Verification and Validation of the VANGARD GPU-based Pinwise Core Simulator Code

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1. Introduction

Recently, the pinwise two-step core calculation is getting increased interests as an alternative to the conventional assemblywise two-step calculation owing to its highly accurate pin-level solutions and tolerable computing time achieved by the remarkable advance in the computing power. VANGARD (Versatile Advanced Neutronics code for GPU-Accelerated Reactor Designs) is a pinwise nodal core analysis code characterized by GPU acceleration for the execution on PCs [1]. It employs 8-group pin-homogenized microscopic group constants which are generated from the lattice calculations by the direct whole core calculation code nTRACER [2]. In the nTRACER-VANGARD two-step core calculation system, the group constants are pre-tabulated as a function of fuel temperature, moderator temperature, moderator density, and boron concentration at various burnup steps and 32 nuclides including a lumped nuclide are considered.

The one-node Simplified P3 (SP3) source expansion nodal method (SENM) is employed as the main nodal kernel in VANGARD while the 4-mesh per assembly coarse mesh finite difference (CMFD) formulation is used as the overall framework. For the thermal-hydraulic feedback, a simple T/H solver based on the single-phase closed channel representing a quarter of an assembly is used. The pin-level microscopic depletion, critical boron concentration (CBC) search, and restart/shuffling capabilities are also available, which are necessary for multi-cycle calculations. The pinwise SPH factors are used to resolve the pin-homogenization issues.

In this work, the analysis capability, accuracy, and performance of VANGARD are verified through the cycle depletion calculations for the commercial PWRs, APR1400 and AP1000, and the BEAVRS multi-cycle benchmark problems.

2. Realistic Core Depletion Calculations

The comprehensive assessments of the simulation capability of VANGARD were performed by the comparison against the transport solutions obtained by nTRACER for the estimated CBCs and the power distributions during depletion. For the nTRACER calculations, a ray spacing of 0.04 cm was used, and 16 azimuthal and 4 polar angles were used in the octant of the solid angle sphere in both core transport calculation and lattice calculations. All the core calculations were performed with the quarter-core symmetry. The convergence criterion for the fission source change was set to 10^{-5}.

The performance of the GPU acceleration was also assessed by the comparison with multi-core CPU results. For the CPU calculation, an Intel I9-10900X processor which has 10 cores was employed. The parallelization was implemented with OpenMP. For the GPU calculation, a single NVDIA GeForce RTX 3090 was employed. Most parts of VANGARD were ported on GPU, but only the performance of the major calculations are discussed in this paper.

2.1. AP1000 Initial Core

As one of Generation III reactors, AP1000 core employs advanced core design concepts such as axially heterogeneous fuel loading. The heterogeneity of the core is severe in both radial and axial directions and it thus poses a challenge in modeling and simulation of the core behavior. In this regard, this complicated core was selected first for the verification of the simulation capability of VANGARD. The assemblies are grouped into 5 regions according to fuel enrichment which ranges widely from 0.74 wt% to 4.80 wt%. Region 4 and 5 where the high-enriched fuels are loaded contains two types of absorbers, WABA and IFBA. The WABA in the AP1000 core is inserted in three different depths. This causes a severe heterogeneity in the axial direction.

In the VANGARD model, the core is represented with 31 axial planes including the spacer grids and axial blankets. The core is depleted up to 18 MWD/kgHM, and 23 burnup points in total were simulated. **Figure 1** shows the comparison results for the boron letdown curves. **Figure 2** and **Figure 3** demonstrate the pin power and axial power error distributions, respectively, at the beginning of cycle (BOC), middle of cycle (MOC), and end of cycle (EOC). For both CBC and pin powers, VANGARD shows excellent agreements with nTRACER. The difference of the CBC is kept below 15 ppm throughout the whole burnup steps, and the pin power errors are steadily decreased so that the maximum and RMS pin power errors after MOC stay near 1.0% and less than 0.5%, respectively. The axial power distributions are also reasonable. The maximum error at the initial core occurs at the spacer grid located at the plane where the severe axial heterogeneity is apparent due to the different WABA lengths; near the top end of the intermediate WABA.

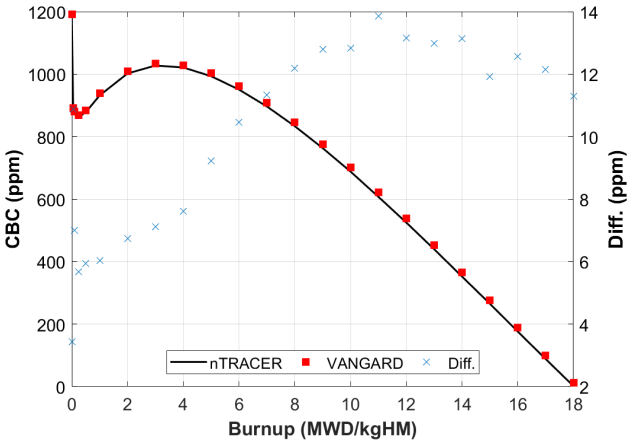

Figure 1. Comparison of boron letdown curves of AP1000 problem.

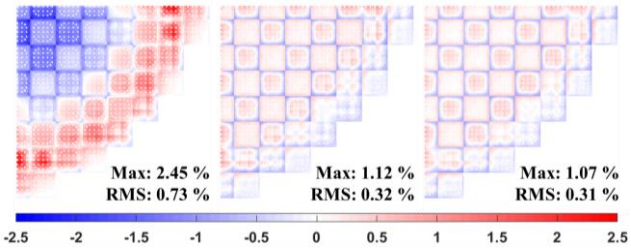

Figure 2. Pin power error (%) distributions at BOC (left), MOC (middle), and EOC (right) of AP1000 problem.

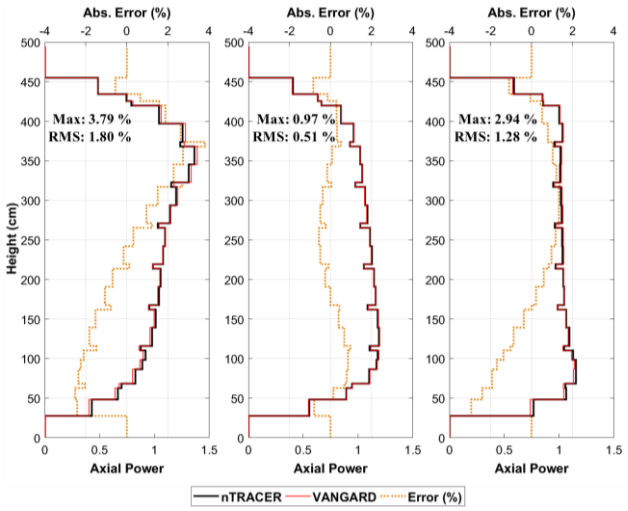

Figure 3. Axial power error (%) distributions at BOC (left), MOC (middle), and EOC (right) of AP1000 problem.

Table 1 summarizes the computing times and the speedup ratios of the GPU-accelerated parts. As the computing time share implies in **Figure 4**, most of the CPU calculation time is taken by the nodal calculation, cross section update, and depletion calculation. Owing to the substantial speedups in these computational hotspots, the total computing time is also notably reduced. Consequently, the cycle depletion calculation could be carried out within 3 minutes.

Table 1. Computing times and speedup ratios.

Calculation	CPU (s)	GPU (s)	Speedup
Nodal	1457.1	70.3	20.7
CMFD	42.5	6.8	6.3
XS	1518.1	47.9	31.7
Depletion	247.8	22.4	11.0
Total	3305.2	168.8	19.6

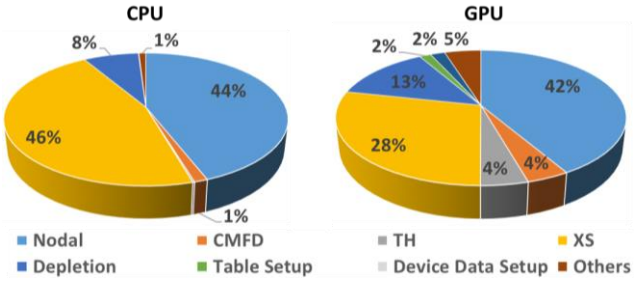

Figure 4. Computing time share comparison.

2.2. APR1400 Initial Core

One of the most significant issues revealed apparently in the pinwise two-step calculations is the inaccuracy of fuel depletion with Gadolinium (Gd). Due to the large spatial self-shielding effect of Gd, a gadolinia fuel presents extremely heterogeneous depletion behavior. However, this intra-pin heterogeneity cannot be simulated elaborately with the use of pin-homogenized group constants. In order to resolve the inaccuracy of gadolinia fuel depletion in the pinwise two-step calculations, we proposed the neighbor-informed burnup correction method and implemented it in VANGARD. This scheme makes a correction of burnups of gadolinia fuel pins using the information of neighbor fuel pins so that accurate cross sections can be used in the gadolinia fuel pins. The thorough analysis on this correction method is under preparation.

In order to verify the accuracy of Gd depletion in VANGARD with the burnup correction method, a cycle depletion calculation was performed for the APR1400 core which has high gadolinia loading. The core is depleted to 18 MWD/kgHM with 21 burnup points. **Figure 5** shows the comparison results of CBC, and **Figure 6** shows the maximum and RMS pin power errors with and without the correction at each burnup step. The pin power error distributions at BOC, MOC, and EOC are demonstrated in **Figure 7**.

With the burnup correction, the negative biases in CBC occurring during Gd depletion are quite well resolved, and the accuracy of the pin powers are significantly improved. Especially, the peculiar errors at the gadolinia fuel pins mostly disappeared with the burnup correction. Consequently, the global power tilt was noticeably reduced. As the result, the maximum and RMS pin power errors are kept below 1.5% and 0.5%,

respectively, throughout the whole burnup steps. As shown in **Figure** 8, the axial power behaviors are also close to the nTRACER while it clearly simulates the fluctuating axial power shapes induced by the non-uniform depletion of Gadolinium.

The computing time comparisons is summarized in **Table 2**. Significant speedups were achieved, especially, for the cross section update which takes the most parts of the total computing time with a speed up of ~40. Finally, the total calculation time was reduced from about 1 hour 15 minutes to less than 200 seconds.

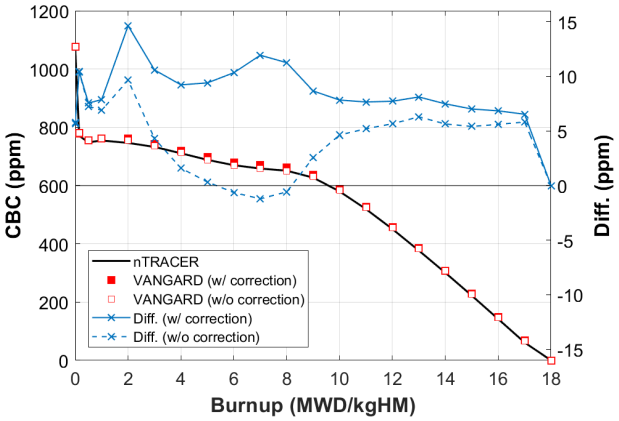

Figure 5. Comparison of boron letdown curves of APR1400 problem.

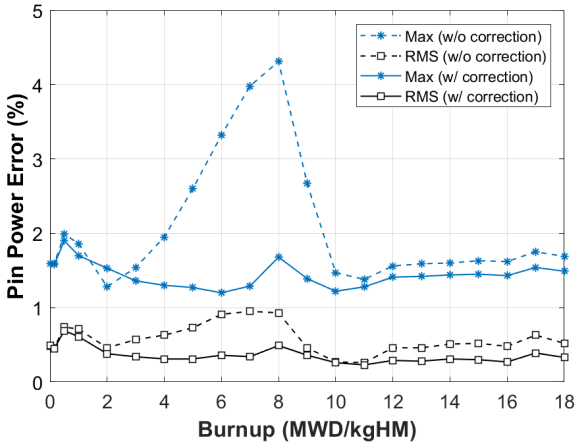

Figure 6. Comparison of pin power errors (%) between with and without correction.

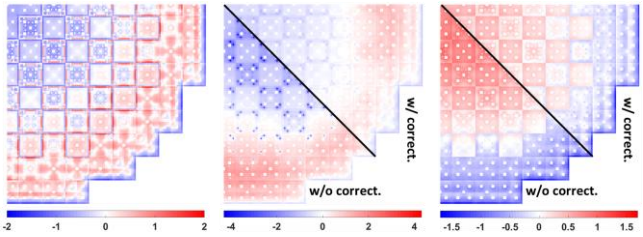

Figure 7. Pin power error (%) distributions at BOC (left), MOC (middle), and EOC (right) of APR1400 problem.

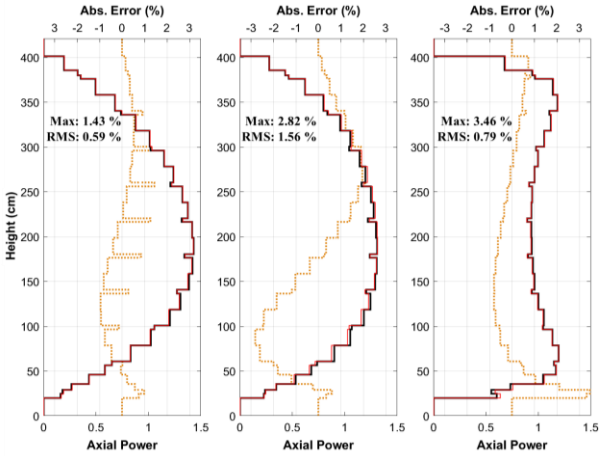

Figure 8. Axial power error (%) distributions at BOC (left), MOC (middle), and EOC (right) of APR1400 problem.

Table 2. Computing time comparisons of APR1400 problem.

Calculation	CPU (s)	GPU (s)	Speedup
Nodal	1586.9	72.4	21.9
CMFD	51.8	8.5	6.1
XS	2450.2	55.9	43.9
Depletion	348.5	31.2	11.2
Total	4488.3	196.6	22.8

2.3. BEAVRS Cycles 1 and 2

In order to verify the restart and loading pattern shuffling capabilities of VANGARD, BEAVRS Cycle 1 and Cycle 2 depletion calculations were performed under the constant power level of 100%. For the CBCs, as shown in **Figure 9**, the comparison with the measurements were made as well as the code-to-code comparison. For Cycle 1, both nTRACER and VANGARD solutions were estimated lower than the measurements with the maximum difference of 35 ppm, however, it is acceptable in that it does not exceed the design criterion of 50 ppm. On the other hand, the CBC differences between VANGARD and nTRACER are negligible in that the largest difference is 7 ppm. The excellent agreements between the two codes are verified in the pin power comparisons as well, as demonstrated in **Figure 10**.

In Cycle 2 depletion, the predicted boron letdown curves follow much closer to the measurements as opposed to Cycle 1. The maximum difference of VANGARD solutions from the measurements and nTRACER solutions is estimated only 19 and 14 ppm, respectively. The pin powers also match well with nTRACER. At all burnup steps except for the BOC, the maximum and RMS pin power errors are within 1.5 % and 0.5 %, respectively, which proves the soundness of the restart and reloading capability of VANGARD for the multi-cycle calculations. There are many factors to

cause the large pin power errors at the BOC for the reloaded core in two-step calculations because it is unlikely that each fuel pin will be depleted in the same condition with the lattice calculation. Therefore, further investigations to resolve the inaccuracy noted at the BOC of Cycle 2 are needed.

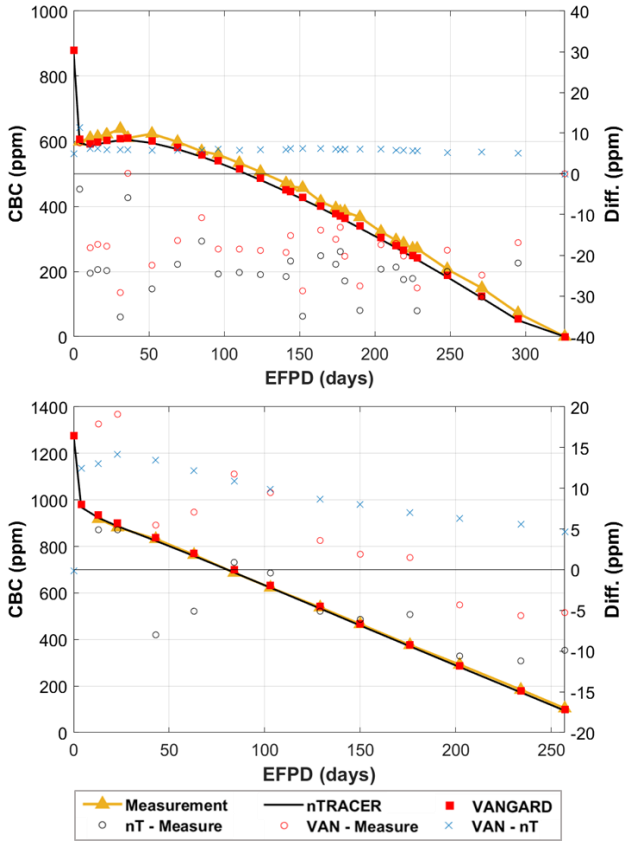

Figure 9. Comparison of Boron letdown curves of BEAVRS Cycle 1 (top) and Cycle 2 (bottom) problem.

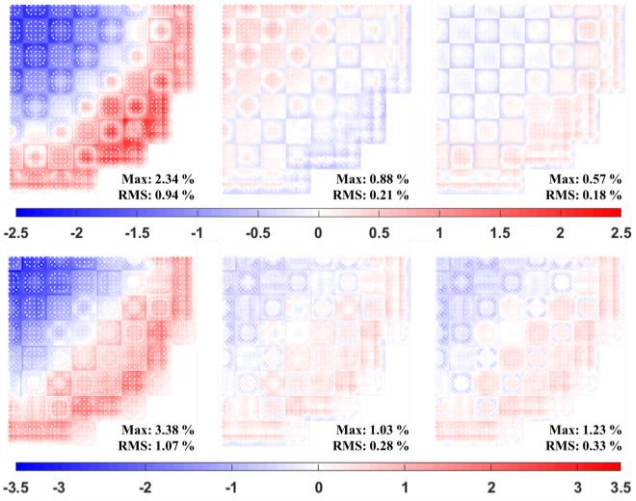

Figure 10. Pin power error distributions (%) at BOC (left), MOC (middle), and EOC (right) of BEAVRS Cycle 1 (top) and Cycle 2 (bottom) problem.

Table 3 represents the computing time comparisons for the BEAVRS Cycle 1 depletion calculation. The total computing time for simulating 30 burnup points was reduced from 1 hour 20 minutes to less than 4 minutes.

Table 3. Computing times and speedup ratios of BEAVRS Cycle 1 calculation.

Calculation	CPU (s)	GPU (s)	Speedup
Nodal	2157.5	84.3	25.6
CMFD	53.1	7.3	7.3
XS	2132.6	56.1	38.0
Depletion	339.6	30.2	11.3
Total	4740.0	205.3	23.1

4. Conclusions

The simulation capability and the performance of the GPU-accelerated pinwise nodal core analysis code VANGARD were comprehensively verified with the cycle depletion calculations for three different problems. The simulation capabilities and the solution accuracy of VANGARD were assessed by the comparison with the transport solutions obtained from nTRACER. Through the analysis of AP1000 core with severe radial and axial heterogeneity, the accuracy for a reactor with advanced core design was confirmed. Additionally, the neighbor-informed burnup correction method was presented for accurate prediction of Gadolinia fuel depletion, and the significant effects of correction were confirmed with the APR1400 depletion calculation. The restart/shuffling capabilities were also verified with the BEAVRS multi-cycle calculations. The substantial improvements in performance obtained with the GPU acceleration was proved by the comparison with the multi-core CPU calculation results. In all problems, the total computing time for the cycle depletion calculations does not exceed 4 minutes. It is sufficiently fast to perform repeated core calculations required for nuclear design on PCs, which makes the practical pinwise core design feasible.

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