

Preliminary Simulation Results of VERA Problems 6 and 7 Using NECP-X/SUBSC

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INTRODUCTION

With the improved understanding of the governing physical mechanism and the steady growth of computing capability, especially the development of massively parallel processing system, the coupling of high-fidelity neutronics and thermal-hydraulics becomes more and more popular worldwide. Serpent 2/SUBCHANFLOW [1], MC21/CTF [2] and RMC/CTF [3] are several famous Monte Carlo methods based coupling codes. All of them are capable of dealing with large-scale problems, including the BEAVRS benchmark [4] and VERA #7 [5]. Still, the computational burden of the Monte Carlo methods is too large compared to the deterministic based methods. For example, MC21 required 6.8 days using 1024 cores while MPACT only took 57 minutes using 464 cores for one Picard iteration [2]. Therefore, the deterministic based coupling codes, including nTRACER/MATRA [6], MPACT/CTF [2] and NECP-X/SUBSC [7] are much more competitive from efficiency viewpoint. This paper summarizes the recent work about applying NECP-X/SUBSC to VERA #6 and VERA #7.

COUPLING NECP-X TO SUBSC**NECP-X**

A three-dimensional direct whole-core transport code NECP-X is being developed in Xi'an Jiaotong University (XJTU), capable of ultrafine geometry description, multi-group library generation, local-global resonance calculation, large-scale parallel 2D/1D transport calculation, pin-by-pin coupling of neutronics and thermo-hydraulics and transient calculation. More details about NECP-X can refer to [8-11].

SUBSC

SUBSC is also an in-house code developed in XJTU intended to be applied for large-scale thermal-hydraulics calculation. A restart GMRES algorithm with an incomplete LU factorization preconditioning was implemented for solving the mass conservation equation in order to improve efficiency of SUBSC code. More details about SUBSC can refer to [12-13].

Coupled Method

Generally, there are two methods for coupling two separate codes into one integrated system: external coupling and internal coupling. For the external coupling method, the transfer of coupling parameters is usually realized through external files. An extra coupling script is needed to execute the coupling calculation. This coupling approach is flexible and simple to incorporate mature codes without adapting them. For the internal coupling method, the neutronics code and T/H code are integrated based on a same framework as two separate modules, where the coupling parameters are transferred in memory. However, due to different parallel performance of the two codes, the computational resource will be wasted. Specifically, NECP-X utilizes 2056 cores while SUBSC only uses 1 core for VERA #7. When the coupling code performs T/H calculation, the extra cores will be waiting until the main core finished T/H calculation. To resolve this problem, an external method was used via Python script to call neutronics and T/H solvers respectively.

Fig. 1 provides flow chat of NECP-X/SUBSC. Before coupling iteration, the universal input processing tools in NECP-X are used to generate SUBSC input card as well as mesh mapping information which maps results between NECP-X and SUBSC. With NECP-X and SUBSC model initialization and mesh mapping complete, Picard iteration is performed. First, NECP-X is solved to get the linear power of each fuel rod to update input card of SUBSC. Second, SUBSC is executed to generate fuel and cladding temperatures as well as subchannel temperatures and densities. All these T/H parameters are saved in HDF5 files. Third, NECP-X reads these HDF5 files to update temperature and density of each material region. Fourth, NECP-X is executed with updated T/H conditions. The Picard iteration is repeated until convergence is achieved.

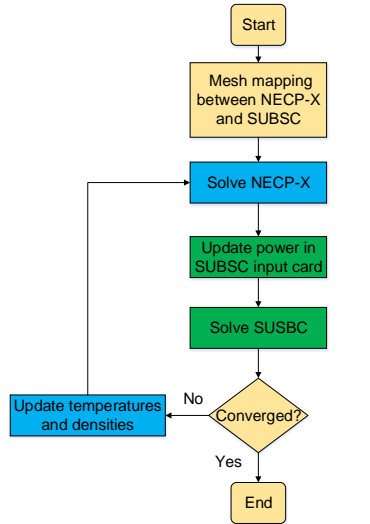


Fig. 1. Flow chat of NECP-X/SUBSC

An Effective Relaxation Method

Since the computational burden is rather large for the high-fidelity coupling calculation, especially the full core coupling calculation. A relaxation method was implemented with the goal of speeding up the convergence behavior.

The traditional relaxation method [8] consists in weighting the results of the actual simulation step with the ones of the previous step by applying relaxation factor x . Take the fuel temperature as an example, the actual temperature is obtained as follows:

$$T_{fuel,i}^{weighted} = (1-x) \cdot T_{fuel,i-1}^{th} + x \cdot T_{fuel,i}^{th} \quad (1)$$

Where $T_{fuel,i-1}^{th}$ is the fuel temperature from the T/H code of the previous step. $T_{fuel,i}^{weighted}$ is used for the neutronics calculation of the current step; x is the relaxation factor whose value is recommended to be 0.5. In this paper, a new relaxation method is proposed by weighting the results of two “relaxed” ones of current and previous steps, since the “relaxed” one is newer. The actual temperature can be obtained as follows:

$$T_{fuel,i}^{weighted} = (1-x) \cdot T_{fuel,i-1}^{weighted} + x \cdot T_{fuel,i}^{th} \quad (2)$$

If we set x to be 0.5, equation (2) can be rewritten in a recursion form as:

$$T_{fuel,n}^{weighted} = 0.5^1 \cdot T_{fuel,n}^{th} + 0.5^2 \cdot T_{fuel,n-1}^{weighted} + \dots + 0.5^{n-1} \cdot T_{fuel,2}^{weighted} + 0.5^{n-1} \cdot T_{fuel,1}^{weighted} \quad (3)$$

The new relaxation method considers contributions from the current step combined with all previous steps. Both

the traditional and new relaxation methods were implemented in the NECP-X/SUBSC coupling code.

RESULTS

VERA #6

VERA #6 is a PWR fuel assembly at HFP conditions. The convergence criteria are summarized in Table I. The parameters used include the eigenvalue and the maximum change in the fuel over a single fuel rod of an axial mesh for the reason that the fuel temperature shows largest oscillations during the coupled run [14]

TABLE I. Convergence criteria

Parameters	Criteria
Δk_{eff}	2 pcm
ΔT_{fuel}	2.0 K

Fig. 2 compares the convergence curves of the fuel temperature for the traditional relaxation method ($x=0.5$) and the new relaxation method ($x=0.5$ -new) when the relaxation factor is set to be 0.5. Table II compares the iteration numbers. We can conclude that the new relaxation method not only stabilizes the coupling calculation but also accelerates it significantly. The iteration process of NECP-X/SUBSC with new relaxation method is shown in Table III.

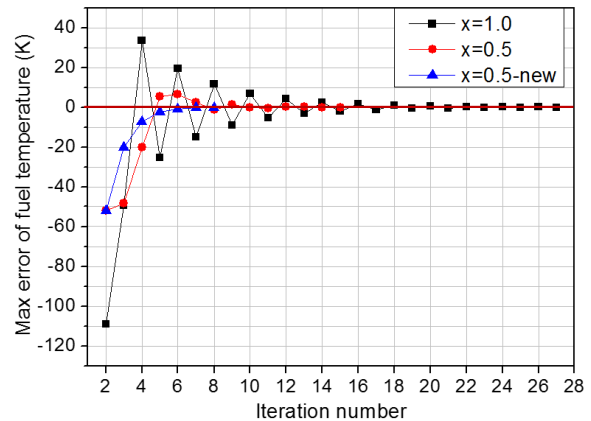


Fig. 2. Comparison of the convergence curves

TABLE II. Comparison of iteration number

Relaxation	Iteration number
1.0	27
0.5	15
0.5-new	8

TABLE III. Comparison of iteration number

Iteration	k_{eff}	Δk_{eff} [pcm]	ΔT_{fuel} [K]
1	1.16732	-	-
2	1.16566	-166	-50.02
3	1.16367	-199	-43.69
4	1.16386	19	-20.80
5	1.16393	7	5.10
6	1.16389	-3	6.92
7	1.16389	0	-3.41
8	1.16389	0	-1.36

Table IV shows eigenvalues of several kinds of coupling codes [2]. Compared to MPACT/CTF, NECP-X/SUBSC overestimates eigenvalue by 28 pcm. Table V presents difference of axially integrated normalized pin power between NECP-X/SUBSC and MPACT/CTF with the maximum relative difference to be 0.15%. Table VI presents difference of subchannel exit coolant temperatures between NECP-X/SUBSC and MPACT/CTF with the maximum difference to be 0.6 K.

TABLE IV. Comparison of iteration number

Code	Eigenvalue
MC21/CTF	1.16424±0.00003
MPACT/CTF	1.16361
NECP-X/SUBSC	1.16389

TABLE V. Difference of axially integrated normalized pin power between NECP-X/SUBSC and MPACT/CTF

	-0.17	-0.17		-0.14	-0.13		-0.10	-0.03
-0.17	0.04	0.04	-0.15	0.06	0.05	-0.09	0.09	0.06
-0.17	0.03	0.02	-0.16	0.05	0.06	-0.09	0.10	0.07
	-0.16	-0.17		-0.11	-0.15		-0.01	0.00
-0.14	0.06	0.05	-0.13	0.11	-0.02	-0.01	0.10	0.05
-0.14	0.05	0.07	-0.16	-0.01		-0.07	0.03	0.05
	-0.12	-0.09		0.00	-0.08	0.10	0.12	0.09
-0.08	0.09	0.08	-0.03	0.10	0.05	0.12	0.15	0.12
-0.03	0.06	0.06	-0.02	0.04	0.03	0.08	0.10	0.11

TABLE VI. Difference of subchannel exit coolant temperatures between NECP-X/SUBSC and MPACT/CTF

0.52	0.40	0.52	0.50	0.40	0.56	0.50	0.47	0.41
0.40	0.37	0.42	0.42	0.41	0.36	0.41	0.41	0.41
0.52	0.42	0.56	0.53	0.36	0.46	0.51	0.43	0.36
0.50	0.42	0.53	0.55	0.34	0.44	0.56	0.43	0.45
0.40	0.41	0.36	0.34	0.44	0.53	0.40	0.44	0.43
0.56	0.36	0.46	0.44	0.53	0.49	0.44	0.41	0.41
0.50	0.41	0.51	0.56	0.40	0.44	0.41	0.43	0.37
0.47	0.41	0.43	0.43	0.44	0.41	0.43	0.45	0.36
0.41	0.41	0.36	0.45	0.43	0.41	0.37	0.36	0.40

VERA #7

VERA #7 represents Watts Bar Unit 1 at BOC, HFP, equilibrium xenon conditions, with different fuel enrichments of 2.11% (red), 2.619% (yellow), and 3.10% (blue), respectively. Table VII provides some key parameters.

TABLE VII. VERA #7 key parameters

Parameter	Value
Inlet Coolant Temperature	565 K
Reactor Pressure	2250 psia
Rated Power (100%)	3411 MW
Rated Coolant Mass Flow (100%)	131.7 Mlbs/hr
RCCA Bank D Position (steps withdrawn)	215

NECP-X is run with 2056 cores parallel while SUBSC is run with only 1 core since SUBSC is a serial subchannel code at present. Table VIII shows eigenvalues of the two coupling codes. Compared to MC21/CTF, NECP-X/SUBSC underestimates eigenvalue by 482 pcm. Fig. 3 presents difference of axially integrated assembly relative power between NECP-X/SUBSC and MC21/CTF with the maximum relative difference to be 1.95%.

TABLE VIII. Comparison of eigenvalue

Code	Eigenvalue
MC21/CTF	0.99994±0.00001
NECP-X/SUBSC	0.99512

1.27	1.29	1.06	0.76	0.40	0.22	0.02	-0.27
1.29	1.22	1.05	0.66	0.39	0.10	-0.15	-0.37
1.06	1.05	0.77	0.47	0.12	-0.05	-0.16	-0.41
0.76	0.66	0.47	0.11	-0.16	-0.33	-0.54	-0.81
0.40	0.39	0.12	-0.16	-0.69	-0.68	-1.09	
0.22	0.10	-0.05	-0.33	-0.68	-1.18	-1.95	
0.02	-0.15	-0.16	-0.54	-1.09	-1.95		
-0.27	-0.37	-0.41	-0.67				

Fig. 3. Difference of axially integrated assembly relative power

CONCLUSION

An external coupling method is used to couple the high-fidelity neutronics code NECP-X to a subchannel code SUBSC via Python script. An effective relaxation method which takes all previous steps results into consideration is adopted to accelerate the coupling calculation. This kind of relaxation method shows excellent performance for VERA #6. Calculated eigenvalue, axially integrated normalized pin and subchannel exit coolant temperatures by NECP-X/SUBSC agree well with that provided by MC21/CTF. Then the NECP-X/SUBSC coupled code is applied to VERA #7. The eigenvalue and axially integrated assembly relative power calculated for VERA #7 are compared to that of MC21/CTF. Compared to MC21/CTF, NECP-X/SUBSC underestimates eigenvalue by 482 pcm. The maximum relative difference of axially integrated assembly relative power is 1.95%. Work is still on the way to analyze the difference between NECP-X/SUBSC and MC21/CTF.

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REFERENCES

1. DAEUBLER M, IVANOV A, et al. "High-fidelity coupled Monte Carlo neutron transport and thermal-hydraulic simulations using Serpent 2/SUBCHANFLOW," *Annals of Nuclear Energy*, 83, pp. 352-375(2015).
2. KELLY III D J, et al. "MC21/CTF and VERA multiphysics solutions to VERA core physics benchmark progression problems 6 and 7," *Nuclear Engineering and Technology*, 49, pp. 1326-1338(2017).
3. GUO J, LIU S, et al. "Coupled neutronics/thermal-hydraulics analysis of a full PWR core using RMC and CTF," *Annals of Nuclear Energy*, 109, pp. 327-336(2017).
4. N. HORELIK, et al., "Benchmark for Evaluation and Validation of Reactor Simulations (BEAVRS)," *Proc. Int. Conf. M&C 2013, Sun Valley, ID, USA, May 5-9, 2013* (2013).
5. GODFREY A T. "VERA core physics benchmark progression problem specifications," Oak Ridge National Laboratory, CASL-U-2012-0131-004, 2013.
6. JUNG Y S, et al. "Practical numerical reactor employing direct whole core neutron transport and subchannel thermal/hydraulic solvers," *Annals of Nuclear Energy*, 62, pp. 357-374 (2013).
7. LIU Z, et al. Development and verification of the high-fidelity neutronics and thermal-hydraulic coupling code system NECP-X/SUBSC[J]. *Progress in Nuclear Energy*, 103, pp. 114-125(2018).
8. JUN CHEN, et al. A new high-fidelity neutronics code NECP-X[J]. *Annals of Nuclear Energy*[J]. 116, pp. 417-28(2018).
9. CHEN ZHAO, et al. Hongchun Wu. Improved leakage splitting method for the 2D/1D transport calculation[J]. *Progress in Nuclear Energy*[J]. 105, pp. 202-210(2018).
10. ZHOUYU LIU, et al. Improvement and optimization of the pseudo-resonant-nuclide subgroup method in NECP-X[J]. *Progress in Nuclear Energy*, 103: 60-73(2018).
11. ZHOUYU LIU, et al. The pseudo-resonant-nuclide subgroup method based global-local self-shielding calculation scheme[J]. *Journal of Nuclear Science and Technology*, 2018, 55(2): 217-228.
12. JUN CHEN, et al. Development of Subchannel Code SUBSC for high-fidelity multi-physics coupling application[J]. *Energy Procedia*, 2017, 127: 264-274.
13. JUN CHEN, etc. Development and Steady Validation of Subchannel Code SUBSC[J]. *Atomic Energy Science and Technology*, v 51, n 6, p 1030-1037(2017).
14. IVANOV A, et al. Development of a coupling scheme between MCNP5 and SUBCHANFLOW for the pin-and fuel assembly-wise simulation of LWR and innovative reactors[C] *M&C 2011, Rio de Janeiro, RJ, Brazil, May 8-12, 2011* (2011).