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A Versatile Method of Coupled Neutronics/Thermal-hydraulics Based on HDF5

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Abstract - *This paper introduces a powerful and efficient method to improve the versatility of the hybrid coupling between the Monte Carlo code RMC and the sub-channel code CTF. This method is accomplished based on the HDF5 file which can be produced by CTF, by using the hierarchical data format to store data. The neutronics and thermal-hydraulics coupling between RMC and CTF has been achieved and applied to the BEAVRS benchmark previously by the REAL group of Tsinghua University. To broaden the scope of applications of the previous coupling codes, the method mentioned in this paper is proposed. The new versatile coupling code system that uses the HDF5 file is applied to the BEAVRS benchmark again to test and verify the versatility and high efficiency of the versatile coupling codes. This paper firstly introduces the HDF5 file and coupling codes RMC and CTF briefly, and then explains the versatile coupling method in details. Besides, the modeling of the BEAVRS benchmark is also presented in this paper. Next, this paper presents the results and analysis of coupling calculation. The conclusions and the future work are introduced finally.*

I. INTRODUCTION

With the rapid development of the high performance computers, the high fidelity multi-physics codes have more improvement space and more practical application value. The neutronics and thermal-hydraulics coupling attracts wide concern in the fission nuclear research field, and has great importance on the reactor design, performance and fuel arrangement. Currently, many research groups have already developed the coupling code systems based on different reactor physics codes or thermal-hydraulics codes, such as the sub-channel code CTF and deterministic code MPACT coupling code system in VERA by the Consortium of Advanced Simulation for Light water reactor (CASL). Many previous work related to the coupling of neutronics and thermal-hydraulic codes can be found in References [2-5].

Recently, the continuous-energy Monte Carlo code RMC and sub-channel code CTF have accomplished the hybrid coupling using BEAVRS benchmark [6]. The hybrid coupling between RMC and CTF was done by adding some scripts to RMC. The scripts have two important functions, one is to read the output data of CTF and assign new data to the variables stored in RMC, and another one is to transfer the power data produced by RMC to CTF. This coupling code system has been validated effective and stable, but it is only suitable for BEAVRS full-core problem. To calculate other benchmarks or problems, the previous coupling code must be changed because the IO files in the RMC are relevant to the geometry of the reactor core and the number of the CTF output files. This disadvantage of the code system results in the complex work of modeling, so the versatile coupling method is in great request.

In this paper, a versatile method of coupling RMC and CTF has been proposed. This method is based on HDF5, which uses hierarchical data format. By using HDF5, the data transfer including reading and writing is more flexible and extensible. And this versatile code system is applied to BEAVRS benchmark again to validate the reliability of this method. The results show that this method has great advantages of solving the poor versatility of external and hybrid coupling.

II. INTRODUCTION TO HDF5

HDF5 is the shorten name of hierarchical data format which is for storing scientific data [7]. It is proposed to store and organize all kinds of data as well as to overcome a limit problem on number and the size of the objects in the file. HDF5 has the distinct advantages of flexible I/O library, efficient storage and availability on almost all platforms. In addition, HDF5 can be expediently opened by the software HDFView, and the scientific data of the HDF5 file can be flexibly accessed by C, F90, C++, and Java APIs.

Through the software HDFView, the detailed data structure and data management in the HDF5 files can be seen intuitively. With the basis of fully knowing the characteristic of the HDF5 file, any data or array in it can be then easily accessed. While, the dimension and information of any dataset in the HDF5 files can be obtained by the specific functions. Thus, even though the data dimension or information is not known in advance, they can be distinctly accessed by the functions of the codes. The structure of the HDF5 is shown in Fig.1.

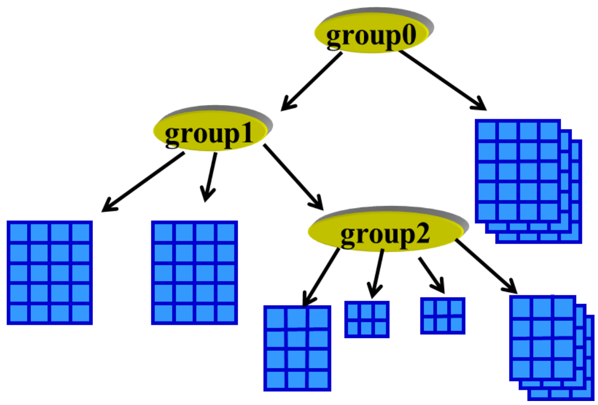

Fig. 1. The data structure instructions of HDF5 file

As is seen from Fig.1, every file starts with a root group which is the top-level structure of the data file. Every group can have any kind of attributes, but the name of an HDF5 attribute must be unique in the scope of the HDF5 item.

For example, the HDF5 file produced by CTF for the BEAVRS benchmark is shown in Fig 2. The h5 file has three groups, "CORE", "INPUT", and "STATE_0001", respectively. Moreover, all the calculation results used in the coupling process are all structured as dataset in the group "STATE_0001", including coolant temperature dataset "channel_liquid_temps [C]", coolant density dataset "liquid_density", and fuel temperature dataset "pin_fueltemps [C]". Besides, the group "STATE_0001" also includes a group "QOI" which has five dataset.

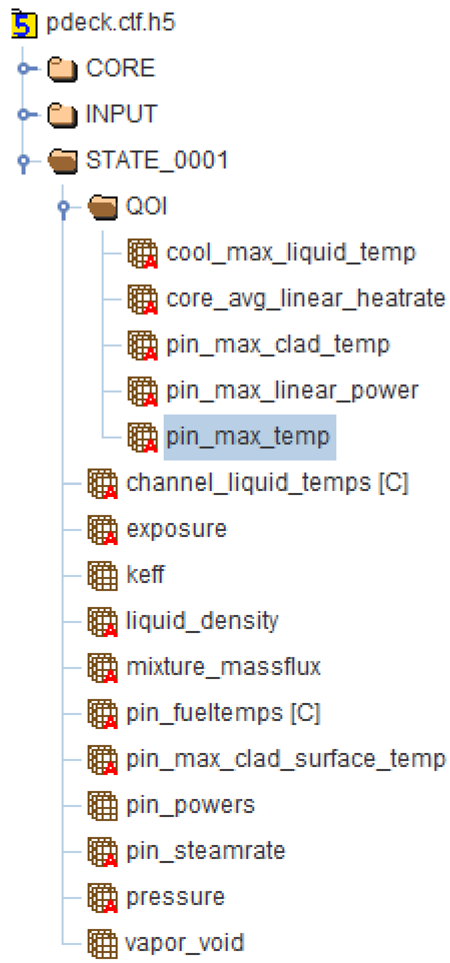

Fig. 2. The HDF5 file for the BEAVRS benchmark by CTF

III. COUPLING CODES

1. Monte Carlo code RMC

RMC is a continuous-energy Reactor Monte Carlo neutron and photon transport code being developed by Department of Engineering Physics at Tsinghua University, Beijing [8]. The code RMC intends to solve reactor analysis problems, and is able to deal with complex geometry, using continuous energy point-wise cross sections of different materials and temperatures. As one of the new generation Monte Carlo codes, RMC is aimed at achieving full core calculations and analysis with high fidelity and efficiency by means of advanced methodologies and algorithms as well as high performance computing techniques.

2. Sub-channel code CTF

CTF is the shortened name given to the version of COBRA-TF (Coolant Boiling in Rod Arrays-Two Fluid) being developed and improved by the Consortium for Advanced Simulation of Light Water Reactors (CASL) and the Reactor Dynamics and Fuel Management Group (RDFMG) at the Pennsylvania State University (PSU) [9]. CTF is a thermal–hydraulic simulation code designed for light water reactor (LWR) vessel analysis. It uses a two-fluid, three-field modeling approach and can solve the detailed full core case in parallel using the domain decomposition method [9]. Owing to its powerful functions and rapid development, CTF has been widely used internationally.

IV. VERSATILE COUPLING METHOD

The previous coupling work with RMC and CTF in reference 6 uses the hybrid coupling method, and this method transfers data by the memory of RMC and the output files of CTF. But, this coupling has two main disadvantages, the complexity of accessing data and the poor versatility of the code. The first one is that there are many CTF output files for RMC code to access because of the CTF domain decomposition parallel technology, so it is error-prone. Fortunately, CTF has the function of producing HDF5 files, and this must be the most appropriate solution to solve the first problem. For the second problem of poor versatility to other benchmarks or cases, there are some changes to the RMC input files and coupling codes.

The main change work is changing all the fixed geometry contents to the variables in the coupling codes. Besides, the second change is adding all the power and geometry information to the RMC input file to be a new input card, just as the Fig.2 shows. This is because in the coupling process RMC will produce the power input file of the code CTF, and this input file needs the geometry and power information, such as the full core map of the reactor and the total operating power.

```
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.2 Partial information of RMC input file

Another important change is reading thermal data from HDF5 files instead of text output files by CTF. And the advantages of this change has been illustrated above.

On the basis of these changes of the coupling code, only the input files of CTF and RMC need to be modified when changing the calculation benchmarks. This is exactly the most important advantage of the versatile coupling.

Another necessity of using the HDF5 file is that all the needed thermal information output by CTF are all in this file. In addition, the parameters are assigned in accordance with assembly, and thus it is very convenient to read data from HDF5 file other than reading a lot of text output files.

As shown in Fig 3, RMC calculates first and produces the power input file of CTF, and then CTF calculates and produces the HDF5 output file. After this process, RMC reads data of this HDF5 file and recalculates.

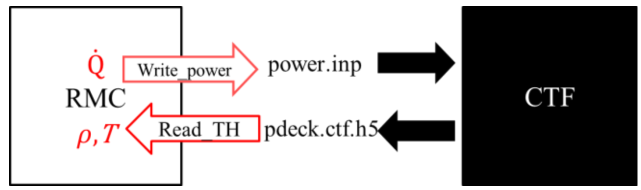

Fig 3 Schematic diagram of hybrid coupling

In this coupling process, the moderator temperature and density are averaged using the data from CTF.

Each coupled calculation begins with a RMC run employing the initialized thermal data, the variation of the averaged node power is used for checking the convergence, and is used as an estimate for the convergence,

$$\delta_{\mathrm{m}}^{n} = \left| \frac{P_{\mathrm{m}}^{n}}{P_{\mathrm{m}}^{n-1}} - 1 \right| \quad (1)$$

$$\delta_{\mathrm{ave}}^{n} = \sqrt{\frac{(\delta_1^n)^2 + (\delta_2^n)^2 + \cdots + (\delta_{\mathrm{N}}^n)^2}{N}} \quad (2)$$

where P_{m}^{n} is the power of $\mathrm{m_{th}}$ mesh in $\mathrm{n_{th}}$ iteration, δ_{m}^{n} is just the power change delta of $\mathrm{m_{th}}$ mesh. So the average variation of all the meshes are shown by the equation (2). It should be taken into consideration that Monte Carlo method has statistical uncertainties affecting the power profile distribution. In general, the averaged uncertainty of all meshes powers is chosen as convergence criterion.

The scheme about the RMC/CTF coupling process is shown in Fig 4.

It is worth to mention that this coupling approach of using HDF5 files is flexible and versatile to treat different problems when the input files of RMC and CTF are prepared.

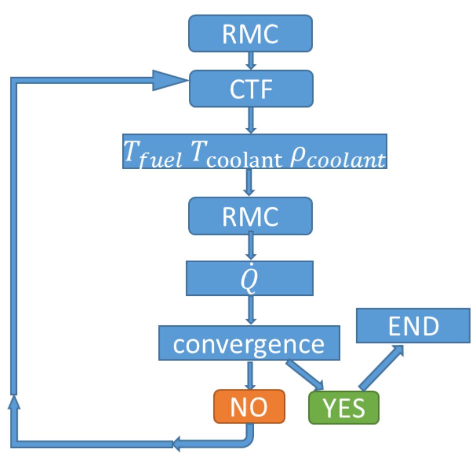

Fig.4 RMC and CTF coupling algorithm flow chart

Ⅴ. BEAVRS BENCHMARK MODELING

BEAVRS is a new benchmark based on a commercial reactor in the United States in the 1960s with detailed core construction parameters and operating measurement data for the verification of reactor analysis tool, which is proposed and released by the Computational Reactor Physics Group of MIT [10]. This benchmark is based on a PWR with 193 fuel assemblies, where each assembly is 17×17 configuration including 264 fuel rods with three different ^{235}U enrichments of 3.1%, 2.4% and 1.6%. As shown in Fig.5, fuel rods of enrichment 3.1% are put in the border of the core, and other rods of enrichment 2.4% and 1.6% are configured like a checkerboard in the middle of reactor core. In the coupling simulations, eight spacer grids in BEAVRS seen in Fig.6 are also modeled to consider the impact of grid mixing on coolant flow, which influences the heat transfer between coolant and clad. The power distribution of RMC calculation is influenced hence.

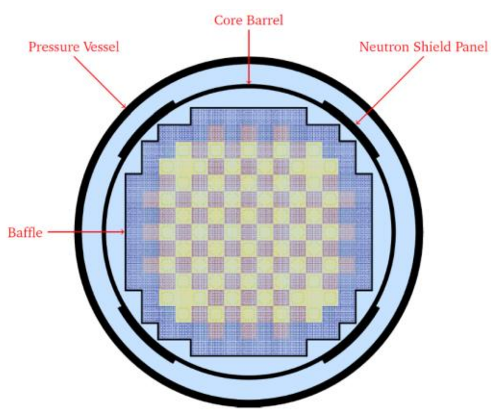

Fig. 5 Radial cross section of BEAVRS core [10]

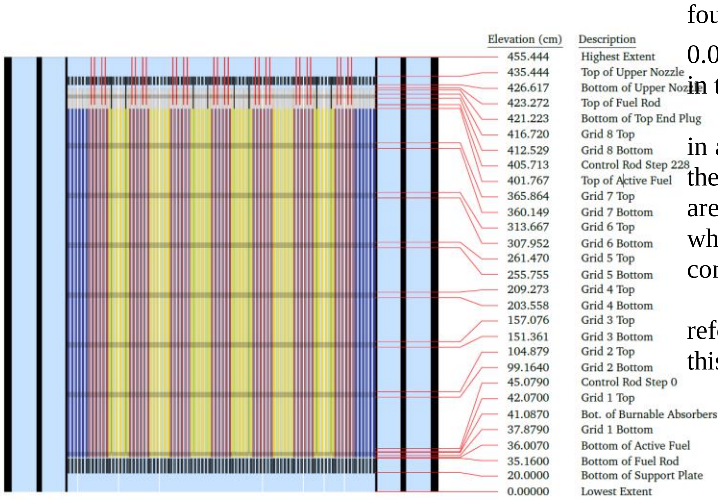

Fig. 6 Axial cross section of the BEAVRS core[10]

The BEAVRS full core model in this paper is the same with the model in reference 6 that the active core is divided into 10 axial segments and 255×255 radial meshes both in RMC and CTF. The meshes in the radial direction in the CTF thermal-hydraulics model resolved the geometry to the pin level with each polygon between four rods as a channel. The BEAVRS benchmark geometry then had a total of 56288 channels over the full core. The data used in all coupled calculations in this paper is listed in Tables I and II.

Table III Nominal value of Thermal Hydraulics condition

Item	Value	Units
Total power	3411	MW
Initial mass flow rate	17083	kg/s
Reference pressure	15.517	Mpa
Inlet water temperature	292.78	℃
Outlet water temperature	310	℃

Table IV Assembly size information

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

Ⅵ. RESULTS AND ANALYSIS

In the coupling simulation, 720 parallel threads of “Tianhe-2” super computer are used for RMC calculation, and 193 cores for CTF calculation. Fig 7 shows the convergence criteria against coupled iterations, and it can be found that after 4 hours’ calculation δ^{n}_{ave} is smaller than 0.0412, indicating that the convergence criteria is achieved in the 8th iteration.

Fig 8 shows the axial power distribution against height in active length with different coupled iterations. Except for the first three iterations, the other profiles of the iterations are almost overlapping especially after the 6_{th} iteration, which means the axial power distribution is meeting the convergence criteria.

Comparing to the previous coupling results in reference 6, all the output data is the same, indicating that this versatile coupling method is correct and effective.

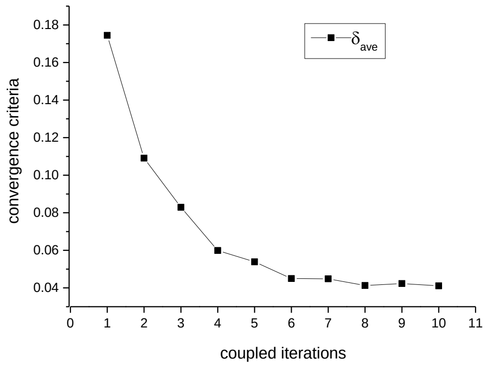

Fig 7 The convergence criteria δ_{ave}^{n} against coupled iterations

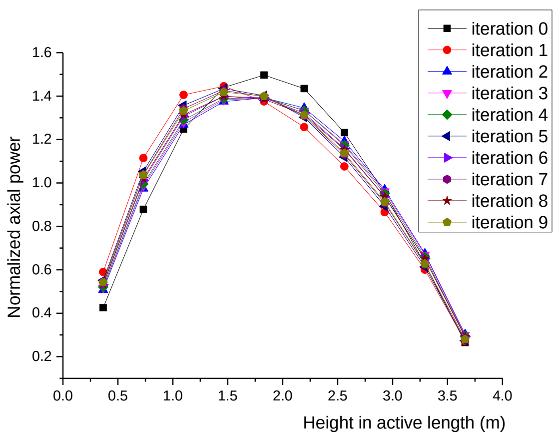

Fig 8 Full core axial power distribution with different iterations

To test and verify the improvement of the new coupling code system efficiency, the previous and current coupling code calculation time of different parts in the whole coupling process for BEAVRS benchmark is also counted, including the neutronics calculation time, the time of the data transfer process “write power” and “read TH”, and the CTF runtime. Besides, the “Write power” means the process that RMC transfers the power data to CTF. The “read TH” means the process that RMC reads the thermal parameters from CTF. The counted time of different parts by using two coupling code systems is listed in table Ⅲ.

Table Ⅲ BEAVRS benchmark calculation time by using two different coupling codes

Cost time	Neutronics calculation (min)	Write power (s)	Read TH (s)	CTF runtime (min)	One iteration (min)
Previous code	14.20	76.76	25.11	11.90	27.80
Current code	14.25	67.20	0.48	10.02	25.40

The counted time in table Ⅲ belongs to the first iteration of the coupled calculation by both the previous code and the current code. 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 has no change because the data transfer is only influenced by the size of data and the data file format. In the simulations, the Doppler broadening effect of the target nucleus influence the nucleus cross sections, thus the temperature and power distribution change in the coupling process. On the contrary, the data size that transferred in the simulation is always the same. So, the decrement of the calculation time benefits from reading the HDF5 file.

From the counted time in table Ⅲ, it is easily found that the calculation time of different codes is almost the same except the “Read TH” process. The previous coupling code reads data from CTF through 193 text output files, but the current coupling code reads data from CTF by one HDF5 file. So, the “Read TH” process by using current versatile coupling code costs less time. Therefore, the calculation results prove that the versatile coupling code based on HDF5 file can save time to some extent.

Ⅶ. CONCLUSIONS AND FUTURE WORK

In this paper, the versatile coupling based on HDF5 file with Monte Carlo code RMC and sub-channel code CTF has been developed. With the comparison of the coupling results by using HDF5 file and the previous coupling work in reference 6, the same coupling results show the reliability and availability of this versatile coupling method. Besides, the new coupling codes also have the advantage of efficiency by comparing the calculation time with the old version of coupling codes.

This versatile coupling code system provides a powerful solution for the coupling between the N-TH codes. And more benchmark tests will be performed to further testify the versatility of the code systems.

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