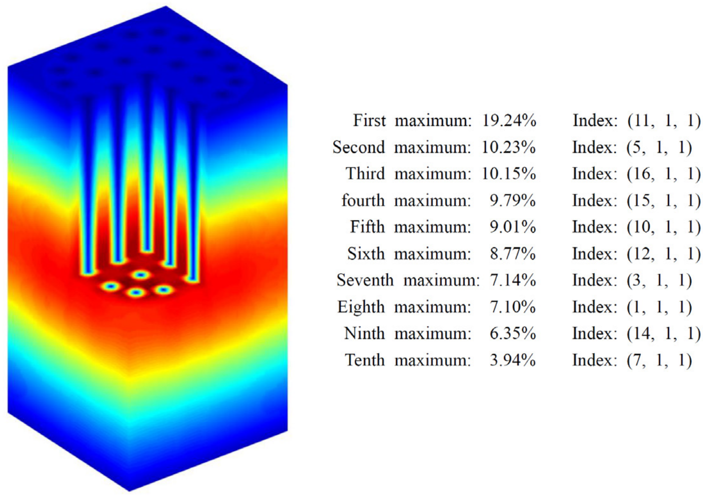

Figure 3. spatial power distribution of the assembly (17×17×100 meshes).

Table 1. Comparison of calculation time, memory and average standard deviation of the two calculation methods.

Using method	Simulation time(minutes)	Data storage	std
FET method: 6th order Legendre and 17×17 meshes	3.26	O(7+289)	0.8%
mesh method: 1×17×17 meshes	3.13	O(289)	0.3%
mesh method: 100×17×17 meshes	4.44	O(28900)	2.4%

Furthermore, under the same conditions of particle histories and calculation cycles, the FET coupling method exhibits a reduction of more than half in terms of standard deviation compared to the mesh-tally coupling method. This reduction in standard deviation signifies that the FET method yields more precise tally results for the MC method, enhancing the accuracy of the calculations.

3.2 Burn-up Calculation of Nuclear Thermal-Physics Coupling of Full-Core

The VERA Core Physics Benchmark Problem ♯7 represents an operating reactor in full geometry detail at beginning-of-cycle (BOC), hot-full-power (HFP), nominal flow conditions, and equilibrium xenon isotopic which has 193 assemblies. In this section, we use a PWR case based on VERA♯7, with the only difference that the number of assemblies is 157. Fig. 4 displays the PWR case's schematic diagram.

The FET method employs 255×255 radial meshes and 6th order Legendre polynomials for the axial direction in the active core region of 365.76 cm within the RMC and Sub-chan models. The FET results are then compared with results obtained using different axial meshes. The mesh number of 255 here comes as $17 \times 15 = 255$, by noting that each assembly has 17×17 rods, and the 157 assemblies of the full-core are distributed in 15×15 meshes. So the whole core is divided into 255×255 meshes.

RMC uses neutron ACE cross sections data from ENDF/B-VII.0 evaluation library and the on-the-fly doppler broadening (OTFDB) is utilized to consider the doppler broadening

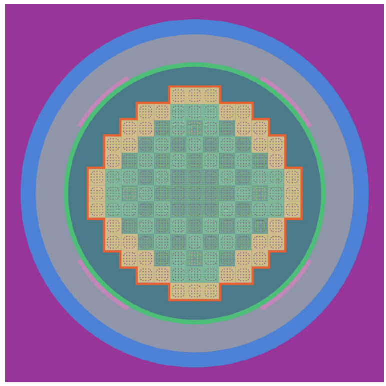

Figure 4. PWR case model.

effect from the temperature changes from the thermal-hydraulic feedback. For MC calculations, 1,000,000 particles are tracked in 50 inactive cycles and 300 active cycles. For large problems like the whole core problem, OpenMP is used with 14 threads for each process and 200 MPI processes is applied.

The results of FET coupling method including the convergent eigenvalue k-effective, the spatial power distributions (radial and axial) and the calculation time, memory and average standard deviation, are compared with the mesh-tally based RMC/SUBCHAN results.

The radial, axial and spatial power distribution of the assembly results are shown in Fig. 5 and 6. What's more, the boron-drop curve of the PWR core is also shown in Fig. 6.

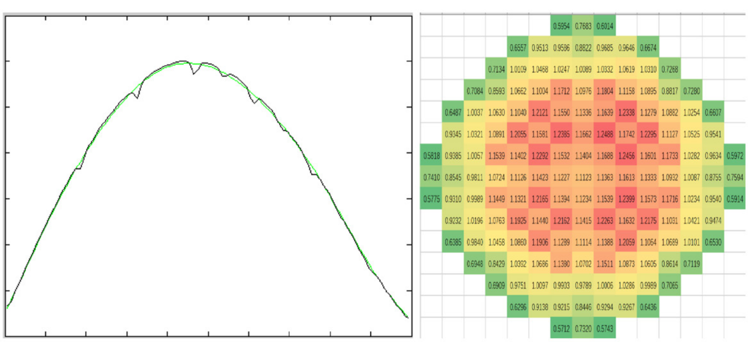

Figure 5. radial and axial power distribution of the PWR core.

In Fig. 5, the radial assemblies power distributions obtained from the two methods exhibit complete consistency. The axial assembly power distribution obtained from the FET method is compared with the results obtained using 100 meshes. The green line represents the FET method, while the black line represents the mesh-tally method. These two lines demonstrate good agreement, indicating a high level of agreement between the FET method and the finely mesh-tally method.

From Fig. 6 we can know that, the average error of the two methods is 0.33%. It can prove the consistency of the results and the correctness of the FET method. And in Figure 6, the boron-drop curve of concentrations is depicted, showcasing a comparison between

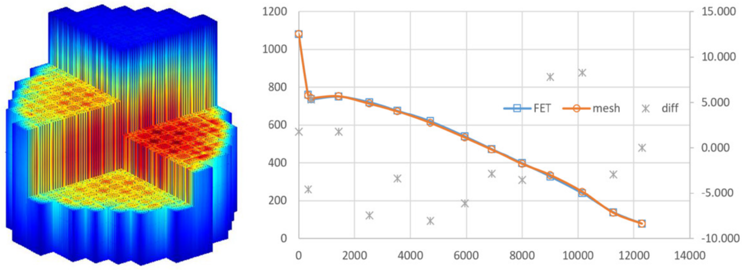

Figure 6. spatial power distribution and boron-drop curve of the PWR core (255×255×100 meshes).

Table 2. Comparison of calculation time, memory and average standard deviation of the two calculation methods.

Using method	Simulation time (per burn-up point, minutes)	Data storage	std
FET method: 6th order Legendre and 255×255 meshes	7.24	O(7+65025)	0.1%
mesh method: 1×255×255 meshes	5.71	O(65025)	0.8%
mesh method: 100×255×255 meshes	10.86	O(6502500)	7.6%

the two coupling methods. The agreement between the two methods is within 10 parts per million (ppm), indicating excellent statistical consistency in terms of eigenvalues and critical boron concentrations. This agreement reinforces the reliability and consistency of the results obtained from the FET coupling method.

Moreover, the calculation time, memory and average standard deviation of the two methods are compared. The results are shown in Table 2.

Table 2 clearly demonstrates that the FET coupling method, when compared with the traditional mesh-tally coupling data transmission method, offers partial acceleration and significantly reduces the memory footprint required for data transmission.

Moreover, under identical conditions of particle histories and calculation cycles, the FET coupling method exhibits a reduction in standard deviation by one order of magnitude compared to the mesh-tally coupling method. This significant decrease in standard deviation indicates that the FET method provides much more precise tally results. The improved accuracy offered by the FET coupling method enhances the reliability of the calculations and contributes to more accurate analysis and predictions.

4 CONCLUSIONS

In this paper, we apply the FET method to achieve nuclear thermal-physics coupling in both RMC and SUBCHAN, showcasing its ability to produce highly accurate and efficient numerical results.

The following conclusions can be taken from the calculation results in section 3:

1. A no-mesh continuous fission energy distribution can be obtained by the FET thermal-physics coupling method.

2. Comparing with traditional mesh-tally coupling method is to prove the correctness of FET coupling method. The FET method excels in obtaining a continuous fission

energy distribution without the need for mesh discretization, making it well-suited for handling complex meshes such as hexagonal and unstructured meshes. Additionally, the FET method yields more accurate tally results, further highlighting its superiority over the traditional method.

3. Additionally, the computational memory can be minimized by substituting the data from numerous mesh power distribution data points with the coefficients of the function.

In conclusion, the FET method provides a notable advantage over the traditional mesh tally method by producing more accurate source distribution and fission energy distribution. This enhanced accuracy is particularly beneficial in nuclear thermal-physics coupling, where it leads to improved results.

References

[1] Nease, Brian and Brown, Forrest B and Ueki, Taro, "Dominance ratio calculations with MCNP" *Proc. Int. Topical Mtg. on Physics of Reactors*. 14–19 (2008).

[2] An, Nan and Pan, Qingquan and Guo, Xiaoyu and Huang, Shanfang and Wang, Kan, "A new functional expansion tallies (FET) method based on cutting track-length estimation in RMC code" *Nuclear Engineering and Design*, **391**. 111736 (2022).

[3] Wang, Kan and Li, Zeguang and She, Ding and Xu, Qi and Qiu, Yishu and Yu, Jiankai and Sun, Jialong and Fan, Xiao and Yu, Ganglin and others, "RMC–A Monte Carlo code for reactor core analysis" *Annals of Nuclear Energy*, **82**. 121–129 (2015).

[4] Jiyang, Yu and Songtao, Wang and Baoshan, Jia, "Development of sub-channel analysis code for CANDU-SCWR" *Progress in Nuclear Energy*, **49**. 334–350 (2007).

[5] Ellis, Matthew and Gaston, Derek and Forget, Benoit and Smith, Kord, "Preliminary coupling of the Monte Carlo code OpenMC and the multiphysics object-oriented simulation environment for analyzing doppler feedback in Monte Carlo simulations" *Nuclear Science and Engineering*, **185**. 184–193 (2017).

[6] Han, Zhuoran and Forget, Benoit and Smith, Kord, "Using Generalized Basis for Functional Expansion" *Multidisciplinary Digital Publishing Institute*, **2**. 161–167 (2021).

[7] Novak, April and Romano, Paul and Wendt, Brycen and Rahaman, Ronald and Merzari, Elia and Kerby, Leslie and Permann, Cody and Martineau, Richard and Slaybaugh, Rachel N, "Preliminary coupling of OpenMC and Nek5000 within the MOOSE framework" *Proceedings of PHYSOR*, **4**. 2018 (2018).

[8] Valtavirta, Ville and Viitanen, Tuomas and Leppänen, Jaakko, "Internal neutronics-temperature coupling in Serpent 2" *Nuclear Science and Engineering*, **177**. 193–202 (2014).

[9] Kerby, Leslie and Tumulak, Aaron and Leppanen, Jaakko and Valtavirta, Ville, "Preliminary serpent-MOOSE coupling and implementation of functional expansion tallies in serpent" *Mathematics & Computational Methods 2017*, **1**. 2017 (2017).

[10] Pan, Qingquan and Lv, Huanwen and Tang, Songqian and Xiong, Jinbiao and Liu, Xiaojing, "Pointing probability Driven semi-analytic Monte Carlo Method (PDMC)–Part I: Global variance reduction for large-scale radiation transport analysis" *Computer Physics Communications*, **291**. 108850 (2023).

[11] Pan, Qingquan and Wang, Lianjie and Cai, Yun and Liu, Xiaojing and Xiong, Jinbiao, "Density-extrapolation Global Variance Reduction (DeGVR) method for large-scale radiation field calculation" *Computers & Mathematics with Applications*, **143**. 10–22 (2023).

[12] Guo, Juanjuan and Liu, Shichang and Shang, Xiaotong and Huang, Shanfang and Wang, Kan, "Coupled neutronics/thermal-hydraulics analysis of a full PWR core using RMC and CTF" *Annals of Nuclear Energy*, **109**. 327–336 (2017).

[13] Andrew T.Godfrey, "VERA core physics benchmark progression problem specifications" *Consortium for Advanced Simulation of LWRs*, **4**. 2014 (2014).

[14] Pan, Qingquan and Lv, Huanwen and Tang, Songqian, "MAGIC-GPS Global Variance Reduction Method for Large-scale Shielding Calculation" *Nuclear Engineering and Design*, **414**. 112581 (2023).