Multi-physics Pin-by-Pin Core Analysis with Sub-channel T/H calculation

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1. Introduction

Much effort of nuclear community is now a day directed to perform high-fidelity and high-resolution reactor analyses. One of the ways to achieve the high fidelity is by coupling interacting physics, like reactor neutronics and thermal hydraulics. At the same time, the high resolution can be obtained by refining the mesh to fuel pin level. Development of tools to obtain such results in a reasonable amount of time with limited computational resources is a challenge.

In our research group, efforts have been made to develop tools to carry out pin-by-pin reactor analyses in a reasonable amount of time by effective parallel computing. First, a new algorithm termed as the Hybrid Coarse-Mesh Finite Difference (HCMFD) algorithm [1] to carry out pin-by-pin neutronics calculations in a reasonable amount of time has been suggested. Similarly, the START code [2] provides capability to carry out sub-channel based thermal hydraulics calculations for large LWR core in a relatively short time. In this study, HCMFD algorithm based code has been coupled with the START code to perform whole-core pin-by-pin neutronics/thermal-hydraulics coupled calculations for a large LWR core. Preliminary results for this effort are presented here.

2. Methodology

2.1 HCMFD Algorithm

In the HCMFD algorithm, two CMFD (Coarse-Mesh Finite Difference) methods are nonlinearly coupled with the nodal expansion method (NEM) applied on pin-level. To enable an efficient parallel computing, the whole domain is decomposed into subdomains, the fuel assemblies in a LWR.

The global balance is governed by solving the global eigenvalue problem with the one-node CMFD method, represented by Eq. (1).

$$A_{cmfd}^{global}\Phi_{cmfd}^{global}=\frac{1}{k}F_{cmfd}^{global}\Phi_{cmfd}^{global}, \quad (1)$$

Φ_{cmfd}^{global} : global node-averaged fluxes,
A_{cmfd}^{global} : global system matrix,
F_{cmfd}^{global} : global fission source operator,
k : multiplication factor.

Then the global balance information is transferred to each subdomain in terms of the boundary conditions, the fixed fission source and incoming currents on the boundary.

At the same time, the local fixed source problems, represented by Eq. (2), are solved by the conventional two-node CMFD method based on NEM, with the given boundary conditions.

$$M_i^{local}\phi_i^{local}=S_i^{local}, i=1,2,...N, \quad (2)$$

ϕ_i^{local} : i-th node local fluxes,
M_i^{local} : i-th node local system matrix,
S_i^{local} : i-th node local fixed source.

The solutions of the local problems are then homogenized for the following global calculation.

In this HCMFD framework, the whole-core pin-by-pin analysis can be performed very effectively by an efficient parallel computing in a local-global non-linear iterative scheme as shown in Fig. 1. Whole-core pin-by-pin neutronics calculations for a large PWR core only take ~10 seconds with 40 cores on Intel Xeon Gold 6148 CPUs (2.40 GHz). More details of the work can be found in the reference [1].

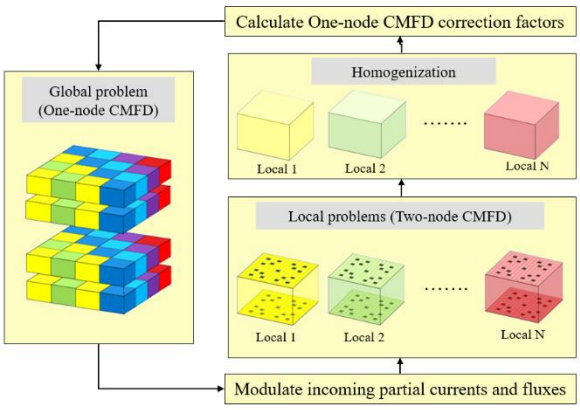

Fig. 1: Schematic diagram of the HCMFD algorithm

2.2 START code

The START (Steady and Transient Analyzer for Reactor Thermal Hydraulics) code is an in-house developed code to perform sub-channel thermal hydraulics analyses for LWRs. The START code is written in modern Fortran in a modular fashion. Special emphasis is on fast execution of the code to perform coupled neutron physics/thermal hydraulics analysis in a reasonable time. OpenMP parallelization is applied to several parts of the code. Good parallel efficiency of almost 80% is achieved. Whole core calculations for a large size PWR (241 assemblies of 17x17 matrix) takes approximately one minute with 40 cores.

The START code is based on homogeneous two-phase model. Basic conservation equations (mass, momentum

and energy), based on sub-channel formulation, are solved using marching algorithm. Newton-Raphson iterations determine pressure drop for axial and radial pressure drop used in axial and lateral momentum equations. Time-dependent solution is based on an implicit scheme. The START code solution has been validated against PSBT. Capability of code to predict quality and void fraction in different geometrical configurations has been carried out. Both steady-state and transient scenarios have been modeled by the code and compared with experimental data. Good agreement is seen between calculated and experimental results. More details of the work can be found in the reference [2]. Various correlations and model used in the START code are given in Table I.

Table I: Correlations and models used in START code

Parameter	Correlation
Two-phase friction multiplier	Armand Correlation
Grid spacer pressure drop	K. Rehme Model
Sub-cooled boiling	Lellouche
Void Fraction	Armand-Massena
HTC (Single phase/subcooled and saturated nucleate boiling)	Dittus-Boelter/ Dittus+Thom

2.3 HCMFD/START Coupled Analysis

As the START code is written in a modular form, the START code has been integrated into the HCMFD code as a T/H module. The main program and START module continuously interchange required data in each neutronics and T/H calculation and do feedbacks for a converged multi-physics solution. Detailed list of data interchanged is introduced in Table II.

Table II: Flow of data in coupled analysis

Data flow	List of data
HCMFD → START	Pin-by-pin linear power.
START → HCMFD	Coolant temperature, Coolant density, Fuel temperature.

To correctly transfer the data between HCMFD and the START code, coolant-centered sub-channel calculated quantities by the START code are converted to rod-centered quantities by taking appropriate weighted average.

Meanwhile, a module for fuel temperature analysis has been added. It performs a 1-D cylindrical fuel temperature analysis using the rod-centered coolant temperature and corresponding surface heat transfer coefficient. The effective fuel pin temperature is simply calculated by using a 30/70 weighted average of fuel centerline and fuel surface temperature [3]. The obtained pin-by-pin fuel temperature data is then transferred to HCMFD for the T/H feedback. The cross-section feedback is done by Eq. (1) with the cross-section derivatives prepared in advance.

$$\Sigma(T_f, T_c, D_c) = \Sigma^{ref} + \frac{\partial \Sigma}{\partial \sqrt{T_f}} \Delta \sqrt{T_f} + \frac{\partial \Sigma}{\partial T_c} \Delta T_c + \frac{\partial \Sigma}{\partial D_c} \Delta D_c + \frac{\partial^2 \Sigma}{\partial D_c^{\,2}} (\Delta D_c)^2 \quad (1)$$

The coupled analysis is initiated by the first HCMFD code with constant values for fuel temperature, coolant temperature and coolant density. After every START run, convergence is checked for coolant temperature and density, fuel temperature and linear power. Iterations continue until the convergence criteria is met. Flow chart for coupled calculations is shown in Fig. 2.

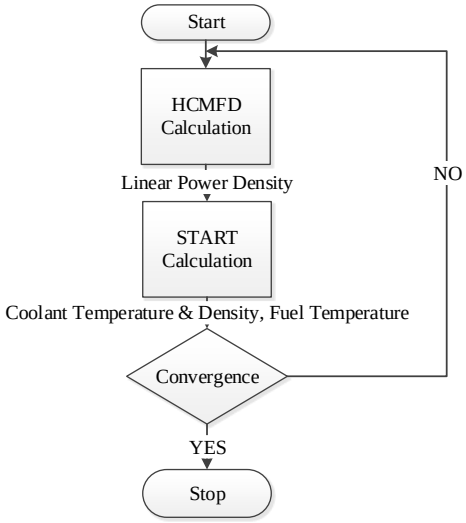

Fig. 2: Flow chart for coupled calculations

Unfortunately, we could not find any benchmark problem or numerical result for a combination of pin-wise diffusion analysis and sub-channel T/H analysis to verify the coupled calculation results since the pin-by-pin whole-core diffusion analysis is not so common. Instead, each part of the integrated code, the HCMFD part and the START code, has been verified individually.

2. Numerical Results

To assess the computational performance of coupled codes, an OPR-1000 core was analyzed [4]. The loading pattern is that of Cycle 1, and is shown in Fig. 3. Total of 177 fuel assemblies of 16 by 16 fuel pins are present in the core. Core has an active height of 3.81 m which is divided into 19 axial segments. Radial mesh is equal to fuel pin pitch.

For convergence criteria, it is observed that maximum linear power error shows slowest convergence. Especially the points near the bottom or top of reactor core, where the power density is small, show larger deviations in relative error. For a maximum linear power error of less than 1%, maximum deviation in coolant temperature & density and fuel temperature is already below 1%. So from all the nodes, maximum linear power error needs to be below 1% in order for coupled calculations to stop.

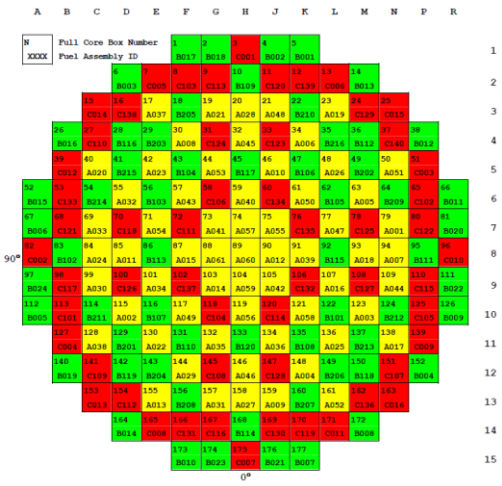

Fig. 3. Fuel loading pattern for Cycle 1

For speedy convergence and avoiding oscillations in the solutions, under relaxation factor (URF) is applied when thermal hydraulics parameters are transferred to HCMFD. Initially, a URF value of 0.5 is applied. Hence when transferring TH parameters to HCMFD, half of previous iteration value and half of current iteration value is used. This helps dampening the oscillations in power profile, as shown by previous studies [5]. Using the under relaxation factor also helps in obtaining convergence in less number of coupled iterations. The variation in linear power density (radial average value) for the 19 axial nodes during coupled process is shown in Fig. 4.

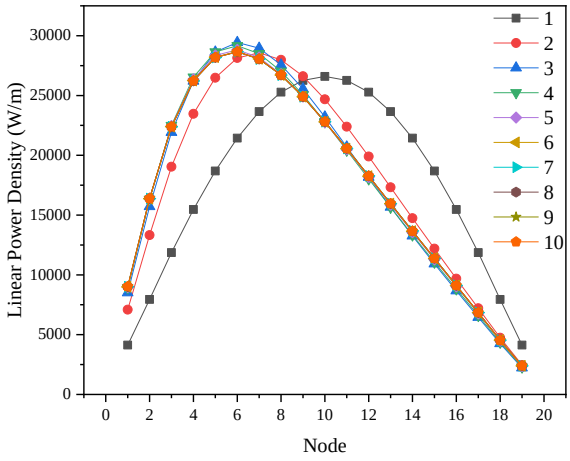

Fig. 4: Linear power density variation during iterations

It is seen that after fourth iteration, the values are quite close to each other showing convergence of solution is being approached. Fig. 4 also shows the effect of coupled studies on linear power density profile. It can be seen that 1st iteration profile is perfectly chopped cosine type, which we expect due to use of constant TH parameters, as compared to top skewed profile obtained after convergence of coupled solution.

Convergence behavior of various parameters with iteration number is shown in Fig. 5. For better presenting the behavior near the convergence, data plotted is from 5th iteration onward.

It is evident from Fig. 5 that maximum error of linear power density is the last one to achieve convergence criteria of 1% relative error. Coolant temperature and density are already showing values which are much less than 1% relative error at 5th iteration point. Although as per 1% convergence criteria, convergence is achieved at 7th iteration. To see the simulation behavior, it was carried on to 10 iterations.

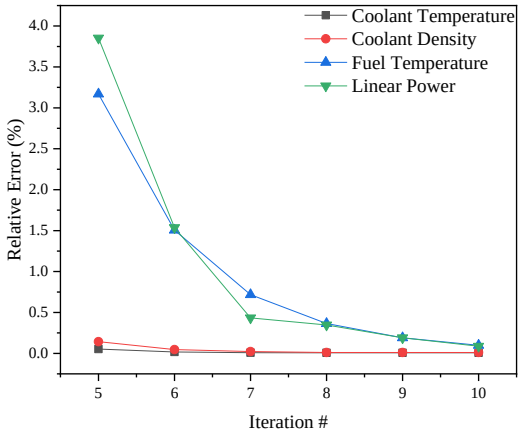

Fig. 5: Convergence behavior of various key parameters

Variation of reactivity with iteration # is shown in Fig. 6. It is seen that reactivity, shown in pcm, shows a value of 15 pcm at 7th iteration. This value continues to decrease with number of iterations. For 10th iteration, a reactivity difference of less than 2 pcm is obtained. The accumulated variation in k-eff is 1082.4pcm from the initial condition.

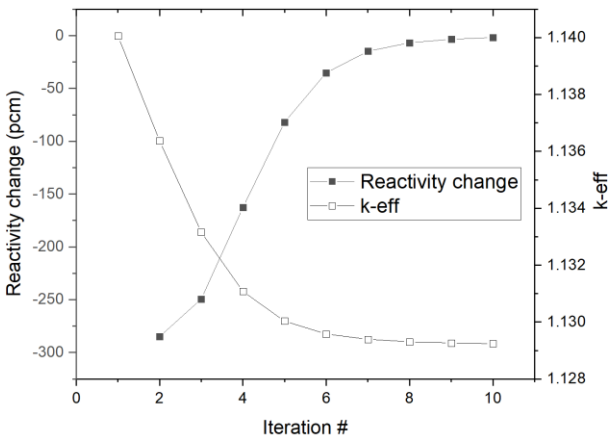

Fig. 6: Convergence behavior of reactivity

Radial power shape comparison for initial and converged solution is shown in Fig. 7. Looking at the scale of initial and converged solution, we see that power is now more evenly spread in the core rather than just peaking at the center and then falling off quickly for peripheral assemblies. Radial assembly peaking factor values of 1.46 and 1.26 are obtained for initial core and converged core respectively.

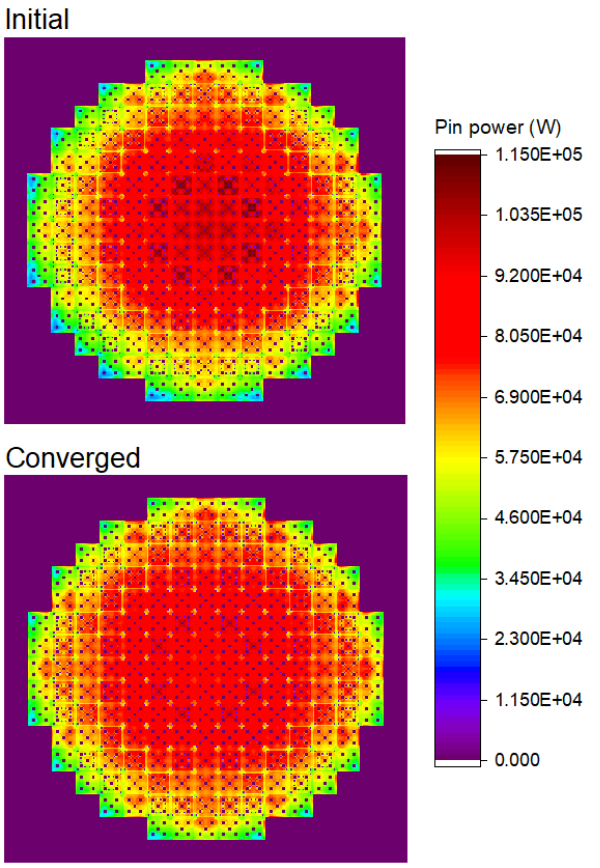

Fig. 7: Initial and converged radial power profile

Calculation time for the simulation are of particular interest as mentioned in the introduction section. Both the codes, HCMFD and the START code, have computational times less than a minute for whole core calculation. In order to further decrease the computational time, part of thermal hydraulic solution (flow rates and pressure drops) from previous iteration was used as an initial guess for current iteration. This caused a significant decrease in computational time once the solution started to reach near convergence.

Individual code timing in each iteration, reported in Table III, confirms this. The overall calculation time for coupled codes to produce a converged solution turn out to be less than 160 seconds for 7 coupled iterations. Calculation time for fuel temperature analysis module is negligible (approx. 1.0 sec for 10 iterations) showing very good parallel performance.

Table III: Computing time

Iteration #	**HCMFD CPU time (sec)**	**START CPU time (sec)**
1	11.89	15.57
2	14.27	13.44
3	12.71	11.45
4	8.50	10.68
5	9.97	10.36
6	9.11	10.24
7	7.02	10.20
Total	155.41	

4. Conclusions

Whole-core pin-by-pin coupled neutron physics/thermal hydraulics simulation for an OPR-1000 core has been carried out using in-house codes. Pin-by-pin neutron physics calculations are carried out using HCMFD algorithm while sub-channel thermal hydraulics solution is carried out using the START code. The simulations have shown that within a very reasonable time (~2.5 minutes), with a small commercial HPC system, pin-by-pin scale coupled simulations are possible. Coupled solution effect can be seen in radial power profile which is showing a radial power peaking value of 1.26 for converged core as compared to 1.46 for initial core. Clearly top-skewed axial power profile as compared to assumed chopped-cosine type one also shows need and importance of coupled calculations for design and safety analyses.

ACKNOWLEDGMENTS

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