Development of a Neutronics and Thermal-Hydraulics Coupling System with RMC and SUBCHAN

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Abstract

The continuous-energy Reactor Monte Carlo code, RMC, was coupled with a sub-channel thermal-hydraulic analysis code, SUBCHAN, using a loose-coupling scheme with an in-house coupling framework by Python scripts. The newly developed coupling system was validated using the VERA core physics benchmark problems 6 and 7. The converged RMC/SUBCHAN solutions were compared with that of the RMC/CTF coupling code which has been validated by multiple benchmarks. A good agreement was achieved on the solution of VERA #6 with the absolute difference of the eigenvalue of 7 pcm and maximum relative difference of 0.11% for the fuel pin fission rate. Besides, the relative difference of the radial power distributions from the two code suites are almost within [-3RSD, 3RSD]. The thermal-hydraulic parameters including the fuel temperatures and the coolant temperatures and densities, agree very well with only a slight overestimation for the averaged outlet coolant temperature by 1K from RMC/SUBCHAN. Excellent agreements with a solution of VERA #7 were also demonstrated for the eigen values and the integral assembly power distributions.

1. Introduction

Simulations of the multi-physics coupling phenomena with a Monte Carlo (MC) physics code coupled with a subchannel thermal-hydraulic (TH) have been commonly applied in nuclear reactors designs and optimizations. In the neutronics and thermal-hydraulics (N-TH) coupling, the MC code can provide the spatial power distribution of high fidelity while the sub-channel code will solve for flow and temperature distributions as feedback. This paper describes a N-TH system composed of the Reactor Monte Carlo code (RMC) [1] and the sub-channel TH analysis code SUBCHAN [2] using a loose-coupling scheme with a in-house coupling framework by Python scripts. The newly developed coupling system are used to simulate the CASL VERA Core Physics Benchmark Progression Problems 6 and 7. The solutions are compared with that of the RMC/CTF coupling code which has been validated by multiple benchmarks [3,4,5] and also the VERA solutions (MPACT/CTF).

2. RMC/SUBCHAN coupling

In this section, the two calculation modules in the RMC/SUBCHAN coupling system are described. The loose coupling scheme with an in-house coupling framework is illustrated detailly.

2.1 RMC and SUBCHAN codes

The Reactor Monte Carlo code, RMC, is an in-house developed stochastic 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.

The sub-channel thermal-hydraulic analysis code, SUBCHAN, features four partial differential equations and can simulate a single-component two-phase mixture. The code uses the Industrial Formulation 1997 as the water properties 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.

2.2 Loose-coupling scheme

Previous work reported the coupling of RMC and COBRA-TF (CTF) [6] 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 complex 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 same 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-Fig. 2 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 physical model with some necessary coupling parameters, especially the convergence criteria. The primary obstacle manifests during the construction of the thermal-hydraulic input model of SUBCHAN. It is well recognized that establishing the interconnections between fuel rods and subchannels represents a highly intricate endeavor. Typically, a subchannel input model for a physical reactor core entails the management of an extensive textual input consisting of nearly several hundred thousand lines. Hence, the development of a preprocessor that can interpret some basic parameters and automatically generate subchannel input cards becomes imperative in order to streamline the process. In this work, a preprocessor called *subchan-preproc* is designed to read a *preproc.yaml* file in YAML format and generate a *SUBCHAN.inp* for the following execution of SUBCHAN. Some basic parameters that include the core assembly layout, the fuel rod and guide tube layout, the initial thermal hydraulic parameters, and some necessary controlling parameters must be specified in the preprocessor input.

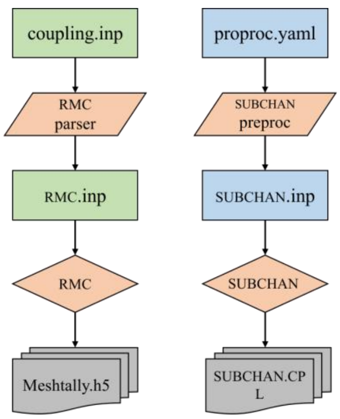


Fig. 1. RMC and SUBCHAN preprocessing flowchart.

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 a power tally file, *MeshTally.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 file, *MeshTally.h5,* which is the input of the next Picard iteration. The Picard iteration in the loose-coupling scheme is repeated until the convergence criteria is achieved.

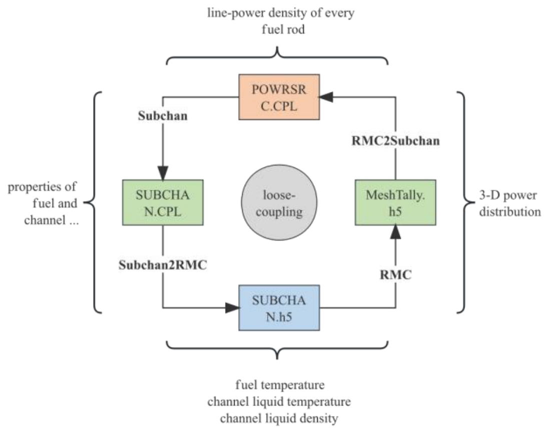


Fig. 2. The flowchar of RMC/SUBCHAN coupling scheme.

3. Validation and analyses

The newly developed RMC/SUBCHAN coupling system is validated using the VERA Core Physics Benchmark Problem 6 and 7. All the calculations are performed on the Tianhe-3 high performance computing cluster with 64 cores of 2.3GHz FT2000+ processor with 128GB of RAM in one node.

3.1 VERA Core Physics Benchmark Problem 6

VERA Problem #6 is a single Westinghouse 17×17 type PWR fuel assembly at the beginning-of-cycle (BOC) and hot-full-power (HFP) conditions, whose material compositions and geometry information can be referred in the official specifications [7]. There are 264 fuel rods, 24 guide tubes and 1 instrument tube, and 324 coolant subchannels, no burnable poison rods or no control rod clusters. All the fuel pins, guide tubes and moderator subchannels are explicitly modeled in RMC and SUBCHAN.

There are 17×17 radial meshes and 49 axial meshes in the active core region of 365.76 cm in RMC and SUBCHAN models. 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 MC calculations, 500000 particles are tracked in 200 inactive cycles and 1000 active cycles.

The results including the convergent eigenvalue k_{eff}, the spatial power distributions and the fuel and coolant temperatures distributions, are compared with solutions from MPACT/CTF (VERA-CS), MC21/CTF, and the RMC/CTF results.

Maximum ten coupled iterations are simulated to converge RMC and SUBCHAN. Throughout one iterative coupling process, the MC simulation necessitates 16 minutes with 5600 MPI processes, whereas the TH analysis computation merely demands 3 seconds with one process. The computational time for coupling interface remains within the order of seconds and the memory footprint of the coupling files amounts to merely 350KB. RMC eigenvalue trajectory during the ten iterations is presented in Fig. 3, which indicates that the iteration converges in the 6th index. The eigenvalues predicted by RMC/SUBCHAN with and without DBRC (Doppler-Broadening Rejection Correction) are compared with previous results in Table I. The difference between RMC/SUBCHAN and RMC/CTF is 7 pcm, which is considered to be statistically good agreement. The difference from MPACT/CTF (VERA-CS) is a little large of 97 pcm, which can be explained by the difference of a deterministic and a stochastic solver and that of the nuclear database. It is noted that the OTFDB with DBRC has been demonstrated to offer more precise solutions than that without DBRC. Consequently, the eigenvalue from RMC/SUBCHAN with DBRC is more convincible despite a discernible difference of -81ppm. Nevertheless, in order to facilitate a more rigorous comparison with the previous results from MPACT/CTF and MC21/CTF, the following evaluations are performed exclusively on the solutions without DBRC.

Table I Calculated eigenvalues of different coupling system for VERA Problem #6.

Coupling system	eigenvalue $k_{eff} \pm std$	difference / pcm
MPACT/CTF	1.16361	-
MC21/CTF	1.16424±2.6E-05	63
RMC/CTF	1.16465±6.7E-05	104
RMC/SUBCHAN	1.16458±4.0E-05	97
RMC/SUBCHAN (DBRC)	1.16280±4.0E-05	-81

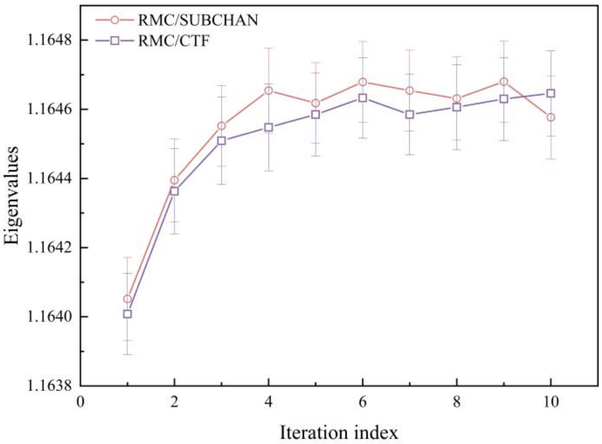


Fig. 3. RMC eigenvalues over the coupling iterations for VERA Problem #6.

Fig. 4 compares the axially-integrated fission rate distributions in the assembly from RMC/SUBCHAN and RMC/CTF. The maximum relative difference of 0.11% and average one of 0.03% of the fission rate distributions indicate a pretty good agreement. The normalized axial power distribution in a single pin with index (16, 16) is also compared with results from RMC/CTF in Fig. 5. The power values are normalized by an average power of 0.939 in Fig. 4 and the black dash curves present the triple relative standard deviation (RSD). The axial power density curves from the two coupling systems agree very well with each other with almost the relative different within [-3RSD, 3RSD].

	1.0360 1.0357 0.02%	1.0369 1.0358 0.11%		1.0343 1.0349 -0.06%	1.0313 1.0316 -0.03%		1.0115 1.0121 -0.06%	0.9775 0.9775 0.00%	RMC/CTF RMC/SUBCHAN difference
1.0365 1.0362 0.02%	1.0095 1.0091 0.04%	1.0096 1.0093 0.04%	1.0364 1.0362 0.02%	1.0086 1.0085 0.00%	1.0057 1.0050 0.07%	1.0255 1.0260 -0.05%	0.9887 0.9891 -0.04%	0.9735 0.9734 0.01%	
1.0365 1.0362 0.03%	1.0096 1.0094 0.01%	1.0099 1.0103 -0.04%	1.0380 1.0380 0.00%	1.0109 1.0112 -0.03%	1.0087 1.0087 0.00%	1.0271 1.0270 0.01%	0.9886 0.9884 0.02%	0.9727 0.9730 -0.03%	maximum 0.11%
	1.0367 1.0367 0.00%	1.0385 1.0383 0.02%		1.0443 1.0443 0.00%	1.0449 1.0440 0.09%		1.0117 1.0111 0.06%	0.9750 0.9751 -0.01%	average 0.03%
1.0343 1.0353 -0.10%	1.0086 1.0086 0.00%	1.0112 1.0112 0.00%	1.0442 1.0443 0.00%	1.0315 1.0312 0.03%	1.0502 1.0504 -0.01%	1.0357 1.0355 0.02%	0.9834 0.9837 -0.02%	0.9654 0.9657 -0.03%	
1.0311 1.0313 -0.03%	1.0052 1.0058 -0.06%	1.0090 1.0086 0.04%	1.0444 1.0445 -0.01%	1.0506 1.0498 0.07%		1.0171 1.0166 0.05%	0.9651 0.9649 0.02%	0.9559 0.9563 -0.04%	
	1.0257 1.0260 -0.03%	1.0272 1.0271 0.01%		1.0356 1.0354 0.02%	1.0167 1.0164 0.03%	0.9733 0.9729 0.05%	0.9482 0.9483 -0.01%	0.9466 0.9472 -0.06%	
1.0118 1.0120 -0.02%	0.9882 0.9885 -0.03%	0.9883 0.9880 0.03%	1.0109 1.0111 -0.01%	0.9831 0.9833 -0.02%	0.9651 0.9647 0.05%	0.9482 0.9485 -0.03%	0.9394 0.9393 0.01%	0.9432 0.9432 0.00%	
0.9771 0.9778 -0.07%	0.9727 0.9733 -0.07%	0.9726 0.9726 0.00%	0.9751 0.9749 0.02%	0.9655 0.9659 -0.04%	0.9563 0.9562 0.01%	0.9471 0.9470 0.01%	0.9430 0.9432 -0.02%	0.9488 0.9497 -0.10%	

Fig. 4. Comparison of the axially-integrated radial fission rate distributions for the VERA Problem #6 assembly predicted by the RMC/SUBCHAN and the RMC/CTF.

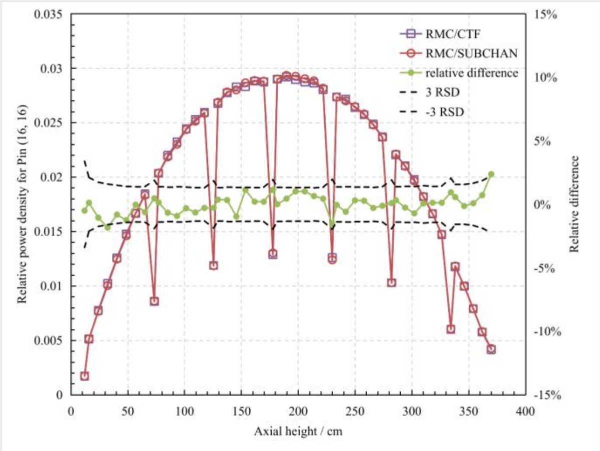
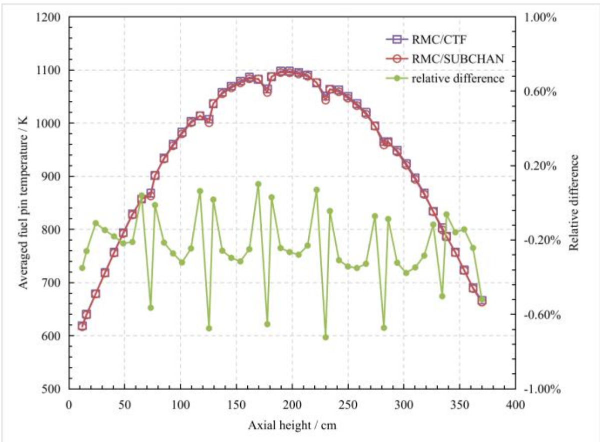
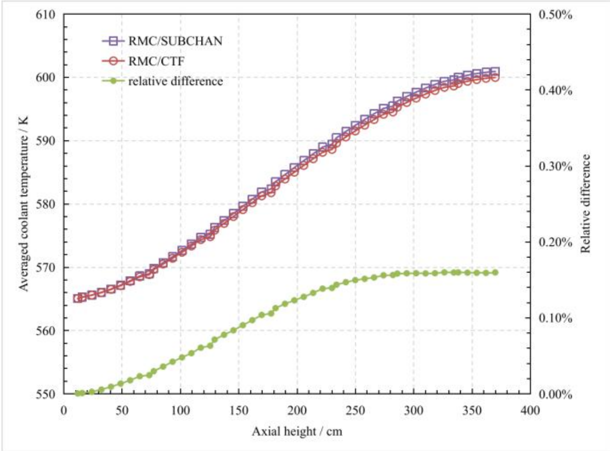


Fig. 5. Comparison of the normalized axial pin power profiles for fuel rod (16,16) predicted by RMC/SUBCHAN and the RMC/CTF.

Fig. 6 compares the axial volume-averaged fuel pin and coolant temperatures distributions for both code suites. RMC/SUBCHAN predicts a similar temperature distribution with RMC/CTF at this axial direction with the difference within [-7.6K, 1.1K]. The axial volume-averaged coolant temperatures from the two coupling systems agree very well with only a slight overestimation of the averaged outlet coolant temperature by 1K from RMC/SUBCHAN. The results demonstrate that SUBCHAN, despite utilizing a four-equations model compared to the nine-equations by CTF, can ensure an adequate level of accuracy for the steady-state subchannel thermal-hydraulic analyses.



(a) fuel temperature



(b) coolant temperature

Fig. 6 Axial volume-averaged fuel pin and coolant temperature profile in VERA Problem #6 assembly from RMC/SUBCHAN and RMC/CTF.

3.2 VERA Core Physics Benchmark Problem 7

VERA Core Physics Benchmark Problem #7 represents an operating reactor in full geometry detail at BOC, HFP, nominal flow conditions, and equilibrium xenon isotopic. The mesh grids of $17 \times 17 \times 49$ meshes and neutron ACE libraries for VERA #7 are identical to that of VE*R*A #6, and OTFDB is also applied to consider the temperature feedback from thermal hydraulics calculations. More neutrons of 1000000 particles per cycle are simulated with 200 inactive cycles and 600 total cycles for the convergence of fission source in the full core.

For large problems like the whole core problem of VERA #7, OpenMP is used with 14 threads for each process and 400 MPI processes is applied. In this case, the MC calculation time remains at 13 minutes due to the less active cycles, while the TH analysis computation time increases to 90 seconds. Furthermore, the memory usage of the coupling files expands to 15MB.

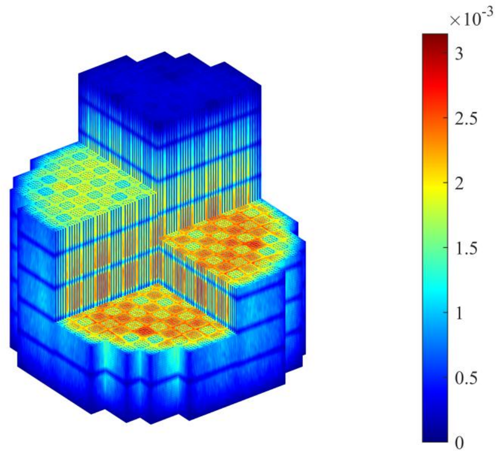


Fig. 7. Three-Dimensional power distributions with 3411MW from RMC/SUBCHAN of VERA Problem#7.

Table II illustrates the final critical boron concentrations from RMC/SUBCHAN, RMC/CTF, and the previous results. Agreement between the two coupling systems is about 4ppm which shows excellent statistical consistency for eigenvalues and critical boron concentrations.

Table II The critical boron concentration different coupling system for VERA Problem #7.

Coupling system	critical boron concentration / ppm	difference / ppm
MPACT/CTF	854	-
MC21/CTF	859	5
RMC/CTF	848	6
RMC/SUBCHAN	852	2

Fig. 7 presents a 3-D view of the pin power distribution from RMC/SUBCHAN where the maximum power peaking factor (PPF) is 1.975. The good agreement of 5.5% relative difference is achieved with the maximum PPF of 1.986 from RMC/CTF. Fig. 8 presents a quarter-symmetric relative power of each assembly in a 1/4 core layout. Assembly powers agree within [-0.33%, 0.58%] with the average relative difference of 0.16%, which demonstrates great agreements for the power distributions from the two codes.

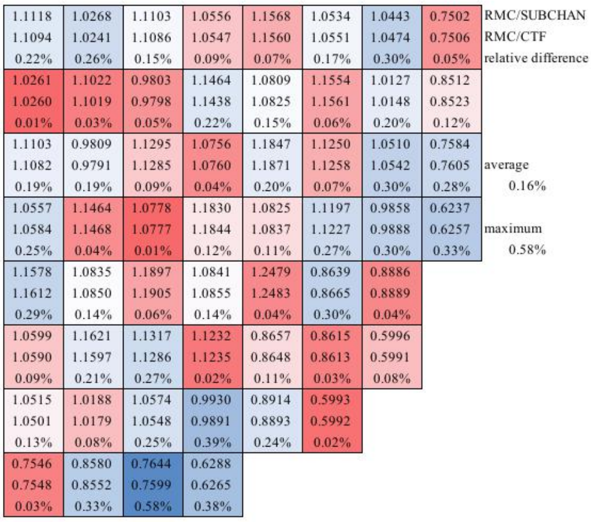


Fig. 8. Axially-integrated assembly relative power from RMC/SUBCHAN and RMC/CTF for VERA Problem #7.

Table III The computation time from SUBCHAN and CTF for VERA Problem #6 and VERA Problem #7.

Time / s	VERA #6	VERA #7
SUBCHAN	2.9	90
CTF	37.9	3154
CTF parallel(mpi)	-	59

4. Conclusions

The continuous-energy Monte Carlo code RMC was coupled with a subchannel thermal hydraulic code SUBCHAN for the multi-physics analyses of the nuclear reactor. The newly developed coupling system was validated using the CASL VERA Core Physics Benchmark Progression Problems 6 and 7. Excellent agreements were demonstrated with the solutions of VERA #6 and VERA #7 from the two coupling systems for eigenvalues, the power distributions, fuel temperatures, and the coolant temperatures and densities. Overall, comparing with solutions from RMC/CTF, RMC/SUBCHAN achieved a comparable level of accuracy for steady-state TH analyses with less time spent on TH calculations, as illustrated in Table III. It is noticed that CTF achieved less computational time for VERA #7 because of the parallel processing with 193 MPI cores. The implementation of MPI parallelism in SUBCHAN will be investigated in the future.

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