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## 공학박사 학위논문

# Development of a GPU-based Practical Pinwise Nodal Core Analysis Code VANGARD for Nuclear Design Applications <br> 핵설계 적용을 위한 GPU 기반 실용적 봉단위 노달 노심 해석 코드 VANGARD 개발 

2023년 2월

> 서울대학교 대학원
> 에너지시스템공학부

전 서 윤

# Development of a GPU-based Practical Pinwise Nodal Core Analysis Code VANGARD for Nuclear Design Applications 

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| 위 원 장 | 김 응 수 | (인) |
| :--- | :--- | :--- |
| 부위원장 | 심 형 진 | (인) |
| 위 | 원 | 주 한 규 |
| (인) |  |  |
| 위 | 원 | 이 은 기 |
| (위 | (인) |  |
| 원 | 이 현 철 | (인) |

## Abstract

A GPU-based pinwise two-step nodal core calculation code named VANGARD (Versatile Advanced Neutronics code for GPU-Accelerated Reactor Designs) is developed. It is featured by the GPU acceleration employing a consumer-grade GPU which can be mounted on a personal computer to realize practical next-generation pinwise nuclear designs. This research presents the development of the essential capabilities for real nuclear designs and integration of them to constitute a fully capable core analysis system. It includes primary solvers such as nodal - CMFD coupled flux solver, thermal-hydraulic (T/H) solver, and depletion solver as well as the capabilities of restart/reloading for multi-cycle calculations, control rod movement during depletion, and load follow operation. The pinwise transient simulation capability is also developed.

The code employs the Source Expansion Nodal Method (SENM) to solve Simplified $\mathrm{P}_{3}\left(\mathrm{SP}_{3}\right)$ equations so that the severe intra-pin thermal flux gradients can be effectively captured with the use of hyperbolic functions while the 4-mesh per assembly coarse mesh finite difference (CMFD) formulation is used as the overall framework. For the T/H calculation, a simple T/H solver based on the single-phase closed channel representing a quarter of an assembly is used for practical applications. A massively parallelized depletion scheme based on the Chebyshev Rational Approximation Method (CRAM) is implemented. The GPU acceleration is applied to almost all of the calculation modules to render feasible simulation times enough to be utilized commercially.

Not limited to the implementation of calculation capabilities and application of GPU acceleration, this research resolves many issues and overcomes challenges revealed in performing the pinwise two-step nodal core calculations on GPU, which have not
been tackled or even known previously, and suggests resolutions for them with newly developed elaborate methods and schemes. To resolve too significant memory burden of the pinwise group constants to be ported on limited GPU device memory, the burnup window scheme is introduced, and the cross section compression technique employing the SVD and LRA are applied. The neighbor-informed burnup correction method is proposed as a practical means to resolve the severe inaccuracy in gadolinia fuel depletion which is apparently observed in pinwise two-step calculations. The numerical stability and significant computing time reduction are achieved by a new CMFD-based pinwise partial current update scheme.

The results of this research confirm the high accuracy and significant computing performance of VANGARD. For the verification, two commercial PWR cores of APR1400 and AP1000 and the BEAVRS multi-cycle benchmark problems were analyzed. For all target problems, VANGARD showed significantly high accuracy compared to nTRACER transport solutions. The CBC differences were within 15 ppm , and the maximum and RMS pin power errors were within $2.0 \%$ and $0.6 \%$, respectively, throughout the whole burnup steps. Meanwhile, substantial speedups were achieved by GPU acceleration in every calculation module. Finally, for all the target problems, a cycle depletion calculation that took more than an hour with 10 CPU cores could be completed within 3 minutes on a consumer-grade GPU. It is corresponding to that core calculation time spent per each state is less than 10 seconds. These comprehensive verification results ensure that VANGARD satisfies both accuracy and computing time requirements to be commercially utilized, which confirms the feasibility of practical pinwise core designs.

Through all of these works, VANGARD has become the first and the only GPUbased full-featured pinwise two-step nodal core calculation code that guarantees accurate pin-level solutions in a feasible simulation time. All of these achievements
presented the high potential of practical pinwise nuclear designs, and this research can serve as a good precedent for future developments of two-step pinwise core calculation systems which will become a trend in the worldwide reactor core design analysis institutes.

## Keywords: Pinwise Two-Step Calculation $\mathrm{SP}_{3}$ SENM GPU Acceleration VANGARD

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## Chapter 1. Introduction

The conventional assemblywise two-step core calculation has been the primary nuclear design method in industries owing to its significantly high computational efficiency. In terms of accuracy, it can meet the safety margin even though employing assembly-homogenized group constants cannot consider the intra-assembly heterogeneity so it inherently entails severe inaccuracy, because the conservative regulatory requirements were applied in the conventional reactor designs and safety analyses.

Recently, however, more precise and accurate core analysis is strongly required as safety regulations have been further tightened, the margin for safety analysis has become increasingly insufficient due to the deterioration of the aging nuclear power plant, and advanced reactors with severe heterogeneity have been actively developed. This requirement cannot be met with the conventional assemblywise two-step method which cannot provide accurate pin-level solutions, therefore, the fidelity of nuclear design tools needs to be enhanced.

As a means of high-fidelity reactor analysis, various direct whole core calculation (DWCC) codes have been actively developed by worldwide research groups which include DeCART of KAERI [1], nTRACER of Seoul National University (SNU) [2], and MPACT of Oak Ridge National Laboratory [3]. Furthermore, the feasibility of the direct whole core analysis method has been greatly improved by the remarkable advances in high-performance computing (HPC) technologies. However, it still relies on large parallel computers and is too expensive to be practically utilized for routine nuclear designs in the industries.

In this regard, the pinwise two-step method using pin-homogenized group constants is getting increased attention as a compromise that can serve as a bridge technology between the assemblywise two-step method developed decades ago and whole core transport solution method which will take decades to be industrially
utilized. The pinwise two-step method has a high potential to be a next-generation nuclear design method that can satisfy both accuracy and performance requirements. With the employment of pin-homogenized cross sections, intra-assembly heterogeneities can be explicitly considered, and it requires far less computational costs compared to DWCCs. Especially, it is more suitable for modern light water reactors (LWRs) and small modular reactors (SMRs) design and analysis in which a detailed pin-level solution is necessary as core designs are more and more complex and heterogeneous.

Based on this background, a new pinwise two-step nodal core calculation code named VANGARD ( $\underline{\text { Versatile }} \underline{\mathbf{A} d v a n c e d ~ \underline{N} \text { eutronics code for } \underline{\mathbf{G}} P U-\underline{A} c c e l e r a t e d ~}$ Reactor Designs) [4] was developed. It is featured by the GPU acceleration using a consumer-grade GPU to achieve practical simulation time even on personal computers (PCs) while retaining practicality. The NVIDIA CUDA [5] was chosen as the GPU development framework for high applicability and ease of coding. The pinwise group constants for VANGARD are generated from lattice calculations by the DWCC code nTRACER to constitute the nTRACER/VANGARD pinwise twostep code system.

In the following sections, previous researches on the pinwise two-step core calculations leading up to this research will be explained, and the purpose and scope of this research, which are specified to overcome the limitations of the previous researches and to resolve previously undiscovered problems, are detailed. Then, the outline of the research is given.

### 1.1 Previous Researches

Various pinwise nodal core calculation codes have been actively developed in both industries and academic institutes, and the feasibility and high accuracy of pinwise nodal core calculation have been continuously demonstrated. Since the early 2000s, Nuclear Fuel Industries (NFI) company in Japan has been utilizing the AEGIS/SCOPE2 code system [6]. In academic institutes, the DYN3D code of Helmholtz-Zentrum Dresden-Rossendorf (HZDR) in Germany [7], the NECPBamboo2.0 code system of Xi'an Jiaotong University (XJTU) in China [8], and the HCMFD code of KAIST in Korea [9] are being developed. All of these previous researches have demonstrated the high potential of pinwise two-step calculation code as an alternative tool for future nuclear designs.

At Seoul National University (SNU) as well, researches on the pinwise two-step core calculations have been conducted step-by-step. At first, Yoon [10] addressed the need for pinwise two-step calculation for practical nuclear design analyses, and based on this, he developed a new pinwise two-step core calculation code employing the 2-dimensional(2D)/1-dimensional(1D) coupled finite difference method (FDM) solver for diffusion equation to maximize computational efficiency. Following that, Cho developed the SPHINCS (Simplified $P_{3}$ Pin Homogenized Innovative Neutronics Core Simulator) code [11] which solves $\mathrm{SP}_{3}$ equations employing the FDM. According to the thorough and systematical analysis of the error sources in pinwise multi-group core calculations by Hong [12] following the above two previous researches, however, FDM is suffered from severe discretization errors and refined meshes are required. However, the fine mesh FDM leads to a significant computing burden, which weakens the original strength of FDM of high computational efficiency. In this regard, he finally suggested Source Expansion Nodal Method (SENM) solver employing $\mathrm{SP}_{3}$ theory as the most optimal solver for retaining both accuracy and practicality, which is in turn adopted as the primary
nodal kernel of VANGARD.
In spite of much cheaper computational costs of the pinwise two-step calculation compared to the DWCC, it is still computationally too demanding to be practically utilized for nuclear designs which involve hundreds of thousands of core calculations. This inherent limitation is relevant to all of the aforementioned pinwise two-step codes. To overcome the non-negligible computational burdens of pin-level calculation, almost all of the pinwise two-step calculation codes ever developed exploit massive CPU parallelism employing OpenMP or Message Passing Interface (MPI). However, the performance enhancement of CPUs is stagnant due to the power and memory barriers. Namely, satisfying the computing time requirement with CPUbased pinwise calculations, especially with nodal solver, to substitute the legacy conventional two-step methods is challenging.

In this regard, the application of GPU acceleration to the pinwise nodal core calculation was devised. GPUs can be a desirable computing resource to substitute multi-core CPU parallelism in that they contain a substantial number of simple arithmetic cores which can deliver significant floating point computing power enabling massive parallelism. The fact that the performance is still being improved exponentially is another undeniable advantage of the employment of GPUs. In fact, there has been an earlier work on applying GPU acceleration to pinwise core calculations in the SCOPE2 code [13] in 2011. Yet, it had limited scope and verification results, and no further work has been performed, supposedly due to the difficulties in porting a large CPU-based legacy code that has been developed for a long time and the limited capabilities and capacity of GPU hardware at that time. For the decade, however, the performance and memory have been continuously and drastically developed, and SNU has cleverly exploited these advanced modern GPUs for practical high-fidelity nuclear analyses and succeeded in application to two codes: the direct whole core calculation code nTRACER [14] and continuous energy Monte Carlo Code PRAGMA [15].

Motivated by these previous successful experiences, VANGARD adopts GPU as the main computing resource. Owing to the increased memory capacity compared to when the GPU acceleration to SCOPE2 was conducted, most parts of VANGARD were ported to GPU. Furthermore, it has been developed with careful considerations of the advantages and limitations of GPU from the very beginning of the development. Therefore, all the algorithms are elaborately optimized to be efficiently executed on GPUs. All these things will allow substantial feasibility and practicality to be achieved which none of the pinwise two-step core calculation codes ever developed could have completely achieved.

### 1.2 Objectives and Scope of the Research

This research aims to develop a fast yet accurate GPU-based pinwise two-step nodal core calculation code for practical applications in nuclear designs and analyses. To accomplish it, the following objectives are achieved in this research.

The first objective is to develop the essential capabilities required for real nuclear designs and integrate them to constitute a fully capable core analysis system. In addition to the neutronics solver employing nodal - CMFD coupled calculation, various capabilities for practical applications are developed as follows:

1) Inline $T / H$ feedback module with the simplified model
2) Pinwise microscopic depletion and B-10 depletion
3) Critical Boron Concentration (CBC) search
4) Xenon equilibrium and transient feedback
5) Restart/Reloading for multi-cycle calculations
6) Control rod movements and load follow operation

The transient calculation capability was also developed to make VANGARD a practical pinwise core design code, for which time-dependent nodal - CMFD solver
and $\mathrm{T} / \mathrm{H}$ solver were additionally developed.
The second objective is to apply GPU acceleration to the calculation modules and attain sufficiently high computational efficiency so that it can be practically utilized in industries. VANGARD was developed to be executed on both CPU and GPU platforms, and the CPU calculation module was also optimized, but in this thesis the optimization requirements for GPU calculation are mainly dealt with in detail since VANGARD is featured by uncommonly fast execution with the use of GPUs. The requirements for exploiting GPU performance are as follows, and all the GPU acceleration modules were implemented to meet the requirements as far as possible.

1) Vectorization:

GPU is specialized at SIMD (Single Instruction Multiple Data) parallelism, therefore, branches should be minimized.
2) Memory Coalescing:

A group of threads should read and write contiguous memory.
3) Local Memory Use:

Access to the main memory should be minimized and frequently used data should be saved in high-bandwidth memories such as cache and register.

Besides the implementation of essential calculation capabilities and GPU acceleration for them to achieve substantial computational efficiency, the novelty of this research comes from that it is also dedicated to resolving severe issues which are newly confronted by shifting the nuclear design method from the legacy assemblywise calculation to pinwise calculation and by introducing the GPU acceleration which is limited by insufficient memory. None of the previous researches on the pinwise two-step method has addressed these issues and suggested the proper resolutions. Thus, this work can serve as a pioneer of GPU-based pinwise two-step calculation method.

The final objective is to confirm the high accuracy and significant computing performance of VANGARD. Since it targets to be applied to real core designs, the
target problems for the comprehensive assessments of VANGARD steady-state calculation capabilities are a series of real cores - APR1400 initial core, AP1000 initial core, and BEAVRS Cycle 1 and 2 cores. - For the verification of the transient calculation modules, NEACRP rod ejection benchmark problems are analyzed. Basically, the accuracy of VANGARD solutions is assessed by comparison with the transport solutions of nTRACER, and if available, measurements and the Monte Carlo solutions of PRAGMA are also used as the references.

### 1.3 Outline of the Thesis

In Chapter 2, the nTRACER/VANGARD two-step code system is introduced including the group constant generation procedure. In Chapter 3, all the details of the full implementation for steady-state calculation capabilities are spelled out. The detailed rationale for the selection of nodal kernel, which is the one-node $\mathrm{SP}_{3}$ SENM kernel, and derivation of it are presented. The coarse mesh finite difference (CMFD) acceleration to enhance the fission source convergence is also treated. Following the neutronics solvers for flux update, all the auxiliary capabilities which are necessary for core design listed in the previous section are detailed. The transient calculation capabilities are addressed in Chapter 4. For computational efficiency and ease of implementation, most of the modules which were pre-established for steady-state calculation are shared with transient calculation as far as possible. This section will specifically describe additionally developed solutions for transient calculation, focusing on the time-dependent nodal - CMFD coupled solver and time-dependent T/H solver. Chapter 5 presents all the details of the GPU acceleration strategies including numerous elaborated computational methods for cleverly utilizing the GPU computing technologies. Chapter 6 covers the challenges of pinwise two-step core calculations and suggests the resolutions for them. Specifically, resolutions of
numerical instability and inaccuracy and resolutions of memory burden are proposed. Chapter 7 presents comprehensive assessments of the simulation capabilities and solution accuracy of VANGARD. In Chapter 8, the effectiveness of the GPU accelerations is demonstrated with noticeable speedups over 10-core CPU calculations for all problems. Chapter 9 concludes the thesis with remarks on the value of this research.

## Chapter 2. nTRACER/VANGARD Two-Step Code System

This chapter will introduce the details of nTRACER/VANGARD two-step code system. The procedure of generating pinwise multi-group constants as well as the SPH factors are spelled out in Section 2.1. The lists of the nuclides considered in the VANGARD code are explained in Section 2.2. The characteristics and the advantages of the hierarchical data format for group constant storage are addressed in Section 2.3.

### 2.1 Group Constant Generation

The pinwise group constants for VANGARD calculations are generated by the nTRACER single assembly depletion calculations. As is done in the conventional two-step calculations, branch calculations are performed at various burnups for each assembly to generate the group constant table as a function of fuel temperature, moderator temperature, moderator density, and boron concentration. Note that for generating group constants of reflector assemblies which do not contain fissile materials, fuel-reflector local problems are solved as described in Figure 2.1, and reflector group constants do not have a dependency on burnup.


Figure 2.1 Fuel-reflector local configurations.

After generating a group constant file for a single assembly through nTRACER calculations, the pinwise and groupwise SuperHomogenization (SPH) factors for
alleviating the homogenization errors are also generated from the combined nTRACER/VANGARD lattice calculations for each assembly. Given the reference pinwise flux information and pin-homogenized cross sections provided by the nTRACER lattice calculations, VANGARD runs iterations to determine the SPH factors for all the burnup points and branch points. This procedure is done only once for each assembly type, and the SPH factors are stored in the pre-generated group constant file.

### 2.2 List of Nuclides in VANGARD

VANGARD group constant considers 32 nuclides, whose list is shown in Table 2.1. There are a few nuclides specially treated in the VANGARD cross section system that require explanations. First of all, the B-10 nuclide is separately defined depending on whether it is used as soluble boron (5000) or burnable absorber (5010) as they require separate treatments in T/H feedback, critical boron search, and depletion calculations. The lumped nuclides are imaginary nuclides that represent more than one elementary nuclide. Three lumped nuclides are for specific materials, and the remaining one (0) incorporates all the other auxiliary nuclides of nTRACER that are not explicitly considered in VANGARD.

Table 2.1 List of the nuclides considered in the VANGARD group constant.

| Type | ZID |
| :---: | :---: |
| Boron | $5000(\mathrm{~B}-10$ in soluble boron), |
|  | $5010(\mathrm{~B}-10$ in burnable poison) |
|  | $93135,54135,60147,61147,61148,61149,62149$ |
| Actinide | $92234,92235,92236,92237,92238$ |
|  | $93237,93238,93239$ |
|  | $94238,94239,94240,94241,94242$ |
| $95241,95242,95243$ |  |
|  | $96242,96243,96244$ |
| Lumped | 0 (Other), 1000 (Moderator), 40000 (Zirconium), |
|  | 64000 (Gadolinium) |

The lumped nuclide for moderator (1000) represents the $\mathrm{H}_{2} \mathrm{O}$ molecule. It is defined to separately treat the scattering matrix of the moderator. In the VANGARD group constant, scattering matrices of every nuclide but $\mathrm{H}_{2} \mathrm{O}$ are merged and stored as a single macroscopic scattering matrix in order to reduce memory usage and enhance computational efficiency. It is valid because the energy migration of neutrons through scattering in LWRs is dominated by the light nuclides in the moderator, especially hydrogen. Namely, it is a waste to store all the microscopic scattering matrices of heavy nuclides to accurately calculate their scattering matrices that are insignificant.

The lumped nuclide for zirconium (40000) incorporates all the zirconium isotopes. It is defined to simulate the removal of burnable poison rods during reloading. In many commercial PWRs, removable burnable poison rods such as Pyrex or WABA are inserted for excess reactivity control which have the lifetime of a single cycle and are removed in the subsequent cycle. However, the group constants for an assembly are generated for the lifetime of the assembly which usually spans three cycles, and it is difficult to consider the extraction of burnable poison rods in the group constants in advance. In VANGARD, therefore, the removal of burnable poison rods is modeled by forcing the number density of the lumped nuclide as well as 5010 to zero during reloading, which is equivalent to removing all the poison and structural materials contained in the burnable poison rods. In order to prevent the guide tube material from being removed together as lumped nuclide, therefore, zirconium is separately treated.

Finally, the lumped nuclide for gadolinium (64000) incorporates all the gadolinium isotopes. A gadolinia fuel presents highly heterogeneous depletion behaviors that cannot be accurately modeled in the pinwise two-step calculations due to spatial homogenization. As the result, a special treatment for gadolinia fuels is introduced in VANGARD in which the gadolinium isotopes are treated as a single fictitious nuclide that is not depleted, which will be elaborated in Section 6.1.2.

### 2.3 Hierarchical Data Format for Group Constants

The VANGARD group constants are stored in the Hierarchical Data Format (HDF) [16] in single precision, although they are cast into double precision in calculations for accuracy. Pinwise group constants are significantly larger in size than the conventional assemblywise group constants, so efficient storing and parsing are important. The HDF format is basically a binary format, so it has a smaller size and much faster parsing speed than the ASCII format. In addition, the HDF format has a hierarchical structure that resembles a file system and allows random access to a specific data, whereas the ASCII format or the ordinary binary format needs to be processed sequentially. Furthermore, the HDF format is readable via external programs unlike the ordinary binary format, which makes troubleshooting easier for programmers and users. Thus, the HDF format is appropriate for dealing with large, hierarchical, and jagged data including the pinwise group constants. Figure 2.2 illustrates the layout of a group constant file of VANGARD visualized by an HDF viewer program.


Figure 2.2 Layout of a group constant file.

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## Chapter 3. Steady-State Calculation Capability

This chapter introduces the full implementation details of the steady-state calculation capabilities of VANGARD. Section 3.1 covers the flux solvers which are most primary in the code. VANGARD employs the one-node simplified $\mathrm{P}_{3}\left(\mathrm{SP}_{3}\right)$ source expansion nodal method (SENM) as the main nodal kernel while the 4-mesh per assembly coarse mesh finite difference (CMFD) formulation is used as the overall framework. This section presents the pinwise nodal solution method including the selection of the nodal kernel and the CMFD acceleration scheme. Section 3.2 introduces the feedback algorithm. In this section, the solution scheme of a lightweight, inline thermal-hydraulic solver for practical applications is explained, which comprises the solution of the heat convection equation for the coolant channel and the heat conduction equation for the fuel pellet. In addition, this section also explains the xenon transient/equilibrium feedback algorithm. In Section 3.3, the depletion algorithm is described. VANGARD employs pinwise microscopic depletion scheme using a depletion chain consisting of 44 nuclides which is extracted from nTRACER such that only important nuclides are explicitly traced and the others are treated macroscopically as a lumped nuclide. This section explains the burnup system solutions for the Bateman equation as well as the B-10 depletion scheme for considering the soluble boron depletion. Section 3.4 presents the overall flowchart of the steady-state calculation for a cycle depletion.

### 3.1 Flux Solvers

This section presents the rationale for determining the one-node $\mathrm{SP}_{3}$ SENM kernel as the optimal pinwise nodal kernel, followed by the derivation of it. In addition, the coarse mesh finite difference method for accelerating the fission source distribution convergence is presented. All these elements constitute the efficient and accurate neutronics solver of VANGARD.

### 3.1.1 Selection of the Pinwise Nodal Kernel

The SENM [17] is employed to solve the $\mathrm{SP}_{3}$ equation in VANGARD in that it can capture severe flux gradients more accurately than other nodal methods owing to the use of hyperbolic functions as well as polynomials for flux expansion. Because the intra-assembly heterogeneities are explicitly considered in the pinwise calculations and the intra-pin flux shapes change severely in low energy groups, the SENM is suitable for the accurate representation of the flux shapes even in pinwise calculations.

VANGARD is based on the $\mathrm{SP}_{3}$ transport approximation in that it is superior in capturing the transport effects to the diffusion approximation by accounting for higher order of the angular flux expansion. Therefore, the $\mathrm{SP}_{3}$ calculation can produce more accurate solutions than the diffusion calculation especially in problems where spatial flux variation is severe, which is challenging for the diffusion approximation.

The superiority of the SENM to the NEM and of the $\mathrm{SP}_{3}$ to the diffusion were confirmed through the actual core calculations. The BEVRS [18] benchmark cores with ARO and with the control rod bank $\mathrm{D}, \mathrm{C}, \mathrm{B}$, and A in under the HZP condition were simulated, and the pin power distributions were compared with the nTRACER transport solutions. Note that for all calculations, the pinwise and groupwise SPH
factors are employed. As shown in Figure 3.1 and Table 3.1, the SENM solution shows definitely better accuracy than the NEM solution. Especially, in the rodded case where the flux gradients are severe, the NEM solver cannot catch the flux variation accurately to have the maximum and RMS pin power error of $7.1 \%$ and $2.6 \%$, respectively, while those in the SENM calculation are only $2.6 \%$ and $0.8 \%$. The accuracy superiority of the $\mathrm{SP}_{3}$ solution over the diffusion solution is also clearly confirmed, as presented in Figure 3.2 and Table 3.2. For both unrodded and rodded cases, the $\mathrm{SP}_{3}$ solutions show better accuracy than the diffusion solutions.

The one-node kernel was chosen to avoid the use of a pinwise $\mathrm{SP}_{3}$ CMFD solver. Although the two-node kernel has better convergence characteristics by reflecting the relations between the interface current and the two node average fluxes simultaneously, it is not favorable in the pinwise $\mathrm{SP}_{3}$ core calculations since it relies on the CMFD updates of the pinwise node average values of the second angular flux moment which can cause numerical instability due to its potential negativity. Furthermore, pinwise $\mathrm{SP}_{3}$ CMFD is computationally expensive. In this regard, the pin-level one-node $\mathrm{SP}_{3}$ SENM kernel is finally chosen as the optimal nodal solution employed within the assembly-level diffusion CMFD formulation with 4 meshes per assembly.


Figure 3.1 Pin power error (\%) distribution comparison between NEM and SENM calculations.

Table 3.1 Comparison of maximum and RMS pin power errors between NEM and SENM calculations.

| Case | Pin power error <br> $(\%)$ | NEM | SENM |
| :---: | :---: | :---: | :---: |
| ARO | Max | 3.9 | 1.4 |
|  | RMS | 2.0 | 0.6 |
| D, C, B, A in | Max | 7.1 | 2.6 |
|  | RMS | 2.6 | 0.8 |



Figure 3.2 Pin power error (\%) distribution comparison between diffusion and $\mathrm{SP}_{3}$ calculations.

Table 3.2 Comparison of maximum and RMS pin power errors between diffusion and $\mathrm{SP}_{3}$ calculations.

| Case | Pin power error <br> $(\%)$ | Diffusion | $\mathrm{SP}_{3}$ |
| :---: | :---: | :---: | :---: |
| ARO | Max | 6.7 | 1.4 |
|  | RMS | 3.1 | 0.6 |
| $\mathrm{D}, \mathrm{C}, \mathrm{B}, \mathrm{A}$ in | Max | 10.3 | 2.6 |
|  | RMS | 4.7 | 0.8 |

### 3.1.2 Derivation of the One-node $\mathrm{SP}_{3}$ SENM Kernel

The derivation of the one-node SENM kernel starts from the transverse-integrated one-dimensional within-group neutron diffusion equation in the following:

$$
\begin{equation*}
-\frac{4 D}{h_{u}^{2}} \frac{d^{2}}{d \xi_{u}^{2}} \phi\left(\xi_{u}\right)+\Sigma_{r} \phi\left(\xi_{u}\right)=Q\left(\xi_{u}\right) \tag{3.1}
\end{equation*}
$$

where $h_{u}$ denotes the node size in the $u$-direction and $\xi_{u}$ represents the coordinate variable normalized in the range of $[-1,1]$ such that the origin of the coordinate is located at the center of the node; namely

$$
\begin{equation*}
\xi_{u}=\frac{2 u}{h_{u}} \tag{3.2}
\end{equation*}
$$

For brevity, the subscript for the direction will be omitted in the following. In the $4^{\text {th }}$ order SENM, the source term $Q$ determined as the sum of the fission, scattering, and transverse leakage sources is expanded up to $4^{\text {th }}$ order using the Legendre polynomials as:

$$
\begin{equation*}
Q(\xi)=\frac{\chi}{k_{e f f}} \psi(\xi)+S(\xi)-L(\xi) \cong \sum_{i=0}^{4} q_{i} P_{i}(\xi) . \tag{3.3}
\end{equation*}
$$

Note that the transverse leakage is approximated as a quadratic function using the node-average leakages of three adjacent nodes, which is the conventional way. By inserting Eq. (3.3) into Eq. (3.1) and solving for the flux, the analytic solution for the flux can be obtained as follows:

$$
\begin{align*}
\phi(\xi) & =\phi_{H}(\xi)+\phi_{P}(\xi) \\
& =A \sinh (\kappa \xi)+B \cosh (\kappa \xi)+\sum_{i=0}^{4} c_{i} P_{i}(\xi) \tag{3.4}
\end{align*}
$$

where the subscripts $H$ and $P$ denote the homogeneous solutions with hyperbolic functions and particular solutions with $4^{\text {th }}$ order polynomials, respectively, and

$$
\begin{gather*}
\kappa=\frac{h}{2} \sqrt{\frac{\Sigma_{r}}{D}},  \tag{3.5}\\
c_{1}=\frac{1}{\Sigma_{r}}\left(q_{1}+\frac{15}{\kappa^{2}} q_{3}\right), c_{2}=\frac{1}{\Sigma_{r}}\left(q_{2}+\frac{35}{\kappa^{2}} q_{4}\right), c_{3}=\frac{q_{3}}{\Sigma_{r}}, c_{4}=\frac{q_{4}}{\Sigma_{r}} .
\end{gather*}
$$

The flux in Eq. (3.4) is also expanded by approximating the homogeneous solutions using the Legendre polynomials, which yields the following expression for the flux:

$$
\begin{equation*}
\phi(\xi)=\bar{\phi}+\sum_{i=1}^{4} a_{i} P_{i}(\xi) . \tag{3.6}
\end{equation*}
$$

From the orthogonality of the Legendre polynomials, the flux expansion coefficients are obtained as follows:

$$
\begin{align*}
& a_{1}=c_{1}+\frac{3}{\kappa}\left(\cosh (\kappa)-\frac{\sinh (\kappa)}{\kappa}\right) A, \\
& a_{2}=c_{2}-5\left(\frac{3 \cosh (\kappa)}{\kappa^{2}}-\left(1+\frac{3}{\kappa^{2}}\right) \frac{\sinh (\kappa)}{\kappa}\right) B, \\
& a_{3}=c_{3}+\frac{7}{\kappa}\left(\left(1+\frac{15}{\kappa^{2}}\right) \cosh (\kappa)-\left(6+\frac{15}{\kappa^{2}}\right) \frac{\sinh (\kappa)}{\kappa}\right) A,  \tag{3.7}\\
& a_{4}=c_{4}-9\left(\frac{5}{\kappa^{2}}\left(2+\frac{21}{\kappa^{2}}\right) \cosh (\kappa)-\left(1+\frac{45}{\kappa^{2}}+\frac{105}{\kappa^{4}}\right) \frac{\sinh (\kappa)}{\kappa}\right) B .
\end{align*}
$$

By imposing the partial incoming currents as the boundary conditions at the two surfaces of the node, the coefficients $A$ and $B$ of the homogeneous solution are determined as:

$$
\begin{align*}
& A=\frac{\left(J^{r-}-J^{l-}\right) / 2-(\mu+\beta) c_{1}-(\mu+6 \beta) c_{3}}{\beta \kappa \cosh (\kappa)+\mu \sinh (\kappa)},  \tag{3.8}\\
& B=\frac{-\mu \bar{\phi}+\left(J^{r-}+J^{l-}\right) / 2-(\mu+3 \beta) c_{2}-(\mu+10 \beta) c_{4}}{\beta \kappa \sinh (\kappa)+\mu(\cosh (\kappa)-\sinh (\kappa) / \kappa)}
\end{align*}
$$

where $J^{l-}$ and $J^{r-}$ represent the incoming currents at the left and right surfaces of
the node, respectively, and $\mu$ is the surface even moment fraction which is differently determined for the summed flux and the $2^{\text {nd }}$ flux moment in the $\mathrm{SP}_{3}$ SENM equations. Once the homogeneous solution is determined, the net current can be obtained by taking the derivative of the node average flux as follows:

$$
\begin{align*}
J(\xi) & =-\frac{2 D}{h} \frac{d \phi(\xi)}{d \xi} \\
& =-2 \beta \kappa(A \cosh (\kappa \xi)+B \sinh (\kappa \xi))-2 \beta \sum_{i=1}^{4} c_{i} P_{i}^{\prime}(\xi) \tag{3.9}
\end{align*}
$$

Substitution of the net current to the nodal balance equation yields the final solution for the node average flux as:

$$
\begin{equation*}
\bar{\phi}=\frac{\bar{s}+\sum_{u=x, y, z}\left(\Sigma_{D}^{u}\left(\frac{1}{2} \tau^{u}\left(J_{u}^{l-}+J_{u}^{r-}\right)+\left(3-\tau^{u}\left(\mu+3 \beta^{u}\right)\right) c_{2}^{u}+\left(10-\tau^{u}\left(\mu+10 \beta^{u}\right)\right) c_{4}^{u}\right)\right)}{\Sigma_{r}+\sum_{u=x, y, z} \Sigma_{D}^{u} \mu \tau^{u}} \tag{3.10}
\end{equation*}
$$

where

$$
\begin{equation*}
\tau=\frac{\kappa \sinh (\kappa)}{\beta \kappa \sinh (\kappa)+\mu\left(\cosh (\kappa)-\frac{\sinh (\kappa)}{\kappa}\right)} \tag{3.11}
\end{equation*}
$$

Using the updated node average flux, the outgoing currents can be obtained as follows:

$$
\begin{align*}
& J^{r+}=\mu \phi(1)+\frac{1}{2} J(1)=\alpha^{s} A+\alpha^{c} B+\mu\left(\bar{\phi}+\tilde{\phi}^{P}(1)\right)+\frac{1}{2} \tilde{J}^{P}(1), \\
& J^{l+}=\mu \phi(-1)-\frac{1}{2} J(-1)=-\alpha^{s} A+\alpha^{c} B+\mu\left(\bar{\phi}+\tilde{\phi}^{P}(-1)\right)-\frac{1}{2} \tilde{J}^{P}(-1) \tag{3.12}
\end{align*}
$$

where

$$
\begin{align*}
& \alpha_{s}=-\beta \kappa \cosh (\kappa)+\mu \sinh (\kappa), \\
& \alpha_{c}=-\beta \kappa \sinh (\kappa)+\mu\left(\cosh (\kappa)-\frac{\sinh (\kappa)}{\kappa}\right), \\
& \tilde{\phi}^{P}(\xi)=\sum_{i=1}^{4} c_{i} P_{i}(\xi),  \tag{3.13}\\
& \tilde{J}^{P}(\xi)=-\frac{2 D}{h} \frac{d \tilde{\phi}^{P}(\xi)}{d \xi}=-2 \beta \sum_{i=1}^{4} c_{i} P^{\prime}(\xi) .
\end{align*}
$$

The $\mathrm{SP}_{3}$ formulation for SENM [19] is derived in the analogous manner to the diffusion formulation starting from the following transverse integrated $\mathrm{SP}_{3}$ equations:

$$
\begin{align*}
& -\frac{4 D_{0}}{h^{2}} \frac{d^{2}}{d \xi^{2}} \hat{\phi}_{0}+\Sigma_{r 0, g} \hat{\phi}_{0}=Q_{0},  \tag{3.14}\\
& -\frac{4 D_{2}}{h^{2}} \frac{d^{2}}{d \xi^{2}} \phi_{2}+\Sigma_{r 2, g} \phi_{2}=Q_{2}
\end{align*}
$$

where

$$
\begin{align*}
& \hat{\phi}_{0}=\phi_{0}+2 \phi_{2}, \\
& D_{0}=\frac{1}{3 \Sigma_{t r}}, \quad D_{2}=\frac{3}{7 \Sigma_{t}},  \tag{3.15}\\
& \Sigma_{r 0}=\Sigma_{r}, \quad \Sigma_{r 2}=\frac{4}{3} \Sigma_{r}+\frac{5}{3} \Sigma_{t} .
\end{align*}
$$

The source terms in Eq. (3.14) are also separately defined for the summed flux $\left(\hat{\phi}_{0}\right)$ and $2^{\text {nd }}$ flux moment ( $\phi_{2}$ ) equations using the node average source ( $\bar{s}$ ) induced from the $0^{\text {th }}$ flux moment, namely the node average flux, as:

$$
\begin{align*}
& Q_{0}=\bar{s}+2 \Sigma_{r}-L_{0}, \\
& Q_{2}=-\frac{2}{3} \bar{s}+\frac{2}{3} \Sigma_{r} \phi_{0}-L_{2} \tag{3.16}
\end{align*}
$$

where

$$
\begin{equation*}
\bar{s}=\frac{\chi}{k_{e f f}} \sum_{g^{\prime}} \nu \Sigma_{f} \phi_{0}+\sum_{g^{\prime}} \Sigma_{s} \phi_{0} . \tag{3.17}
\end{equation*}
$$

The $\mathrm{SP}_{3}$ SENM equations are solved for the summed flux and the $2^{\text {nd }}$ flux moment with differently defined coefficients: diffusion coefficients, removal cross sections, and surface even moment fraction $\mu$. The value of $\mu$ is set to $1 / 4$ and $7 / 16$ for the summed flux and the $2^{\text {nd }}$ flux moment equations, respectively.

Note that the equations for the summed flux and the $2^{\text {nd }}$ flux moment are written in the same form. Only the specific data - diffusion coefficients, removal cross sections, and source terms - are different. Namely, the solution schemes for the two equations are identical. It allows to share the same compute kernels across the two coupled equations in the $\mathrm{SP}_{3}$ formulation, which is favorable for the vectorization on a GPU that is optimized for the operations exploiting SIMD parallelism.

Figure 3.3 shows the within-group solution sequence of the one-node SENM kernel. Operations colored in blue are performed for each direction, and they are implemented such that the operation for one direction is independent from others. Namely, it is possible to use different types of nodal kernels and expansion orders across different directions. In case of the expansion order, $2^{\text {nd }}$ order is applied to the radial direction while $4^{\text {th }}$ order is applied to the axial direction. For the radial direction, applying $4^{\text {th }}$ order expansion to the pin-sized fine mesh incurs stability issues [19] and is basically overkill. On the other hand, the axial solution requires full $4^{\text {th }}$ order expansion since the axial mesh size is relatively large. In this manner, kernels of different orders are adaptively used in different directions for efficient pinwise nodal core calculations.


Figure 3.3 Solution sequence for each group in the one-node SENM kernel.

### 3.1.3 Coarse Mesh Finite Difference Acceleration

In VANGARD, the assembly-level multi-group (MG) diffusion CMFD calculation is performed with the 4-mesh per assembly to accelerate the convergence of fission source distribution. The conventional CMFD acceleration method is employed where the linear system is set for the homogenized coarse meshes and the unknown is the global 3D coarse mesh scalar fluxes. The CMFD calculation begins with generating spatially homogenized MG cross sections and fission spectra on the coarse meshes. The coarse mesh cross sections are calculated as the flux-volumeweighted average of the fine mesh cross sections while the coarse mesh fission spectra are computed by using the fission source distribution instead of the flux distribution. Thus, for each energy group $(g)$, the spatially homogenized macroscopic cross section for the reaction type of $x$ and the fission spectra are obtained as follows:

$$
\begin{equation*}
\Sigma_{g, I}^{x}=\frac{\sum_{i \in I} \Sigma_{g, i}^{x} \phi_{g, i} V_{i}}{\sum_{i \in I} \phi_{g, i} V_{i}}, \quad \chi_{g, I}=\frac{\sum_{i \in I} \chi_{g, i} \psi_{i} V_{i}}{\sum_{i \in I} \psi_{i} V_{i}} \tag{3.18}
\end{equation*}
$$

where $I$ is the coarse mesh index, and $i$ is the fine mesh index.
The current correction coefficient $(\hat{D})$ is introduced so that it preserves the net current at the interface between two coarse meshes, which makes equivalent between CMFD and nodal solutions, as follows:

$$
\begin{equation*}
J_{I+1 / 2}^{n e t}=-\tilde{D}_{I+1 / 2}\left(\phi_{I+1}-\phi_{I}\right)-\hat{D}_{I+1 / 2}\left(\phi_{I}+\phi_{I+1}\right) . \tag{3.19}
\end{equation*}
$$

From the correlation between the net current at the interface which can be obtained from the high-order solution, in this case the nodal solution, and the two coarse mesh scalar fluxes, the correction coefficient of each coarse mesh is computed for each direction as follows:

$$
\begin{equation*}
\hat{D}_{I+1 / 2}=\frac{-\tilde{D}_{I+1 / 2}\left(\phi_{I+1}-\phi_{I}\right)-J_{I+1 / 2}^{n e t}}{\phi_{I}+\phi_{I+1}} . \tag{3.20}
\end{equation*}
$$

With the net current relation in Eq. (3.19), the finite difference form of the diffusion equation for each coarse mesh $(I)$ of each energy group $(g)$ is represented as follows:

$$
\begin{align*}
& \sum_{u}\left(-\tilde{D}_{u, g}-\hat{D}_{u, g}\right) \phi_{I, g}^{u} A_{I, u}+\left(\Sigma_{r, g} V_{I}+\sum_{u}\left(\tilde{D}_{u, g}-\hat{D}_{u, g}\right) A_{I, u}\right) \phi_{I, g}-V_{I} \sum_{g^{\prime} \neq g} \Sigma_{g^{\prime} g} \phi_{I, g^{\prime}} \\
= & \frac{1}{k_{e f f}} \chi_{g} V_{I} \sum_{g^{\prime}} v \Sigma_{f, g^{\prime}} \phi_{I, g^{\prime}} \tag{3.21}
\end{align*}
$$

where $A_{u}$ is the coarse mesh area at the $u$-th surface, and V is the coarse mesh volume. Resultantly, the global 3D CMFD linear system is setup in the matrix form as:

$$
\begin{equation*}
\left(\mathbf{M}-\boldsymbol{\Sigma}_{s}\right) \boldsymbol{\varphi}=\frac{1}{k_{e f f}} \chi \mathbf{F} \boldsymbol{\varphi} \tag{3.22}
\end{equation*}
$$

Here, the node major ordering scheme is used so that a $G \times G$ block matrix is formed
for each coarse mesh and the overall structure becomes a block septa diagonal matrix.
The solutions obtained from the CMFD power iteration are the global 3D coarse mesh fluxes, which are fed back to the nodal solver by modulating the fine mesh fluxes using the ratio of the coarse mesh fluxes determined in the previous nodal CMFD calculation as follows:

$$
\begin{equation*}
\phi_{i}^{(l)}=\phi_{i}^{(l-1)}\left(\frac{\phi_{I, \text { CMFD }}^{(l)}}{\phi_{I, \text { Nodal }}^{(l-1)}}\right), \quad i \in I \tag{3.23}
\end{equation*}
$$

where
$\phi_{i}^{(l)}=$ fine mesh flux obtained from the $l$-th CMFD calculation
$\phi_{I, N o d a l}^{(l-1)}=$ coarse mesh flux obtained from the ( $l-1$ )-th nodal calculation
$\phi_{I, C M F D}^{(l)}=$ coarse mesh flux obtained from the $l$-th CMFD calculation.

### 3.2 Feedback Calculations

Consideration of the T/H feedback effects is essential in analyzing operating reactors, but it is typically achieved by coupling an independent $\mathrm{T} / \mathrm{H}$ code with the neutronics code, which is cumbersome. VANGARD has a lightweight built-in T/H solver that uses a simplified yet reasonably accurate model suited for practical applications. Equilibrium and transient xenon feedback schemes were also introduced to prevent numerical xenon oscillations. This section spells out the $\mathrm{T} / \mathrm{H}$ feedback and xenon feedback calculations.

### 3.2.1 T/H Feedback

In the simplified T/H model employed in VANGARD, it is assumed that each axial segment of a fuel rod is an axially infinite and azimuthally symmetric cylinder. Namely, the axial heat conduction between the segments is neglected and only the
radial 1 D heat conduction within each segment is solved. This is valid because the axial temperature distribution in a fuel rod presents much milder variations than the radial one so the axial heat flux is small. For the coolant, each flow channel is treated as closed so that there is no flow mixing between the flow channels. All the other hydraulic effects of coolant such as the pressure drop are also neglected, and only the axial enthalpy rise by the heat transferred from the contained fuel rods is considered.

Under these assumptions, the steady-state heat conduction equation for the fuel and cladding is given as:

$$
\begin{equation*}
-\frac{1}{r} \frac{\partial}{\partial r}\left(r k(r) \frac{\partial T}{\partial r}\right)=(1-\gamma) q^{\prime \prime \prime} \tag{3.24}
\end{equation*}
$$

where $q^{\prime \prime \prime}$ is the volumetric heat generation and $\gamma$ denotes the direct heating ratio which is the fraction of the heat directly released to the coolant as gamma rays. The correlations for the thermal conductivity $k$ of fuel and cladding are adopted from the fuel performance analysis code FRAPCON [20].

The heat convection equation for the gas gap is given as:

$$
\begin{equation*}
q^{\prime \prime}=h_{g} \Delta T \tag{3.25}
\end{equation*}
$$

The gap conductance $h_{g}$ can be either specified by the user as a single value or computed using a look-up table derived from the fuel performance analysis code ROPER [21] in which the gap conductance is given as a function of linear power rate and burnup.

The heat conduction equations are numerically solved with the finite difference method. Figure 3.4 illustrates the discretization schematics of a fuel rod for the finite difference calculation. Points are positioned with equidistance in each region. The number of points in the fuel pellet $n$ excluding the center point can be arbitrarily determined by the user, and two and three points are used for the gap and cladding,
respectively.


Figure 3.4. Discretization of a fuel rod for the finite difference scheme.

The discretized equations for solving the heat conduction equations are shown through Eq. (3.26) to Eq. (3.31). Boundary conditions are imposed by the zero temperature gradient condition at the center and the coolant temperature $T_{\text {bulk }}$ at the periphery. The equations at the region interfaces are derived by the assumption that the temperature profiles in the pellet and cladding can be expressed as quadratic functions.

At the center of a pellet $(i=0)$ :

$$
\begin{equation*}
\frac{4 k_{0}}{\Delta r_{f}^{2}}\left(T_{0}-T_{1}\right)=(1-\gamma) q^{\prime \prime \prime} \tag{3.26}
\end{equation*}
$$

At the interior of a pellet $(1 \leq i<n)$ :

$$
\begin{equation*}
-\frac{1}{\Delta r_{f}^{2}}\left[k_{i-\frac{1}{2}}\left(1-\frac{\Delta r_{f}}{2 r_{i}}\right) T_{i-1}-\left(k_{i-\frac{1}{2}}+k_{i+\frac{1}{2}}+\frac{\Delta r_{f}}{2 r_{i}}\left(k_{i+\frac{1}{2}}-k_{i-\frac{1}{2}}\right)\right) T_{i}+k_{i+\frac{1}{2}}\left(1+\frac{\Delta r_{f}}{2 r_{i}}\right) T_{i+1}\right]=(1-\gamma) q^{\prime \prime \prime} \tag{3.27}
\end{equation*}
$$

At the surface of a pellet $(i=n)$ :

$$
\begin{equation*}
-\frac{1}{\Delta r_{f}^{2}}\left[2 k_{n} T_{n-1}-\left(2 k_{n}+h_{g} \Delta r_{f}\left(3+\frac{1}{n}-\frac{k_{n-1}}{k_{n}}\right)\right) T_{n}+h_{g} \Delta r_{f}\left(3+\frac{1}{n}-\frac{k_{n-1}}{k_{n}}\right) T_{n+1}\right]=(1-\gamma) q^{\prime \prime \prime} \tag{3.28}
\end{equation*}
$$

At the gap side of a cladding $(i=n+1)$ :

$$
\begin{equation*}
\frac{1}{t_{c}^{2}}\left[8 k_{n+1}\left(T_{n+2}-T_{n+1}\right)+4 t_{c} h_{g} \frac{r_{n}}{r_{n+1}}\left(T_{n}-T_{n+1}\right)\right]-h_{g} \frac{r_{n}}{r_{n+1}}\left[\frac{1}{r_{n+1}}+\frac{2}{t_{c}}\left(\frac{k_{n+2}}{k_{n+1}}-1\right)\right]\left(T_{n}-T_{n+1}\right)=0 \tag{3.29}
\end{equation*}
$$

At the middle of a cladding $(i=n+2)$ :

$$
\frac{1}{\Delta r_{c}^{2}}\left[k_{i-\frac{1}{2}}\left(1-\frac{\Delta r_{c}}{2 r_{n+2}}\right) T_{n+1}-\left(k_{i-\frac{1}{2}}+k_{i+\frac{1}{2}}+\frac{\Delta r_{c}}{2 r_{n+2}}\left(k_{i+\frac{1}{2}}-k_{i-\frac{1}{2}}\right)\right) T_{n+2}+k_{i+\frac{1}{2}}\left(1+\frac{\Delta r_{c}}{2 r_{n+2}}\right) T_{n+3}\right]=0
$$

At the wall side of a cladding $(i=n+3)$ :

$$
\begin{equation*}
-\frac{8 k_{n+3}}{t_{c}{ }^{2}} T_{n+2}+\left[\frac{8 k_{n+3}}{t_{c}{ }^{2}}+\frac{4 h_{w}}{t_{c}}+h_{w}\left(\frac{1}{r_{n+3}}+\frac{2}{t_{c}}\left(1-\frac{k_{n+2}}{k_{n+3}}\right)\right)\right] T_{n+3}=\left[\frac{4 h_{w}}{t_{c}}+h_{w}\left(\frac{1}{r_{n+3}}+\frac{2}{t_{c}}\left(1-\frac{k_{n+2}}{k_{n+3}}\right)\right)\right] T_{b u l k} \tag{3.31}
\end{equation*}
$$

where
$h_{w}=$ wall heat transfer coefficient,
$t_{c}=$ thickness of the cladding,
$\Delta r_{f}=\quad$ size of meshes in the pellet,
$\Delta r_{c}=$ size of meshes in the cladding,
$k_{i \pm \frac{1}{2}}=\quad$ average thermal conductivity of point $i$ and $i \pm 1$.

The fuel temperature of each cell used to determine the cross sections is defined by the Doppler temperature, which is expressed as the weighted sum of the centerline and surface temperatures as described in Eq. (3.32). The weighting factor $\alpha$ is set to $\frac{5}{9}$ [22] by default, while it can be specified by the user.

$$
\begin{equation*}
T_{\text {Doppler }}=(1-\alpha) T_{0}+\alpha T_{n} . \tag{3.32}
\end{equation*}
$$

The coolant temperature of each axial segment of a channel is determined by the simple enthalpy conservation equation in the axial direction with the constant mass flux assumption, which is given as:

$$
\begin{equation*}
[\rho h v]_{\text {out }}=[\rho h v]_{i n}+q^{\prime} \Delta z \tag{3.33}
\end{equation*}
$$

where $q^{\prime}$ and $\Delta z$ are the linear heat generation rate and the thickness of the axial segment, respectively. The average enthalpy of inlet and outlet is used to determine the coolant temperature of the level.

To compensate the lack of cross-flow mixing effects between channels in the closed-channel model, pinwise channels are lumped into coarser channels called macro-channels, as described in Figure 3.5. All the fuel rods belonging to the same macro-channel share the same coolant temperature. VANGARD can divide each assembly into arbitrary $N \times N$ macro-channels. The number of divisions can be specified by the user, and $2 \times 2$ division is used as default.


Figure 3.5. Pinwise channels (left) and macro-channels (right).

### 3.2.2 Xenon Feedback

Since the depletion calculation proceeds with relatively large time steps, shorttime xenon transient cannot be taken into account properly, which incurs xenon oscillations that lead to severe changes in flux and power distributions between burnup steps. To prevent this, the number density of xenon is not calculated by the depletion solver but is determined by a nonlinear iteration between the neutronics solution and the analytic solution of the xenon-iodine chain in the following:

$$
\begin{align*}
& \frac{d N_{I}(t)}{d t}=\gamma_{I} \Sigma_{f} \bar{\phi}-\lambda_{I} N_{I}(t),  \tag{3.34}\\
& \frac{d N_{X_{e}}(t)}{d t}=\gamma_{X_{e}} \Sigma_{f} \bar{\phi}+\lambda_{I} N_{I}(t)-\lambda_{X_{e}} N_{X e}(t)-\sigma_{a}^{X e} N_{X e}(t) \bar{\phi}
\end{align*}
$$

where $\gamma$ is the fission product yield.
The widely used assumption is the equilibrium xenon assumption in which the number density of xenon is always at the equilibrium state. The equilibrium number densities of xenon and iodine can be calculated by forcing the time derivative terms to zero in Eq. (3.34), which yields:

$$
\begin{align*}
& N_{I}=\frac{\gamma_{I} \Sigma_{f} \bar{\phi}}{\lambda_{I}} \\
& N_{X e}=\frac{\left(\gamma_{I}+\gamma_{X e}\right) \Sigma_{f} \bar{\phi}}{\lambda_{X e}+\sigma_{a}^{X e} \bar{\phi}} \tag{3.35}
\end{align*}
$$

However, in conditions where the reactor power level changes over time, the equilibrium xenon assumption is not valid. In such cases, VANGARD can employ a transient xenon assumption as well. Keeping the time derivative terms remained in Eq. (3.34) and solving the system of ODEs yields:

$$
\begin{align*}
& N_{I}(t)=\frac{a}{b}+k_{1} e^{-b t}, \\
& N_{X_{e}}(t)=\frac{a+c}{d}-b k_{1} e^{-t(b+d)} \frac{e^{d t}-e^{b t}}{b-d}+k_{2} e^{-d t} \tag{3.36}
\end{align*}
$$

where $t$ is the time step and

$$
\begin{align*}
a & =\gamma_{I} \Sigma_{f} \bar{\phi}, \\
b & =\lambda_{I}, \\
c & =\gamma_{X e} \Sigma_{f} \bar{\phi}, \\
d & =\lambda_{X e}+\sigma_{a}^{X e} \bar{\phi},  \tag{3.37}\\
k_{1} & =N_{I}(0)-\frac{a}{b}, \\
k_{2} & =N_{X e}(0)-\frac{a+c}{d} .
\end{align*}
$$

Note that the flux solution used for the transient xenon is that of the current burnup step, but the flux level normalizer is calculated using the average power level of the two burnup steps.

### 3.3 Depletion Solvers

Depletion calculation is crucial for predicting the long-term behavior of a reactor. For an accurate depletion, a pinwise microscopic depletion solver is implemented in VANGARD which employs a simplified burnup chain derived from nTRACER. The VANGARD depletion solver can model not only the transmutation of nuclides during operation but also the long-term cooling effect during inspection and reloading by nuclide decay. This section introduces the depletion calculation algorithm of VANGARD, which encompasses the solution scheme for the burnup chain and B-10 depletion model to track the isotopic changes in the soluble boron during operation.

### 3.3.1 Solution of Burnup Systems

The burnup chain of VANGARD consists of 44 nuclides. For actinides, 29 major nuclides from uranium $(\mathrm{Z}=92)$ to curium $(\mathrm{Z}=96)$ are considered. Figure 3.6 illustrates the burnup chain of actinides where only important decay and reaction are shown. The remaining 15 nuclides include B-10 in burnable poison (5010) and fission products related to xenon/samarium poisoning (I, Xe, Nd, Pm, and Sm). Only four major fissile nuclides (U-235, U-238, Pu-239, and Pu-241) have fission product yield information.


Figure 3.6 Burnup chain of actinides in VANGARD.

The depletion calculation is governed by the Bateman equation which is written as follows:

$$
\begin{equation*}
\frac{d N_{i}(t)}{d t}=\sum_{\substack{j=1 \\ j \neq i}}^{N} l_{i j} \lambda_{j} N_{j}(t)+\bar{\phi} \sum_{\substack{j=1 \\ j \neq i}}^{N} \gamma_{i j} \bar{\sigma}_{j} N_{j}(t)-\left(\lambda_{i}+\bar{\sigma}_{i} \bar{\phi}\right) N_{i}(t) \tag{3.38}
\end{equation*}
$$

where

$$
\begin{aligned}
N_{i}(t) & =\text { Atomic number density of nuclide } i \\
l_{i j} & =\text { Yield fraction of nuclide } i \text { from the decay of nuclide } j \\
\gamma_{i j} & =\text { Yield fraction of nuclide } i \text { from the reaction of nuclide } j
\end{aligned}
$$

$$
\begin{aligned}
\lambda_{i} & =\text { Decay constant of nuclide } i, \\
\bar{\sigma}_{i} & =\text { One-group absorption cross section of nuclide } i, \\
\bar{\phi} & =\text { One-group neutron flux } .
\end{aligned}
$$

Eq. (3.38) can be expressed as a system of ordinary differential equations (ODE) in a matrix form:

$$
\begin{equation*}
\frac{d \overrightarrow{\mathbf{N}}(t)}{d t}=\mathbf{A} \overrightarrow{\mathbf{N}}(t) \tag{3.39}
\end{equation*}
$$

whose solution is expressed in terms of matrix exponential:

$$
\begin{equation*}
\overrightarrow{\mathbf{N}}(t)=e^{\mathbf{A} t} \overrightarrow{\mathbf{N}}(0) \tag{3.40}
\end{equation*}
$$

Eq. (3.40) is solved by the Chebyshev Rational Approximation Method (CRAM) [23], which reduces it to:

$$
\begin{equation*}
\overrightarrow{\mathbf{N}}(t)=\alpha_{0} \overrightarrow{\mathbf{N}}(0)+2 \operatorname{Re}\left(\sum_{j=1}^{k / 2} \alpha_{j}\left(\mathbf{A} t-\theta_{j} \mathbf{I}\right)^{-1} \overrightarrow{\mathbf{N}}(0)\right) \tag{3.41}
\end{equation*}
$$

where $k$ is the order of the CRAM, which is set to 16 as default in VANGARD, and $\alpha$ and $\theta$ are the complex residues and poles, respectively.

To obtain the solution of Eq. (3.41) which entails matrix inversion, iterative linear system solution schemes are employed in VANGARD. In the CPU calculation, C++ Eigen linear algebra package [24] is utilized for the complex matrix and vector operations. The Gauss-Seidel iteration method is employed for the matrix inversion and the burnup system of each cell is solved independently by OpenMP parallelization. However, the CRAM solver is implemented manually for GPUs due to the lack of library support.

### 3.3.2 B-10 Depletion

The soluble boron is commonly utilized to control the excess reactivity of reactors. It is dissolved in the Reactor Coolant System (RCS) by the Chemical and Volume Control System (CVCS) in the form of boric acid. The natural boron consists of B10 and B-11, and B-10 takes approximately $20 \%$ of isotopic fraction. Since B-10 has a significantly larger absorption cross section than $\mathrm{B}-11, \mathrm{~B}-10$ is mostly removed while the content of B-11 remains constant during the operation. For this reason, the boron depletion in the RCS is implemented only for the B-10 with the change of B11 regarded negligible. The variation of the number density of B-10 is given as follows:

$$
\begin{equation*}
\frac{d N_{B 10}(t)}{d t}=-N_{B 10}(t) \frac{\int_{V_{C \text { cort }}} \int \sigma_{a}^{B 10}(\overrightarrow{\mathbf{r}}, E) \phi(\overrightarrow{\mathbf{r}}, E) d E d \overrightarrow{\mathbf{r}}}{V_{R C S}} \tag{3.42}
\end{equation*}
$$

which can be analytically solved as:

$$
\begin{equation*}
N_{B 10}(t)=N_{B 10}(0) \exp \left(-\frac{\int_{V_{\text {Core }}} \int \sigma_{a}^{B 10}(\overrightarrow{\mathbf{r}}, E) \phi(\overrightarrow{\mathbf{r}}, E) d E d \overrightarrow{\mathbf{r}}}{V_{R C S}} t\right) \tag{3.43}
\end{equation*}
$$

where $N_{B 10}$ is the number density of B-10 and $V_{\text {Core }}$ and $V_{R C S}$ are the volume of the coolant in the core and the RCS, respectively. $V_{\text {Core }}$ is calculated by the code, and $V_{R C S}$ is derived from the user-specified relative volume of the core coolant to the RCS coolant.

It should be noted that performing B-10 depletion requires a caution in the cross section treatment, because the lattice calculations for the group constant generation are performed with the natural boron composition. Namely, the boron concentrations in the group constants become inconsistent with the simulation value when $B-10$ is
depleted. Thus, assuming the impact of B-11 is negligible, the simulated boron concentration is adjusted to the equivalent value in the group constants as follows:

$$
\begin{equation*}
\mathrm{ppm}:=\operatorname{ppm} \times \frac{f_{B 10}^{\text {depleeded }}}{f_{B 10}^{\text {natural }}} \tag{3.44}
\end{equation*}
$$

where $f_{B 10}^{\text {natural }}$ and $f_{B 10}^{\text {depleted }}$ are the abundance of B-10 in natural and depleted boron, respectively. Note that the adjusted value is only used internally for the cross section interpolation and not shown in the output.

### 3.4 Overall Flowchart of Steady-State Calculation

Figure 3.7 illustrates the overall calculation flow of VANGARD employing GPUs. Calculations accelerated by GPU are colored in green and calculations performed on CPU are colored in blue. Note that almost all of the calculation modules were offloaded to GPU. Only the table setup which determines the burnup range required for the core state of each burnup step and organizes a sub-table containing group constants of the specified burnup points is performed on CPU, which will be elaborated in Section 6.2.1.

The calculation begins with initializing the burnup table and cross sections, followed by the initial CMFD calculation which provides the initial guess. If the core is fresh, namely not reloaded, the burnup table will contain only one burnup point. After the initial CMFD calculation, the neutronics iteration loop is initiated. First, each nodal sweep performs 5 outer iterations where each outer iteration is again composed of 6 inner iterations. The iteration counts were empirically chosen to be optimal. After the nodal sweep, T/H feedback, boron update, and Xenon update are carried out consecutively. Then, the cross sections are newly calculated and the CMFD calculation is performed to accelerate the convergence. This procedure is repeated until the neutronics iteration is converged. The converged neutronics
solution is then fed to the depletion solver and used to update the core compositions. The updated core compositions are again fed back to the neutronics solver, which constitutes the global iteration loop involving successive feedbacks between the neutronics and the depletion solvers.


Figure 3.7 Steady-state calculation flow chart of VANGARD.

## Chapter 4. Transient Calculation Capability

The need for a fast and accurate pin-level core analysis is particularly emphasized in the transient analysis. The assemblywise two-step calculation employing assembly-homogenized cross sections cannot catch the severe intra-assembly flux gradients occurring near the perturbed rod during a transient, therefore, the use of detailed pin-level solutions is essential in the transient analysis. Furthermore, one of the significant challenges of transient analysis is excessive computational burdens because it requires repetitive core calculations for more than hundreds of time steps.

In this respect, as a part of the development to make VANGARD a practical pinwise core design code, the transient calculation capabilities have been developed. VANGARD can be a completely suitable core transient analysis tool in terms of accuracy and practicality in that it targets to achieve tolerable computing time even on a PC by exploiting gaming GPUs while yielding accurate pin-level solutions.

Basically, the transient solutions are originated from the same governing equations with the steady-state solutions, but the time derivative term which has been imposed to be zero in the steady-state solution is retained. Therefore, efficient implementation is possible without modifying the pre-established solvers for steady-state analysis. Once the steady-state solvers are implemented, only a few modifications are additionally needed to account for the time-dependent characteristics.

This chapter covers the solvers of time-dependent equations for the flux and T/H feedback. In Section 4.1, the time-dependent $\mathrm{SP}_{3}$ formulation is derived and the CMFD linear system for the time-dependent diffusion equation is presented. In Section 4.2, the solution of the time-dependent heat convection equation for the coolant channel and the solution of the time-dependent heat conduction equation for the fuel pellet are described in detail.

### 4.1 Flux Solvers

### 4.1.1 Time-dependent $\mathrm{SP}_{3}$ Formulation

In this section, the time-dependent nodal solution of the diffusion and $\mathrm{SP}_{3}$ equations are derived briefly. The detailed derivations including definitions of the terms can be found in [25][26].

The time-dependent multi-group neutron diffusion equation as well as the precursor balance equation are written as follows:

$$
\begin{gather*}
\frac{1}{v_{g}} \frac{\partial \phi_{g}}{\partial t}=\chi_{g}(1-\beta) \psi+\sum_{g^{\prime}=1}^{G} \Sigma_{g^{\prime} g} \phi_{g^{\prime}}+\sum_{k=1}^{6} \chi_{d g k} \lambda_{k} C_{k}-\left(\nabla \cdot J_{g}+\Sigma_{r g} \phi_{g}\right),  \tag{4.1}\\
\frac{d C_{k}(t)}{d t}=\beta_{k} \psi(t)-\lambda_{k} C_{k}(t) . \tag{4.2}
\end{gather*}
$$

For the temporal discretization, the theta method is applied, which writes Eq.
where $R_{g}^{n}$ denotes the RHS terms of Eq. (4.1) at the time step $n$.

$$
\begin{equation*}
\frac{\phi_{g}^{n+1}-\phi_{g}^{n}}{v_{g} \Delta t_{n+1}}=\theta R_{g}^{n+1}+(1-\theta) R_{g}^{n} . \tag{4.3}
\end{equation*}
$$

In order to obtain the precursor density of the new time step $(n+1)$, a quadratic variation of the fission source is assumed, which expresses it in terms of the two known fission sources of the previous and current time step and the one unknown fission source of the new time step as follows:

$$
\begin{equation*}
C_{k}^{n+1}=\kappa_{k} C_{k}^{n}+\frac{\beta_{k}}{\lambda_{k}}\left(\Omega_{k}^{n-1} \psi^{n-1}+\Omega_{k}^{n} \psi^{n}+\Omega_{k}^{n+1} \psi^{n+1}\right) \tag{4.4}
\end{equation*}
$$

where

$$
\begin{align*}
& \Omega_{k}^{n-1}=\frac{1}{\lambda_{k} \Delta t_{n}(\gamma+1)}\left(\frac{2 \bar{\kappa}_{k}}{\lambda_{k} \Delta t_{n}}-\gamma\left(\kappa_{k}+1\right)\right), \\
& \Omega_{k}^{n}=\frac{1}{\lambda_{k} \Delta t_{n}}\left(\kappa_{k}+1+\frac{\bar{\kappa}_{k}}{\gamma}\left(1-\frac{2}{\lambda_{k} \Delta t_{n}}\right)\right)-\kappa_{k},  \tag{4.5}\\
& \Omega_{k}^{n+1}=1-\frac{2}{\lambda_{k} \Delta t_{n}(\gamma+1)}+\frac{\bar{\kappa}_{k}}{\lambda_{k} \Delta t_{n} \gamma(\gamma+1)}\left(\frac{2}{\lambda_{k} \Delta t_{n}}-1\right), \\
& \gamma=\frac{\Delta t_{n+1}}{\Delta t_{n}}, \kappa_{k}=e^{-\lambda_{k} \Delta t_{n+1}}, \text { and } \bar{\kappa}_{k}=1-\kappa_{k} .
\end{align*}
$$

By combining Eq. (4.1), (4.3), and (4.4), the transverse-integrated time-dependent neutron diffusion equation for each direction can be represented as follows:

$$
\begin{align*}
-\frac{4 D_{g}}{h^{2}} \frac{d \phi_{g}^{n+1}}{d \xi^{2}}+\Sigma_{r g} \phi_{g}^{n+1}= & \left(\chi_{p g}(1-\beta)+\omega^{n+1}\right) \psi^{n+1}+\sum_{\substack{g^{\prime}=1 \\
g^{\prime} \neq g}}^{G} \Sigma_{g^{\prime} g} \phi_{g^{\prime}}^{n+1}  \tag{4.6}\\
& +\frac{\phi_{g}^{n}-\phi_{g}^{n+1}}{\theta v_{g} \Delta t_{n+1}}+\tilde{s}_{d g}^{n}-L^{n+1}+\Theta R_{g}^{n},
\end{align*}
$$

where

$$
\begin{align*}
& \tilde{s}_{d g}^{n}=\sum_{k=1}^{6} \chi_{d g k}\left(\lambda_{k} \kappa_{k} C_{k}^{n}+\beta_{k}\left(\Omega_{k}^{n-1} \psi^{n-1}+\Omega_{k}^{n} \psi^{n}\right)\right), \\
& \omega_{g}^{n+1}=\sum_{k=1}^{6} \chi_{d g k} \beta_{k} \Omega_{k}^{n+1}, \Theta=\frac{1-\theta}{\theta} \tag{4.7}
\end{align*}
$$

For the efficient implementations, the equation is rearranged to have the same form as the steady-state equation, and the final form of the time-dependent transverseintegrated neutron diffusion equation is represented as Eq. (4.8). The only difference from the steady-state solution is that the transient source $\left(s_{t r, g}^{n+1}\right)$ needs to be additionally calculated. This reformulation enables most of the pre-established nodal solvers for the steady-state solutions to be directly used for the transient solutions without any modifications.

$$
\begin{equation*}
-\frac{4 D_{g}}{h^{2}} \frac{d^{2} \phi_{g}^{n+1}}{d \xi^{2}}+\Sigma_{r g} \phi_{g}^{n+1}=\chi_{g} \psi^{n+1}+\sum_{g^{\prime}=1}^{g^{\prime}=G} \Sigma_{g^{\prime} g} \phi_{g^{\prime}}^{n+1}-L_{g}^{n+1}+s_{t r}^{n+1} \tag{4.8}
\end{equation*}
$$

where

$$
\begin{align*}
& s_{t r, g}^{n+1}=s_{\text {fixed }, g}^{n}+\Delta \chi_{g} \psi^{n+1}-\frac{\phi_{g}^{n+1}}{\theta v_{g} \Delta t_{n+1}}, \\
& s_{f i x e d, g}^{n}=\tilde{s}_{d g}^{n}+\frac{\phi_{g}^{n}}{\theta v_{g} \Delta t_{n+1}}+\Theta R_{g}^{n},  \tag{4.9}\\
& \Delta \chi_{g}=-\chi_{g}+\left(\chi_{p g}(1-\beta)+\omega_{g}^{n+1}\right) .
\end{align*}
$$

Note that the fixed source ( $s_{f i x e d, g}^{n}$ ) is determined only by the current time step solutions which are known so that it is constant during the current time step. Therefore, it is calculated only once per each time step.

The $\mathrm{SP}_{3}$ formulation is derived in an analogous manner with the diffusion formulation. The equations are defined for the summed flux and $2^{\text {nd }}$ flux moment with differently defined diffusion coefficients and removal cross sections.

$$
\begin{align*}
& -\frac{4 D_{0, g}}{h^{2}} \frac{d^{2}}{d \xi^{2}} \hat{\phi}_{0, g}+\Sigma_{r 0, g} \hat{\phi}_{0, g}=s_{0, g}+s_{t r, 0, g},  \tag{4.10}\\
& -\frac{4 D_{2, g}}{h^{2}} \frac{d^{2}}{d \xi^{2}} \phi_{2, g}+\Sigma_{r 2, g} \phi_{2, g}=s_{2, g}+s_{t r, 2, g}
\end{align*}
$$

where

$$
\begin{align*}
& \hat{\phi}_{0, g}=\phi_{0, g}+2 \phi_{2, g}, \\
& D_{0, g}=\frac{1}{3 \Sigma_{t r, g}}, D_{2, g}=\frac{3}{7 \Sigma_{t, g}},  \tag{4.11}\\
& \Sigma_{r 0, g}=\Sigma_{r, g}, \Sigma_{r 2, g}=\frac{4}{3} \Sigma_{r, g}+\frac{5}{3} \Sigma_{t, g} .
\end{align*}
$$

As in the steady-state formulation, the source terms are also separately defined. In the same manner as the diffusion equation, the total source terms in the $\mathrm{SP}_{3}$ equations are easily obtained by the addition of the transient sources to the steady-state formulations as follows:

$$
\begin{align*}
& s_{0, g}=\bar{s}_{g}+2 \Sigma_{r, g} \phi-L_{0, g}, s_{2, g}=-\frac{2}{3} \bar{s}_{g}+\frac{2}{3} \Sigma_{r, g} \hat{\phi}_{0, g}-L_{2, g}, \\
& s_{t r, 0, g}=\tilde{s}_{d g}^{n}+\Delta \chi_{g} \psi^{n+1}+\frac{\phi_{0, g}^{n}-\phi_{0, g}^{n+1}}{\theta v_{g} \Delta t_{n+1}}+\Theta R_{0, g}^{n},  \tag{4.12}\\
& s_{t r, 2, g}=-\frac{2}{3} s_{t r, 0, g}+\frac{5}{3}\left(\frac{\phi_{2, g}^{n}-\phi_{2, g}^{n+1}}{\theta v_{g} \Delta t_{n+1}}+\Theta R_{2, g}^{n}\right) .
\end{align*}
$$

### 4.1.2 CMFD for Transient Calculation

In the steady-state CMFD calculation, the fission source calculated in the previous CMFD power iteration serves as the fixed source. The fixed source is updated during iterations at a CMFD calculation, therefore, it runs iterations until it meets the convergence criteria. In the transient calculation, on the other hand, the fission source is included in LHS for better convergence, and the CMFD linear system for the new time step $(n+1)$ sets the transient fixed source in RHS which comprises the current time step ( $n$ ) solutions. Resultantly, the final CMFD fixed source problem is set as Eq. (4.13). Since the fixed source is determined only once per each time step and is not variant during the current time step, the linear system is solved only once per each CMFD calculation.

$$
\begin{equation*}
\left(\mathbf{M}^{n+1}-\boldsymbol{\Sigma}_{s}^{n+1}-(\chi+\Delta \chi) \mathbf{F}^{n+1}+\frac{1}{\theta v \Delta t} \mathbf{I}\right) \boldsymbol{\varphi}^{n+1}=\mathbf{s}_{\text {fixed }}^{n} \tag{4.13}
\end{equation*}
$$

where

$$
\begin{equation*}
\mathbf{s}_{\text {fixed }}^{n}=\tilde{\mathbf{s}}_{d}^{n}+\frac{1}{\theta v \Delta t_{n+1}} \boldsymbol{\varphi}^{n}+\Theta \mathbf{R}^{n} \tag{4.14}
\end{equation*}
$$

### 4.2 T/H Feedback

### 4.2.1 Transient Heat Convection Solution for Channel

As in the steady-state solution, the heat convection equations are solved for each axial segment of a channel. The derivation of the transient heat convection solution is started from the mass conservation and energy conservation equations as follows:

$$
\begin{gather*}
\frac{\partial \rho}{\partial t}+\frac{\partial \rho v}{\partial z}=0  \tag{4.15}\\
\frac{\partial \rho h}{\partial t}+\frac{\partial \rho h v}{\partial z}=q \tag{4.16}
\end{gather*}
$$

The volume-integrated mass conservation and energy conservation equations with temporal differencing by the Theta method are represented as follows:

$$
\begin{align*}
& \frac{\rho^{(n+1)}-\rho^{(n)}}{\Delta t}+\theta \frac{[\rho v]_{\text {out }}^{(n+1)}-[\rho v]_{\text {in }}^{(n+1)}}{\Delta z}+\bar{\theta} \frac{[\rho v]_{\text {out }}^{(n)}-[\rho v]_{\text {in }}^{(n)}}{\Delta z}=0,  \tag{4.17}\\
& \frac{[\rho h]^{(n+1)}-[\rho h]^{(n)}}{\Delta t}+\theta \frac{[\rho h v]_{\text {out }}^{(n+1)}-[\rho h v]_{\text {in }}^{(n+1)}}{\Delta z}+\bar{\theta} \frac{[\rho h v]_{\text {out }}^{(n)}-[\rho h v]_{\text {in }}^{(n)}}{\Delta z}  \tag{4.18}\\
= & \theta q^{(n+1)}+\bar{\theta} q^{(n)} .
\end{align*}
$$

Note that the variables without any subscript denoting inlet or outlet represent the node-averaged quantities. The volumetric heat source $(q)$ of each axial segment of a channel is defined as the sum of the heat provided through the wall and the direct heating as follows:

$$
\begin{equation*}
q=q^{\prime \prime} \frac{\zeta}{A_{c}}+\gamma q_{c}^{\prime \prime \prime} . \tag{4.19}
\end{equation*}
$$

By dividing by $\frac{\theta}{\Delta z}$ and setting all the knowns to the RHS except for the time
derivative terms, Eq. (4.17) and (4.18) are represented as follows:

$$
\begin{gather*}
\frac{\Delta z}{\theta \Delta t}\left(\rho^{(n+1)}-\rho^{(n)}\right)+[\rho v]_{\text {out }}^{(n+1)}=[\rho v]_{\text {in }}^{(n+1)}-\frac{\bar{\theta}}{\theta}\left([\rho v]_{o u t}^{(n)}-[\rho v]_{i n}^{(n)}\right),  \tag{4.20}\\
\frac{\Delta z}{\theta \Delta t}\left([\rho h]^{(n+1)}-[\rho h]^{(n)}\right)+[\rho h v]_{\text {out }}^{(n+1)} \\
=[\rho h v]_{\text {in }}^{(n+1)}-\frac{\bar{\theta}}{\theta}\left([\rho h v]_{o u t}^{(n)}-[\rho h v]_{i n}^{(n)}\right)+\Delta z\left(q^{(n+1)}+\frac{\bar{\theta}}{\theta} q^{(n)}\right) \tag{4.21}
\end{gather*}
$$

Here, five variables are unknown including two average values ( $\rho, h$ ) and three outlet values $\left(\rho_{\text {out }}, h_{\text {out }}, v_{\text {out }}\right)$ of the time step $(n+1)$, which are the targets to be solved. Using auxiliary state equations as

$$
\begin{gather*}
\rho^{(n+1)}-\rho^{(n)}=\left.\frac{d \rho}{d h}\right|^{(n)}\left(h^{(n+1)}-h^{(n)}\right),  \tag{4.22}\\
{[\rho h]^{(n+1)}-[\rho h]^{(n)}=\left.\frac{d[\rho h]}{d h}\right|^{(n)}\left(h^{(n+1)}-h^{(n)}\right) .} \tag{4.23}
\end{gather*}
$$

the time derivative terms in LHS of the Eq. (4.20) can be expressed in terms of volume enthalpy change as:

$$
\begin{equation*}
[\rho v]_{\text {out }}^{(n+1)}=\underbrace{-\left.\frac{\Delta z}{\theta \Delta t} \frac{d \rho}{d h}\right|^{(n)}}_{\equiv \alpha} X+\underbrace{[\rho v]_{i n}^{(n+1)}-\frac{\bar{\theta}}{\theta}\left([\rho v]_{\text {out }}^{(n)}-[\rho v]_{i n}^{(n)}\right)}_{\equiv \beta} \equiv \alpha X+\beta \tag{4.24}
\end{equation*}
$$

where

$$
\begin{equation*}
X \equiv h^{(n+1)}-h^{(n)} . \tag{4.25}
\end{equation*}
$$

By assuming the node-averaged enthalpy to be the average of the inlet and outlet enthalpies and combining with Eq. (4.24) and (4.25), $[\rho h v]_{\text {out }}^{(n+1)}$ can be represented as a quadratic equation in terms of the enthalpy change $(X)$ as follows:
soll wional unezan

$$
\begin{align*}
{[\rho h v]_{\text {out }}^{(n+1)} } & =[\rho v]_{\text {out }}^{(n+1)} h_{\text {out }}^{(n+1)} \\
& =(\alpha X+\beta)\left(2 X+2 h^{(n)}-h_{\text {in }}^{(n+1)}\right)  \tag{4.26}\\
& =2 \alpha X^{2}+\gamma X+\delta
\end{align*}
$$

where

$$
\begin{align*}
h^{(n+1)} & =h^{(n)}+X=\frac{1}{2}\left(h_{o u t}^{(n+1)}+h_{i n}^{(n+1)}\right), \\
\gamma & =\alpha\left(2 h^{(n)}-h_{i n}^{(n+1)}\right)+2 \beta,  \tag{4.27}\\
\delta & =\beta\left(2 h^{(n)}-h_{i n}^{(n+1)}\right) .
\end{align*}
$$

A pair of the analytic solutions of Eq. (4.26) can be easily obtained. To choose the final solution out of the two ones, a linear formulation is introduced which starts from approximating the outlet enthalpy of the time step $(n+1)$ to that of the time step (n) so that $[\rho h v]_{\text {out }}^{(n+1)}$ is expressed as a linear equation in terms of the enthalpy change as:

$$
\begin{equation*}
[\rho h v]_{\text {out }}^{(n+1)}=[\rho v]_{\text {out }}^{(n+1)} h_{\text {out }}^{(n+1)} \cong[\rho v]_{\text {out }}^{(n+1)} h_{\text {out }}^{(n)}=(\alpha X+\beta) h_{\text {out }}^{(n)} \tag{4.28}
\end{equation*}
$$

With the above relation and additionally introduced auxiliary state equation as

$$
\begin{equation*}
[\rho h]^{(n+1)}-[\rho h]^{(n)}=\left.\frac{d[\rho h]}{d h}\right|^{(n)}\left(h^{(n+1)}-h^{(n)}\right), \tag{4.29}
\end{equation*}
$$

the LHS of Eq. (4.21) which consists only of the unknowns can be reformulated as a linear equation in terms of enthalpy change, the solution of which also can be directly obtained.

Out of the two solutions of Eq. (4.26), the one closer to the solution of the linear formulation is selected as the final solution. Finally, the volume enthalpy change is obtained and it resultantly updates the enthalpy of the new time step $(n+1)$, with which the two average unknowns of the new time step composing the time derivative terms of the Eq. (4.20) and (4.21) are updated as follows:

$$
\begin{align*}
& \rho^{(n+1)}=\rho\left(h^{(n+1)}\right)  \tag{4.30}\\
& {[\rho h]^{(n+1)} \simeq \rho^{(n+1)} h^{(n+1)} .}
\end{align*}
$$

The final solutions for the mass conservation and energy conservation equations are then obtained as follows:

$$
\begin{align*}
& {[\rho v]_{\text {out }}^{(n+1)}=[\rho v]_{\text {in }}^{(n+1)}-\frac{\Delta z}{\theta \Delta t}\left(\rho^{(n+1)}-\rho^{(n)}\right)-\frac{\bar{\theta}}{\theta}\left([\rho v]_{\text {out }}^{(n)}-[\rho v]_{\text {in }}^{(n)}\right) . }  \tag{4.31}\\
& {[\rho h v]_{\text {out }}^{(n+1)}=} {[\rho h v]_{\text {in }}^{(n+1)}-\frac{\Delta z}{\theta \Delta t}\left([\rho h]^{(n+1)}-[\rho h]^{(n)}\right) } \\
&-\frac{\bar{\theta}}{\theta}\left([\rho h v]_{\text {out }}^{(n)}-[\rho h v]_{\text {in }}^{(n)}\right)+\Delta z\left(q^{(n+1)}+\frac{\bar{\theta}}{\theta} q^{(n)}\right) . \tag{4.32}
\end{align*}
$$

By dividing Eq. (4.32) by Eq. (4.31), the outgoing enthalpy of the time step ( $n+1$ ) can be updated, with which the average enthalpy is subsequently updated. From the average enthalpy, the node average channel bulk temperature can be calculated, from which the heat transfer coefficient can be updated. All of them are then fed back to the calculation of the fuel pellet temperature profile.

### 4.2.2 Transient Heat Conduction Solution for Fuel

As in the steady-state calculation, one-dimensional cylindrical finite difference heat conduction equation is solved for each axial plane. The time-dependent heat conduction equation is described as Eq. (4.33) where $q^{\prime \prime \prime}$ is the volumetric heat generation rate.

$$
\begin{equation*}
C_{p} \frac{\partial T}{\partial t}=\frac{1}{r} \frac{\partial}{\partial r}\left(r k \frac{\partial T}{\partial r}\right)+q^{\prime \prime \prime}=f(r, t) \tag{4.33}
\end{equation*}
$$

With temporal differencing by the Theta method, the heat conduction equation can be expressed as follows:

$$
\begin{equation*}
C_{p} \frac{T^{(n+1)}-T^{(n)}}{\Delta t^{(n+1)}}=\theta f^{(n+1)}+(1-\theta) f^{(n)} \tag{4.34}
\end{equation*}
$$

Here, the spatial derivative term of $f$ is identical to that in the steady-state calculation. This equation is setup for each fuel region with finite difference approximation. As in the channel equations, all the known values are set on RHS which results in a tridiagonal linear system as Eq. (4.35). Note that the spatial derivative term of $f$ which determines the lower and upper diagonal elements, $l_{i}$ and $u_{i}$ respectively, as well as $d_{i}$ is identical with those in the steady-state calculation, so most of the steady-state calculation routines can be reused. Only the time derivatives applied to the target fuel mesh (i) need to be additionally considered.

$$
\begin{align*}
& l_{i}^{(n+1)} T_{i-1}^{(n+1)}+\left(d_{i}^{(n+1)}-\frac{C_{p}}{\theta \Delta t}\right) T_{i}^{(n+1)}+u_{i}^{(n+1)} T_{i+1}^{(n+1)}  \tag{4.35}\\
& =q_{i}^{\prime \prime \prime(n+1)}+\frac{\bar{\theta}}{\theta} q_{i}^{\prime \prime(n)}+g\left(T_{i-1}^{(n)}, T_{i}^{(n)}, T_{i+1}^{(n)}\right)-\frac{C_{p}}{\theta \Delta t} T_{i}^{(n)} .
\end{align*}
$$

## Chapter 5. GPU Acceleration Strategies

GPU can be a desirable computing resource to substitute multi-core CPU parallelism in that they contain a substantial number of simple arithmetic cores which can deliver significant floating point computing power, enabling massive parallelism. In particular, this characteristic can be a great remedy for the critical downside of the pinwise two-step calculation that a tremendous amount of pinwise data should be treated. In this research, the NVIDIA CUDA [5] was chosen as the GPU programming tool kit to take advantages of its general applicability and ease of coding. In order to achieve high performance of GPU, memory optimization is particularly important. Three fundamental optimization requirements are presented in the following, which all the GPU calculation modules in VANGARD are developed to meet as far as possible.

1) Vectorization:

GPU is a subset of vector processors and is specialized in SIMD (Single Instruction Multiple Data) parallelisms, namely, the efficiency is maximized when threads in each warp perform SIMD operation. Therefore, braches that can make a part of threads inactive should be minimized.
2) Local memory use:

A GPU contains a substantial number of simple arithmetic cores, which can deliver significant floating point computing power. However, it is bounded by the performance of the relatively slow main memory, so a GPU contains several types of small but fast local memories to buffer the main memory accesses. Therefore, access to the main global memory should be minimized and frequently used data should be saved in high-bandwidth memories such as cache and register to have high performance.
3) Memory coalescing:

Even though the global memory access is required to be minimized due to its poor bandwidth, it is inevitable. In this case, a group of threads should read and write contiguous memory, which is called memory coalescing, so that the memory access in a warp that is the computational unit for the memory read and write operations should be concentrated.

Besides, numerous strategies were devised and introduced for the optimal and efficient GPU calculation for each solver. This chapter describes all details of the GPU acceleration strategies for the computational hotspots - nodal, CMFD, T/H, and depletion calculations - which take most parts of the total computing time.

### 5.1 Nodal Calculation

The characteristics of the nodal method make it suitable for GPU acceleration. First of all, the iteration scheme is highly regular and parallelizable in that every cell and energy group are solved independently with the same algorithm. The memory layout is also very much regular and contiguous, which enables coalesced memory accesses. In addition, the nodal kernel involves a lot of arithmetic operations for the calculation of expansion coefficients, and these variables are stored as local variables. Namely, the operational intensity and the local memory utilization are high. Costly exponential calculations in the SENM that were considered as a drawback can also be effectively handled on GPUs by exploiting the Special Function Units (SFU) of GPUs which provide hardware-level fast approximate single precision evaluations of some special math functions including exponentials.

In GPU implementation, exploiting single precision is highly desirable in terms of arithmetic performance and memory utilization. One of the key characteristics of the consumer-grade GPUs on which VAGNARD targets to be executed is that they are
dedicated to single precision arithmetic, while the support for double precision arithmetic is minimal. Hence, every arithmetic operation of the GPU nodal kernel needs to use single precision to achieve the maximum performance. However, using single precision can harm the accuracy and lead to numerical instabilities when handling large exponential terms which arise in the axial solution. To elaborate, the problem occurs when calculating the flux expansion coefficients in Eq. (3.7) where hyperbolic terms are involved. The term inserted to the hyperbolic functions is proportional to the mesh size, and it can lead to extremely large hyperbolic values when solving the axial direction which has a relatively large mesh size. To resolve this, a mixed precision scheme is employed, in which precisions are mixed in the axial 4th order kernel while single precision is employed entirely for the radial 2nd order kernel that does not suffer from the instability issues. In the axial kernel, double precision is employed for the ordinary arithmetic - namely the coefficients calculations - where a cascade effect of round-off errors may occur, while expensive hyperbolic functions are still computed in single precision. In this way, an optimal combination of precision is found with respect to performance, accuracy, and stability.

To confirm if this mixed precision technique is optimal, a sensitivity study was carried out with the APR1400 3D core problem, in which five different combinations of precisions are tested. The combinations of precisions for each test case are shown in Table 5.1. In the table, 'arithmetic' denotes the plain arithmetic operations other than the hyperbolic function calculations. Figure 5.1 presents the relative nodal computing time of each case with respect to the full single precision case (Case 1) and the maximum pin power error of each case compared to the results of the full double precision case (Case 5). In all cases, the impact of the choice of precisions on the accuracy is negligible, where the maximum pin power errors are way less than $0.0001 \%$. This verifies that the mixed precision approach is valid. Regarding the performance, the case in which double precision is used only for the arithmetic in
the axial kernel (Case 2) is the optimal except for Case 1, which can be easily expected. It can be also seen that employing single precision selectively for the hyperbolic functions renders much better performance than blindly using double precision. Thus, it is proved that Case 2 which is the current mixed precision approach is optimal since Case 1 incurs a stability problem.

Table 5.1 Tested combinations of precisions.

|  | Case 1 | Case 2 | Case 3 | Case 4 | Case 5 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Radial <br> Arithmetic | FP32 | FP32 | FP64 | FP32 | FP64 |
| Axial <br> Arithmetic | FP32 | FP64 | FP64 | FP64 | FP64 |
| Radial <br> Hyperbolic | FP32 | FP32 | FP32 | FP32 | FP64 |
| Axial <br> Hyperbolic | FP32 | FP32 | FP32 | FP64 | FP64 |



Figure 5.1 Relative nodal computing time and maximum pin power error of each case.

### 5.2 CMFD Calculation

All of the CMFD calculation modules are offloaded to GPU. Homogenization, linear system setup, power iteration, and pinwise solution update are all performed on GPU. Note that the CMFD calculation on GPU is performed entirely in double precision for the numerical stability of linear system solution. For the linear system solver, a preconditioned BiCGSTAB solver developed with the cuBLAS [27] and cuSPARSE [28] libraries are used, where the zero fill-in incomplete LU (ILU0) preconditioner provided by the cuSPARSE library is applied. The linear system matrix is stored in the Block Compressed Sparse Row (BSR) format whose block size is the number of energy groups. The BSR format inevitably contains some zeros and may result in a waste of memory and computations compared to the ordinary Compressed Sparse Row (CSR) format, but it makes the parallel matrix construction on GPU easier and may expose more parallelism to the libraries due to its more explicit block structure.

### 5.3 T/H Feedback Calculation

In the steady-state calculation, the T/H feedback calculation is very cheap because it uses a simplified model and it solves the coolant heat transfer equation only once per T/H calculation, owing to the fixed heat source with the concept that all heat generated in the pellet must be delivered to the coolant without accumulation in the fuel. As the result, T/H calculation takes only a little part of the total computing time.

On the contrary, in the transient calculation, the heat source for the coolant transfer equation is determined by the fuel temperature profile. It requires coupled iterative solutions, leading to repetitive steam table calculations for the coolant channel as well as linear system solutions for the intra-pellet temperature of each pin. Thus, the

T/H calculation time in the transient core analysis is non-negligible. Actually, when the T/H calculation was still performed on CPUs while the other time-consuming calculations such as nodal and cross section calculations were performed on a GPU, it was observed that the portion of the $\mathrm{T} / \mathrm{H}$ calculation becomes significantly large, taking the largest portion of the total computing time in transient analysis. For this reason, the $\mathrm{T} / \mathrm{H}$ modules were ported on GPU.

For the fuel heat conduction solution, a linear system is set up for each fuel cell and directly solved by the manually implemented tri-diagonal LU linear system solver by taking advantage of the pre-described tri-diagonal matrix format of the heat conduction equation solution. Since the linear system is solved independently for each fuel cell, straightforward parallelization is possible such that each thread solves a linear system of each fuel cell. Given the coolant bulk temperature as the boundary condition, intra-pellet temperature profile of each fuel cell is obtained by each thread.

For the coolant channel heat transfer solution, on the other hand, the fine-grained parallelization cannot be applied. The axial heat transfer calculation for a coolant channel is the representative sequential calculation which requires the solutions of the lower channel mesh as the boundary conditions. Therefore, it is not desired to parallelize the axial planes. Considering that VANGARD uses the assembly-level macro channel, as the result, the target mesh of the coolant channel calculation would be 3D assembly-level mesh. With coarse-grained parallelism, the GPU acceleration is not much effective. On the contrary, it was noted in Figure 5.2, which shows the speedup of a single GPU calculation time over 10-core CPU calculation time for the NEACRP HZP rod ejection problem on the quarter core, that the GPU calculation took more computing time than the 10 -core CPU calculation for the assembly channel and 4-box mesh channel which VANGARD adopts as the default channel option. Moreover, offloading the T/H channel calculation on GPU is cumbersome due to the lack of library support for the steam table which is readily usable in the CPU calculation.

For all of these reasons, the fuel pellet calculation is accelerated by GPU while the coolant channel calculation remained to be performed on CPU multi cores even in the GPU calculation mode. This kind of hybrid calculation requires the data transfer between the host and GPU device for the coupled heat conduction for fuel pellet heat convection for coolant channel equation solutions. Specifically, the coolant bulk temperature obtained in the channel calculation should be fed back to the pellet conduction solution as the boundary condition, and the heat flux obtained by the solution of the pellet fuel temperature profile should be transferred to the channel calculation to compose the heat source. In spite of the repetitive data transfer, the additional time for this is not that significant because the data size is small, which is dependent on the macro-level coolant channel meshes.


Figure 5.2 Speedup of coolant channel calculation time according to the number of divisions per assembly.

### 5.4 Depletion Calculation

The entire procedure of depletion calculation, including one-group reaction rate calculation and burnup system construction as well as the CRAM solver, is fully parallelized on GPU. All the operations on GPU employ double precision as the
range of the values treated in the depletion calculation is too wide for single precision to cover. The primary operation in the CRAM is the matrix inversion in Eq. (3.41), and VANGARD utilizes the Gauss-Seidel method for efficient inversion. The depletion calculation is essentially solving a large batch of cell-wise independent burnup systems possessing the same sparsity pattern, which is highly parallelizable and vectorizable. Thus, parallelization is applied to the cells, and each thread runs the Gauss-Seidel iteration for its cell for a prescribed number of times. The burnup matrices are stored in the non-zero major ordering scheme [29], which takes advantage of the common sparsity pattern and contiguously stores the matrix elements of all cells for each non-zero position, as described in Figure 5.3. As the result, accesses to the burnup matrices across the cells are fully coalesced. The matrices are stored in the CSR format except the diagonals whose inverses are separately stored as vectors for efficient Gauss-Seidel calculation, and the sparsity pattern is searched only once at the initialization stage. The vectors for representing the sparsity pattern are stored in a common and fast-access memory of GPU such as constant memory.


Figure 5.3 Schematics of the non-zero major ordering scheme for burnup matrices.

# Chapter 6. Challenges of Pinwise Two-Step Core Calculation and Resolutions 

### 6.1 Resolutions of Numerical Instability and Inaccuracy

There are many issues apparently observed in the pinwise two-step core calculation which have not been problematic in the conventional assemblywise twostep core calculation. This section will cover two methodological issues and the resolutions for them for practical and accurate pin-level core analyses.

One is numerical instability in the one-node pinwise nodal - assemblywise CMFD coupled calculation. The one-node nodal kernel requires both incoming currents and node average flux as the boundary conditions. However, the pinwise incoming currents cannot be directly updated from the assembly-level CMFD calculation while the pinwise average fluxes can be readily obtained by the CMFD solutions. It causes a lagging between the pinwise flux and the pinwise incoming currents, which in turn deteriorates the convergence and often incurs instability. To resolve this, the CMFD-Based Partial Current Update Scheme was devised which recalculates the pinwise partial currents using the CMFD solution so that not only the pinwise fluxes but also the pinwise partial currents reflect the CMFD calculation results.

The other is the depletion inaccuracy of gadolinia fuel. It originates from retaining the intra-assembly heterogeneities. Gadolinia fuels exhibit highly heterogeneous depletion behaviors inside the pellet which is induced by the large spatial selfshielding effect of Gadolinium (Gd). Since the heterogeneity information is completely lost during the homogenization process, naively depleting the Gd isotopes using the pin-homogenized quantities induces nonacceptable errors. To accurately predict the depletion of gadolinia fuels in the pinwise two-step core
calculations, a simple yet effective scheme was proposed. This scheme makes a correction of burnups of gadolinia fuel pins using the information of neighboring general fuel pins so that accurate cross sections can be used in the gadolinia fuels.

In the following subsections, these two methodological issues and resolutions for each are addressed in detail. The effectiveness of each resolution is also examined with the APR1400 [30] 2D core depletion calculation results.

### 6.1.1 CMFD-Based Partial Current Update Scheme

## Methodology

In the conventional assemblywise nodal codes, the nodal mesh and the CMFD mesh are neatly aligned, and two-node kernels whose only boundary condition is the node average flux are typically used. Therefore, the CMFD solver does not have to update the surface currents. In VANGARD, however, the radial CMFD mesh size is chosen much bigger than the nodal meshes to achieve higher computational efficiency in three-dimensional (3D) CMFD calculation. Specifically, a quarter of an assembly is taken as the radial CMFD mesh size so that a CMFD mesh consists of several tens of pin-sized nodal meshes. The linear system is set for the coarse meshes and the solutions obtained from the CMFD power iteration are the coarse mesh fluxes. Since the one-node kernel requires incoming partial currents which are to be updated by the CMFD solution, a special measure has to be devised to determine the nodewise partial current from the coarse mesh fluxes. Note that updating the pinwise average fluxes is trivial since the level of the pinwise fluxes can be adjusted by the ratio of the updated coarse mesh flux to the previous one. However, the pinwise incoming currents cannot be updated directly from the coarse mesh CMFD results.

To reflect the CMFD solution in the update of pinwise partial current, two types of CMFD current correction factors are employed. One is the standard CMFD net
current correction factor which is determined at the coarse mesh interface using the homogenized nodal solutions and is used for constructing the CMFD linear system for power iteration:

$$
\begin{equation*}
\hat{D}_{I+1 / 2}=\frac{-\tilde{D}_{I+1 / 2}\left(\bar{\phi}_{I+1}-\bar{\phi}_{I}\right)-J_{I+1 / 2}^{n e t}}{\bar{\phi}_{I}+\bar{\phi}_{I+1}} . \tag{6.1}
\end{equation*}
$$

The other is the outgoing partial current correction factor defined in the modified partial current based CMFD formulation, mp-CMFD [31], calculated at the fine mesh:

$$
\begin{equation*}
\hat{\hat{D}}_{i+1 / 2}^{+}=\frac{4 J_{i+1 / 2}^{+}+2 \tilde{D}_{i+1 / 2}\left(\phi_{i+1}-\phi_{i}\right)-\left(\omega_{i} \phi_{i}+\left(1-\omega_{i}\right) \phi_{i+1}\right)}{4 \phi_{i}} \tag{6.2}
\end{equation*}
$$

Note that the mp-CMFD correction factor is not used in the CMFD power iteration. It is only used to determine the pinwise outgoing currents from the modulated pinwise fluxes determined from the CMFD coarse mesh flux update. Namely, the pinwise outgoing partial current is not incorporated in the CMFD linear system but is used only for the subsequent nodal calculation. The following relation is used for the partial current update:

$$
\begin{equation*}
J_{i+1 / 2}^{+}=-\frac{1}{2} \tilde{D}_{i+1 / 2}\left(\phi_{i+1}-\phi_{i}\right)+\frac{1}{4}\left(\omega_{i} \phi_{i}+\left(1-\omega_{i}\right) \phi_{i+1}\right)+\hat{\hat{D}}_{i+1 / 2}^{+} \phi_{i} . \tag{6.3}
\end{equation*}
$$

Figure 6.1 schematically describes the two-level correction of surface partial currents where the detailed calculation procedure is given as follows:

1) Calculate the mp-CMFD outgoing partial current correction factors at the surfaces of each pin.
2) Homogenize pins into coarse meshes and calculate the standard CMFD net current correction factors for each coarse mesh.
3) Perform 3D CMFD calculation and update coarse mesh fluxes.
4) Modulate the pinwise fluxes using the updated coarse mesh fluxes.
5) Recalculate the outgoing currents for each pin using the pinwise mp-CMFD outgoing partial current correction factors and the modulated pinwise fluxes.
6) 


2)

3)

4)

5)


Figure 6.1 Schematic procedure of the two-level correction in the CMFD acceleration.

Figure 6.2 describes the overall algorithm of the nodal - CMFD iteration. The nodal sweep is done in red-black ordering in space and Jacobi in energy to expose a high degree of parallelism. The transverse leakage update is performed at each outer iteration instead of each inner iteration for stability, which turned out to have a negligible impact on the convergence rate. The nodal sweeper performs a fixed number of iterations at each nodal solve: 5 times of outer iterations with 6 times of inner iterations per outer iteration. On the other hand, the CMFD convergence criteria are imposed on error reductions. For the inner iteration in which the BiCGSTAB method is utilized as the linear system solver, relative residual reduction of 0.01 is used as the escape criterion. The outer iteration escapes when the $l_{2}$-norm of the relative fission source change reduces to below 0.5 times of its initial value
with minimum of 5 iterations, and the Wielandt shift scheme is applied. All the criteria were empirically determined to be optimal.

```
DO WHILE (!CONV)
    Update fission source
    DO Nodal outer iteration
        Update transverse leakage
        DO Nodal inner iteration
        DO Red-black sweep
            DO Node sweep
                DO Group sweep
                        Nodal kernel calculation
                END DO Group sweep
            END DO Node sweep
            Update incoming current
            END DO Red-black sweep
    END DO Nodal inner iteration
    Update fission source
    Update eigenvalue
END DO Nodal outer iteration
Homogenize for CMFD
Set CMFD linear system
Solve CMFD linear system
Update eigenvalue
Update fine-mesh flux
Update fine-mesh partial current
END DO
```

Figure 6.2 Nodal - CMFD iteration algorithm.

## Effects of CMFD-Based Partial Current Update Scheme

The effect of the partial current update was examined with an APR1400 2D core depletion calculation. $\mathrm{T} / \mathrm{H}$ feedback and CBC search were not carried out to prevent them from affecting the convergence. Figure 6.3 shows the fission source error at each nodal outer iteration at the beginning of cycle (BOC) with and without the partial current update. Note that in both cases the pinwise fluxes are updated by the

CMFD calculation. The CMFD calculation is performed for every 5 nodal outer iterations, and the partial current update follows after each CMFD calculation. It can be seen that the convergence rate is significantly improved with the partial current update, and as the result, the total number of the nodal and CMFD outer iterations for the entire depletion calculation are also substantially reduced, as presented in Table 6.1 which shows the total number of outer iterations during a depletion calculation consisting of 22 steps. In the table, the average number of outer iterations per step is given in parentheses. Approximately $60 \%$ of the iterations could be reduced by the partial current update.


Figure 6.3 Comparison of nodal outer fission source error reduction at the BOC.

Table 6.1 Comparison of the number of outer iterations in the depletion calculations.

| CMFD-based <br> partial current update | Nodal | CMFD | Ratio |  |
| :---: | :---: | :---: | :---: | :---: |
|  |  |  | Nodal | CMFD |
| off | $1135(51.6)$ | $4549(207)$ | 1.0 | 1.0 |
| on | $485(22.0)$ | $1901(86.4)$ | 0.43 | 0.42 |

### 6.1.2 Neighbor-Informed Burnup Correction Method

For the accurate prediction of Gd pin depletion, using the correct burnup of the Gd pin is very important. Since the capture reaction rates of Gd isotopes change sensitively with burnup, a small difference in burnup can significantly change the result. However, it is quite difficult to determine the burnup of a Gd pin correctly so that nontrivial errors can be induced in the core depletion calculation. In this regard, the so-called neighbor-informed burnup correction (NIBC) method is introduced in this section. The problem of using the own burnup of a Gd pin is identified in the next subsection and the rationale and procedure of the NIBC method will be presented in the second subsection.

## Problem Identification

In order to demonstrate the problem associated with Gd depletion, a 2D model of the APR1400 core, which is a commercial core loaded with a large amount of gadolinia for reactivity control, is analyzed under a fixed thermal-hydraulic (T/H) and boron condition. The core configuration is shown in Figure 6.4. The pin burnup distributions of VANGARD are compared with those of nTRACER whole-core transport calculation results.


Figure 6.4 Core configuration of APR1400 [32]

Figure 6.5 shows the maximum relative pin burnup errors for the APR1400 core. One is for all fuel pins, and the other is only for ordinary fuel pins while excluding Gd pins in the same core. This figure demonstrates that the maximum pin burnup errors occur at the Gd pins at most burnup steps. Figure 6.6 illustrates the pin burnup error distributions at the burnup of $0.05 \mathrm{MWD} / \mathrm{kg}, 10 \mathrm{MWD} / \mathrm{kg}$, and $18 \mathrm{MWD} / \mathrm{kg}$, which correspond to the beginning-of-cycle (BOC), middle-of-cycle (MOC), and end-of-cycle (EOC) steps, respectively. In early burnup steps, large errors occur at the ordinary fuel pins located at the core periphery while the errors at Gd pins are not noticeable. Only the environmental effects are dominant. However, the errors at Gd pins continuously grow as the core depletes. It is most dominant at MOC which involves a global tilt in the error distribution. Even with the global tilt, however, the maximum errors of the ordinary fuel pins remain below $3 \%$.

The opposite depletion behaviors of gadolinia and ordinary fuel pins can be explained by the self-regulation mechanism between burnup and power. In an ordinary fuel pin, lower burnup results in more fissile materials left, thereby leading to higher power. As the result, if an ordinary fuel pin was predicted to have less power than the normal value at a certain burnup step, the burnup is underestimated and it would increase the power at the next burnup step, which in turn increases burnup and suppresses power sequentially. In this manner, the burnup and power are continuously self-regulated by negative feedback during depletion in the case of ordinary fuel pins. In contrast, a lower burnup in a Gd pin results in more absorber materials left which would further suppress power. As the result, positive feedback occurs in the Gd pins: if a Gd pin is less depleted at a certain burnup step, not only the burnup but also the power is reduced in the next burnup step, and this continues until all the absorber materials are exhausted. In short, the burnup error of a Gd pin at the beginning is propagated throughout depletion and accumulated in a monotonous way.


Figure 6.5. Maximum relative pin burnup errors (\%) computed with and without gadolinia fuel pins at each burnup step.


Figure 6.6. Relative pin burnup error (\%) distributions at BOC (left), MOC (middle), and EOC (right).

## Rationale and Procedure of NIBC

Based on the above observation, it can be concluded that an accurate estimation of the Gd pin burnup using its own power history cannot be achieved due to the underlying physics and that it is necessary to introduce an external correction. In this regard, the NIBC method which is to utilize the average burnup of the neighboring

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ordinary fuel pins in representing the burnup state of a Gd pin is devised in this work. The rationale is that the Gd pin and its neighboring fuel pins would have been depleted under a similar environment, and the burnups of ordinary fuel pins can be predicted with high accuracy. Thus, the average burnup of its neighboring fuel pins can be a reliable indicator of the depletion state. The procedure for applying the NIBC method is set as follows:

1) In the group constant table, the XSs of each Gd pin are functionalized with the average burnup of its surrounding 8 ordinary fuel pins instead of its own burnup. If a neighboring pin is not an ordinary fuel pin, it is excluded from the average.
2) In the depletion calculation, the burnup of every pin is first updated normally. For the Gd pins, however, their own burnups are overridden by the average of the updated burnups of their neighboring fuel pins in the XS interpolation.

## Effects of the NIBC

As noted in Figure 6.7 which shows the reference multiplication factors of nTRACER and the errors of VANGARD solutions and Figure 6.8 which shows the maximum and RMS pin power errors at each burnup step, the NIBC method noticeably reduces the errors in the gadolinia depletion for both multiplication factor and pin powers. The negative biases in the multiplication factor which is as large as nearly 200 pcm at the MOC are clearly reduced to less than 20 pcm throughout the cycle. The improvements in the pin power errors are also meaningful in that the maximum pin power error of nearly $8 \%$ is reduced to well below $3 \%$ and the largest RMS error of over $2 \%$ is reduced to $0.7 \%$. Figure 6.9 illustrates the pin power error distributions at $9 \mathrm{MWD} / \mathrm{kg}$ where the peak pin power errors are observed. The peculiar errors at the Gd pins mostly disappear with the NIBC method. As the consequence, global error tilt is considerably reduced as well.


Figure 6.7 Comparison of multiplication factors.


Figure 6.8 Comparison of pin power errors between with and without NIBC.


Figure 6.9 Pin power error distributions (\%) at $9 \mathrm{MWD} / \mathrm{kgHM}$.

### 6.2 Resolutions of Memory Limitation

One of the significant issues accompanied with the pinwise two-step core calculation is the considerable memory requirement by the group constant (GC) data. The microscopic cross sections are tabulated for each pin, reaction type, energy group, and nuclide at each burnup step, and at some selected burnup steps, extra tabulations for branch points are further required. Therefore, the 8 G pinwise microscopic GC tables adopted in VANGARD result in tremendous data size. Actually, the size is more than 1,000 times larger than the 2 G assemblywise GC data. It thus imposes a significant restriction on offloading onto a GPU of which the available memory capacity is limited, and extremely deteriorates the practicality of the code. Thus, it is necessary to overcome the significant memory limitation of the GPU to exploit it to achieve feasible computing time.

This section describes two methods to reduce the memory burden and effectively
offload the pinwise group constant data to the limited memory of the GPU. One is the burnup window scheme with adaptively resizing sub-table which offload the group constant data only for the required burnup points for the current core state, and the other is the GC data compression scheme by the dimensionality reduction technique utilizing Singular Value Decomposition (SVD) and Low Rank Approximation (LAR).

### 6.2.1 Burnup Window Scheme with Adaptively Resizing Sub-table

It is practically impossible to store the entire group constant data on a GPU whose memory is very much limited, which prevents achieving the goal of VANGARD to be executed on PCs with consumer-grade GPUs. Thus, the burnup window scheme is introduced for an efficient porting of the group constant data to GPUs. In this scheme, a burnup window and a cross section sub-table are defined for each assembly type. In a core, assemblies of the same type are located at multiple positions and will have different burnup exposure with each other, but they will still share the same group constant data. The burnup window of an assembly type is defined by the minimum and maximum burnup exposures of the assemblies of that type in the core. Then, the cross section sub-table of the assembly type is defined such that it only contains the cross sections of the burnup range specified by the burnup window, which is then ported to GPU. As the result, only the cross section data of the burnup points necessary at the current core state are ported. The burnup windows and accordingly the cross section sub-tables are updated at each burnup step by scanning the burnup exposures of assemblies. Figure 6.10 shows an example of the burnup window of an arbitrary group constant data.


Figure 6.10 Example of burnup window (indicated as red-dotted box).

In the implementation of the cross section sub-table, the double-ended queue (deque) container of the $\mathrm{C}++$ Standard Template Library (STL) is utilized, which can be flexibly resized by adding and deleting elements at both front and back. It is preferred to the standard queue as a burnup window can occasionally move "forward" between predictor and corrector steps within a burnup step. Figure 6.11 schematically illustrates the adaptive resizing of a cross section sub-table by drawing necessary data from the group constant table and dropping unused data. The cross section data of each burnup point are first wrapped into a class object (packet) and pushed to the sub-table. When a packet is being pushed, its internal data are ported to GPU and only the pointers to the GPU data are kept in the sub-table. When a packet is being popped, its destructor is invoked which automatically wipes out its containing GPU data. Once the sub-table for a burnup step is established, its elements are cast into plain arrays of device pointers and provided to GPU because the deque container is not directly usable on the GPU side.


Figure 6.11 Implementation of a cross section sub-table with the deque container of the $\mathrm{C}++$ STL.

Even though the burnup window scheme alleviates the memory burden of GPUs, however, its effectiveness is decreased in the later burnup steps where the required burnup range is widened due to the non-uniform depletion of fuels across the core. It is apparent for the types of assemblies which are loaded in both interior and periphery of the core. The interior assemblies have high burnups while the peripheral ones have low burnups, but because they utilize the same group constant data, the burnup window has to cover both low and high burnups.

### 6.2.2 Cross Section Data Compression by Dimensionality Reduction

The burnup window scheme can alleviate the memory burden of GPUs by selectively porting only the necessary data at each burnup step, but it does not resolve the storage burden completely. In this regard, another measure to reduce the memory for GC table storage is implemented in VANGARD. It is the XS data compression technique proposed by Yamamoto et al. [33]. This technique makes an algebraic compression of the microscopic XS matrix off-line by an LRA and reconstructs the microscopic XSs on-the-fly. Note that the group constant data such as the
macroscopic scattering matrices, SPH factors, and fission spectra, which are defined macroscopically, are not compressed because their data sizes are not that large.

Consider an arbitrary $m \times n$ matrix $\mathbf{A}$ where $m \geq n$. The SVD of a matrix A is expressed as:

$$
\begin{equation*}
\mathbf{A}=\mathbf{U} \mathbf{\Sigma} \mathbf{V}^{T} \tag{6.4}
\end{equation*}
$$

where $\mathbf{U}(m \times m)$ and $\mathbf{V}(n \times n)$ are the orthogonal matrices whose columns are the left and right singular vectors of $\mathbf{A}$, respectively, and $\boldsymbol{\Sigma}(m \times n)$ is the diagonal matrix whose elements are the singular values arranged in the descending order. The magnitude of a singular value is related to the contribution of the corresponding singular vectors to the original matrix and typically the first a few singular values are dominant. This implies that the singular vectors corresponding to small singular values can be neglected. Using this fact, the LRA reduces the size of $\mathbf{U}, \mathbf{V}$, and $\mathbf{\Sigma}$ by eliminating the singular values smaller than the $k$-th singular value, where $k$ is the reduced rank, and their corresponding singular vectors. Consequently, the low-rank approximated matrix $\mathbf{A}_{k}$ is represented as:

$$
\begin{equation*}
\mathbf{A}_{k}=\mathbf{U}_{k} \boldsymbol{\Sigma}_{k} \mathbf{V}_{k}^{T} . \tag{6.5}
\end{equation*}
$$

By multiplying the left singular vector matrix $\mathbf{U}_{k}(m \times k)$ and the singular value matrix $\boldsymbol{\Sigma}_{k}(k \times k)$, the coefficient matrix $\mathbf{F}_{k}(m \times k)$ can be defined as:

$$
\mathbf{F}_{k}=\left(\begin{array}{ccc}
u_{11} & \cdots & u_{1 k}  \tag{6.6}\\
\vdots & \ddots & \vdots \\
u_{m 1} & \cdots & u_{m k}
\end{array}\right)\left(\begin{array}{ccc}
s_{1} & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & s_{k}
\end{array}\right)=\left(\begin{array}{ccc}
f_{11} & \cdots & f_{1 k} \\
\vdots & \ddots & \vdots \\
f_{m 1} & \cdots & f_{m k}
\end{array}\right) .
$$

Thus, $\mathbf{A}_{k}$ can be expressed as the multiplication of $\mathbf{F}_{k}$ and the right singular vector matrix $\mathbf{V}_{k}(n \times k)$ as:

$$
\mathbf{A}_{k}=\left(\begin{array}{c}
\mathbf{a}_{1}  \tag{6.7}\\
\vdots \\
\mathbf{a}_{m}
\end{array}\right)=\left(\begin{array}{ccc}
f_{11} & \cdots & f_{1 k} \\
\vdots & \ddots & \vdots \\
f_{m 1} & \cdots & f_{m k}
\end{array}\right)\left(\begin{array}{c}
\mathbf{v}_{1}^{T} \\
\vdots \\
\mathbf{v}_{k}^{T}
\end{array}\right)
$$

In consequence, each row vector of $\mathbf{A}_{k}$ can be represented as the linear combination of the coefficients and the right singular vectors as follows:

$$
\begin{equation*}
\mathbf{a}_{i}=f_{i, 1} \mathbf{v}_{1}^{T}+\cdots+f_{i, k} \mathbf{v}_{k}^{T} \tag{6.8}
\end{equation*}
$$

It is important to note that only $\mathbf{F}_{k}$ depends on the pins and state points since $\mathbf{V}_{k}$ can be constructed such that it depends only on the XS type, the energy group, and the nuclide type. Once $\mathbf{V}_{k}$ is constructed, the singular vectors can be reused at every pin and state point. This is a good feature for vectorization. The linear combination coefficients in Eq. (6.8) are recalculated by interpolating the coefficients in $\mathbf{F}_{k}$ at every iteration in which the core state is changed. It is assumed that the coefficients will have a similar dependency on the state point parameters as the XSs do. Thus, the conventional XS interpolation method is applied directly to the coefficients as well to yield:

$$
\begin{align*}
f_{i, j}\left(T_{m}, T_{f}, \rho, p p m\right)= & f_{i, j}\left(T_{m 0}, T_{f 0}, \rho_{0}, p p m_{0}\right) \\
& +\frac{\partial f_{i, j}}{\partial T_{m}} \Delta T_{m}+\frac{\partial f_{i, j}}{\partial \sqrt{T_{f}}} \Delta \sqrt{T_{f}}+\frac{\partial f_{i, j}}{\partial \rho} \Delta \rho+\frac{\partial f_{i, j}}{\partial(p p m)} \Delta(p p m) \tag{6.9}
\end{align*}
$$

For the decomposition, all the microscopic cross section data are first weighted by the corresponding flux and number densities and then cast into a single cross section matrix. Each row of the matrix contains the weighted microscopic cross sections of all the nuclides, energy groups, and reaction types at each pin and state point. The reason for weighting is to reflect the importance of each cross section element in terms of the actual contribution to the reaction rates so that the quality of the LRA is
improved. Also, it is important to note that $\kappa \sigma_{f}$, where $\kappa$ is the energy release per fission, should not be included in the matrix, as it is extremely prone to numerical errors due to its small magnitude which is lower by several orders than those of other cross sections. Errors in $\kappa \sigma_{f}$ lead to inaccurate power calculation and can have a substantial impact on depletion calculations as the flux normalization factors used in the depletion calculations rely on the calculated power. Therefore, $\kappa$ is stored separately and only $\sigma_{f}$ and $v \sigma_{f}$ are included in the matrix for the decomposition.

The XS matrix is constructed to be optimal considering the access patterns of $\mathbf{F}_{k}$ and $\mathbf{V}_{k}$ on GPU, as described in Figure 6.12 and Figure 6.13. The order of elements in each column, which determines the order of rows in $\mathbf{F}_{k}$, is arranged such that the outermost parameter is the burnup point, and for each burnup point, the XS vectors of the base condition and the branch conditions, if available, are arranged. In each XS vector, pins are arranged sequentially. They are located innermost because the interpolation of coefficients described by Eq. (6.9) is pinwise parallelized and it is desired to have adjacent threads access contiguous memory for coalescing on a GPU. The order of elements in each row, which determines the order of rows in $\mathbf{V}_{k}$, is arranged such that the outermost parameter is the reaction type, followed by the energy groups and nuclides. The linear combination in Eq. (6.8) is fully parallelizable over reaction types, energy groups, and nuclides although there are cases where only the XSs of a specific reaction type are required or energy groups need to be swept sequentially for one-group reaction rate calculation. However, the operations on the nuclides are always parallelizable in any case, thus it is desirable to locate the nuclides innermost.


Figure 6.12 Column structure of the cross section matrix.


| Group | Group | Group | $\ldots$ | Group |  |  | Group | Group |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 2 | 3 | $\cdots$ | $g$ | $\cdots$ | $N_{g}-2$ | $N_{g}-1$ | $N_{g}$ |


| Nuclide | Nuclide |  |  |  |  |
| :---: | :---: | :--- | :---: | :--- | :--- | :---: |
| 1 | 2 | Nuclide <br> $i$ |  |  | Nuclide <br> $N_{\text {nucl }}$ |

Figure 6.13 Row structure of the cross section matrix.

For a VANGARD group constant file containing 256 pins and 138 state points, the dimension of the XS matrix would be:

$$
\begin{aligned}
& m=256[\text { pins }] \times 138[\text { state points }]=35,328, \\
& n=32[\text { nuclides }] \times 8[\text { groups }] \times 5[\text { reactions }]=1,280
\end{aligned}
$$

which would require 172.5 MB of memory in single precision. After applying the compression technique with the reduced rank of 128, only $\mathbf{F}_{k}$ and $\mathbf{V}_{k}$ need to be stored, whose dimensions are:

$$
\begin{aligned}
& \mathbf{F}_{k}: m \times k=35,328 \times 128, \\
& \mathbf{V}_{k}: n \times k=1,280 \times 128
\end{aligned}
$$

which would require only 17.9 MB of memory. Consequently, nearly $90 \%$ of memory is reduced.

## Determination of the SVD Rank

In the dimensionality reduction technique employing the SVD and the LRA, the reduced rank for the LRA should be pre-determined. We have set the criterion to determine the reduced rank such that the sum of the cutoff singular values becomes less than $10^{-6}$ of the total, and the criterion was examined with the APR1400 basic fuel assembly group constants, whose results are shown in Figure 6.14. Following the result, we determined to globally use the first 128 singular values, which is the smallest multiple of 32 (the size of warp in CUDA) that satisfies the criteria of all types of assemblies.


Figure 6.14 Required rank of each assembly type.

## Effects of the Microscopic Cross Section Compression

The accuracy of the cross section reconstruction after the compression was investigated by comparing the APR1400 core depletion calculation results with the reference solutions obtained by using the original cross sections. Figure 6.15 presents the difference in critical boron concentration (CBC) and the maximum pin power
error at each burnup step in the core depletion calculation. Here, the group constants of not only the basic fuel assemblies but also the assemblies with spacer grids and the radial and axial reflector assemblies were compressed. In all burnup steps, the differences of CBC were less than 0.002 ppm , and the maximum pin power errors are of $0.0001 \%$ order. It confirms that the solution accuracy is unchanged after the compression even in core calculations.


Figure 6.15 CBC and pin power differences in the core depletion calculations.

Figure 6.16 shows the comparison of GPU memory usage at each burnup step. The memory usage changes at each burnup step due to the burnup window scheme. However, it should be noted that the burnup window scheme is not applied to the compressed cross sections; namely, the coefficient matrix of the entire burnup range and the right singular vector matrix are stored on GPU as a whole, and only the uncompressed group constant data such as the macroscopic scattering cross section matrices, SPH factors, and fission spectra are subject to the burnup window scheme and ported adaptively. Nevertheless, it does not serve as a large memory burden as the compression is done very effectively. On the contrary, as the decomposed matrices are ported only once at the initialization stage and employed throughout the rest of the calculation, the overhead of constructing the cross section sub-tables at

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each burnup step is reduced. In addition, the GPU memory usage becomes stable and predictable as most of the required memory is reserved at the initialization stage, which eliminates the risk of running out of memory during calculation. Consequently, the peak GPU memory usage is reduced from $\sim 17 \mathrm{~GB}$ to $\sim 9.2 \mathrm{~GB}$. As shown in Table 6.2, the group constant file size for each fuel assembly type is also substantially reduced by the compression technique to yield a $73 \%$ reduction in memory.


Figure 6.16. Comparison of GPU memory usages.

Table 6.2 Comparison of group constant file sizes.

|  | Original | Compressed |
| :---: | :---: | :---: |
| File Size (MB) | 236.8 | 64.8 |

## Chapter 7. Verifications and Validations

The solution accuracy and simulation capabilities of VANGARD were comprehensively examined through cycle depletion calculations for a series of real cores of APR1400 [30], AP1000 [34], and BEAVRS benchmark [18] problems. For all core problems, nTRACER direct whole core depletion calculations were performed to generate the reference solution such that consistent comparisons are possible with the same multi-group cross section library for both VANGARD and nTRACER calculations. In the VANGARD calculations, the pinwise and groupwise SPH factors are employed which are functionalized in the same way as the regular cross sections. In the following sections through $7.1-7.3$, the specification of each core is given and the accuracy of VANGARD is then assessed by the comparison with the nTRACER direct whole core calculation results and, if needed, measured data and the PRAGMA Monte Carlo calculation results are also used as the reference. For all cores, the axial structures were explicitly modeled as precisely as possible. Group constants for the assemblies bearing spacer grids and the axial reflector assemblies were separately generated and used. The transient solution accuracy was examined by the HZP rod ejection problems of the NEACRP benchmark in Section 7.4. As in the core cycle depletions, the results of VANGARD are compared with the nTRACER solutions.

### 7.1 APR1400 Initial Core Depletion

APR1400 is a Generation III large power reactor of Korea. The core is loaded with 241 fuel assemblies of $16 \times 16$ lattice and extensively utilizes the gadolinia burnable absorbers to control excess reactivity. The initial core of APR1400 is loaded with nine types of fuel assemblies that are classified according to the fuel enrichment and
the gadolinia content, as illustrated in Figure 7.1 along with the loading pattern. This core was chosen as the target problem for the verification of VANGARD due to its representativeness of typical PWRs, its large size that increases the computational complexity, and the existence of gadolinia fuels that enables to examine the gadolinia fuel depletion scheme of VANGARD.


Figure 7.1 Initial core loading pattern of the APR1400 core [32].

The core was depleted up to $18 \mathrm{MWD} / \mathrm{kgHM}$, and 21 burnup steps including the BOC were simulated in total with and without the NIBC option. Figure 7.2 shows the 3D power distributions calculated by VANGARD with NIBC at the BOC, MOC ( $8 \mathrm{MWD} / \mathrm{kgHM}$ ), and EOC.

The CBC letdown curves ant the errors are shown in Figure 7.3. It seems that the CBC errors are larger with the NIBC method, however, it can be easily found that it is merely due to error cancellation. Without NIBC, the gadolinia burnable absorbers are depleted slower than they should be, which can be confirmed by the large negative pin power errors noted for the Gd pins at the MOC illustrated in Figure 7.4. This introduces a significant negative bias in reactivity, which cancels out with the baseline positive reactivity errors. In terms of the power distributions, the improvement of errors with the burnup correction is clearer. At the MOC where the
peak pin power error occurs, the maximum and RMS pin power errors are substantially reduced from $4.3 \%$ and $0.9 \%$ to $1.7 \%$ and $0.5 \%$, respectively, as presented in Figure 7.5. As the peculiar errors at the gadolinia fuel pins are removed, global power distributions are improved as well, which can be seen clearly by the notable reduction of the global power error tilt at the MOC shown in Figure 7.4. The axial power distributions and error distributions with NIBC are shown in Figure 7.6. The axial power distributions are also significantly improved where the peak maximum and RMS errors are reduced from $8 \%$ and $4.8 \%$ to $2.9 \%$ and $1.8 \%$, respectively, as shown in Figure 7.7.

As a whole, VANGARD presents fairly good agreements with nTRACER. CBC differences are kept below 15 ppm , and the maximum and RMS pin power errors do not exceed $2 \%$ and $0.5 \%$, respectively. The axial power demonstrates slightly higher degree of errors, as the maximum and RMS errors reach $4 \%$ and $2 \%$, respectively. Nonetheless, considering that the axial core structures were explicitly modeled in detail which tend to be smeared in the conventional design codes, the errors are considered acceptable.


Figure 7.2. APR1400 power distributions at BOC, MOC, and EOC.


Figure 7.3. CBC letdown curves and errors for the APR1400 initial core.


Figure 7.4. Pin power error (\%) distributions at BOC (left), MOC (middle), and EOC (right) for the APR1400 initial core.


Figure 7.5. Maximum and RMS pin power errors at each burnup step for the APR1400 initial core.


Figure 7.6 Axial power and error (\%) distributions with NIBC at BOC (left), MOC (middle), and EOC (right).

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Figure 7.7. Maximum and RMS axial power errors at each burnup step for the APR1400 initial core.

### 7.2 AP1000 Initial Core Depletion

AP1000 is the representative Generation III + advanced nuclear power plant developed by the Westinghouse Electric Company. Its core employs many advanced design concepts such as fuel enrichment zoning, axial blankets with annular fuels for accommodating fission gas release, and combination of multiple types of burnable absorbers: Wet Annular Burnable Absorbers (WABA) of different axial lengths and Integral Fuel Burnable Absorbers (IFBA). The initial core loading pattern is illustrated in Figure 7.8. The core is loaded with 157 fuel assemblies of $17 \times 17$ lattice which are grouped into five regions according to the enrichment ranging widely from 0.74 to $4.8 \mathrm{wt} \%$. IFBAs and WABAs are contained in the region 4 and 5 where high-enriched fuels are loaded. The WABAs are classified as short, intermediate, and long WABAs depending on the length of the absorber regions, as described in Figure 7.9, and they are all inserted at the same time, which causes severe heterogeneity in the axial direction. As the result, the core is highly
heterogeneous in both radial and axial directions, posing challenges in modeling and simulation. Such complexity makes the core suitable for verifying the solution capability of VANGARD.

|  | H | G | F | E | D | C | B | A |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 2 | 4 | 2 | 4 | 2 | 4 | 5B | 3 |
| 2 | 4 | 2 | 4 | 2 | 4 | 2 | 5A | 1 |
| 3 | 2 | 4 | 2 | 4 | 2 | 5C | 3 |  |
| 4 | 4 | 2 | 4 | 2 | 5C | 3 | 1 |  |
| 5 | 2 | 4 | 2 | 5C | 2 | 3 |  |  |
| 6 | 4 | 2 | 5C | 3 | 3 |  |  |  |
| 7 | 5B | 5A | 3 | 1 |  |  |  |  |
| 8 | 3 | 1 |  |  |  |  |  |  |

Figure 7.8 Initial core loading pattern of the AP1000 core [35].


Figure 7.9 Axial configurations of fuel rods and WABAs of the AP1000 core [35].

The core was depleted up to $18 \mathrm{MWD} / \mathrm{kgHM}$ using 23 burnup steps including the BOC. Figure 7.10 shows the 3D power distributions calculated by VANGARD at the BOC, MOC, and EOC. The CBCs match closely within 14 ppm as shown in Figure 7.11, and the agreement in the pin power distributions is also quite good as shown in Figure 7.12 and Figure 7.13 in that the largest maximum and RMS errors which occur at BOC are only $1.76 \%$ and $0.54 \%$, respectively. The errors smoothly decrease by annealing to nearly $0.9 \%$ and $0.3 \%$ at the EOC, respectively. The axial power reveals slightly larger errors than radial pin power, especially at the early stage of the
cycle where the maximum and RMS errors reach $3.8 \%$ and $2.3 \%$, respectively, as seen in Figure 7.14 and Figure 7.15. However, given the extreme axial heterogeneity introduced by the WABAs of different lengths, the errors are within an acceptable level for a two-step design code. Rather, it should be emphasized that such detailed axial representation is possible with VANGARD to yield reasonable accuracy.


Figure 7.10 AP1000 power distributions at BOC, MOC, and EOC.


Figure 7.11. CBC letdown curves and errors for the AP1000 initial core.

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Figure 7.12. Maximum and RMS pin power errors at each burnup step for the AP1000 initial core.


Figure 7.13. Pin power error (\%) distributions at BOC (left), MOC (middle), and EOC (right) for the AP1000 initial core.

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Figure 7.14. Maximum and RMS axial power errors at each burnup step for the AP1000 initial core.


Figure 7.15. Axial power and error (\%) distributions at BOC (left), MOC (middle), and EOC (right) for the AP1000 initial core.

### 7.3 BEAVRS Benchmark Problems

BEAVRS (Benchmark for Evaluation And Validation of Reactor Simulations) [18] benchmark provides detailed descriptions of the two operational cycles of a commercial nuclear power reactor as well as the measured data including HZP physics test results, boron letdown curves, and detector signals. A series of problems of BEAVRS benchmark is quite suitable for comprehensively verifying the extensive capabilities of VANGARD such as the restart/reloading, control rod movements during depletion, and load follow calculation capabilities.

The BEAVRS cores are loaded with 193 fuel assemblies of $17 \times 17$ lattice which are specified according to the enrichments and burnable absorber (BA) configurations. The fuel loading pattern of the Cycle 1 is shown in Figure 7.16 where the indices on several assemblies denote the number of BA pins. The shuffling pattern for the Cycle 2 core is shown in Figure 7.17.

As in the previous two core cases, the comparisons were made mainly against the nTRACER transport solutions, however, in the case that nTRACER cannot provide the reference solutions due to the lack of simulation capabilities such as control rod movements and load follow operation, PRAGMA solutions were used as the reference. Furthermore, BEAVRS provides measurements, therefore, if measurements are available, they were also used as the references. This section covers the HZP physics tests, HFP depletion, and load follow operation for each cycle.


Figure 7.16 Loading pattern of the BEAVRS Cycle 1 core [18].


Figure 7.17 Shuffling pattern of the BEAVRS Cycle 2 core [18].

### 7.3.1 Hot Zero Power Physics Tests

The critical boron concentrations under various control rod bank insertion conditions for the Cycle 1 are compared in Table 7.1. The estimated CBC of VANGARD matches well with measurements in that the maximum difference occurring in the most intensely rodded case is only 24 ppm . Considering that the design review criterion (DRC) of the CBC in a typical HZP physics test is 50 ppm [36], this difference is quite acceptable. In code-to-code comparisons with PRAGMA and nTRACER, it shows much better accuracy for all cases. Especially compared with nTRACER solutions, the differences for all cases are within 2 ppm .

The control rod bank worth (CRBW) for the full insertion sequence is calculated by the difference of reactivity between before and after inserting the target control rod in the core with the earlier inserted rods loaded under the critical condition made by the pre-calculated CBC for each rodded case. The VANGARD solutions for the Cycle 1 are compared with those of nTRACER and PRAGAM as well as measurements, as shown in Table 7.2. Compared with the measurements, the estimated CRBWs show good agreements. For all cases, the maximum absolute and relative errors do not exceed 50 pcm and $5.0 \%$, respectively. They are far less than the DRC for the individual bank worths which are defined as the smaller one between 100 pcm and $15 \%$. As in the CBC comparisons, VANGARD solutions for CRBW agree well with those of PRAGMA and nTRACER within 20 pcm and $3.0 \%$.

The isothermal temperature coefficient (ITC) is compared in Table 7.3. In all codes, it is calculated in the same manner by making the $5^{\circ} \mathrm{F}$ perturbation to the inlet temperature. On the contrary to the CBCs and CRBWs, VANGARD shows significantly large differences in the ITCs from the measurements. VANGARD tends to underestimate the ITCs, but this tendency is observed in two other code calculation results. Meanwhile, it still shows good agreements with the solutions of PRAGMA and nTRACER with negligible errors.

Table 7.1 Comparison of HZP critical boron concentrations (ppm) of BEAVRS Cycle 1.

| Case | Measured <br> $(\mathrm{M})$ | PRAGMA <br> $(\mathrm{p})$ | nTRACER <br> $(\mathrm{n})$ | VANGARD <br> $(\mathrm{V})$ | $\mathrm{V}-\mathrm{M}$ | $\mathrm{V}-\mathrm{P}$ | $\mathrm{V}-\mathrm{n}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ARO | 975 | 978 | 969.43 | 967.90 | -7 | -10 | -1.53 |
| D in | 902 | 917 | 908.67 | 907.06 | 5 | -10 | -1.61 |
| C, D in | 810 | 817 | 810.24 | 809.16 | -1 | -8 | -1.08 |
| B, C, D in | - | 725 | 719.14 | 717.39 | - | -8 | -1.75 |
| A, B, C, D in | 686 | 679 | 673.46 | 672.69 | -13 | -6 | -0.77 |
| A, B, C, D, SE, in | - | 638 | 633.45 | 633.63 | - | -4 | 0.18 |
| A, B, C, D, SE, SD in | - | 575 | 570.92 | 571.15 | - | -4 | 0.23 |
| A, B, C, D, SE, SD, SC in | 508 | 486 | 484.36 | 483.77 | -24 | -2 | -0.59 |

Table 7.2 Comparison of HZP control rod bank worths (pcm) of BEAVRS Cycle 1.

| Case | Measured <br> $(\mathrm{M})$ | PRAGMA <br> $(\mathrm{p})$ | nTRACER <br> $(\mathrm{n})$ | VANGARD <br> $(\mathrm{V})$ | V -M | V -P | V -n |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| D in | 788 | 783 | 781 | 781 | -7 <br> $(-0.9 \%)$ | -2 <br> $(-0.2 \%)$ | 0 <br> $(0.0 \%)$ |
| C with D in | 1203 | 1255 | 1246 | 1239 | 36 <br> $(3.0 \%)$ | -16 <br> $(-1.3 \%)$ | -7 <br> $(-0.6 \%)$ |
| B with D, C in | 1171 | 1220 | 1210 | 1217 | 46 <br> $(3.9 \%)$ | -3 <br> $(-0.3 \%)$ | 6 <br> $(0.5 \%)$ |
| A with D, C, B in | 548 | 587 | 585 | 570 | 22 <br> $(4.1 \%)$ | -17 <br> $(-2.9 \%)$ | -15 <br> $(-2.6 \%)$ |
| SE with D, C, B, A in | 461 | 497 | 494 | 482 | 21 <br> $(4.6 \%)$ | -15 <br> $(-3.0 \%)$ | -12 <br> $(-2.5 \%)$ |
| SD with D, C, B, A, SE in | 772 | 784 | 778 | 777 | 5 <br> $(0.6 \%)$ | -7 <br> $(-0.9 \%)$ | -1 <br> $(-0.1 \%)$ |
| SC with D, C, B, A, SE, SD in | 1099 | 1115 | 1097 | 1104 | 5 <br> $(0.5 \%)$ | -11 <br> $(-1.0 \%)$ | 7 <br> $(0.7 \%)$ |

Table 7.3 Comparison of HZP isothermal temperature coefficients ( $\mathrm{pcm} /{ }^{\circ} \mathrm{F}$ ) of BEAVRS Cycle 1.

| Case | Measured <br> $(\mathrm{M})$ | PRAGMA <br> $(\mathrm{p})$ | nTRACER <br> $(\mathrm{n})$ | VANGARD <br> $(\mathrm{V})$ | $\mathrm{V}-\mathrm{M}$ | $\mathrm{V}-\mathrm{P}$ | $\mathrm{V}-\mathrm{n}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ARO | -1.75 | -2.98 | -2.80 | -3.00 | -1.25 | -0.02 | -0.20 |
| D in | -2.75 | -4.56 | -4.40 | -4.40 | -1.65 | 0.16 | 0.00 |
| D, C in | -8.01 | -9.43 | -9.40 | -9.40 | -1.39 | 0.03 | 0.00 |

Since the nTRACER code is not capable of elaborate load follow calculation and control rod movements during depletion, the comparisons against nTRACER solutions cannot be made for the Cycle 2. Instead, the VANGARD solutions were compared with the measurements and the PRAGMA solutions, which are shown in Table 7.4 - Table 7.6. In the reloaded cores as well, the CBC differences from the measurements are sufficiently small within 20 pcm . The differences from PRAGMA solutions are entirely negligible. In the case of CRBWs, the errors from the measurements were still within the design criterion in that for all cases the absolute and relative errors are smaller than 50 pcm and $15 \%$. The error of total CRBW of $4.1 \%$ is also smaller than the DRC of $8.0 \%$. The ITC for the Cycle 2 ARO case was estimated larger than the measurement by $0.9 \mathrm{pcm} /{ }^{\circ} \mathrm{F}$, but the difference from the PRAMGA solutions is sufficiently small.

Table 7.4 Comparison of HZP critical boron concentrations (ppm) of BEAVRS
Cycle 2.

| Case | Measured <br> $(\mathrm{M})$ | PRAGMA <br> $(\mathrm{P})$ | VANGARD <br> $(\mathrm{V})$ | $\mathrm{V}-\mathrm{M}$ | $\mathrm{V}-\mathrm{P}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| ARO | 1405 | 1390.5 | 1390.8 | -14.3 | 0.3 |
| C in | 1273 | 1289.3 | 1289.5 | 16.5 | 0.2 |

Table 7.5 Comparison of HZP control rod bank worths (pcm) of BEAVRS Cycle 2.

| Case | Measured <br> $(\mathrm{M})$ | PRAGMA <br> $(\mathrm{P})$ | VANGARD <br> $(\mathrm{V})$ | $\mathrm{V}-\mathrm{M}$ | $\mathrm{V}-\mathrm{P}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| D in | 426 | 480.3 | 475.2 | 49.2 <br> $(11.6 \%)$ | -5.0 <br> $(-1.1 \%)$ |
| C in | 1014 | 1027.4 | 1027.4 | 13.4 <br> $(1.3 \%)$ | 0.0 <br> $(0.0 \%)$ |
| B in | 716 | 734.4 | 711.0 | -5.0 <br> $(-0.7 \%)$ | -23.3 <br> $(-3.2 \%)$ |
| A in | 420 | 399.6 | 408.7 | -11.3 <br> $(-2.7 \%)$ | 9.1 <br> $(2.3 \%)$ |
| SE in | 438 | 440.9 | 444.0 | 6.0 <br> $(1.4 \%)$ | 3.0 <br> $(0.7 \%)$ |
| SD in | 305 | 360.3 | 348.2 | 43.2 <br> $(14.2 \%)$ | -12.1 <br> $(-3.4 \%)$ |
| SC in | 307 | 358.3 | 346.2 | 39.2 <br> $(12.8 \%)$ | -12.1 <br> $(-3.4 \%)$ |
| SB in | 781 | 821.7 | 808.5 | 27.5 <br> $(3.5 \%)$ | -13.2 <br> $(-1.6 \%)$ |
| SA in | 326 | 374.4 | 359.3 | 33.3 <br> $(10.2 \%)$ | -15.1 <br> $(-4.0 \%)$ |
| Total | 4733 | 4997.3 | 4928.5 | 195.5 <br> $(4.1 \%)$ | -68.8 <br> $(-1.4 \%)$ |

Table 7.6 Comparison of HZP isothermal temperature coefficients ( $\mathrm{pcm} /{ }^{\circ} \mathrm{F}$ ) of BEAVRS Cycle 2.

| Case | Measured <br> $(\mathrm{M})$ | PRAGMA <br> $(\mathrm{P})$ | VANGARD <br> $(\mathrm{V})$ | $\mathrm{V}-\mathrm{M}$ | $\mathrm{V}-\mathrm{P}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| ARO | 1.71 | 0.69 | 0.80 | -0.91 | 0.11 |

### 7.3.2 Hot Full Power Depletions

The Cycle 1 and 2 depletion calculations under the constant power level of $100 \%$ were performed. Since the measured data for CBC are provided, the CBC at each burnup step of both cycles was compared with measurements as well as with the nTRACER solution.

Figure 7.18 shows the 3D power distributions calculated by VANGARD at the BOC, MOC, and EOC. For the Cycle 1, both nTRACER and VANGARD estimate CBCs lower than the measurement with the maximum difference of 37 ppm , as presented in Figure 7.19. However, it is still in an acceptable range. On the other hand, the CBC differences between VANGARD and nTRACER are negligible throughout the whole burnup steps where the largest difference is only 6 ppm .

The pin power distributions and the axial power distributions were compared with those of nTRACER. The maximum and RMS pin power error trends along the burnup are shown in Figure 7.20, and the pin power error distributions at BOC, MOC, and EOC are demonstrated in Figure 7.21. The excellent agreements between the two codes are verified in the pin power comparisons where the maximum and RMS pin power errors are kept below $0.8 \%$ and $0.3 \%$, respectively, during the depletion except for at the BOC. The axial power distributions are also estimated close to those of nTRACER, as demonstrated in Figure 7.22 and Figure 7.23. At all burnup steps, the maximum and RMS axial power errors are within $3 \%$ and $1 \%$. However, the axial power errors are increasing with significant oscillation especially near the EOC, which turned out to be caused by the xenon oscillation. Thus, further investigation to alleviate this effect is needed to ensure consistently high accuracy in axial power distributions.


Figure 7.18 BEAVRS Cycle 1 power distributions at BOC, MOC, and EOC under the HFP condition.


Figure 7.19 CBC letdown curves and errors for the BEAVRS Cycle 1 core under the HFP condition.

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Figure 7.20 Maximum and RMS pin power errors at each burnup step for the BEAVRS Cycle 1 core under the HFP condition.


Figure 7.21 Pin power error (\%) distributions at BOC (left), MOC (middle), and EOC (right) for the BEAVRS Cycle 1 core under HFP condition.


Figure 7.22 Maximum and RMS axial power errors at each burnup step for the BEAVRS Cycle 1 core under the HFP condition.


Figure 7.23 Axial power and error (\%) distributions at BOC (left), MOC (middle), and EOC (right) for the BEAVRS Cycle 1 core under HFP condition.
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The 3D power distributions and burnup distributions of the Cycle 2 calculated by VANGARD at the BOC, MOC, and EOC are illustrated in Figure 7.24 and Figure 7.25 , respectively. For the Cycle 2 as well, The CBCs estimated by VANGARD match well with the measurements and with the nTRACER solutions within 20 ppm and 15 ppm , respectively, as shown in Figure 7.26. The pin powers are in good agreement with nTRACER as demonstrated in Figure 7.27 and Figure 7.28. At all burnup steps except for the BOC, the maximum and RMS pin power errors are within $1.5 \%$ and $0.5 \%$, respectively. The axial power distributions are also in good agreement with nTRACER throughout the whole burnup steps, as shown in Figure 7.29 and Figure 7.30. For most burnup steps, the maximum and RMS axial power errors are lower than $3 \%$ and $1 \%$, respectively. The high solution accuracy for the Cycle 2 calculation proves the soundness of the restart and reloading capability of VANGARD.

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. The most significant factor is the environment effect caused by inter-assembly heterogeneity. This effect is introduced more severely in the Cycle 2 core where high-enriched fresh fuel assemblies are loaded between shuffled assemblies from the Cycle 1. As noted in Figure 7.25, there must be severe gradients in burnup in the reloaded core. However, this cannot be elaborately predicted in two-step core calculations which employ pregenerated pin-homogenized cross sections from lattice calculations. Another factor to cause errors only to reloaded cores is the inability to rigorously consider the history effect of BA-withdrawn assemblies where the BA rods are loaded in the Cycle 1 core but withdrawn in the Cycle 2 core. In order to rigorously simulate the extraction of BA rods between cycles, it should use group constants generated from an unnatural lattice calculation where an assembly is depleted with BA rods until a certain burnup corresponding to the end of Cycle 1 and then depleted without BA
rods. However, it is practically impossible because the group constants for an assembly are generated for the lifetime of the assembly which spans three cycles at once. Therefore, in VANGARD, for the Cycle 2 calculation of those BA-withdrawn assemblies, the group constants of the corresponding base assembly which has the same enrichment but does not contain BA rods are used. It entails an inevitable limitation that the depletion history with BA rods loaded of the previous cycle cannot be incorporated in the group constants.


Figure 7.24 BEAVRS Cycle 2 power distributions at BOC, MOC, and EOC under the HFP condition.


Figure 7.25 BEAVRS Cycle 2 burnup distributions at BOC, MOC, and EOC under the HFP condition.


Figure 7.26 CBC letdown curves and errors for the BEAVRS Cycle 2 core under the HFP condition.


Figure 7.27 Maximum and RMS pin power errors at each burnup step for the BEAVRS Cycle 2 core under the HFP condition.


Figure 7.28 Pin power error (\%) distributions at BOC (left), MOC (middle), and EOC (right) for the BEAVRS Cycle 2 core under the HFP condition.


Figure 7.29 Maximum and RMS axial power errors at each burnup step for the BEAVRS Cycle 2 core under the HFP condition.


Figure 7.30 Axial power and error (\%) distributions at BOC (left), MOC (middle), and EOC (right) for the BEAVRS Cycle 2 core under the HFP condition.

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### 7.3.3 Load Follow Calculations

BEAVRS benchmark provides measured data for boron letdown curves and detector signals along with power history and the control rod bank positions at each burnup step. Due to the lack of capability of control rod movement during depletion and load follow calculation of nTRACER, the code-to-code comparisons in this section were made with PRAGMA solutions.

Based on the actual power history, the power level model was simplified so that total 31 burnup points were determined to be simulated which consists of burnup points at which the measured data are provided and the burnup points right before and after the reactor trip where the power level drastically changes, as presented in Figure 7.31. Note that for the T/H feedback and xenon feedback calculation within a specific burnup step, the core power provided at that burnup point is used, and for the depletion calculation, the average core power during the burnup step is used.

The CBC letdown curves are compared in Figure 7.32. Compared to the measurements, the non-negligible differences are observed at the later burnup steps, which exceeds the acceptance criterion, 50 ppm , but this trend is observed in PRAGMA results as well. The large errors at the later burnup steps are also noted in the core follow results of another deterministic transport code nTER [37]. Considering that the large differences from the measurements at the later burnup steps are commonly observed in the various code calculations, these errors might be originated from the uncertainties of measurements and the inability to simulate the actual power history accurately. Meanwhile, the differences between VANGARD and PRAGMA solutions are kept below 15 ppm during depletion. Not only in CBCs but also in pin powers, VANGARD shows excellent agreements with PRAGMA as shown in Figure 7.33 and Figure 7.34. The largest maximum and RMS pin power errors during the depletion are only $2.2 \%$ and $0.5 \%$, respectively.

The comparisons of detector signals at BOC, MOC, and EOC are demonstrated through Figure 7.35 - Figure 7.37, and those at all burnup steps are summarized in Table 7.7. As in the CBC comparisons, large differences from the measurements are observed at the later burnup steps in which the maximum error of the detector signal reaches nearly $7.5 \%$. Nonetheless, the maximum errors do not exceed $5 \%$ except for the EOC, and the RMS errors are kept below $2.5 \%$, which results in the average RMS error throughout the whole burnup steps of $1.6 \%$. Through the code-to-code comparison with PRAGMA, the high accuracy was confirmed in that the maximum errors are within $2.5 \%$, and the average RMS error of all burnup steps is only $0.6 \%$.


Figure 7.31 Power history and control rod bank positions of the Cycle 1 load follow operation.


Figure 7.32 CBC letdown curves and errors for the BEAVRS Cycle 1 core under the load follow operation.


Figure 7.33 Maximum and RMS pin power errors at each burnup step for the BEAVRS Cycle 1 core under the load follow operation (ref.: PRAGMA).

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Figure 7.34 Pin power error (\%) distributions at BOC (left), MOC (middle), and EOC (right) for the BEAVRS Cycle 1 core under the load follow operation (ref.: PRAGMA).


|  | H | G | F | E | D | C |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 8 | 0.9423 0.9386 -0.37\% |  |  |  |  |  |
| 9 | $\begin{array}{r\|} \hline 0.7845 \\ 0.7804 \\ -0.41 \% \\ \hline \end{array}$ | $\begin{array}{r} \hline 1.0368 \\ 1.0314 \\ -0.54 \% \\ \hline \end{array}$ |  |  | PRAGMA VANGARD Diff. |  |
| 10 | $\begin{aligned} & 1.0836 \\ & 1.0814 \end{aligned}$ | $\begin{aligned} & 0.9075 \\ & 0.9044 \end{aligned}$ | $\begin{aligned} & 1.1597 \\ & 1.1585 \end{aligned}$ |  | RMS | 0.34\% |
|  | -0.23\% | -0.31\% | -0.12\% |  | Max | 1.16\% |
| 11 | 0.9369 <br> 0.9351 <br> 0.18\% | 1.1665 <br> 1.1623 <br> -0.42\% | $\begin{gathered} \hline 0.9823 \\ 0.9790 \\ -0.33 \% \\ \hline \end{gathered}$ | $\begin{array}{r} 1.2655 \\ 1.2619 \\ -0.36 \% \\ \hline \end{array}$ |  |  |
| 12 | $\begin{array}{c\|} \hline 1.1637 \\ 1.1646 \\ 0.09 \% \\ \hline \end{array}$ | $\begin{gathered} \hline 0.9658 \\ 0.9640 \\ -0.18 \% \end{gathered}$ | $\begin{gathered} \hline 1.2146 \\ 1.2126 \\ -0.20 \% \end{gathered}$ | $\begin{array}{r\|} \hline 1.0593 \\ 1.0581 \\ -0.12 \% \\ \hline \end{array}$ | 1.3006 1.3122 $1.16 \%$ |  |
| 13 | $\begin{array}{c\|} \hline 0.9352 \\ 0.9332 \\ -0.19 \% \end{array}$ | $\begin{gathered} \hline 1.1993 \\ 1.2024 \\ 0.31 \% \end{gathered}$ | $\begin{array}{r} 0.9722 \\ 0.9703 \\ -0.19 \% \\ \hline \end{array}$ | 1.3510 <br> 1.3546 <br> 0.36\% | 1.1836 <br> 1.1800 <br> -0.36\% | $\begin{array}{r} 0.8381 \\ 0.8350 \\ -0.31 \% \\ \hline \end{array}$ |
| 14 | $\begin{aligned} & \hline 1.2599 \\ & 1.2634 \\ & 0.35 \% \\ & \hline \end{aligned}$ | $\begin{gathered} \hline 0.8618 \\ 0.8594 \\ -0.24 \% \\ \hline \end{gathered}$ | $\begin{gathered} \hline 1.2570 \\ 1.2600 \\ 0.29 \% \end{gathered}$ | $\begin{array}{\|c\|} \hline 0.9267 \\ 0.9258 \\ -0.09 \% \\ \hline \end{array}$ | $\begin{gathered} \hline 0.9315 \\ 0.9380 \\ 0.65 \% \\ \hline \end{gathered}$ | $\begin{array}{c\|} \hline 0.6897 \\ 0.6876 \\ -0.21 \% \\ \hline \end{array}$ |
| 15 | $\begin{array}{\|r\|} \hline 0.7623 \\ 0.7639 \\ 0.16 \% \end{array}$ | $\begin{gathered} \hline 0.7929 \\ 0.7966 \\ 0.37 \% \end{gathered}$ | $\begin{array}{c\|} \hline 0.7098 \\ 0.7117 \\ 0.19 \% \end{array}$ | $\begin{array}{r\|} \hline 0.5794 \\ 0.5805 \\ 0.10 \% \\ \hline \end{array}$ |  |  |

Figure 7.35 Comparisons of the Cycle 1 detector signals at BOC.


|  | H | G | F | E | D | C |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 8 | 1.2083 |  |  |  |  |  |
|  | 1.2231 |  |  |  |  |  |
|  | 1.48\% |  |  |  |  |  |
| 9 | 1.0645 | 1.2891 |  |  | PRAGMA <br> VANGARD Diff. |  |
|  | 1.0621 | 1.2845 |  |  |  |  |
|  | -0.23\% | -0.46\% |  |  |  |  |
| 10 | 1.2815 | 1.1031 | 1.2889 |  |  | 0.65\% |
|  | 1.2927 | 1.0973 | 1.2996 |  | RMS |  |
|  | 1.11\% | -0.58\% | 1.07\% |  | Max | 1.48\% |
| 11 | 1.1013 | 1.3026 | 1.1027 | 1.2999 |  |  |
|  | 1.0964 | 1.2959 | 1.0963 | 1.2948 |  |  |
|  | -0.49\% | -0.66\% | -0.64\% | -0.51\% |  |  |
| 12 | 1.2704 | 1.0877 | 1.2808 | 1.0756 |  |  |
|  | 1.2804 | 1.0828 | 1.2754 | 1.0732 | $\begin{aligned} & 1.0834 \\ & 1.0942 \end{aligned}$ |  |
|  | 1.00\% | -0.49\% | -0.54\% | -0.24\% | 1.08\% |  |
| 13 | 1.0407 | 1.2377 | 1.0286 | 1.2202 | 1.01641.0149 | 0.7188 |
|  | 1.0406 | 1.2497 | 1.0279 | 1.2323 |  | 0.7160 |
|  | -0.02\% | 1.20\% | -0.08\% | 1.21\% | -0.16\% | -0.27\% |
| 14 | 1.1754 | 0.8519 | 1.1374 | 0.8110 | 0.7186 | 0.5299 |
|  | 1.1866 | 0.8503 | 1.1474 | 0.8097 | 0.7259 | 0.5299 |
|  | 1.13\% | -0.16\% | 1.00\% | -0.13\% | 0.73\% | 0.00\% |
| 15 | 0.6670 | 0.6784 | 0.6217 | 0.5033 |  |  |
|  | 0.6676 | 0.6781 | 0.6226 | 0.5050 |  |  |  |
|  | 0.06\% | -0.03\% | 0.09\% | 0.17\% |  |  |  |

Figure 7.36 Comparisons of the Cycle 1 detector signals at MOC.


|  | H | G | F | E | D | C |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 8 | 1.1144 <br> 1.1348 <br> 2.04\% |  |  |  |  |  |
| 9 | 1.0178 <br> 1.0085 <br> -0.93\% | $\begin{array}{\|} \hline 1.1971 \\ 1.1822 \\ -1.49 \% \end{array}$ |  |  | PRAGMA VANGARD Diff. |  |
| 10 | $\begin{aligned} & 1.1677 \\ & 1.1871 \end{aligned}$ | $\begin{aligned} & 1.0413 \\ & 1.0283 \end{aligned}$ | $\begin{aligned} & 1.1788 \\ & 1.1966 \end{aligned}$ |  | RMS | 1.40\% |
|  | 1.94\% | -1.31\% | 1.78\% |  | Max | 2.48\% |
| 11 | 1.0536 <br> 1.0381 <br> -1.55\% | $\begin{array}{c\|} \hline 1.2211 \\ 1.2031 \\ -1.79 \% \\ \hline \end{array}$ | $\begin{array}{r\|} \hline 1.0637 \\ 1.0487 \\ -1.50 \% \\ \hline \end{array}$ | $\begin{array}{r} 1.2473 \\ 1.2346 \\ -1.28 \% \\ \hline \end{array}$ |  |  |
| 12 | 1.2049 <br> 1.2248 <br> 1.98\% | 1.0718 <br> 1.0601 <br> -1.18\% | $\begin{array}{r\|} \hline 1.2486 \\ 1.2344 \\ -1.43 \% \\ \hline \end{array}$ | $\begin{array}{r\|} \hline 1.0840 \\ 1.0781 \\ -0.59 \% \\ \hline \end{array}$ | $\begin{array}{r\|} \hline 1.0805 \\ 1.1030 \\ 2.25 \% \\ \hline \end{array}$ |  |
| 13 | $\begin{gathered} \hline 1.0745 \\ 1.0705 \\ -0.40 \% \end{gathered}$ | $\begin{array}{c\|} \hline 1.2314 \\ 1.2544 \\ 2.29 \% \end{array}$ | $\begin{gathered} \hline 1.0698 \\ 1.0651 \\ -0.47 \% \end{gathered}$ | $\begin{gathered} 1.2243 \\ 1.2491 \\ 2.48 \% \end{gathered}$ | $\begin{array}{c\|} \hline 1.0667 \\ 1.0681 \\ 0.14 \% \end{array}$ | $\begin{gathered} 0.7983 \\ 0.7948 \\ -0.35 \% \end{gathered}$ |
| 14 | $\begin{array}{r\|} \hline 1.2042 \\ 1.2286 \\ 2.44 \% \end{array}$ | 0.9244 <br> 0.9191 <br> -0.54\% | $\begin{gathered} \hline 1.1713 \\ 1.1941 \\ 2.28 \% \end{gathered}$ | $\begin{gathered} \hline 0.8675 \\ 0.8648 \\ -0.28 \% \end{gathered}$ | 0.7400 <br> 0.7576 <br> $1.76 \%$ | $\begin{gathered} \hline 0.5550 \\ 0.5554 \\ 0.05 \% \end{gathered}$ |
| 15 | $\begin{array}{c\|} \hline 0.7083 \\ 0.7043 \\ -0.39 \% \end{array}$ | $\begin{array}{\|c\|} \hline 0.7193 \\ 0.7136 \\ -0.57 \% \\ \hline \end{array}$ | $\begin{array}{\|c\|} \hline 0.6658 \\ 0.6638 \\ -0.20 \% \\ \hline \end{array}$ | $\begin{gathered} \hline 0.5389 \\ 0.5391 \\ 0.02 \% \end{gathered}$ |  |  |

Figure 7.37 Comparisons of the Cycle 1 detector signals at EOC.

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Table 7.7 Summary of the detector signal comparisons of the Cycle 1 load follow calculation.

| Measured Point |  | Power (\%) | VANGARD vs. Measured (\%) |  | VANGARD vs. PRAGMA (\%) |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Day | EFPD |  | Max | RMS | Max | RMS |
| 0 | 0.00 | 0.71 | 4.62 | 1.86 | 1.16 | 0.34 |
| 18 | 1.15 | 20.31 | 4.14 | 1.70 | 0.71 | 0.30 |
| 54 | 4.36 | 32.42 | 3.65 | 1.67 | 0.64 | 0.28 |
| 62 | 7.52 | 48.69 | 3.68 | 2.11 | 0.98 | 0.42 |
| 66 | 9.09 | 48.90 | 3.03 | 1.47 | 1.15 | 0.36 |
| 81 | 17.02 | 74.04 | 3.52 | 1.25 | 0.80 | 0.35 |
| 82 | 17.76 | 73.17 | 3.57 | 1.73 | 0.74 | 0.32 |
| 88 | 22.40 | 89.47 | 2.74 | 1.17 | 1.08 | 0.46 |
| 92 | 26.03 | 98.67 | 4.60 | 2.21 | 0.97 | 0.45 |
| 161 | 33.76 | 64.66 | 4.38 | 2.04 | 1.07 | 0.35 |
| 169 | 40.07 | 99.78 | 3.11 | 1.25 | 0.95 | 0.44 |
| 187 | 56.33 | 99.98 | 2.67 | 1.20 | 0.98 | 0.43 |
| 218 | 82.55 | 93.78 | 2.31 | 1.13 | 1.00 | 0.46 |
| 251 | 114.50 | 99.60 | 2.14 | 1.14 | 1.13 | 0.54 |
| 323 | 147.79 | 63.65 | 4.92 | 2.12 | 1.08 | 0.51 |
| 339 | 159.56 | 99.70 | 2.50 | 0.98 | 1.48 | 0.65 |
| 368 | 184.14 | 99.30 | 2.41 | 1.25 | 1.76 | 0.77 |
| 403 | 212.61 | 99.86 | 3.78 | 1.46 | 1.65 | 0.88 |
| 434 | 238.90 | 99.51 | 2.54 | 1.26 | 1.60 | 0.88 |
| 468 | 269.85 | 99.91 | 3.12 | 1.41 | 2.04 | 1.11 |
| 504 | 301.55 | 99.79 | 2.79 | 1.44 | 2.18 | 1.21 |
| 551 | 314.91 | 84.48 | 4.53 | 2.20 | 2.35 | 1.32 |
| 573 | 331.80 | 69.86 | 7.45 | 2.49 | 2.48 | 1.40 |
|  |  |  | Average 1 | Error: <br> 。 | Average | Stror: \% |

For the Cycle 2 load follow calculation, VANGARD solutions show excellent agreements with references. For CBCs as noted in Figure 7.38, the differences from the measurements and PRAGMA are within 60 ppm and 4 ppm , respectively. In the case of pin powers, as shown in Figure 7.39 and Figure 7.40, the maximum and RMS pin power errors are consistently lower than $2 \%$ and $0.5 \%$, respectively, except for at BOC, which shows the same behavior in the Cycle 2 HFP calculation. For the detector signal comparisons as well, as presented through Figure 7.41 - Figure 7.43 and in Table 7.8, the high accuracy of VANGARD solutions is confirmed where the average RMS errors are at the level of $1 \%$.

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Figure 7.38 CBC letdown curves and errors for the BEAVRS Cycle 2 core under the load follow operation.


Figure 7.39 Maximum and RMS pin power errors at each burnup step for the BEAVRS Cycle 2 core under the load follow operation (ref.: PRAGMA).


RMS: 0.83\%


RMS: 0.29\%


Figure 7.40 Pin power error (\%) distributions at BOC (left), MOC (middle), and EOC (right) for the BEAVRS Cycle 2 core under the load follow operation (ref.: PRAGMA).


|  | H | G | F | E | D | C |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 8 | 1.1958 <br> 1.1969 <br> 0.12\% |  |  |  |  |  |
| 9 | 1.1334 <br> 1.1100 <br> -2.33\% | $\begin{array}{r} 1.1193 \\ 1.0883 \\ -3.10 \% \\ \hline \end{array}$ |  |  | PRAGMA <br> VANGARD <br> Diff. |  |
| 10 | $\begin{aligned} & 1.0864 \\ & 1.0794 \end{aligned}$ | $\begin{aligned} & 1.1330 \\ & 1.1111 \end{aligned}$ | $\begin{aligned} & 1.1562 \\ & 1.1534 \end{aligned}$ |  | RMS | 1.25\% |
|  | -0.70\% | -2.20\% | -0.27\% |  | Max | 3.10\% |
| 11 |  | $\begin{aligned} & 1.1629 \\ & 1.1453 \\ & -1.76 \% \end{aligned}$ | $\begin{array}{r} 1.0695 \\ 1.0642 \\ -0.53 \% \\ \hline \end{array}$ |  |  |  |
| 12 | $\begin{aligned} & 1.1002 \\ & 1.1003 \\ & 0.01 \% \\ & \hline \end{aligned}$ | 1.0978 <br> 1.0903 <br> -0.75\% | $\begin{array}{r} 1.1186 \\ 1.1042 \\ -1.44 \% \\ \hline \end{array}$ | $\begin{array}{r} 0.9667 \\ 0.9703 \\ 0.36 \% \\ \hline \end{array}$ | $\begin{array}{c\|} \hline 0.9989 \\ 1.0106 \\ 1.17 \% \\ \hline \end{array}$ |  |
| 13 | $\begin{gathered} 1.0713 \\ 1.0681 \\ -0.32 \% \end{gathered}$ | $\begin{array}{c\|} \hline 1.1013 \\ 1.1023 \\ 0.10 \% \end{array}$ | $\begin{gathered} 1.0623 \\ 1.0641 \\ 0.18 \% \end{gathered}$ | $\begin{gathered} \hline 1.0778 \\ 1.0899 \\ 1.20 \% \end{gathered}$ | $\begin{gathered} 1.0288 \\ 1.0393 \\ 1.05 \% \end{gathered}$ | $\begin{array}{\|r\|} \hline 0.9726 \\ 0.9884 \\ 1.59 \% \end{array}$ |
| 14 | $\begin{aligned} & \hline 1.0575 \\ & 1.0722 \\ & 1.47 \% \end{aligned}$ | $\begin{array}{r} \hline 1.0880 \\ 1.0843 \\ -0.38 \% \end{array}$ | $\begin{gathered} \hline 1.0336 \\ 1.0462 \\ 1.26 \% \end{gathered}$ | $\begin{aligned} & \hline 1.0595 \\ & 1.0705 \\ & 1.10 \% \end{aligned}$ | 0.8379 0.8595 2.16\% | 0.4526 <br> 0.4527 <br> 0.00\% |
| 15 | $\begin{array}{\|r\|} \hline 0.9586 \\ 0.9736 \\ 1.50 \% \end{array}$ | $\begin{array}{r\|} \hline 0.9544 \\ 0.9650 \\ 1.06 \% \end{array}$ | $\begin{gathered} \hline 0.8007 \\ 0.8102 \\ 0.96 \% \end{gathered}$ | $\begin{gathered} \hline 0.4770 \\ 0.4760 \\ -0.09 \% \end{gathered}$ |  |  |

Figure 7.41 Comparisons of the Cycle 2 detector signals at BOC.


|  | H | G | F | E | D | C |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 8 | $\begin{array}{r\|} \hline 1.185 \\ 1.2067 \end{array}$ |  |  |  |  |  |
| 9 | $\begin{array}{r\|} \hline 1.0572 \\ 1.0500 \\ -0.72 \% \\ \hline \end{array}$ | $\begin{array}{r} 1.0623 \\ 1.0452 \\ \hline-1.70 \% \\ \hline \end{array}$ |  |  | PRAGMA <br> VANGARD <br> Diff. |  |
| 10 | $\begin{aligned} & 1.0322 \\ & 1.0445 \end{aligned}$ | $\begin{aligned} & 1.0906 \\ & 1.0800 \end{aligned}$ | $\begin{aligned} & 1.1992 \\ & 1.2105 \end{aligned}$ |  | RMS | 1.01\% |
|  | 1.23\% | -1.05\% | 1.12\% |  | Max | 2.17\% |
| 11 | 1.0730 <br> 1.0609 <br> -1.21\% | $\begin{gathered} 1.1925 \\ 1.1809 \\ -1.16 \% \end{gathered}$ | $\begin{aligned} & \hline 1.0778 \\ & 1.0705 \\ & -0.73 \% \end{aligned}$ | $\begin{aligned} & \hline 1.2580 \\ & 1.2422 \\ & -1.58 \% \end{aligned}$ |  |  |
| 12 | $\begin{array}{r} 1.1146 \\ 1.1298 \\ 1.52 \% \end{array}$ | $\begin{gathered} 1.0921 \\ 1.0849 \\ \hline-0.72 \% \end{gathered}$ | $\begin{aligned} & 1.2334 \\ & 1.2185 \end{aligned}$ $-1.50 \%$ | $\begin{gathered} 1.0394 \\ 1.0364 \\ -0.30 \% \end{gathered}$ | $\begin{array}{l\|} \hline 1.1274 \\ 1.1438 \\ 1.64 \% \end{array}$ |  |
| 13 | $\begin{aligned} & \hline 1.0400 \\ & 1.0370 \end{aligned}$ | $\begin{aligned} & 1.1264 \\ & 1.1361 \end{aligned}$ | $\begin{aligned} & 1.0505 \\ & 1.0475 \end{aligned}$ | $\begin{aligned} & 1.1702 \\ & 1.1856 \end{aligned}$ | $\begin{aligned} & 1.0543 \\ & 1.0551 \end{aligned}$ | $\begin{aligned} & \hline 0.9174 \\ & 0.9206 \end{aligned}$ |
| 14 | $\begin{aligned} & 0.9880 \\ & 1.0040 \end{aligned}$ | $\begin{aligned} & 1.0390 \\ & 1.0328 \end{aligned}$ $-0.61 \%$ | $\begin{aligned} & 1.0250 \\ & 1.0371 \end{aligned}$ | $\begin{aligned} & 1.0003 \\ & 1.0035 \end{aligned}$ $0.32 \%$ | $\begin{aligned} & 0.8103 \\ & 0.8274 \end{aligned}$ | 0.5085 0.5070 $-0.15 \%$ |
| 15 | $\begin{array}{r\|} \hline 0.8212 \\ 0.8263 \\ 0.51 \% \\ \hline \end{array}$ | $\begin{array}{r} 0.8351 \\ 0.8387 \\ 0.37 \% \\ \hline \end{array}$ | $\begin{array}{r\|} \hline 0.7368 \\ 0.7425 \\ 0.56 \% \\ \hline \end{array}$ | $\begin{array}{r} 0.5262 \\ 0.5246 \\ -0.16 \% \\ \hline \end{array}$ |  |  |

Figure 7.42 Comparisons of the Cycle 2 detector signals at MOC.



Figure 7.43 Comparisons of the Cycle 2 detector signals at EOC.

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Table 7.8 Summary of the detector signal comparisons of the Cycle 2 load follow calculation.

| Measured Point |  | Power <br> (\%) | VANGARD vs. Measured (\%) |  | VANGARD vs. PRAGMA (\%) |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Day | EFPD |  | Max | RMS | Max | RMS |
| 5 | 0.43 | 29.11 | 5.33 | 2.07 | 3.10 | 1.25 |
| 10 | 3.01 | 80.47 | 5.47 | 1.78 | 2.50 | 1.01 |
| 13 | 5.49 | 99.99 | 4.69 | 1.83 | 2.25 | 0.95 |
| 35 | 27.25 | 99.68 | 2.34 | 1.13 | 2.67 | 0.81 |
| 42 | 34.25 | 65.00 | 3.83 | 1.85 | 1.57 | 0.72 |
| 65 | 51.31 | 100.16 | 1.87 | 0.95 | 1.90 | 0.94 |
| 93 | 77.17 | 99.90 | 1.58 | 0.85 | 1.93 | 0.88 |
| 126 | 97.48 | 100.08 | 1.80 | 0.92 | 2.20 | 0.98 |
| 156 | 125.78 | 99.75 | 1.83 | 0.78 | 2.17 | 1.01 |
| 191 | 156.89 | 99.91 | 1.83 | 0.85 | 2.23 | 1.12 |
| 220 | 185.78 | 99.96 | 3.35 | 1.07 | 2.47 | 1.16 |
| 251 | 209.85 | 99.55 | 1.97 | 0.89 | 2.28 | 1.23 |
| 266 | 224.83 | 99.91 | 2.51 | 0.98 | 2.28 | 1.30 |
| 296 | 251.30 | 99.92 | 2.08 | 0.84 | 2.59 | 1.46 |
|  |  |  | Average | Error: <br> \% | Average | Error: |

### 7.4 NEACRP Rod Ejection Problems

The NEACRP benchmark [38] core is composed of 157 fuel assemblies. Each assembly contains 264 fuel rods arranged in $17 \times 17$ array, and consists of 18 axial planes including axial reflectors. For all cases, the rod ejection time is 0.1 seconds.

First of all, sensitivity tests were performed on time step size for VANGARD. The results obtained from VANGARD employing the fully implicit method for temporal discretization with time step size of 1 ms were used as reference solutions. As demonstrated in Figure 7.44, the transient solutions obtained from the CrankNicholson (CN) method with time step size of 5 ms and 10 ms match well with the reference solutions for all problems. Thus, the time step size of VANGARD calculation is set to 10 ms , and the Crank-Nicolson method is employed for the temporal discretization. In nTRACER calculation, on the other hand, the fully implicit method is employed with time step size of 5 ms .


Figure 7.44 Comparison of core power behavior according to time step sizes.

Figure 7.45 - Figure 7.47 show the 3D power distributions of the A1, B1, and C1 problem calculated by VANGARD at the steady-state, at the time of core power peak and also at 1.0 second. They clearly show the significant localized pinwise power increase near the rod-ejected position during the transient, which demonstrates the
transient simulation capability of VANGARD. Table 7.9 summarizes the calculation results of VANGARD compared with those of nTRACER. Figure 7.48 shows the core power behaviors of each problem, and the maximum Doppler temperature and the maximum moderator temperature behaviors of each problem are in Figure 7.49.

Prior to the analysis of transient results, the steady-state solutions were assessed for the ejected rod worth. For the B1 and C1 problems, the rod worth of VANGARD agrees with that of nTRACER within 1 pcm . For the A1 problem, however, a relatively large overestimation of 3 pcm is noted due to the severe heterogeneity which leads to a much earlier peak in the core power. Even the small difference has a nontrivial impact on core power because the transient core power behavior is strongly dependent on the ejected rod worth [26].

Meanwhile, for the other cases which do not suffer from the mismatch of the initial condition, all the transient results including the core power and T/H parameters are quite close to the nTRACER results, which verifies the soundness of the transient simulation capability of VANGARD.


Figure 7.45 Power distributions of A1 problem at the steady state (left), core power peak (middle), and 1.0 s (right).


Figure 7.46 Power distributions of B1 problem at the steady state (left), core power peak (middle), and 1.0 s (right).


Figure 7.47 Power distributions of C 1 problem at the steady state (left), core power peak (middle), and 1.0 s (right).

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Table 7.9 Comparison between VANGARD and nTRACER results for the NEACRP HZP rod ejection cases.

| Parameter | Solver | A1 | B1 | C1 |
| :---: | :---: | :---: | :---: | :---: |
| Ejected Rod worth (pcm) | nTRACER | 792.67 | 824.15 | 945.97 |
|  | VANGARD | 795.62 | 824.15 | 946.95 |
|  | Diff. | 2.95 | - | 0.98 |
| Max. Core <br> Power (\%) | nTRACER | 69.07 | 236.70 | 397.42 |
|  | VANGARD | 77.87 | 257.76 | 454.18 |
|  | Diff. | 8.80 | 21.06 | 56.76 |
| Peak Time (s) | nTRACER | 0.715 | 0.515 | 0.265 |
|  | VANGARD | 0.700 | 0.520 | 0.260 |
|  | Diff. | -0.015 | 0.005 | -0.005 |
| Max. <br> Doppler Temperature at $5 \mathrm{~s}\left({ }^{\circ} \mathrm{C}\right)$ | nTRACER | 483.12 | 445.70 | 519.28 |
|  | VANGARD | 477.15 | 451.57 | 524.32 |
|  | Diff. | -5.97 | 5.87 | 5.87 |
| Max. <br> Moderator <br> Temperature at $5 \mathrm{~s}\left({ }^{\circ} \mathrm{C}\right)$ | nTRACER | 307.39 | 302.68 | 308.19 |
|  | VANGARD | 307.91 | 303.04 | 308.71 |
|  | Diff. | 0.52 | 0.36 | 0.52 |

<A1>

<B1>


<C1>



Figure 7.48 Comparison of core power behaviors.


Figure 7.49 Comparison of maximum Doppler temperature behaviors (left) and maximum moderator temperature behaviors (right).

## Chapter 8. Computing Time Assessments

The soundness and performance of the GPU calculation modules were examined with a series of core cycle depletion problems and NEACRP control rod ejection problems. The core features and the calculation conditions are all the same as those introduced in Chapter 7 for verifications and validations. In the CPU calculation modules, OpenMP multi-core parallelization is applied and the Eigen [24] linear algebra package is utilized for the matrix and vector operations in the CMFD and depletion calculations. The soundness of the GPU calculation modules was verified by comparing the CBCs and pin powers with those of the CPU calculation modules, and the performance of the GPU calculation modules was evaluated against the multi-core CPU parallel calculation performance. For the CPU calculations, a single Intel i9-10900X CPU with 10 cores was used, and a single NVIDIA GeForce RTX 3090 GPU was used for the GPU calculations. The specifications of the computing resources are shown in Table 8.1.

Table 8.1 Specifications of the computing resources.

| Processor Type | GPU | CPU |
| :---: | :---: | :---: |
| Name | NVIDIA GeForce <br> RTX 3090 | Intel i9-10900X |
| \# of Cores | 10,496 for FP32 <br> 164 for FP64 | 10 |
| Base Core Frequency | 1.40 GHz | 3.70 GHz |
| DRAM Bandwidth | $936 \mathrm{~GB} / \mathrm{s}$ <br> (GDDR6X) | $42 \mathrm{~GB} / \mathrm{s}$ <br> (Dual Channel <br> DDR4-2666) |
| FP32 Performance | $29,389 \mathrm{GFLOPS}$ | $1,184 \mathrm{GFLOPS}$ |
| FP64 Performance | 459 GFLOPS | 592 GFLOPS |
| MSRP | $\$ 1,499$ | $\$ 648-\$ 658$ |

### 8.1 APR1400 Initial Core Depletion

Figure 8.1 presents the CBC letdown curves of the CPU and GPU calculations, and Figure 8.2 shows the pin power differences between the CPU and GPU calculations at the BOC, MOC, and EOC. For a rigorous comparison, tightly converged solutions were obtained with the fission source convergence criterion of $10^{-7}$. Throughout the results, it is confirmed that the GPU calculation modules yield equivalent results to the CPU calculation modules, as the calculated CBCs and pin power distributions are virtually the same. The CBC differences over the entire burnup steps do not exceed 0.01 ppm , and the maximum pin power differences steadily remain below $0.0003 \%$. Additionally, this is another proof of that the mixed precision technique used in the nodal solver does not deteriorate the solution accuracy.


Figure 8.1 Comparison of CBC letdown curves for the APR1400 core case.
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Figure 8.2. Pin power error (\%) distributions at BOC (left), MOC (middle), and EOC (right) for the APR1400.

On the other hand, the performance difference between the CPU and GPU calculations is significant. In the CPU calculation, the three major modules take up to $98 \%$ of the total computing time as shown in Figure 8.3. Substantial speedups for these were achieved with GPU. As summarized in Table 8.2, the nodal, cross section, and depletion calculations were accelerated by 22,44 , and 11 times, respectively. As the result, the total calculation time was reduced from about 75 minutes with 10 CPU cores to the level of 3 minutes with a single GPU. This demonstrates that the GPU accelerations modules of VANGARD were highly efficiently implemented and that the pinwise two-step nodal core calculation can be done with a feasible computing time for the application to routine core design analyses by GPU acceleration.

Meanwhile, an important observation from the results is that reconstructing the compressed XSs is faster than directly interpolating the raw XSs on GPU. It is because the reconstruction calculation has highly regular memory access pattern which is merely composed of element-wise matrix and vector operations, while the raw XS interpolation involves very irregular memory accesses that hinder the coalescing on GPU. Namely, the XS compression technique brings an additional advantage in terms of computing time due to the special characteristics of GPUs.


Figure 8.3 Computing time shares for the APR1400 core depletion case.

Table 8.2 Computing time of the major hotspots and total computing time for the APR1400 core depletion case.

| Calculation | CPU (s) | GPU (Original) |  | GPU (w/ Compression) |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | Time (s) | Speedup | Time (s) | Speedup |
| Nodal | 1586.9 | 72.4 | 21.9 | 72.9 | 21.8 |
| XS | 2450.2 | 55.9 | 43.8 | 29.1 | 84.2 |
| Depletion | 348.5 | 31.2 | 11.2 | 22.1 | 15.8 |
| Total | 4488.3 | 196.6 | 22.8 | 158.9 | 28.2 |

### 8.2 AP1000 Initial Core Depletion

The significant performance of the GPU calculation modules was also reproduced in the AP1000 core case. Figure 8.4 illustrates the computing time shares of the CPU and GPU calculations, and Table 8.3 presents the computing time of the three major hotspots and the total computing time, along with the speedup factors. The nodal, cross section, and depletion calculations were accelerated by 21,57 , and 15 times, respectively, and as the result, the entire cycle depletion calculation for the AP1000 initial core could be carried out within 2.5 minutes with a single GPU which had initially taken about 55 minutes with a deca-core CPU


Figure 8.4 Computing time shares for the AP1000 core depletion case.

Table 8.3 Computing time of the major hotspots and total computing time for the AP1000 core depletion case.

| Calculation | CPU (s) | GPU (Original) |  | GPU (w/ Compression) |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | Time (s) | Speedup | Time (s) | Speedup |
| Nodal | 1457.1 | 70.3 | 20.7 | 70.1 | 20.8 |
| XS | 1518.1 | 47.9 | 31.7 | 26.6 | 57.1 |
| Depletion | 247.8 | 22.4 | 11.1 | 16.3 | 15.2 |
| Total | 3305.2 | 168.8 | 19.6 | 143.2 | 23.1 |

### 8.3 BEAVRS Cycle 1 Core Depletion

The computing times and speedup factors of the computational hotspots and total computing time are summarized in Table 8.4, and the computing time shares of CPU and GPU calculations are presented in Figure 8.5. The nodal calculation and the cross section update were accelerated by 25 and 37 times, respectively, and the depletion calculation was also sped up by over 11 times. Consequently, the total computing time was reduced from about 1 hour 20 minutes to within 3.5 minutes. This computing time is equivalent to that a core calculation for a state can be performed in 6.8 seconds, which is fast enough to be industrially executed.

Table 8.4 Computing time of the major hotspots and total computing time for the BEAVRS Cycle 1 core HFP depletion case.

| Calculation | CPU (s) | GPU (Original) |  | GPU (w/ Compression) |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | Time (s) | Speedup | Time (s) | Speedup |
| Nodal | 2157.5 | 86.5 | 24.9 | 86.2 | 25.0 |
| XS | 2132.6 | 58.3 | 36.6 | 32.6 | 65.5 |
| Depletion | 339.6 | 30.2 | 11.3 | 26.9 | 12.6 |
| Total | 4740.0 | 212.6 | 22.3 | 187.7 | 25.3 |



Figure 8.5 Computing time shares for the BEAVRS Cycle 1 core HFP depletion case.

### 8.4 NEACRP Rod Ejection Problems

The soundness of the GPU-accelerated modules for transient analyses was assessed by the comparison with CPU results for the C 1 problem which was calculated with full core geometry so that it takes the most computing time among the three target problems. Figure 8.6 shows the core power behaviors from the CPU and GPU calculations and the relative errors between the two calculations. The GPU calculation result was confirmed to agree with the CPU calculation result, showing the relative error kept below $0.01 \%$.

Table 8.5 and Table 8.6 summarizes the computing times and speedup ratios of the four major GPU-accelerated parts of A1 quarter core problem and C 1 full core problem, respectively. The computing time share comparisons for them are
demonstrated in Figure 8.7 and Figure 8.8. All the calculations involve 100 transient steps with time step size of 10 ms . With GPU acceleration, substantial speedups were achieved, especially in the nodal solver which took $96 \%$ of the total computing time in the CPU calculation. Owing to this, the total computing time was reduced from 20 minutes to 50 seconds for A1 quarter core problem, and from 75 minutes to 2.5 minutes for C 1 full core problem.


Figure 8.6 Core power comparison between CPU and GPU calculations for the C 1 problem.

Table 8.5 Computing time (s) of the major hotspots and total computing time (s) for the NEACRP A1 problem.

| Calculation | CPU <br> $(10$ cores $)$ | GPU <br> (single) | Speedup |
| :---: | :---: | :---: | :---: |
| Nodal | 1225.8 | 24.7 | 49.7 |
| CMFD | 15.6 | 3.3 | 4.7 |
| XS | 2.7 | 0.2 | 15.2 |
| TH | 27.7 | 14.6 | 1.9 |
| Total | 1285.2 | 50.9 | 25.2 |



Figure 8.7 Computing time shares for the NEACRP A1 problem.

Table 8.6 Computing time (s) of the major hotspots and total computing time (s) for the NEACRP C1 problem.

| Calculation | CPU <br> $(10$ cores $)$ | GPU <br> (single) | Speedup |
| :---: | :---: | :---: | :---: |
| Nodal | 4420.0 | 78.1 | 56.6 |
| CMFD | 55.9 | 6.3 | 8.8 |
| XS | 9.7 | 0.5 | 18.7 |
| TH | 83.9 | 44.0 | 1.9 |
| Total | 4612.1 | 154.4 | 29.9 |



Figure 8.8 Computing time shares for the NEACRP C1 problem.

## Chapter 9. Summary and Conclusions

The pioneering GPU-based pinwise two-step nodal core calculation code VANAGARD has been developed, which leverages modern GPU computing capabilities to realize practical next-generation nuclear designs. As VANGARD targets to be used in commercial nuclear design analyses, a consumer-grade GPU that can be mounted on PCs was adopted as the main computing resource, which ensures affordability and practicality. Since VANGARD has been developed to fully exploit GPU performance from the scratch, almost all parts of the calculation modules including the three major computational hotspots - nodal solver, cross section treatment, and depletion solver - have been ported to GPU. Therefore, unnecessary overheads caused by the data transfer between CPU and GPU, which were not negligible, were minimized.

In VANGARD, the pin-level one-node $\mathrm{SP}_{3}$ SENM was chosen as the primary nodal kernel. SENM was chosen owing to its capability to capture severe flux gradients occurring in the pinwise multi-group calculations with use of its hyperbolic terms. One-node kernel is selected to avoid the pinwise $\mathrm{SP}_{3} \mathrm{CMFD}$ calculation which will lead to deterioration of stability and computing performance. In order to retain both accuracy and computational efficiency, radial $2^{\text {nd }}-$ axial $4^{\text {th }}$ order hybrid flux expansion was used. Besides, a mixed precision technique was devised to maximize the exploitation of powerful single precision computing power of consumer-grade GPU, in which only the simple arithmetic operations in the axial kernel are selectively done in double precision while the rest of operations of the nodal solver are done in single precision. By the sensitivity test, it was demonstrated to be the optimal combination in terms of stability, accuracy, and computing performance.

For the acceleration of fission source distribution convergence, assembly-level diffusion CMFD solver was paired with the nodal kernel. In order to resolve the
instability revealed in one-node pinwise nodal - assemblywise CMFD coupled calculation, CMFD-based partial current update scheme was developed. This method is to reflect the CMFD solutions in the update of pinwise partial currents by using mp-CMFD relation and the modulated pinwise fluxes which are updated from the CMFD coarse mesh flux update. Through the parametric study, the significant effectiveness of the pinwise partial current update was demonstrated.

VANGARD employs 8 -group microscopic group constants which are generated by the lattice calculations of the whole-core transport code nTRACER. To resolve too significant memory burden of the pinwise group constants, two measures were introduced to fit into the limited memory capacity of consumer-grade GPUs. The first one is the burnup window scheme which ports only the group constants which are necessary at each burnup step. The second one is the cross section compression technique which reduces the dimension of the microscopic cross section matrix algebraically by employing the SVD and LRA. This compression technique was confirmed not to harm the accuracy for the 2D core depletion calculation, furthermore, it turned out that not only it reduced the memory usage but also it reduced the computing time on GPU noticeably owing to the regular memory access pattern.

In depletion calculation, an efficient and massively parallel solution of batched burnup system with the CRAM was achieved by employing the cheap Gauss-Seidel method for the matrix inversion. The non-zero major ordering scheme for the matrix storage maximizes the coalescing on GPU. The inaccuracy of gadolinia fuel depletion, which is apparently observed in pinwise two-step core calculations, was resolved by introducing the neighbor-informed burnup correction scheme in which the cross sections of gadolinia fuel pins are functionalized by the average burnup of neighboring general fuel pins, not using their own burnups. The significant accuracy improvement was confirmed by the APR1400 core depletion calculation which is highly loaded with gadolinia fuels.

To constitute a fully capable core analysis system, VANGARD is not limited to developing individual modules but integrates them, and implements various auxiliary capabilities for practical applications, including the inline T/H feedback module with the simplified model and the features like CBC search, B-10 depletion, and xenon equilibrium and transient feedback. In addition, the transient calculation capability was also developed.

The high solution accuracy and execution performance of VANGARD were confirmed by the cycle depletion calculations for two commercial PWR cores of APR1400 and AP1000 and the BEAVRS multi-cycle benchmark problems. In terms of accuracy, VANGARD solutions presented excellent agreements with nTRACER transport solutions in both CBCs and power distributions. For all target problems, CBC differences were within 15 ppm , and the maximum and RMS pin power errors were within $2.0 \%$ and $0.6 \%$, respectively, throughout the whole burnup steps. Meanwhile, substantial speedups were achieved by GPU acceleration in every calculation module. Finally, for all the target problems, a cycle depletion calculation which took more than an hour with 10 CPU cores could be completed within 3 minutes on a consumer-grade GPU. It is corresponding to less than 10 seconds per state. These results ensure that VANGARD satisfies both accuracy and computing time requirements for commercial nuclear designs, which confirms the feasibility of practical pinwise core designs.

For the verification of transient calculation capabilities, NEACRP rod ejection problems were analyzed. All the transient results including the core power and T/H parameters were confirmed to be quite close to the nTRACER results. In terms of computing performance, a single consumer-grade GPU achieved substantial speedups over the 10 -core CPU calculation with 50 and 57 times speedup in the nodal calculation time and 25 and 30 times speedup in the total calculation time, which results in the total calculation time reduced to 50 seconds and 2.5 minutes to
simulate 100 times steps for the A 1 quarter core and C 1 full core problem, respectively.

Through all of these works, VANGARD has become the first and the only GPUbased full-featured pinwise two-step nodal core calculation code that can satisfy both accuracy and computing time requirements to the practical level. Moreover, this research is of value in that it resolved many issues and overcome challenges revealed in performing the pinwise two-step nodal core calculations on GPU, which have not been tackled or even known previously, and in that it suggested resolutions for them with newly developed elaborate methods and schemes. All of these achievements presented the high potential of practical pinwise nuclear designs, and this research can serve as a good precedent for future developments of pinwise two-step core calculation systems which will become a trend in the worldwide reactor core design analysis institutes.

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## 초 록

본 연구에서는 실용적 핵설계 적용을 위한 신속하고 정확한 GPU 기반의 봉단위 2단계 노달 노심 해석 코드 VANGARD를 개발하였다. GPU 가속을 특징으로 하는 이 코드는 PC 에 장착 가능한 소비자용 GPU 를 활용함으로써 실용적인 차세대 봉단위 핵설계를 실현한다.

본 연구는 실제 핵설계에 필요한 필수 기능들을 개발하고 통합하는 과정에서부터 시작한다. 이에 따라 정확한 중성자 해석을 위한 노달 해법을 비롯하여 봉단위 열궤환 계산, 연소 계산 기능을 구현하였고, 다주기 계산을 위한 재장전 및 재시작 기능, 사고 해석을 위한 과도 계산 기능을 구현하였다. 뿐만 아니라 SMR과 같은 차세대 원전 설계 및 해석에 필수적으로 요구되는 제어봉 조정 기능과 부하추종운전 기능을 구현함으로써, 노심 설계 및 해석에 필요한 모든 기능들을 갖춘 봉단위 노심 계산 체계를 구축하였다.

본 연구에서는 $\mathrm{SP}_{3}$ 이론 기반의 선원확장노달법(SENM)을 봉단위 다군 계산을 위한 최적의 해법으로 선정하고 구현하였다. SENM의 쌍곡선함수를 이용하여 핀 내부의 극심한 중성자속을 효과적으로 고려함으로써 코드의 정확도를 확보하고, 집합체 당 4 개의 격자를 사용하는 소격격자 유한차분 가속법을 결합하여 중성자속 계산 체제의 신속성을 확보하였다. 열 궤환 계산에서는 집합체 당 4 개의 격자를 기반으로 하는 1 차원 단상 폐유로 모델을 채택함으로써 실용적 적용이 가능하도록 하였다. 또한, 효율적인 봉단위 연소 계산을 위해 Chebyshev Rational Approximation Method (CRAM) 기반의 대규모 병렬화 연소 기법을

구현하였다. 대부분의 계산 시간을 차지하는 중성자속 계산, 단면적 계산, 열 퀘환 계산, 연소 계산을 비롯한 모든 주요 계산 모듈에 GPU 가속을 적용함으로써 상용 수준의 계산 시간을 달성하는 데 성공하였다.

핵설계 필수 계산 기능의 구현과 GPU 가속 기법의 도입에 그치지 않고, 본 연구는 그 동안 해결되지 않았거나 혹은 알려지지 않았던 GPU를 활용한 봉단위 2 단계 노달 노심 계산을 수행함에 있어 드러나게 되는 다양한 문제들을 해결하고, 새롭게 개발된 정교한 방법론과 체계로 이에 대한 해결책을 제시한다. 제한된 GPU 디바이스 메모리에 방대한 양의 봉단위 군정수를 효과적으로 포팅하기 위해 연소 테이블 방법을 개발 및 적용하였으며, SVD와 LRA를 이용한 차원 축소 기법을 통해 미시 단면적 데이터를 효과적으로 압축하였다. 계산의 전반적인 수렴을 안정화 시키기 위해 봉단위 중성자속뿐만 아니라 봉단위 부분 중성자류 또한 CMFD의 해를 이용하여 재계산 하는 CMFD 기반 부분중성자류 갱신법을 개발 및 적용함으로써 노달 계산의 반복 수와 전체 계산 시간을 효과적으로 감축하였다. 봉단위 2 단계 계산에서 드러나게 되는 극심한 가돌리니아 연료봉 연소 부정확도를 해결하기 위해서는 간단하지만 효과적인 보정 기법인 Neighbor-Informed Burnup Correction 기법을 개발하였고, 성공적으로 적용됨을 확인하였다.

계산의 정확도와 계산 시간에 대한 검증은 상용로 APR1400과 AP1000 초기 노심 및 BEAVRS 검증문제 1 주기, 2 주기 노심에 대한 3 차원 연소 계산을 통해 수행하였다. 검증 결과, nTRACER의 수송해와 비교했을 때, 모든 문제에 대해서, 모든 연소 스텝에서 임계붕소농도 오차가 15 ppm 이내, 봉 출력 최대 오차와 RMS 오차가 각각 $2.0 \%$ 와 $0.6 \%$ 이내로

나타나며 VANGARD의 높은 정확도를 입증하였다. 반면 GPU 가속을 통해 압도적인 계산 성능 향상을 이루어 냄으로써, 모든 검증 문제 대해 멀티 코어 CPU 계산을 통해 한 시간이 넘게 소요 되었던 1 주기 연소 계산을 3 분 내로 수행하는 데 성공하였고, 결과적으로 한 연소 스텝 당 10 초 이내의 계산시간을 달성하였다.

본 연구는 GPU 기반의 봉단위 계산에서 나타나는 여러 난제들을 효과적으로 해결하여 실용적이고 정확한 봉단위 핵설계의 실현이 가능함을 입증했다는 점에서 큰 가치가 있다. 이 연구를 통해 제시된 여러 난제 해결책은 향후 세계 원자로 노심 설계 해석 기관에서 대세가 될 봉단위 2 단계 계산 체제 개발 과정에 좋은 선례로 활용될 수 있을 것이다.

