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Versatility and stabilization improvements of full core neutronics/thermal-hydraulics coupling between RMC and CTF

Juanjuan Guo[a], Shichang Liu[a], Xiaotong Shang[a], Qicang Shen[b], Xiaoyu Guo[a], Shanfang Huang[a,*], Kan Wang[a], Xiaoming Chai[c]

[a] Department of Engineering Physics, Tsinghua University, Beijing 100084, China
[b] Department of Nuclear Engineering and Radiological Sciences, University of Michigan, 2355 Bonisteel Boulevard, Ann Arbor, MI 48109, USA
[c] Science and Technology on Reactor System Design Technology, Nuclear Power Institute of China, Chengdu 610041, China

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ABSTRACT

This paper presents the versatility and stabilization improvements of high fidelity multi-physics coupling of neutronics and thermal-hydraulics. The coupling is accomplished between the Monte Carlo code RMC and the sub-channel code CTF. Target motion sampling method of RMC and the domain decomposition parallel strategy of CTF are used to decrease the memory requirement as well as to improve the calculation efficiency. The hybrid coupling method is adopted in coupled RMC/CTF code, in which CTF is invoked by RMC flexibly. For code versatility and stabilization, the HDF5 (hierarchical data format) file is used to replace text files in data transfer between two coupled codes, and the predictor-corrector method is also proposed to stabilize the coupling. The coupled code is validated as versatile by successfully testing two full-core problems with different scales. The BEAVRS full core calculation results show the efficiency improvement as a result of using the HDF5 file in the versatile coupled code, and the predictor-corrector method used in the simulation is demonstrated to be effective for stabilizing and accelerating the coupling convergence. Moreover, a modified PWR full core problem simulation indicates that the coupling between neutronics and thermal-hydraulic influences the power distribution both radially and axially, because of the Doppler broadening effect and coolant properties feedback.

1. Introduction

High fidelity multi-physics numerical reactor simulations are gaining increasing attention in the nuclear energy area as the high performance computer technology develops rapidly. Realistic nuclear reactors are extremely complex coupled systems involving different kinds of physics, including neutronics, thermal-hydraulics (TH), fuel performance, and chemistry. Thermal-hydraulics is a key influence factor on neutronics calculations and safety analyses due to the temperature and coolant density effect on the core reactivity and power distribution. For high fidelity simulations, the detailed precise reactor core analysis must take into account the interaction between neutronics and thermal-hydraulics (N-TH). Hence, the N-TH coupling has become a major issue and has been extensively studied.

Currently, various kinds of Monte Carlo-TH coupled code systems using different coupling means have been accomplished and improved constantly. The Karlsruhe Institute of Technology (KIT) has externally coupled the well-known Monte Carlo code MCNP (Briesmeister, 2000) with the thermal-hydraulics codes FLICA4 (Aniel et al., 2005) and SubChanFlow (Sanchez et al., 2010) respectively in an advanced platform NURESIM (Hoogenboom et al., 2011). Applications to the fuel pin lattice and clusters cases prove the flexibility of this coupled system. Another coupled code system based on the Monte Carlo code MCNPX (Hendricks et al., 2007) and the sub-channel code COBRA-IV (Wheeler et al., 1976) was achieved externally by Miriam Vazquez at Ciemat (Vazquez et al., 2013), and it was applied to the fuel assembly calculation at the pin level and the full core problem at the assembly level for fast reactors. Besides, the internal coupled code MCNP6 (Goorley, 2013)/CTF (Salko et al., 2015) was also realized at the pin level by North Carolina State University for a full assembly scale simulation (Bennett et al., 2016), in which the sub-channel code CTF was added as a subfolder of the Monte Carlo code MCNP. The new generation of advanced Monte Carlo code RMC (Wang et al., 2015), developed and improved by the Reactor Engineering Analysis Lab (REAL) group in Tsinghua University, was also coupled with several thermal-hydraulics codes in different ways. Li has accomplished the coupling of RMC and the CFD code CFX (Marchisio et al., 2003) externally for the Pebble Bed-Advanced High Temperature Reactor (PB-AHTR) core analysis (Li

* Corresponding author at: LIUQING Building Room 902, Tsinghua University, Beijing 100084, China.
E-mail address: sfhuang@mail.tsinghua.edu.cn (S. Huang).

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et al., 2012a). Moreover, RMC and the sub-channel code COBRA-EN (Basile et al., 1999) were coupled employing the hybrid method by Liu et al. (2015), in which COBRA was invoked by RMC. Recently, the hybrid coupled code RMC/CTF was done by Guo for the complex BEAVRS (Horelik and Herman, 2012) full core pin by pin simulation (Guo et al., 2016). However, the pre-developed coupled code system between RMC and CTF still has some limitations. The main limitation is the versatility problem that this code cannot easily be applied to other all cases.

Moreover, the Picard iteration was used in the pre-developed coupled code system, which is prone to numerical instabilities and low speed of convergence. The instabilities of Picard iteration will be enlarged in Monte Carlo-TH coupling, due to the statistical variance of the Monte Carlo method and strong feedback between N/T-H, etc. Recently, the Newton method combined with Monte Carlo perturbation theory (Aufiero and Fratoni, 2017) was proposed to solve the stabilization problem for Monte Carlo-TH coupling. However, only the coolant density feedback on neutronics was considered in their study, and it is difficult to obtain the Jacobian matrix of power distribution due to the perturbation of thermal/hydraulics fields.

This paper aims to solve the versatility and stabilization problem of the Monte Carlo-TH coupling based on the hybrid RMC/CTF coupled code. The main improvement for code versatility is using the HDF5 (Folk et al., 2011) file rather than the text file as the data transfer interface between the two codes. The HDF5 file uses hierarchical data format for logically storing and managing data, and it provides a flexible and convenient interface for reading data. Besides, the predictor-corrector method (Noor, 2001) for accelerating convergence is also proposed in the coupling to stabilize the power distribution. The improved RMC/CTF coupled code is validated to be versatile by successfully calculating two full-core problems that have different scales. In addition, the predictor-corrector method is also demonstrated to be elegant and effective by significantly stabilizing and accelerating the convergence of the full core coupling.

In this paper, Section 2 introduces coupled codes RMC and CTF briefly. Section 3 describes the most important coupling scheme, and Section 4 explains the Stabilization of the coupling convergence. Further, Section 5 demonstrates the test benchmarks modeling and the simulation results, and Section 6 presents the conclusions and perspectives finally.

2. Computer codes

Computer codes used in the coupling work are the Monte Carlo code RMC and the thermal-hydraulics sub-channel code CTF, which will be introduced in this section. Moreover, some technologies of the two codes play an important role in the coupling work and are also explained in this section.

2.1. Monte Carlo code RMC

RMC (Wang et al., 2015) stands for Reactor Monte Carlo, which is a new Monte Carlo transport code for reactor core analysis. The code RMC has been developed by the Department of Engineering Physics at Tsinghua University, and has the advantages of being able to flexibly treat complex geometry as well as conveniently use continuous energy point-wise cross sections of materials and temperatures. Besides, RMC is also advanced in complete functions and high performing speed (Wang et al., 2011). At present, RMC has the powerful functions of criticality calculation, burnup calculation (She et al., 2013), on-the-fly cross sections processing with temperature (Li et al., 2012b), N-TH coupling (Li et al., 2012a), etc. Furthermore, the functions of parallel calculation (She et al., 2013), source convergence acceleration (She et al., 2012), and domain decomposition (Liang et al., 2012), allow for running fast on high-performance computing platforms.

With high performance and complete functions, RMC is suitable for coupling. The high performance of RMC makes the coupling efficient because coupling needs sufficient iterations to meet the convergence criterion. In the coupling process, RMC runs the criticality calculations to obtain the power profiles using mesh tallies, and it may calculate problems with arbitrary temperatures. For creating cross sections at arbitrary temperatures, the on-the-fly interpolation method (Liu et al., 2016b) and the target motion sampling (TMS) method have been developed in RMC (Liu et al., 2016c). In this paper, the TMS method is used in the coupling.

2.2. Thermal-hydraulics code CTF

CTF (CASL, 2015), representing Coolant Boiling in Rod Arrays-Two Fluid, is a 3D thermal–hydraulic sub-channel code designed for light water reactor (LWR) vessel analyses. It was developed by the Consortium for Advanced Simulation of Light Water Reactors (CASL) and the Reactor Dynamics and Fuel Management Group (RDFMG) at Pennsylvania State University (PSU). In addition, CTF has been improved and validated for both pressurized water reactor (PWR) and boiling water reactor (BWR) analyses. CTF uses a two-fluid, three-field modeling method and is able to effectively calculate the temperature and density distribution of the coolant and the temperature distribution of the fuel and cladding. CTF has been extensively used throughout the nuclear industry due to its powerful functions and rapid development.

2.2.1. PWR preprocessor and domain decomposition

For the high-efficiency hybrid coupling, the PWR preprocessor and the domain decomposition parallel technology (Salko et al., 2015) of CTF are key technologies in the RMC/CTF coupling. Introductions to them can also be seen in Guo et al. (2017a). The PWR preprocessor can both greatly simplify the user input and effectively reduce the input error by automatically generating the input file of CTF code. Moreover, the domain decomposition parallel technique dramatically contributes to the coupling efficiency through dividing the whole model into multiple domains. Compared with serial calculations, parallel calculations can significantly save time and improve the operation efficiency. Therefore, the PWR preprocessor and the domain decomposition technique of CTF allow for efficient and precise thermal-hydraulics simulations for large-scale complex problems, so they support the development of the high-efficiency RMC/CTF coupling.

2.2.2. HDF5 file output function

For the versatility of the RMC/CTF coupled code, the HDF5 file output function of CTF plays a crucial role. Whether running in serial or in parallel, the code CTF used in this coupling is able to output all the calculation results to a HDF5 file if the HDF5 library is correctly installed on the operating platform. Any HDF5 file produced by CTF has the same data arrangement except the name of the root group. The root group name is “deck.ctf.h5” when CTF runs in serial, which is different from the name “pdeck.ctf.h5” in CTF parallel running. The HDF5 file “pdeck.ctf.h5” can be opened by HDFView, and the file data structure is shown in Fig. 1.

The named group “pdeck.ctf.h5” is just the HDF5 root group, containing three HDF5 groups named “CORE”, “INPUT”, and “STATE_0001” (Fig. 1). The “STATE_0001” group has one group and several datasets that store important calculation results. Calculation results needed in the coupling are the coolant temperature and density, and the fuel temperature, which are all structured as datasets “channel_liquid_temps [C]”, “liquid_density”, and “pin_fueltemps [C]”, respectively. Furthermore, all the information in datasets can be flexibly obtained by HDF5 library functions, allowing for the versatility of the coupling.

3. Coupling scheme

For versatile hybrid RMC/CTF coupling, the most important is the

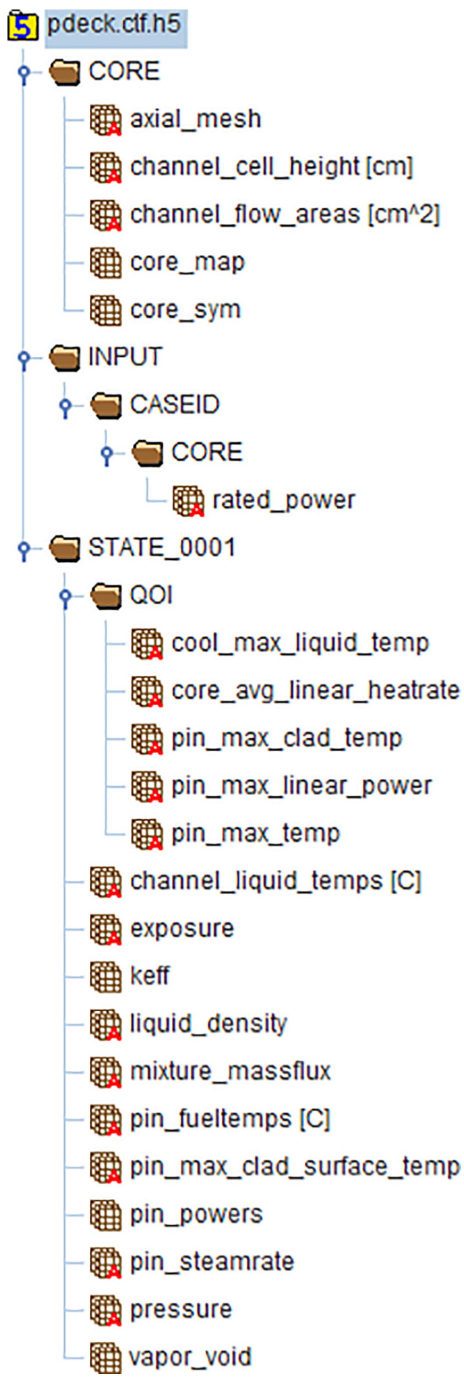


Fig. 1. The data structure of the HDF5 file for the BEAVRS benchmark.

coupling scheme indicating how the coupling is accomplished. In this section, the first part focuses on the basic hybrid coupling method providing information on data transfer process of the coupling. The most essential versatile coupling method introduced in the second part illustrates how the HDF5 file is used for the versatility of the coupling. Besides, the convergence criterion in the coupling is also explained in this section.

3.1. Hybrid coupling method

For convenient and flexible coupling, the hybrid coupling method is used here. Actually, the hybrid method is a new coupling method and has been adopted in the original coupled RMC/CTF code. Traditionally, the neutronics code and the thermal-hydraulics code can be coupled externally or internally. In the external coupling, both codes are invoked by the external scripts or platforms. This method is easy to implement as the codes do not need change, but it cannot support the versatility of the coupling. For example, the neutronics code PARCS and thermal-hydraulics code Relap5 are coupled externally through a parallel virtual machine (PVM) (Wu, et al., 2015). Conversely, internal coupling means integrating the codes into one single code that two codes should be modified greatly. It is complex to realize but has the advantages of good versatility, like the internal MCNP6/CTF coupled code (Bennett et al., 2016). To combine the advantages of the two coupling methods, the hybrid coupling method is proposed. In this section, the hybrid coupling method was reviewed, and the detailed information can be found in Guo et al. (2016).

In the hybrid RMC/CTF coupling, the needed data was transferred through the CTF external output file and the RMC memory, indicating that CTF was invoked by RMC. Some internal scripts were added to RMC for invoking CTF and reading the CTF output file. As the master code, RMC ran firstly and calculated the power profiles in memory. The internal script of RMC then read the power data from the memory, produced the power input file for CTF and invoked CTF. CTF ran and calculated the thermal data, coolant temperature and density, and the fuel temperature. RMC read the data from the CTF output file and ran for a new iteration. This coupling process was repeated until the satisfaction of the convergence criterion, and the coupling algorithm is shown in Fig. 2.

3.2. Versatile coupling method

The code versatility is the main improvement of the coupled RMC/CTF code in this paper. Without any change to codes, the original coupled RMC/CTF code can only simulate problems that have same geometry with the BEAVRS benchmark. To simulate more cases that have different scales, the code versatility is improved. Versatility in this

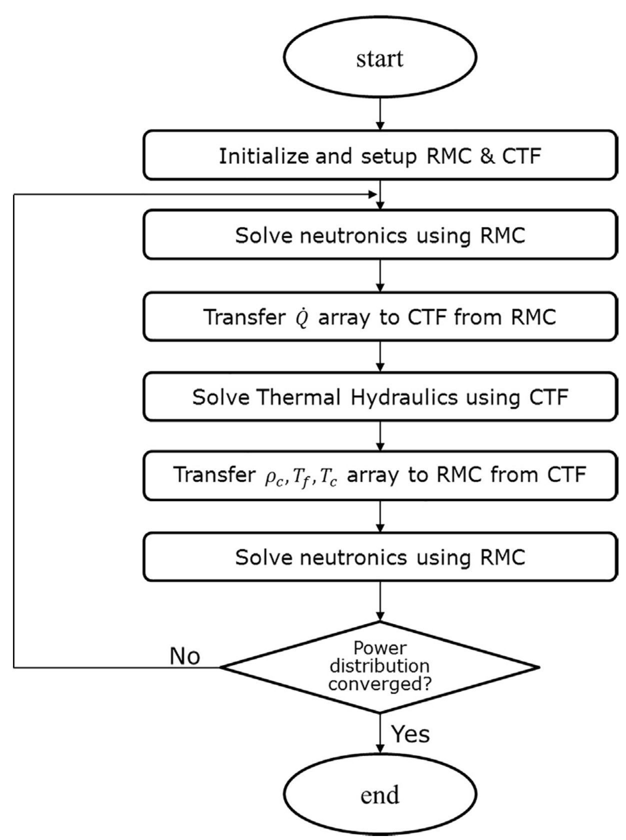


Fig. 2. RMC and CTF coupling algorithm flow chart (Guo et al., 2017a).

paper refers to that the improved coupled code can simulate problems with different scales without any change to the code itself. After the improvement, the coupled code can calculate the problems of the single fuel rod, assembly or full core.

The most important process of the versatile method involves using HDF5 files to replace the text files in the data exchange. Therefore, the HDF5 technology is introduced firstly in this section, and then the implementation of the method is represented in detail.

3.2.1. Introduction to HDF5 technology

HDF5 is the abbreviation of the hierarchical data format for storing and managing scientific data, which contains a data model, a library and a file format. The detailed information of HDF5 technology can be seen in Guo et al. (2017b), so this paper gives a brief review to it.

The HDF5 technology has been developed and improved by the HDF group located at the University of Illinois. It supports all kinds of datatypes for large-volume and complex data with flexible and efficient I/O. Moreover, HDF5 has the advantages of portability and extensibility. In addition, HDF5 can be expediently opened by the software HDFView, and can be flexibly accessed by C, F90, C++, and Java APIs.

The basic component of the HDF5 file is the HDF5 data model. It has the classifications of HDF5 groups, HDF5 datasets, and HDF5 datatype objects, which correspond to the groups, array data, and types in the HDF5 file, respectively.

The HDF5 group, similar to the directory in a file system, is the explicit representation of the relationship between HDF5 groups, HDF5 datasets, and HDF5 datatype objects. Generally, each HDF5 file must have one HDF5 group called the HDF5 root group, and this root group can contain any number of HDF5 groups or HDF5 datasets. HDF5 datasets can be viewed as located content variables, which are arranged logically as a multidimensional array. The detailed datasets information can be captured by the HDF5 dataspace. In addition, the datasets information can also be easily obtained by functions of the HDF5 library which is designed mainly for accessing and managing all kinds of items in the HDF5 file. Using the HDF5 library, the HDF5 dataset can perform various operations, such as reading, creating, updating and deleting.

The arrangement of the data structure is shown in Fig. 3, where the oval shapes represent HDF5 groups and rectangles denote HDF5 datasets.

Every HDF5 file starts with the top-level root group that governs all data of the file (Fig. 3). Every group can contain HDF5 datasets or new groups, but the name of any group or dataset must be unique in the scope of the HDF5 file for the inerrability of attaching data.

HDF5 files are stored in a self-describing format, integrating the data and the primary source of the data. This format "allows one to access the data without knowing anything about the actual representation of the data or the layout of the file" (Kuehn, 1996), which makes it possible to overcome the versatility problem of the original coupled code.

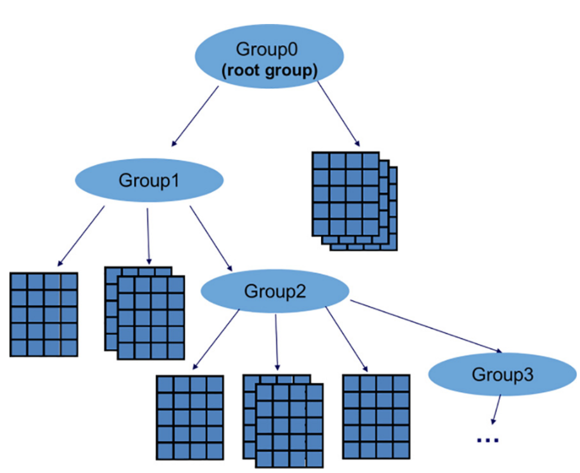


Fig. 3. The data structure instructions of HDF5 file (Guo et al., 2017b).

3.2.2. Versatility achievement

For the code versatility, the coupled RMC/CTF code was improved mainly from three aspects. Firstly, all fixed geometry contents in the coupling code were changed to variables, which supports the code versatility. Another important change was adding all the power and geometry information to the RMC input file to be a new input card, shown as Fig. 4. In the coupling process, RMC was required to produce the CTF power input file, whose information should be previously known. Therefore, all the geometry and the power information included in the power input file, such as the full core map of the reactor and the total operating power, were all written in the RMC input file. Finally, the most significant change is reading thermal data from HDF5 files instead of text output files by CTF. As described in Sections 2 and 3, using the HDF5 file highly supports the versatility of the coupling. Moreover, the change to the code also improved the simulation efficiency. Previously, the CTF output files read by RMC were a collection of text files that each file contained one domain data. In every coupling iteration, RMC read the text files to get data of all domains, consuming more time than reading only one HDF5 file containing all domains data.

With the versatile method used in the coupling, the new version of the coupled RMC/CTF code can be applied to problems that have different scales when the input files of RMC and CTF are prepared.

3.3. Convergence criterion

In the coupling simulation, how to judge its convergence really deserves extensive and detailed study due to random variations of the Monte Carlo method. Recently, different convergence criteria of the Monte Carlo and thermal-hydraulics coupling have been studied and evaluated by Guo et al. (2017a), including the average power relative variation and the power axial offset. In this coupling, the power relative variation between two adjacent iterations is adopted as the convergence criterion. When it is smaller than the average relative error of all power values in the RMC tally file, the coupling is converged. This can be expressed as:

$$\sqrt{\frac{\left(\frac{P_1^n}{P_1^{n-1}}-1\right)^2+\left(\frac{P_2^n}{P_2^{n-1}}-1\right)^2+\ldots+\left(\frac{P_N^n}{P_N^{n-1}}-1\right)^2}{N}} \leqslant \sqrt{\frac{\left(\frac{RE_1^n}{RE_1^{n-1}}-1\right)^2+\left(\frac{RE_2^n}{RE_2^{n-1}}-1\right)^2+\ldots+\left(\frac{RE_N^n}{RE_N^{n-1}}-1\right)^2}{N}}, \tag{1}$$

where P_m^n and RE_m^n represent the power value and the power relative error of the mth mesh in the nth iteration, respectively.

This criterion is validated to be useful and appropriate, and its threshold involves neutronics calculation conditions, including the neutron number, inactive cycles and active cycles. Therefore, the criterion threshold varies from case to case.

4. Stabilization of coupling convergence

4.1. Power oscillations

The power oscillation phenomenon refers to that the power distribution deviates from the normal distribution in coupling iterations. Actually, this problem generally exists in the nonlinear coupling, and it may arise when simulating the coupling of Monte Carlo-TH for full core cases. This section takes the BEAVRS benchmark as an example to account for the power oscillation phenomenon. Moreover, detailed information of the benchmark is represented in Section 5.1.1, so only part information of the benchmark is shown here.

BEAVRS benchmark is based on a PWR reactor design in the United

```
COUPLE_CRITICALITY
PowerSymmetry
POWER Totalpower=3411//Mth double
GEOMETRY COREDIMENSION=15 ASSEMDIMENSION=17   AXIALMESH=10   ASSEMNUMBER=193

   Bound = -161.2773 161.2773 -161.2773 161.2773 36.007 401.767
GUIDETUBE Number=25 Location=
```

Fig. 4. Partial coupling information of the RMC input file.

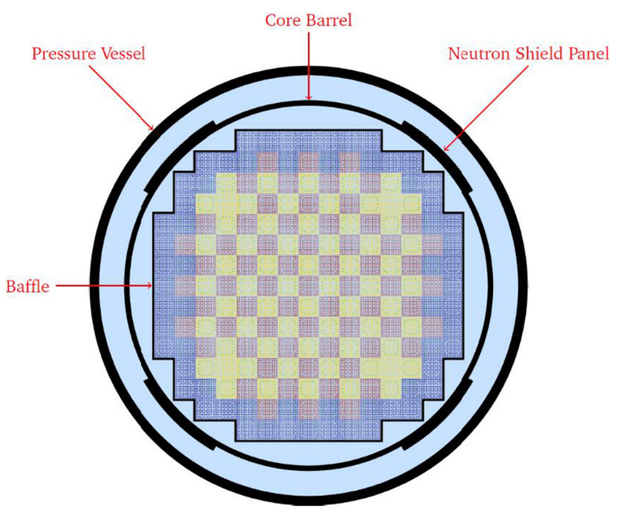


Fig. 5. Radial cross section of the BEAVRS core. The 3.1% enriched assemblies are around the edge with the 2.4% and 1.6% enriched assemblies in the middle.

States with 193 fuel assemblies, and each assembly has a 17 × 17 configuration. As shown in Fig. 5, assemblies have three different ^{235}U enrichments of 3.1%, 2.4% and 1.6% configured like a checkerboard.

This benchmark is simulated by the pre-developed RMC/CTF coupled code without any treatment to the data exchange process, and the power and coolant density distributions in the coupling are shown as Fig. 6.

After several iterations, the power and coolant density distributions become severely asymmetrical and has an opposite trend between two adjacent iterations (Fig. 6). The oscillation phenomenon is mainly due to the uncertainty of the Monte Carlo calculation and the negative feedback of temperature distributions. In the simulation, when an oscillation occurs in one iteration due to the statistical error of the Monte Carlo method, the coolant density and fuel temperature in the next iteration will follow the power oscillation. Afterwards, the following power distribution has an opposite oscillation because of the strong negative Doppler broadening effect and the moderator feedback.

To overcome the power oscillations and converge the simulation in the full core pin level simulation of BEAVRS (Guo et al., 2016), the power distribution generated by RMC has the 1/8 symmetry treatment before being transferred to CTF given that the geometry and the fuel arrangement of the BEAVRS full core is almost 1/8 symmetrical. Moreover, this paper proposes the predictor-corrector method to solve power oscillations effectively.

4.2. Fixed-point iteration of coupling

For convergence stabilization, the predictor-corrector method is proposed in the coupling, which has the advantages of simple implementation and efficient acceleration. To explain this method, the fixed-point iteration of the coupling should be introduced first.

In coupling iterations, the power distribution calculated by the neutronics code involves e.g., the fuel temperature, coolant temperature and density, and the relationship can be expressed as:

$$\varphi = F(T,\rho), \tag{2}$$

where φ represents the power distribution generated by the neutronics code, T and ρ are thermal parameters from the T/H code representing the coolant and fuel temperature and coolant density, and F denotes the function relationship between φ and T, ρ. In coupling iterations, Eq. (2) can be transformed into

$$\varphi^n = F(T^{n-1},\rho^{n-1}) = G(\varphi^{n-1}), \tag{3}$$

where φ^n and φ^{n-1} are power distributions of nth and n − 1th iterations, T^{n-1}, ρ^{n-1} mean the temperature and density of fuel and coolant in the n − 1th iteration, and the function relationship between φ^n and φ^{n-1} is denoted by G. Eq. (3) means that the current power distribution is determined by the previous one. The relationship between φ^n and φ^{n-1} is a negative feedback as a result of the negative Doppler broadening effect, so the converged power distribution exists and can be expressed as:

$$\varphi^* = G(\varphi^*), \tag{4}$$

where φ^* is the converged power distribution in coupling iterations. The coupling process of N-TH is actually a fixed-point iteration, and the data transfer process in iterations can be expressed as Fig. 7.

The relationship of different parameters in one iteration is shown as Fig. 7, where Φ and $R(\Phi)$ represent power distributions transferred to CTF and that generated directly by RMC, respectively. Besides, T represents the matrixes of thermal parameters calculated by CTF, including the coolant temperature and density, and the fuel temperature. The relationship between Φ_{n+1} and $R(\Phi_n)$ varies from different processing methods. In the Picard iteration, Φ_{n+1} is just equal to $R(\Phi_n)$.

4.3. Predictor-corrector method for coupling stabilization

The predictor-corrector method (Noor, 2001) is a commonly-used method to predict initial values for ordinary differential equations and accelerate convergence in Newton iterations.

In ordinary differential equations, the initial value problem refers to the process of solving equations:

$$\begin{cases} \frac{du}{dt} = f(t,u), \quad 0 \leqslant t \leqslant T < +\infty \\ u(0) = u_0 \end{cases}, \tag{5}$$

if $f(t, u)$ is continuous and satisfied of Lipschiz condition, which means that a positive number L allows the establishment of the equation:

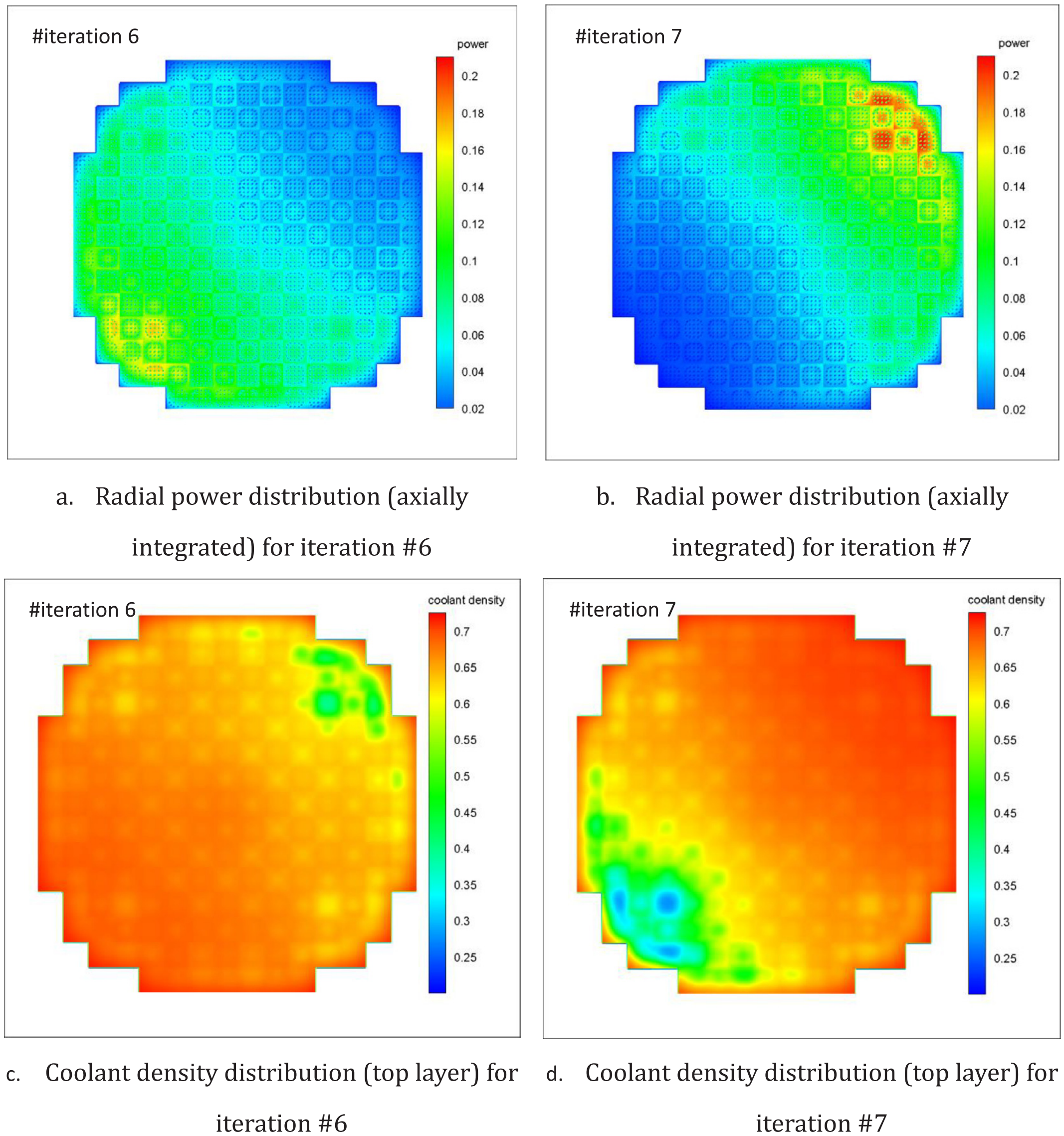
$$|f(t,u_1) - f(t,u_2)| \leqslant L|u_1 - u_2|, \tag{6}$$

ordinary differential equations have the unique solution that meets the initial condition. However, it's difficult to obtain the accurate solution, so calculating the numerical solution is a general method. When solving the initial values with predictor-corrector method, the Euler method is used in advance for obtaining the estimated value of the next nodal point.

For accelerating the convergence in Newton iterations, the predictor-corrector method is based on the opposite power distribution trend between two adjacent iterations, which can be expressed as:

$$\Phi_{n+1} = \frac{\Phi_n + R(\Phi_n)}{2}, \tag{7}$$

where Φ_n and $R(\Phi_n)$ are power distributions of CTF and RMC in the n^{th} iteration, and Φ_{n+1} is the power distribution transferred to CTF in the $n+1$th iteration. This processing procedure is expected to counteract the



a. Radial power distribution (axially integrated) for iteration #6

b. Radial power distribution (axially integrated) for iteration #7

c. Coolant density distribution (top layer) for iteration #6

d. Coolant density distribution (top layer) for iteration #7

Fig. 6. Radial power distribution (axially integrated) and coolant density distribution (top layer) of the BEAVRS full core for iterations #6 (left) and #7(right).

Fig. 7. Data transfer process schematic diagram in #n + 1 coupling iteration.

opposite oscillations of power distributions between Φ_n and $R(\Phi_n)$, which can stabilize and accelerate the coupling convergence.

Power and density oscillations in Section 4.1 demonstrate that power distributions between adjacent iterations in the coupling, namely Φ_n and $R(\Phi_n)$, have the opposite oscillation, because of the uncertainty of Monte Carlo and negative feedback effect. Based on this, the normal power distribution is expected to be obtained by averaging adjacent power distributions. Actually, some other methods for convergence acceleration are similar to the predictor-corrector method expect the coefficient of Φ_n and $R(\Phi_n)$.

The relaxation acceleration method proposed in Bennett et al., (2016) also accounts for the statistical noise. This method defines the distribution as the sum of all the previous distributions as:

$$\Phi_{n+1} = \frac{1}{n}\sum_{i=1}^{n} R(\phi), \tag{8}$$

according to Eq. (8), the error will decrease with increasing number of iterations. Moreover, the Eq. (8) can be rearranged as:

$$\Phi_{n+1} = \left(1-\frac{1}{n}\right)\frac{1}{n-1}\sum_{i=1}^{n-1} R(\phi_i) + \frac{1}{n}R(\phi_n) = \left(1-\frac{1}{n}\right)\phi_n + \frac{1}{n}R(\phi_n), \tag{9}$$

From Eq. (9), the relaxation technique is just a weighted function of the current power distribution $R(\phi_n)$ and the previous distribution ϕ_n. Therefore, the predictor-corrector method has the same weighted coefficient of ϕ_n and $R(\phi_n)$ in all iterations. The acceleration effect of the relaxation method has been shown in Bennett et al., (2016), and this paper demonstrates the acceleration effect of the predictor-corrector method.

5. Results and analyses

The coupled code was tested on two different scales examples. The first test problem involves the BEAVRS full core problem whose modeling is the same as that tested by the pre-developed coupled RMC/CTF code. Moreover, it is calculated to test and verify the accuracy, stability and reliability of this new coupled RMC/CTF code version. Another test problem is a modified realistic reactor, in which geometry and operation parameters are from Qinshan Phase II (Li et al., 2007) and the fuel

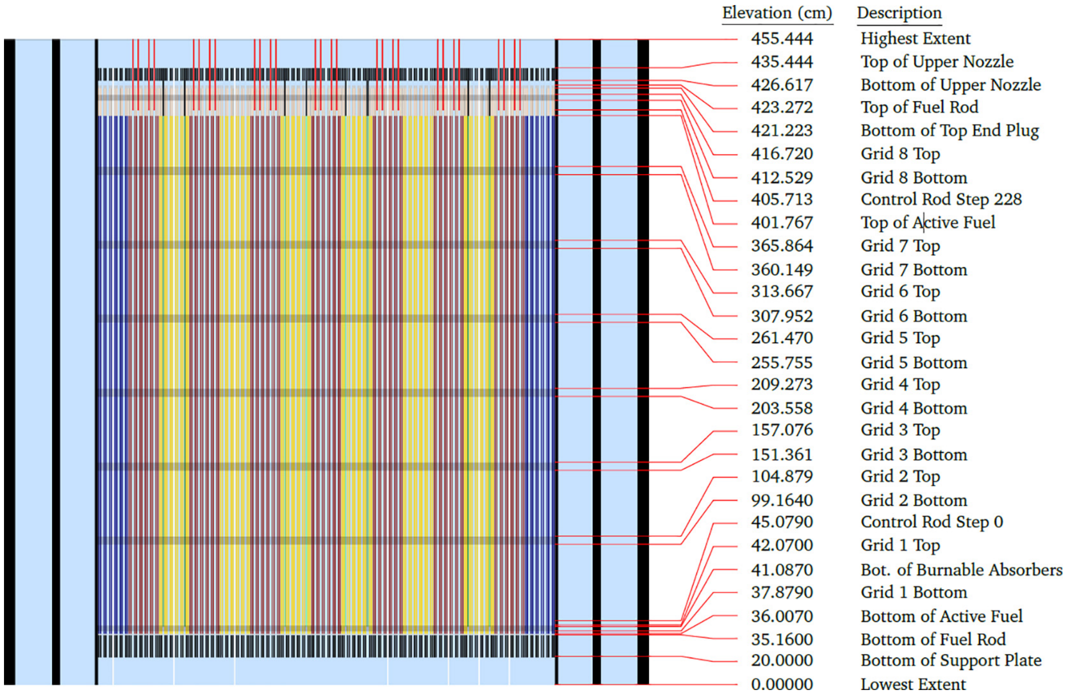


Fig. 8. Axial cross section of the BEAVRS core.

Table 1
Nominal values of the thermal hydraulics conditions for BEAVRS benchmark.

Item	Value	Units
Total power	3411	MW
Initial mass flow rate	17,083	kg/s
Reference pressure	15.517	MPa
Inlet water temperature	292.78	°C
Outlet water temperature	310	°C

Table 2
Assembly geometry for BEAVRS benchmark.

Item	Size
Number of fuel rods	264
Number of guide tube rods	25
Active length (mm)	3657.6
Bundle pitch (mm)	215.04
Fuel rod diameter (mm)	7.84
Cladding inner diameter (mm)	8.00
Cladding outer diameter (mm)	9.14
Pin pitch (mm)	12.60
Guide tube inner diameter (mm)	11.22
Guide tube outer diameter (mm)	12.04

Table 3
Convergence criterion for BEAVRS benchmark CTF calculation.

Item	Value
Outer Iteration Convergence Criterion	0.001
Maximum Number of Outer Iterations	5
Maximum Number of Inner Iterations	40
Global Energy Balance	0.01%
Global Mass Balance	0.01%
Fluid Energy Storage	0.01%
Solid Energy Storage	0.01%
Mass Storage	0.01%

Table 4
BEAVRS benchmark calculation time by using two different coupling codes.

Cost time	Neutronics calculation (min)	Write power (min)	Read TH (min)	CTF runtime (min)	One iteration (min)
Previous code	14.20	1.28	0.42	11.90	27.80
Current code	14.25	1.12	0.008	10.02	25.40

arrangement is from Hoogenboom benchmark (Liu et al., 2016a). It is simulated to validate the versatility of the coupling code, which means that the coupled code in this paper can simulate different scales problems. Besides, power distributions of the two simulations demonstrated in Sections 5.1 and 5.2, have the 1/8 symmetry treatment, which are used as reference results of evaluating the stabilization effect of the predictor-corrector method in Section 5.1.3.

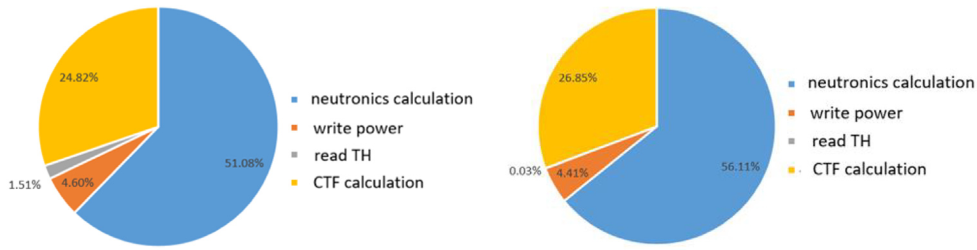
5.1. BEAVRS benchmark

5.1.1. Problem modeling

Benchmark for Evaluation And Validation of Reactor Simulations (BEAVRS) is a famous and commonly used test benchmark for reactor analysis released by the Computational Reactor Physics Group at MIT (Horelik and Herman, 2012). It is based on a 1960s commercial PWR reactor design in the United States with 193 fuel assemblies, with each assembly having a 17 × 17 configuration. As shown in section 4.1, assemblies have three different ^{235}U enrichments of 3.1%, 2.4% and 1.6% configured like a checkerboard.

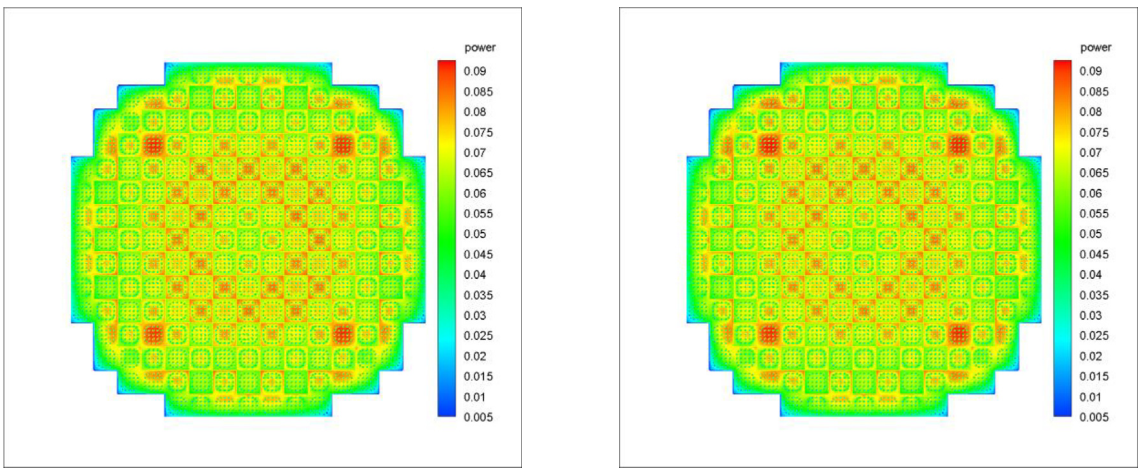
The modeling of this benchmark was the same as that of Guo et al. (2017a). Eight spacer grids were simulated in the coupling, as shown in Fig. 8. Besides, the core was divided into 10 segments axially and 255 × 255 meshes radially. Radial meshes in RMC modeling were resolved to pin level, and each polygon between four rods was a channel in CTF simulation. The BEAVRS benchmark geometry then had a total of 56,288 channels over the full core. The detailed data used in coupled calculations is listed in Tables 1–3.

The calculation conditions were also identical to the simulation using previous coupled RMC/CTF code. Each RMC transport calculation used 200 inactive cycles and 200 active cycles in the first iteration and 500 active cycles in the following iterations. Each cycle simulated one



a. Previous RMC/CTF coupled code calculation b. Current RMC/CTF coupled code calculation

Fig. 9. Calculation time comparison between two different code versions.



a. Predictor-corrector method b. Symmetry method

Fig. 10. Converged radial power distributions of predictor-corrector and symmetry methods (axially integrated).

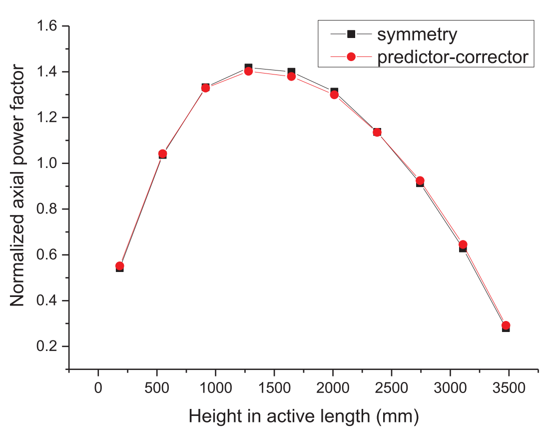


Fig. 11. Converged axial power profiles of symmetry and predictor-corrector methods for the BEAVRS full core case (radially integrated).

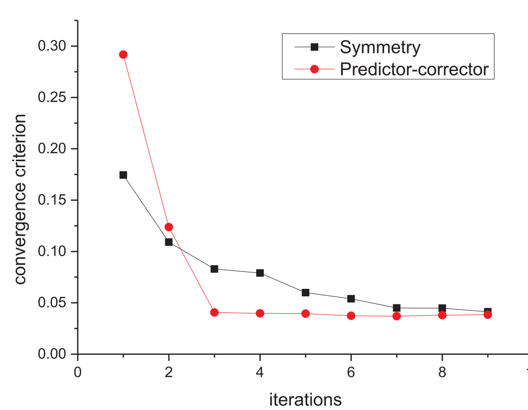


Fig. 12. Convergence criterion profiles of symmetry and predictor-corrector methods for the BEAVRS full core case.

million neutrons, and the boron concentration was 599 ppm. The average relative statistical errors in the power of each fuel pin in RMC for all the meshes was 0.042, so the convergence criterion was set at 0.042.

5.1.2. Results verification and time comparison

In the coupling simulation for BEAVRS full core problem, 720 parallel threads of "Tianhe-2" supercomputer were used for RMC calculations and 193 cores for CTF calculations. This simulation ran for approximately four hours and then converged. All the output data were identical to those using previous coupled RMC/CTF code, indicating that this versatile coupling method was correct, stable and effective. The specific results can be referenced in Guo et al. (2016).

The calculation time for this problem of the previous and current codes were counted to test and verify the efficiency improvement of the new versatile coupled code. The counted time contained the neutronics calculation, the data transfer process "write power" and "read TH", and the CTF calculation. Besides, "Write power" meant the process of RMC transferring the power data to CTF, and "read TH" represented the process of RMC reading thermal parameters from CTF. The counted time of different parts by using two coupling code systems is listed in Table 4, and it is also plotted as Fig. 9.

The counted time in Table 4 belongs to the first iteration of the coupled calculation by both the previous code and the current code.

Table 5
Convergence criterion data against iterations of symmetry and predictor-corrector methods for BEAVRS full core case.

Iterations	Convergence criterion of Symmetry method	Convergence criterion of Predictor-corrector method
1	0.1744	0.2917
2	0.1091	0.1238
3	0.0829	0.0406
4	0.079	0.0398
5	0.0599	0.0395
6	0.0539	0.0374
7	0.045	0.037
8	0.0448	0.0379
9	0.0413	0.0384

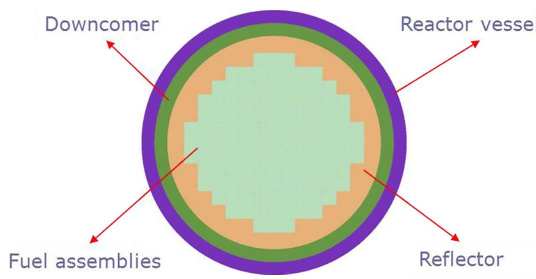


Fig. 13. Radial cross section of the modified Qinshan Phase II reactor core (plotted by RMC). All fuel rods are 1.87% enriched.

Table 6
Nominal values of the thermal hydraulics conditions for modified Qinshan Phase II full core problem.

Item	Value	Units
Total power	1930	MW
Initial mass flow rate	13494.44	kg/s
Reference pressure	15.517	MPa
Inlet water temperature	293.4	°C
Outlet water temperature	329.8	°C

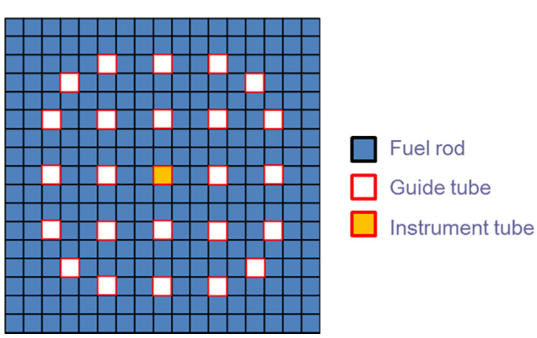


Fig. 14. Assembly layout showing guide tubes and instrument tube placement.

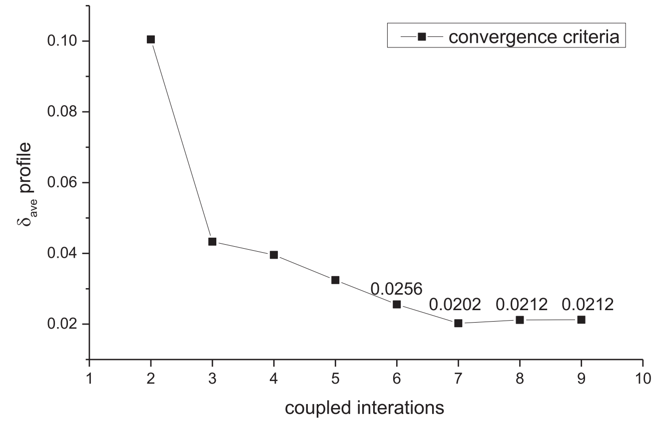


Fig. 15. Convergence of δ_{ave}^{n} in modified Qinshan Phase II reactor core coupling simulation.

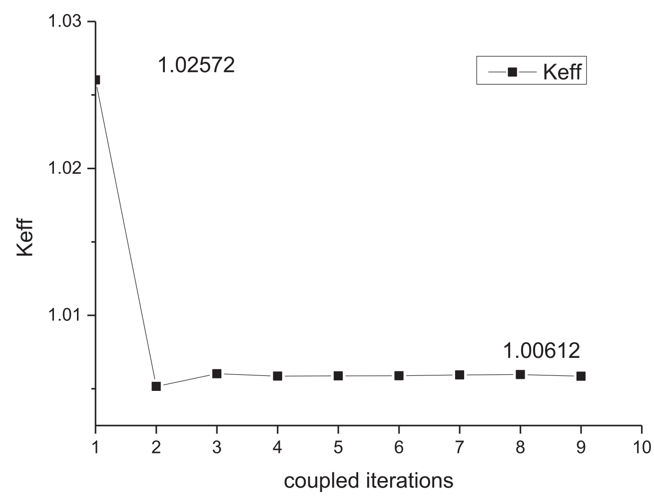


Fig. 16. Variation of Keff during the iterations in modified Qinshan Phase II reactor core coupling simulation.

The neutronics and CTF calculation time of other iterations may be different from the first iteration because the temperature and power distribution may change, but the "Read TH" process time almost had no variation because the data transfer was only influenced by the size of transferred data and the data file format. In the simulations, the transferred data size is always the same.

The versatile coupled code improved the simulation efficiency mainly from reducing the time of "Read TH" process (Table 4 and Fig. 9). Moreover, the CTF runtime also changes from the state of computing resources, but it has no relationship with the data exchange. The previous coupled code read data from CTF through 193 text output files, whereas the current coupling code did it by one HDF5 file. In addition, accessing data in HDF5 file has high efficiency because of the scientific data storage of the HDF5 file. Therefore, the "Read TH" process by using current versatile coupling code cost less time than that of using previous code, proving that the versatile coupling code based on HDF5 file can improve the calculation efficiency. Above all, compared with text files, exchanging data through HDF5 files is more flexible and better for the versatility of the coupled code.

5.1.3. Stabilization improvement using predictor-corrector method

A new simulation for the BEAVRS full core case using the predictor-corrector method was performed, in which all calculation conditions were the same as the 1/8 symmetrical treatment case. To demonstrate the stabilization effect of the predictor-corrector method, the coupling results should be accurate first. The simulation results are presented in Figs. 10 and 11.

The converged radial and axial power distributions of two cases using symmetry and predictor-corrector methods are all identical. Radial power distributions of two methods shown in Fig. 10 are almost the same visually, and the axial power profiles demonstrated in Fig. 11 are also coincident. Simulation results indicate that the predictor-corrector method does not influence the converged coupling results, which is the basis of evaluating its stabilization and acceleration effect. Profiles of the convergence criterion described in Section 3.3 are presented in Fig. 12 and Table 5.

As shown in Fig. 12, the predictor-corrector method can both stabilize and accelerate the coupling convergence compared with the

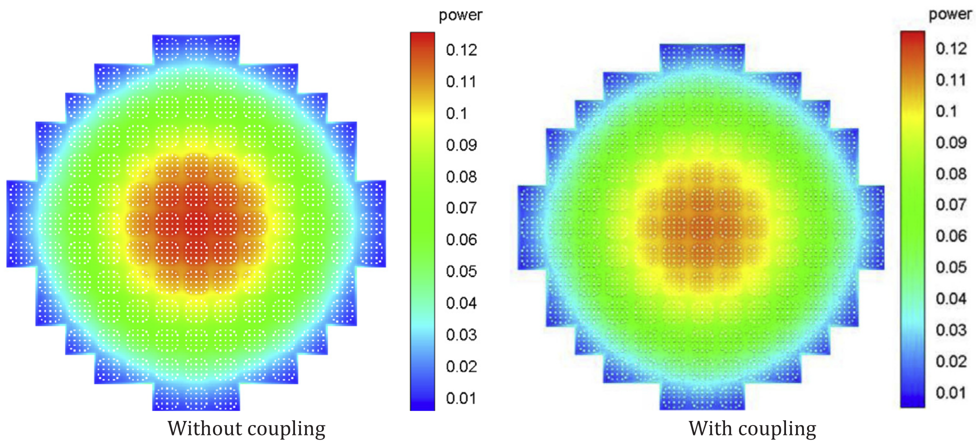


Fig. 17. Radial power distribution in the modified Qinshan Phase II reactor core (axially integrated).

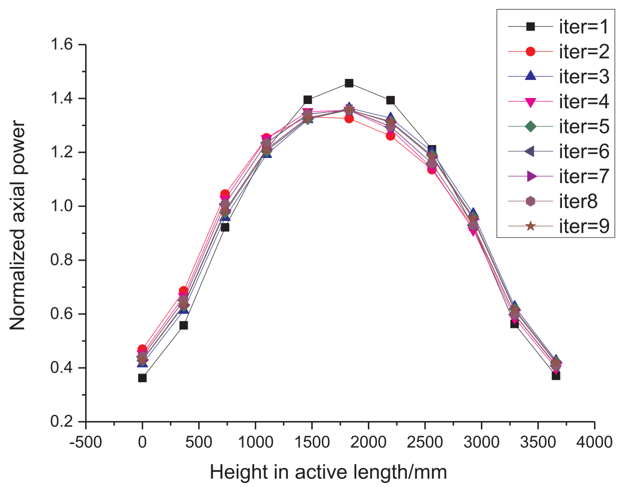


Fig. 18. Axial power distribution in the modified Qinshan Phase II reactor core (radially integrated).

symmetry method. According to the cases, the convergence criterion at conditions described in Section 5.1 is 0.042. From Table 5, iterations needed for convergence of symmetry and predictor-corrector methods are 9 and 3, respectively. Simulation results prove that the predictor-corrector method can not only stabilize the coupling effectively but also accelerate the convergence noticeably. In addition, predictor-corrector method can also be applied to the asymmetrical cases while the symmetry method is only suitable for symmetrical cases, which indicates the versatility of the predictor-corrector method and new version RMC/CTF coupling code.

5.2. Modified PWR full core

5.2.1. Problem modeling

Another test problem whose geometry and meshes are different from the BEAVRS benchmark is also simulated to validate the versatility of the coupled code. It is actually a simple modified PWR full core based on the dimensions and state conditions of the Chinese realistic reactor, namely Qinshan Phase II, and the fuel arrangement of the Hoogenboom benchmark. The full core has 121 assemblies, and each has 17 × 17 pin by pin arrangement with uniform enrichment of 1.87%. In addition, each assembly contains 264 fuel rods, 24 guide tubes and one instrument tube in the center, and no control rods or removable burnable absorber assemblies are modeled in this problem. The radial cross section of this full core and the thermal-hydraulics specifications are shown in Fig. 13 and Table 6, and the geometry specification for the assembly is given in Fig. 14 and Table 2.

The mesh division and calculation conditions for this full core coupling is described in this part. The active core was divided into 10 axial segments and 289 × 289 radial meshes both in RMC and CTF, leading to a total of 31,944 rods and 35,412 channels over the full core. Regarding the calculation condition, each RMC transport used 200 inactive cycles and 600 active cycles with 1000,000 neutrons per cycle, and the boron concentration was 360 ppm. Moreover, the convergence criterion was 0.022, which was the root-mean-square of relative statistical errors tallied by RMC in all meshes.

5.2.2. Calculation results

The coupling simulation ran on the Tianhe-2 supercomputer using 720 parallel cores for RMC calculations and 121 cores for CTF calculations. After running for about six hours, the simulation met the convergence criterion and finished. The profiles of the convergence criterion δ_{ave}^{n} and Keff are shown in Figs. 15 and 16, respectively.

The coupling simulation met the convergence criterion after several iterations (Fig. 15). The convergence criterion δ_{ave}^{n} was smaller than 0.022 from the 7th iteration, indicating the convergence of the simulation. RMC ran firstly using uniform coolant temperature and density, and fuel temperature, resulting in less accurate power distribution. From the second iteration, RMC used the accurate thermal distribution from CTF and calculated again. Therefore, δ_{ave}^{n} was relatively large in the initial iterations, but after several iterations it became small.

K_{eff} in the coupling process was essentially constant after a few iterations (Fig. 16). K_{eff} was large in the first iteration because RMC had no T/H feedback, and it became small after iterations for the Doppler broadening effect of the nuclear target.

Besides δ_{ave}^{n} and K_{eff} profiles, the power distribution was also used to study the coupling effect on the full core directly. Radial distributions with and without coupling are shown in Fig. 17, in which values are axially integrated. Moreover, the axial power distribution radially integrated is shown in Fig. 18.

The radial distribution with coupling was more uniform than that of without coupling (Fig. 17). From Fig. 17, the coupling with T/H feedback decreased the peak value and increased the least value, namely homogenizing the radial power distribution, for the Doppler broadening effect of the nuclear target.

The coupling increased the power at the bottom of the core and reduced the peak power level (Fig. 18). In the coupled iterations, water flowed from the bottom to the top and absorbed the heat from the fuel rod, so the water temperature in the higher position was greater than that of the lower position. On the contrary, the water density in the higher position was smaller than that of the lower position. Therefore, the higher water density near the bottom provided better moderation to neutrons, which increased the power in the lower part of the core and decreased the peak value position. The peak value decreased also because of the Doppler broadening effect.

6. Conclusions and perspectives

This paper presents a versatile and stable coupled neutronics and thermal-hydraulics code based on the Monte Carlo code RMC and subchannel code CTF. The TMS cross sections of RMC are used to simplify the cross section calculations as well as reduce the memory requirement. The coupled code uses the HDF5 file to replace text files in the data transfer process for code versatility and also adopts the predictor-corrector method to stabilize and accelerate the coupling convergence. The coupling uses the hybrid coupling method, enabling the modeling simplification and the versatility of the code system through the use of the neutronics code memory.

The coupled code is tested by two full core problems with different scales to validate its accuracy and versatility. The BEAVRS full core problem is tested against the previous coupled code, and the simulation result shows the accuracy and efficiency improvement of the new versatile coupled RMC/CTF code. In addition, the successful simulation of the modified Qinshan Phase II full core problem indicates the code versatility.

The predictor-corrector method is applied to the BEAVRS full core case, and simulation results reveal its stabilization and acceleration effect on coupling convergence without influencing the coupling results compared with the symmetry method.

Coupling effects on the radial and axial power distribution show the necessity of the coupling between neutronics and thermal-hydraulics. The radial power distribution after coupling becomes more uniform because of the Doppler broadening effect of the nuclear target, demonstrating the coupling homogenization effect. Axially, the power peak decreases for the Doppler broadening effect, and the power peak value position decreases for the coolant density distribution in axial direction.

Further developments of the coupled RMC/CTF code can focus on applications of more cases including VERA problems, and on the coupling for transient and kinetics analysis. In addition, more methods for accelerating the convergence of coupling are being explored.

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