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ABSTRACT

The Griffin code is a Multiphysics Object-Oriented Simulation Environment (MOOSE) based reactor multiphysics analysis application jointly developed by Idaho National Laboratory and Argonne National Laboratory. The code includes a variety of steady-state solvers for fixed-source, k-eigenvalue, adjoint, and subcritical multiplication, as well as transient solvers for point-kinetics, improved quasi-static, and spatial dynamics. The code reads multigroup cross sections in the ISOXML format generated from external deterministic or Monte Carlo cross section generation codes.

The implementation of the cross section generation capability in Griffin was initiated last year by plugging in the cross section application programming interface (CSAPI) and reviewing the methodologies for treating particulate fuels. The focus this year was on improving the CSAPI integration and implementing advanced self-shielding methods for applications to advanced reactor problems with TRISO fuels. First, the process for cross section library generation was updated to accurately and rigorously produce isotopic cross section data. Second, the equivalent Dancoff factor cell method performing slowing down calculations on the fly for the resonance treatment was implemented in CSAPI to improve the accuracy of effective multigroup cross sections in the resonance energy range. Third, the iterative local spatial self-shielding method was implemented under the calculation framework of the equivalent Dancoff factor cell method to accurately deal with the double heterogeneity effect of particulate fuel.

The updated CSAPI with the advanced self-shielding methods, together with the cross section libraries generated based on the improved process, were tested for pin-cell, unit-cell, and fuel assembly problems with various resonance self-shielding conditions based on very high temperature reactor, high temperature test reactor, and Empire benchmark cores, indicating that the updated CSAPI in Griffin is able to produce multigroup cross sections accurately and efficiently. We also showed that the methodology worked well for pebble bed fuel from HTR-10, but the capability still needs to be fully integrated into CSAPI. In the future, further benchmark tests will be performed for various thermal reactor core problems, including particulate fuel-based pebble bed reactors.

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ACRONYMS

0D	Zero-dimensional
1D	One-dimensional
2D	Two-dimensional
3D	Three-dimensional
BP	Burnable Poison
CMFD	Coarse-Mesh Finite Difference
CPM	Collision Probability Method
CSAPI	Cross Section Application Programming Interface
DF	Disadvantage Factor
DFEM	Discontinuous Finite Element Method
EDC	Equivalent Dancoff factor Cell
ENCM	Enhanced Neutron Current Method
ENDF	Evaluated Nuclear Data File
ESSM	Embedded Self-Shielding Method
FSP	Fixed Source Problem
HFEM	Hybrid Finite Element Method
HFG	Hyperfine Group
HTTR	High Temperature Test Reactor
ILSS	Iterative Local Spatial Self-shielding
LWR	Light Water Reactor
MOC	Method of Characteristics
MOOSE	Multiphysics Object-oriented Simulation Environment
MPI	Message Passing Interface
NGNP	Next Generation Nuclear Plant
NR	Narrow Resonance
PTT	Pebble Tracking Transport
PWR	Pressurized Water Reactor

S-P	Sanchez-Pomraning
SN	Discrete Ordinates
SPH	Super-homogenization
VHTR	Very High Temperature Reactor

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1. Introduction

The DOE-NE Nuclear Energy Advanced Modeling and Simulation (NEAMS) program has developed a number of advanced modeling and simulation tools to deploy advanced nuclear energy technologies for industry and government organizations. As part of the effort, a Multiphysics Object-Oriented Simulation Environment (MOOSE)-based reactor physics code for multiphysics applications, named Griffin [1], has been developed jointly by Idaho National Laboratory (INL) and Argonne National Laboratory (ANL), which includes a variety of deterministic steady-state transport solvers for fixed source, k-eigenvalue, adjoint, and subcritical multiplication as well as transient solvers for point-kinetics, improved quasi-static, and spatial dynamics.

In this fiscal year, the performance of the transport solvers in Griffin was significantly improved in terms of accuracy and computation time by implementing a discontinuous finite element method (DFEM)-based discrete ordinate (SN) asynchronous transport sweeper [2] together with the coarse mesh finite difference (CMFD) acceleration for heterogeneous- or homogeneous-geometry applications. A new solver based on the hybrid finite element method (HFEM) spherical harmonics expansion (PN) solver (similar to the variational nodal method) [3] for homogeneous-geometry applications was also added. Details were reported in Reference [4].

For transport calculations in Griffin, multigroup cross sections for fast or thermal reactor problems can be provided from an external file in the ISOXML format [5], which are generated from deterministic or Monte Carlo cross section generation codes. Isotopic or composition-based cross section data are stored hierarchically with the natural XML (eXtensible Markup Language) tree structure, which allows a great flexibility to manage isotopic or composition data with many state points.

Last year, to improve the cross section generation capability in Griffin, we initiated the integration of the cross section application programming interface (CSAPI) [6], which is a portable functional module for generating multigroup cross sections using the subgroup or resonance table method for thermal spectrum problems. CSAPI needs a multigroup cross section library, which is generated for a specific reactor or reactor type of interest. This library contains principal isotopic multigroup cross sections as well as resonance cross section data (or subgroup parameters for the subgroup method) as a function of temperature and background cross section for all isotopes necessary for solving a problem of interest. The CSAPI module by design can be adapted to any transport code with a fixed source solver capability. CSAPI allows transport

solvers to generate self-shielded multigroup cross sections on the fly (online), accounting for the effects of heterogeneous geometry as well as temperature and composition. Plugging CSAPI into Griffin was made successful by adding the Fortran/C++ interfaces for data transfer between Griffin and CSAPI and putting the DFEM-SN-based fixed source solver for escape cross section calculations.

In this fiscal year, the cross section library generation process was updated to better support the advanced resonance self-shielding methods implemented in CSAPI. Initially, all isotopic multigroup cross sections including isotopic scattering matrices were generated from OpenMC [7]. However, in order to provide an alternative and verification option to users, the procedure of using the combination of Serpent2 [8] and NJOY [9] was added, in which the two codes produce isotopic principal cross sections and scattering matrices, respectively.

The resonance self-shielding treatment of the CSAPI module in Griffin was also significantly improved with the on-the-fly slowing down method and the particulate fuel modeling capability. Specifically, the equivalent Dancoff factor cell (EDC) method [10, 11] was implemented as the on-the-fly slowing down methods. The EDC method decouples a multidimensional geometry problem (e.g., a whole core) to multiple one-dimensional (1D) pin-cell problems, preserving Dancoff factors of fuel pins calculated in the multidimensional geometry, and solves the hyperfine group (HFG, $\sim 400,000$ groups) slowing down equation of MC²-3 with the 1D pin-cell geometry using the collision probability method (CPM). The EDC method takes advantage of the accuracy of the on-the-fly slowing down method without degrading computational time since 1D pin-cell problems can be solved in parallel using the computationally cheap 1D CPM solver.

Together with the EDC method, the iterative local spatial self-shielding (ILSS) method [12] was introduced for treating the double heterogeneity effect of particulate fuel. The method approximately accounts for the effect of randomly distributed particles on the particle-to-particle shadowing effect using a homogenized composition region surrounding a particle of interest at the center. The cross section of the homogenized composition region should use the self-shielded one of the particle at the center, both of which are therefore determined iteratively. Particle-cell averaged HFG cross sections are obtained by solving the HFG slowing down equation with the particle self-shielding iteration in a 1D particle cell problem and used in the EDC method to obtain a weighting spectrum of the stochastic-region for condensation.

The enhanced capability of CSAPI in Griffin was tested for a few reactor problems, including HTTR (High Temperature Test Reactor), VHTR (Very High Temperature Reactor), and Empire microreactor problems. In addition, we extended the tests to a preliminary study with pebble fuel problems, not using the

Griffin CSAPI but using MC²-3 [12, 13], to ensure that the ILSS method implemented in CSAPI worked well for PBR (Pebble Bed Reactor) applications.

In this report, Section 2 introduces the cross section data handling capabilities of the ISOXML module and the cross section generation methodologies of the CSAPI module in Griffin, as well as the CSAPI multigroup cross section library generation procedure. Section 3 presents the implementation of the advanced resonance self-shielding methods to the CSAPI module in Griffin. Verification tests and results are discussed in Section 4, followed by conclusions and future work in Section 5 and Section 6, respectively.

2. Cross Section Capabilities in Griffin

2.1 ISOXML

Nuclear data is provided through evaluated nuclear reaction databases (ENDF) [14–18] stored in the ENDF-6 format [19]. The ENDF-6 rules are defined by the U.S. National Nuclear Data Center (NNDC) on behalf of the Cross Section Evaluation Working Group (CSEWG). An ENDF library can contain data for neutron reactions as well as data relating to radioactive decay, fission-product yield spectrum, neutron thermal scattering, photo-atomic interactions, and more. ENDF libraries are the data source for the modeling and simulation of nuclear reactors.

However, cross section data stored in the ENDF-6 format is not directly usable for radiation transport calculations. As a result, the data in the ENDF-6 format must first be processed by ENDF-6 processing codes such as NJOY [20], AMPX [21], ETOE2 [13], CALENDF [22], FRENDY [23], PREPRO [24], and others. The output of such nuclear data processing codes is either 1) in a multigroup format with resonance self-shielding data, such as GENDF with NJOY, for the deterministic path with lattice physics codes, such as DRAGON [25], MC²-3 [13], and TRITON [26], or 2) in an ACE format for continuous energy Monte Carlo codes, such as Serpent [8], MCNP [27], Shift [28], and OpenMC [7]. Both paths can generate reactor-specific multigroup cross section libraries typically without resonance self-shielding data for the final multigroup radiation transport calculations for reactor analysis. The reactor-specific multigroup cross section libraries may require certain equivalence data for regions of interest to account for the spatial homogenization or group condensation effects. The number of energy groups for these multigroup libraries with and without resonance self-shielding/equivalence data can vary from several to thousands. Data used in the deterministic self-shielding codes (Path 1) traditionally employ finer energy group structures (hundreds to thousands of groups) and are tabulated as a function of temperature and other parameters used in the self-shielding methods. Data used in the deterministic full core solvers are typically tabulated with state variables, such as fuel temperature, coolant density, etc., for users to bring in spatial and energy spectrum effects on evaluating local macroscopic cross sections in simulations of engineering-scale geometries. A large number of isotopes, multiple reaction types, and a combination of all state variables can make the multigroup library difficult to manage because of the size of the library. A uniform format for multigroup libraries with resonance self-shielding data/equivalence data for both lattice physics and full-core transport calcula-

tions is desired. Along with the format, the capability to perform operations on the data (self-shielding, interpolation, mixing, etc.) is also desired for users and developers to avoid repeated coding efforts for these operations.

Existing library formats, like ANISN [29], ISOTXS [30], and AMPX [21], were created decades ago and are obscure to use or do not support all functionalities required by the transport calculations. Lattice physics codes that process the multigroup data from ENDF-6 processing codes have their own input library. Lattice physics codes and Monte Carlo codes also generate multigroup libraries in their own formats. There is a need to modernize these formats and extend their functionalities with the latest available computing tools.

The ISOXML module provides the capabilities to process nuclear data from some of these external cross section generation codes and to produce data in the ISOXML format. ISOXML entails a number of library structures and formats for:

- multigroup cross section and kinetic data
- equivalence data
- decay, transmutation, and fission-product yield data.

The ISOXML format is based on the XML (Extensible Markup Language) [31] format. The multigroup cross section library is designed to manage all isotopes at all state points for any type of calculation (e.g., steady state, transient, and depletion). A state point is described by several state variables (e.g., fuel and coolant temperatures, soluble boron concentration, and accumulated burnup). All of the ISOMXL-formatted libraries share several appealing features:

- the general mark-up language for which robust and efficient parsers exist
- data are managed hierarchically with the natural XML tree structure
- the sequence of nodes in an XML file on the same tree level is irrelevant, which gives the library a great flexibility in managing all state points and all isotopes
- it is human readable and writable, although designed for computer-driven data manipulation, which makes the format very accessible to new users when compared to many other formats
- it allows for complete validity checks.

As mentioned previously, it bears repeating that the flexibility and readability of the ISOXML data format is one of its most attractive features. Scientific studies frequently need to modify datasets in the process of their modeling, sometimes to remove unneeded data and other times to correct and update data based on recent experimental results. With the C++ object-oriented programming paradigm, the ISOXML format makes it trivial for users to find, modify, and add data to ISOXML libraries, provided that the overall energy group structure of the library is unchanged (which would necessitate generation of a new multigroup library for a new energy spectrum). By increasing the accessibility of the data format to users who were not directly involved in the development of the format, the format (and the data stored in said format) can be more readily accessed, modified, and implemented for modeling and simulation by other users.

To reduce storage requirements, an XML library can be converted to a binary file with netCDF [32]. It needs to be noted beforehand that all symbols in an XML file are case sensitive. A manipulator of ISOXML in C++ with RapidXML [33] is created. A Fortran interface is going to be provided to facilitate coding efforts in Fortran. With this format, operations, including interpolation and mixing, can be done with a uniform interface. Users and developers are shielded from the complexity of these operations.

The ISOXML module is accessible within Griffin but can also be used as a standalone executable. Currently, the ISOXML module can load and convert a number of files to the ISOXML format:

- Serpent2 result files for cross sections and kinetics parameters
- Serpent2 detector files for reference super-homogenization (SPH) flux solutions
- ISOTXS and PMATRX data files
- ORIGEN-formatted decay and fission-product yield data files
- ENDF-6 isotope decay constants, decay chains, and fission yields
- ACE file format for a continuous-energy slowing down solver in Griffin.

2.2 Generation of the Multigroup Library for CSAPI

Several computer codes are needed to process cross sections and generate the cross section library for CSAPI. Those codes are briefly introduced as follows:

- OpenMC [7]: a Monte Carlo code to solve a pin cell with an isotope of interest with different number densities and temperatures to produce isotopic cross sections for different background cross section and temperature conditions. OpenMC produces principal cross sections and scattering matrices for isotopes.
- Serpent2 [8]: a Monte Carlo code to solve a pin cell with an isotope of interest to produce isotopic cross sections as OpenMC does. This provides an alternative path of generating isotopic cross sections. Serpent2 generates principal cross sections for isotopes, but scattering matrices are provided from NJOY since Serpent2 does not produce them.
- NJOY (Version 2012 or higher) [9]: a nuclear data processing code to produce microscopic cross sections for an isotope of interest. Only fission spectrum and multigroup scattering kernels are generated by NJOY, and scattering matrices are normalized to total scattering cross sections generated from Serpent2.
- GenISOTXS [6]: a code to process the cross sections generated from OpenMC or Serpent2 to edit out the cross sections in the ISOTXS format or the ASCII format required for the cross section library processing.
- MC²-3 [13]: a multigroup cross section generation code to produce self-shielded cross sections for a given composition. For the cross section library generation, the code reads the fluxes and cross sections generated from a Monte Carlo code and performs the transport calculations using the method of characteristics (MOC) to produce background cross sections for each isotope.
- GenCSLIB [6]: a code to process the data that a Monte Carlo code and MC²-3 generate, tabulate cross sections as a function of background cross section and temperature and produce the cross section library in the ASCII format.
- Python scripts: several Python scripts to extract, verify, and convert data at each calculation step.

Multiple calculation steps are needed to produce the cross section library for CSAPI. The cross section library generation process is summarized below.

- Step 1: run a Monte Carlo code for a pin cell representing a reactor of interest. The calculations are repeated by changing the number density of a resonant isotope of interest such that the background

cross sections of the resonant isotope vary. As a Monte Carlo code, we used OpenMC [7] since it produces a complete set of microscopic cross sections including scattering matrices (Path 1 in Fig. 1). However, microscopic cross sections for some isotopes with small number densities could have too large uncertainties, especially in scattering matrices in the low energy range, even using a very large number of particle histories. As an alternative, Serpent2 and NJOY can be used (Path 2 in Fig. 1), in which principal microscopic cross sections are produced from Serpent2 and scattering matrices are provided from NJOY. In the NJOY calculation, the fine-group spectrum from the pin cell calculation of Serpent2 may be input to make the group collapsing of scattering matrices consistent with the pin cell calculation. The total scattering cross sections obtained from NJOY are updated to be the same as those from Serpent2.

- Step 2: extract isotopic cross sections from the Monte Carlo outputs, which are used to calculate the background cross sections for resonant isotopes using a deterministic code. We used the MOC solver of MC²-3, solving the fixed source problems (FSPs) for all the cases solved by a Monte Carlo code. Additionally, the SPH factor may be introduced to force the reaction rates from MC²-3 to match those from a Monte Carlo code.
- Step 3: repeat Steps 1 and 2 with different temperatures and then construct a cross section data library for an isotope with the tabulation of fission, absorption, and scattering resonance cross sections in terms of background cross section and temperature. A cross section data library involves higher order scattering matrices as well. All isotopic cross section data libraries are merged to a single file with an index table.

The process of generating the multigroup library for CSAPI is illustrated in Fig. 1, which involves several Python scripts as well as additional computer codes, as shown in the figure, to generate code inputs and process code outputs for linking the calculation steps.

2.3 Methodologies of CSAPI

In the Griffin CSAPI, there are two resonance treatment methods available: the resonance table method and EDC method. The former belongs to the Bondarenko approach using a heterogeneous resonance table, and the latter belongs to the on-the-fly slowing down method. For the double heterogeneity treatment, the

Figure 1: Process of generating the multigroup library for CSAPI.

recently developed ILSS method was adopted and incorporated in the calculation framework of the EDC method. These three methodologies are explained in detail in this section.

2.3.1 Resonance Table Method

This method is basically the Bondarenko approach [34] that iteratively determines effective cross sections at calculated background cross sections from a pre-generated look-up table. In the conventional equivalence theory [35], resonance integrals are generated by solving slowing down problems in a zero-dimensional (0D) problem and tabulated as a function of background cross section and temperature. Then, effective cross sections of resonant isotope r are calculated as

$$\sigma_{X,g}^r = \frac{RI_{X,g}^r(\sigma_{b,g}^r, T)}{1 - RI_{a,g}^r(\sigma_{b,g}^r, T) / \sigma_{b,g}^r}, \quad (1)$$

where X is a reaction type and a and b mean absorption and background, respectively. The background cross section typically consists of composition background cross section (volumetric source) and escape cross section (surface source) as

$$\sigma_{b,g}^r = \frac{\sum_{i \neq r} N^i \lambda_g^i \sigma_p^i + D / \bar{l}_f}{N^r}, \quad (2)$$

where r and i are isotope indices, p means a potential scattering, λ is the intermediate resonance parameter, N means an atomic number density, D is a Dancoff factor, and $\bar{l}_f$ is the mean chord length of a fuel rod. This formulation holds only for a two-region problem (fuel + moderator), based on the narrow resonance (NR) approximation neglecting the resonance scattering and the one-term rational approximation of the escape probability from a fuel rod [35]. The escape probability in the presence of neighboring fuels is corrected via the Dancoff factor, D , defined as the probability for a neutron escaping fuel rods in a lattice to have its first collision in non-fuel regions at the black (optical thickness) fuel limit. More advanced formulations use N -terms in the rational approximation of the escape probability and determines $2N$ coefficients of the rational form with the least square fitting at $2N - 1$ grey optical thickness points under the constraint that the sum of N term coefficients equals unity [36].

Meanwhile, the resonance table method in the Griffin CSAPI tabulates the effective cross sections of resonant isotope r directly as a function of background cross section and temperature as:

$$\sigma_{X,g}^r = \sigma_{X,g}^r(\sigma_{b,g}^r, T), \quad (3)$$

where the formula of the background cross section differs from Eq. (2) as will be explained later in this section. The Griffin CSAPI does not rely on the rational approximation of the escape probability. Escape probabilities are implicitly considered when solving an FSP at the region-dependent grey optical thicknesses of fuel rods, and thus this formulation holds in a general geometry where equivalence theory fails.

In addition, this approach also has some parallels with other techniques, such as the physical probability table method of the subgroup method based on a heterogeneous table [37] and the embedded self-shielding method (ESSM) [38, 39] in that the consistency between generating and using heterogeneous tables derived by a user is enforced rather than relying on equivalence theory. The Griffin CSAPI approach is, however, considered to be more advanced than others due to the differences in the formulation of the FSP explained below.

Many lattice physics and whole-core transport codes, such as HELIOS [40], DeCART [41], nTRACER [42], MPACT [43], etc., solve the following FSP for isotope r .

$$\vec{\Omega} \cdot \nabla \psi_g^r(\vec{x}, \vec{\Omega}) + \left(N^r(\vec{x}) \sigma_{a,g}^r(\vec{x}) + \sum_i \lambda_g^i \Sigma_{p,g}^i(\vec{x}) \right) \psi_g^r(\vec{x}, \vec{\Omega}) = \frac{1}{4\pi} \sum_i \lambda_g^i \Sigma_{p,g}^i(\vec{x}), \quad (4)$$

where i is an isotope index. Then, the escape cross section for isotope r is calculated as

$$\sigma_{e,g}^r = \sigma_{a,g}^r \frac{\phi_g^r}{1 - \phi_g^r} - \frac{1}{Nr} \sum_i \lambda_g^i \Sigma_{p,g}^i, \quad (5)$$

where $\phi_g^r = \int_{\mathcal{S}} \psi_g^r(\vec{x}, \vec{\Omega}) d\Omega$ with $\mathcal{S}$ being the unit sphere. Although there are slight variations in Eq. (4) among different methods/codes, it should be noted that Eq. (4) ignores the resonance scattering cross section, which means that the true optical thickness is not used. Thus, the physical fuel rod escape probability is not reflected in the flux solution of Eq. (4), resulting in non-negligible errors when directly using equivalence theory. To reduce such errors, the equivalence is enforced between effective (in the pre-generated table) and region-dependent cross sections for a target problem by calculating effective cross sections in the same manner, both in the table generation step and the usage step with a consistent bias. This is called the "enforced equivalence." Due to this nature, the enforced equivalence has a large sensitivity to the representative pin-cell configuration used to generate the table; for example, the enforced equivalence starts to fail in the case that a representative pin-cell and a target pin geometry have different pellet radii [44].

On the other hand, the Griffin CSAPI uses the formulation of the Tone's method [45] for solving an FSP. The Tone's method was originally developed primarily for the resonance treatment of fast reactor calculations. The advantage of this method is that it does not resort to the rational approximation of the escape probability in equivalence theory, but to more accurate collision probabilities implicitly calculated by solving an FSP. By introducing two key approximations that:

1. the scattering interval of neutrons is much larger than the width of the resonance (narrow resonance [NR] approximation),
2. the energy dependence of the collision probability in an energy group relies only on a target region (i.e., the resonance of a target nuclide within the group is assumed constant in source regions),

a spectrum model for resonant isotope r is derived as

$$\phi_k^r(E) = \frac{1}{E} \frac{\sigma_p^r + \sigma_{b,p,k,g}^r}{\sigma_{t,k}^r(E) + \sigma_{b,t,k,g}^r(E)}, \quad (6)$$

where

$$\sigma_{b,p,k,g}^r = \frac{\sum_j P_{g,j \rightarrow k} V_j \sum_{i \neq r} N_j^i \sigma_p^i}{\sum_j P_{g,j \rightarrow k} V_j N_j^r} \text{ and } \sigma_{b,t,k,g}^r(E) = \frac{\sum_j P_{g,j \rightarrow k} V_j \sum_{i \neq r} N_j^i \sigma_t^i(E)}{\sum_j P_{g,j \rightarrow k} V_j N_j^r}, \quad (7)$$

where k and j are region indices, i is an isotope index, and $\sigma_{b,p,k,g}^r$ and $\sigma_{b,t,k,g}^r$ are the potential and total background cross sections, respectively. We adopt the traditional definition for $P_{g,j \rightarrow k}$ as the probability that a neutron born uniformly and isotropically in region j has its first collision in region k . By further neglecting the energy dependence of the total cross section of other isotopes in the background cross section, $\sigma_{b,t,k,g}^r(E)$, and dividing it into composition background cross section and escape cross section, the final expression of the flux model for isotope r and group g becomes

$$\phi_k^r(E) \simeq \frac{1}{E} \frac{\sigma_p^r + \sigma_{b,p,k,g}^r}{\sigma_{t,k}^r(E) + \sigma_{b,k,g}^r}, \quad (8)$$

where

$$\sigma_{b,k,g}^r = \sigma_{0,k,g}^r + \sigma_{e,k,g}^r, \sigma_{0,k,g}^r = \frac{\sum_{i \neq r} N_k^i \sigma_{t,k,g}^i}{N_k^r} \text{ and } \sigma_{e,k,g}^r = \frac{\sum_j P_{g,j \rightarrow k} V_j \sum_{i \neq r} N_j^i \sigma_{t,g}^i}{\sum_j P_{g,j \rightarrow k} V_j N_j^r} - \sigma_{0,k,g}^r. \quad (9)$$

In the Griffin CSAPI, the escape cross section in Eq. (9) is evaluated not by directly calculating collision probabilities but by replacing each of the numerator and the denominator with solutions of the following two FSPs, respectively, which are solved by the DFEM-SN solver in Griffin,

$$\text{Numerator: } \vec{\Omega} \cdot \nabla \psi_{g,1}^r(\vec{x}, \vec{\Omega}) + \left(\sum_i N^i(\vec{x}) \sigma_{t,g}^i(\vec{x}) \right) \psi_{g,1}^r(\vec{x}, \vec{\Omega}) = \frac{1}{4\pi} \sum_{i \neq r} N^i(\vec{x}) \sigma_{t,g}^i(\vec{x}), \quad (10)$$

$$\text{Denominator: } \vec{\Omega} \cdot \nabla \psi_{g,2}^r(\vec{x}, \vec{\Omega}) + \left(\sum_i N^i(\vec{x}) \sigma_{t,g}^i(\vec{x}) \right) \psi_{g,2}^r(\vec{x}, \vec{\Omega}) = \frac{1}{4\pi} N^r(\vec{x}), \quad (11)$$

and

$$\sigma_{e,k,g}^r = \phi_{k,g,1}^r / \phi_{k,g,2}^r - \sigma_{0,k,g}^r. \quad (12)$$

To make this method applicable to equivalence theory, it's assumed that the total cross section of other isotopes is equal to their potential scattering cross section in Eq. (9) to have a consistent background cross section expression and derive the spectrum model equivalent to that in a homogeneous medium. However, since the heterogeneous effective cross section table is employed in the CSAPI library, such an approximation is not required. Instead, the enforced equivalence is imposed as explained previously. It should be noted that the sensitivity of the enforced equivalence to a representative pin-cell configuration would be much smaller than that of the enforced equivalence which resorts to the FSP of Eq. (4). This is because a physically true escape probability is considered in FSPs by using best-estimate total cross sections, not ab-

sorption plus potential cross sections, and the only approximations involved are to neglect the within-group variation of the total cross section of other isotopes in every region, including a target region, and the use of the NR approximation. The NR approximation fails in a lower epithermal energy range where resonances are relatively wide, but this bias is covered by the enforced equivalence. Therefore, although not proved explicitly through numerical experiments, the FSP formulation of the Griffin CSAPI would be more robust than that adopted in other lattice physics and whole-core transport codes listed above.

2.3.2 Equivalent Dancoff Factor Cell (EDC) Method

This method belongs to the on-the-fly slowing down method, which does not involve the pre-tabulation step. A direct method for this category is to solve the transport equation in the whole domain in a slowing down calculation. A resulting spectrum is used as a weighting function for condensation to the target group structure. However, this approximation-free method is not practical at all, and thus many approximated ways have been proposed [10, 11, 46–48], to which the EDC method belongs. Instead of solving the slowing down problem in an explicit heterogeneous lattice geometry using the DFEM-SN solver, the heterogeneous lattice geometry is decoupled to multiple 1D pin-cell problems that preserve the Dancoff factor calculated in the reference geometry using the DFEM-SN solver. The slowing down problem is solved using the 1D CPM solver, which is computationally very cheap. In the Griffin CSAPI, the slowing down calculation scheme of MC²-3 is used [13]; fission and non-elastic scattering sources are assumed to be fixed, and elastic scattering sources are computed recursively on successive HFGs (416,400 groups with equal lethargy width of 1/24000 from 14.191 MeV to 0.414 eV). This approach is basically based on the same idea used in the SCALE procedure that the SCALE Monte Carlo code MCDancoff is used to compute Dancoff factors, which are then used to modify the standard CENTRM two-region 1D unit cell models to account for three-dimensional (3D) lattice heterogeneous effects [10]. This approach was successfully demonstrated for a pressurized water reactor (PWR) assembly problem by another code named Galaxy as well [11].

A Dancoff factor for each fuel pin is calculated using the enhanced neutron current method (ENCM) [49] by solving the following FSP once using the DFEM-SN solver in Griffin.

$$\vec{\Omega} \cdot \nabla \psi(\vec{x}, \vec{\Omega}) + (\Sigma_a(\vec{x}) + \Sigma_p(\vec{x})) \psi(\vec{x}, \vec{\Omega}) = \frac{1}{4\pi} \Sigma_p(\vec{x}), \quad (13)$$

where Σ_a is 10^5 for fuel regions and 0 for other regions and Σ_p is the potential scattering cross section. A

Dancoff factor for a fuel lump, f , is calculated as

$$D_f^{3D} = \bar{l}_f ((\Sigma_{a,f} + \Sigma_{p,f}) \phi_f - \Sigma_{p,f}), \quad (14)$$

where $\bar{l}_f$ is the mean chord length of the fuel lump, f . The superscript 3D means that the FSP is solved in the whole 3D geometry. However, a Dancoff factor is typically calculated in a 2D domain since the resonance treatment is usually performed plane-by-plane without considering the axial leakage effect and the ENCM has not been proved for its applicability to the 3D geometry. This will be briefly discussed again in Section 2.3.4. Note that all the problems solved in this report are 2D cases so that this issue is irrelevant to the results in the verification tests. Once the Dancoff factor is obtained, the equivalent outermost radius of 1D cell of the fuel pin, R_{eq}^{1D} , is determined to preserve the Dancoff factor of the original geometry by solving the following non-linear equation using the binary search.

$$D_f^{1D}(R_{eq}^{1D}) = D_f^{3D}, \quad (15)$$

where the left-hand side is the Dancoff factor calculated using the 1D CPM in the 1D cell of which the outermost radius is R_{eq}^{1D} . Once the Dancoff-factor equivalent 1D cell is determined, the fixed source slowing down calculation is performed to obtain the weighting spectrum for condensation.

The approximation in the EDC method poses constraints on the widths of resonance energy groups in mainly two aspects. First, the Dancoff factor approach itself assumes identical fuels in a lattice, and thus, the neighboring effect of different fuel types and temperatures on a within-group spectrum of a target region cannot be considered. Note that the resonance table approach approximately considers this via escape cross sections by using the average magnitude of different total cross sections in neighboring regions in an FSP. Second, the fuel to moderator ratio is not preserved in an EDC, which does not preserve the resonance escape probability, and in turn, the overall spectrum attenuation over energy. For these two reasons, the widths of the resonance energy groups should not be too coarse. Typically, widths similar to those of major U-238 resonances would be the most practical choice as in the WIMS-69 group structure [50]. Coarser group widths would cause notable errors in a weighting spectrum. Note that this constraint on the energy group structure in the resonance energy range also applies to the resonance table method mainly because the replacement of within-group spectrum information with a single parameter of the background cross section

makes it harder to cover a wide range of variation of the within-group spectrum in larger group widths caused by the resonance interference effect among different isotopes, different lattice heterogeneities, etc.

2.3.3 Iterative Local Spatial Self-shielding (ILSS) Method for Particulate Fuel Modeling

For cross section evaluation of particulate fuels, either the transport solver can be modified to consider the microstructure of particles dispersed in a compact or the compact-averaged cross sections are evaluated and passed to the normal transport solver without its modification. In this work, the latter approach was selected and implemented under the calculation framework of the EDC method. By performing slowing down calculations in an appropriate particle cell model, both energy and spatial self-shielding inside particles are taken into account. There are several possible ways to treat particulate fuels for the resonance table method, which will be considered in future work. Currently, particulate fuels can only be modeled with the EDC method.

The stochastic region-averaged multigroup microscopic cross section of isotope i in energy group g is computed as

$$\bar{\sigma}_{X,g}^i = \frac{1}{\bar{N}^i} \sum_k \left\{ N_k^i v_k \frac{\int_g \sigma_{X,k}^i(E) \phi_k(E) dE}{\int_g \bar{\phi}(E) dE} \right\}, \quad (16)$$

where N_k^i , v_k , and ϕ_k are the atomic density of isotope i , volume fraction, and flux of micro-region k in a compact, respectively, and $\bar{N}^i$ and $\bar{\phi}$ are the average atomic density of isotope i and the average flux in a compact, respectively. To compute the flux at the micro-region k , the true ratio of flux at micro-region k to the average flux of the compact is approximated to the ratio obtained in a simplified particle cell model as

$$\phi_k(E) = \frac{\phi_k(E)}{\bar{\phi}(E)} \bar{\phi}(E) \approx \frac{\phi_k^{\text{p.c.}}(E)}{\bar{\phi}^{\text{p.c.}}(E)} \bar{\phi}^{\text{Lat.}}(E) = d_k^{\text{p.c.}}(E) \bar{\phi}^{\text{Lat.}}(E), \quad (17)$$

where p.c. stands for a particle cell calculation, Lat. means a lattice calculation, and d refers to a disadvantage factor (DF) defined as the ratio of flux at the micro-region to the average flux of the stochastic region. Inserting Eq. (17) into Eq. (16) yields

$$\bar{\sigma}_{X,g}^i = \frac{1}{\bar{N}^i} \sum_k \left\{ N_k^i v_k \frac{\int_g \sigma_{X,k}^i(E) d_k^{\text{p.c.}}(E) \bar{\phi}^{\text{Lat.}}(E) dE}{\int_g \bar{\phi}^{\text{Lat.}}(E) dE} \right\} = \frac{\int_g \bar{\sigma}_X^i(E) \bar{\phi}^{\text{Lat.}}(E) dE}{\int_g \bar{\phi}^{\text{Lat.}}(E) dE}, \quad (18)$$

where

$$\bar{\sigma}_X^i(E) = \frac{1}{\bar{N}^i} \sum_k N_k^i v_k \sigma_{X,k}^i(E) \frac{\phi_k(E)}{\bar{\phi}(E)} \approx \frac{1}{\bar{N}^i} \sum_k N_k^i v_k \sigma_{X,k}^i(E) d_k^{\text{p.c.}}(E). \quad (19)$$

In the energy range where the energy dependence of the cross section and DF cannot be neglected, Eq. (18) is computed in two steps: $d_k^{\text{p.c.}}(E)$ is calculated by solving a particle cell problem in the first step, and $\bar{\phi}^{\text{Lat.}}(E)$ is calculated from a lattice self-shielding formalism using the approximated stochastic region-averaged cross section of Eq. (19) in the second step. In this work, the lattice self-shielding formalism is the EDC method. In the fast and thermal energy range where the energy dependence of the cross section and DF is neglected, $\sigma_{X,k}^i(E)$ and $d_k^{\text{p.c.}}(E)$ are taken out of the integral, and Eq. (18) is approximated to

$$\bar{\sigma}_{X,g}^i = \frac{1}{\bar{N}_i} \sum_k N_k^i v_k \sigma_{X,k,g}^i d_{k,g}^{\text{p.c.}}, \quad (20)$$

which only requires the DF calculation that solves a particle cell problem.

The ILSS method [12] is used for calculating DFs. The uniqueness of this method lies in the way that it considers the stochastic effect on spatial self-shielding inside particles. For the resonance energy groups where the mean free path of neutrons is either comparable to or smaller than the average spacing among particles, the stochastic dispersion of neighboring particles should be considered to estimate spatial self-shielding inside particles. For this, a particle of interest at the center is surrounded by the homogenized composition of fuel particles and matrix, including the particle type of interest, as shown in Fig. 2.

Figure 2: Particle cell model to calculate DFs in the resonance energy range.

The homogenized composition is introduced to model the effect of random particle distribution on the reaction rates in the particle at the center by including the target (center) particle type in it. The most important part is that the homogenized composition cross sections of Fig. 2 use spatially self-shielded cross sections of the particles and matrix, and thus, depend on DFs of them. This makes the N particle cell problems coupled together, and the coupled set of N particle cell problems are solved iteratively until all

DFs converge. Note that, even for $N = 1$, the DF of the particle should be determined iteratively due to the presence of the DF of the particle type itself in the cross section of the homogenized composition. This DF iteration (i.e., spatial self-shielding iteration) is performed inside the energy loop of the slowing down calculation. Once $d_k^{p,c}(E)$ is obtained, pointwise stochastic region-averaged cross sections are obtained using Eq. (19) and used in the lattice self-shielding method to obtain $\bar{\phi}^{\text{Lat.}}(E)$.

Figure 3: Particle cell model to calculate DFs in the fast and thermal energy ranges.

In the fast energy range, neutrons are born from fission in the fuel kernel and leak to the matrix and the moderator region where neutrons disappear through down-scattering. On top of that, the mean free path of neutrons far exceeds an average spacing among particles and even the distance between compacts. In this circumstance, preserving the relative amount of moderator to fuel is more important than considering the stochastic effect in determining the ratio of the flux in the fuel kernel to the average flux of the compact. Thus, the regular particle array model of Fig. 3 is used instead of that of Fig. 2. In the thermal energy range, scattering sources from the matrix and the moderator drive the flux distribution inside a compact. In the absence of a large resonance in the fuel kernel, the regular particle array model is accurate enough in determining the DF in the fuel kernel. The DF in the fuel kernel is not sensitive to the presence of the moderator at the outside of the matrix in Fig. 3. Thus, the flux solution of the particle model of Fig. 3 is utilized to compute DFs in the thermal energy range, too. A detailed investigation is needed in future work to check the validity of the particle cell model of Fig. 3 in the thermal energy range for cases such as a plutonium fuel where large resonances in a particle exist. It should be noted that the N particle-type problems of Fig. 3 are decoupled. Thus, DFs in the fuel particle and matrix are calculated by solving an eigenvalue problem for each particle type in the CSAPI multigroup structure, and stochastic region-averaged multigroup cross sections of Eq. (20) for the fast and thermal energy groups are obtained.

2.3.4 Discussion on Online Cross Section Generation

When generating multigroup cross sections online, there are several points that need to be taken into account and carefully addressed to accurately generate multigroup cross sections for various reactor problems with different conditions.

- Within-group resonance interference effect:

The within-group spectrum is mainly affected by major resonances of resonant isotopes within an energy group. For methods utilizing a pre-tabulated effective cross section set, an error arises from the fact that only resonances of a target resonant isotope are considered in the within-group weighting spectrum used in the generation of the table. The change of the within-group spectrum due to resonances of other resonant isotopes in a target problem is approximately considered by assuming that the resonances of other isotopes are constant within the energy group, and the flux depression due to the resonances of other isotopes occurs uniformly on the average sense in the entire within-group via the background cross section. This causes non-negligible errors, especially in plutonium-dominant regions or in burnable poison or control rod regions that have large resonances in the resonance energy range. On the other hand, the resonance interference effect is naturally accounted for in the on-the-fly slowing down method.

- Non-uniform intra-pellet temperature and burn-up profiles for power reactor:

Intra-pellet variations of temperature and burnup profiles are concerns in power reactors. In order to properly consider this effect in a transport calculation, different cross section zones should be used within a pellet, or properly averaged cross sections over the entire radial zone of the pellet should be used. However, the resonance table approach has two drawbacks. First, when different cross section zones are to be used for radial rings in a pellet, the resonance table approach may have some errors in ring-wise cross sections, mainly because the ring-wise escape probability and the fuel-lump escape probability are different. That is, applying the effective cross section vs. background cross section relation for the fuel lump to ring-wise relations would cause some errors. Note that this holds even for uniform intra-pellet temperature and burnup profile cases. Second, effective cross sections in a resonance table are generated at a uniform intra-pellet temperature and number density, and thus the effect of non-uniform variation within a pellet is missing in the resonance table. There are

some techniques to approximately consider these effects [51, 52], but those techniques have not been applied in this work yet. Note that the on-the-fly slowing down method is able to naturally consider these effects because different HFG cross sections at different rings in a pellet are used in the slowing down calculation.

- Thermal up-scattering:

The thermal up-scattering refers to up-scattering due to the thermal agitation of a target nuclide, which gives the secondary energy distribution of double differential scattering kernel the temperature dependency. This temperature dependency of a scattering kernel becomes stronger for heavier nuclides. This is the reason graphite up-scattering is considered to be more important in a graphite-moderated system than hydrogen up-scattering in a LWR. For example, graphite up-scattering can be prominent even at a few tens of eV energy range for temperatures higher than 1000 K. For even heavier nuclides, such as uranium or plutonium isotopes, this temperature dependency is dramatically affected under strongly varying scattering cross sections [53]. Neglecting this effect causes a huge impact on capture rates of U-238 at resonances in the low energy range [54].

In the current CSAPI multigroup library, the multigroup scattering kernel generated using the Serpent2 + NJOY path has a temperature dependency only up to 10 eV regardless of temperature. This is because NJOY is used to generate the multigroup scattering kernel in the Serpent2 + NJOY path, and 10 eV is the maximum incoming neutron energy in the NJOY THERMR module. Another problem is that the NJOY THERMR module does not take into account the resonance scattering in computing the scattering kernel. That is, the free gas scattering from the $S(\alpha, \beta)$ formulation in the THERMR module is derived under the assumption of the constant scattering cross section [20]. Therefore, work is planned in the next fiscal year to utilize the modification of NJOY made by [55] in which resonance scattering cross section is incorporated in the $S(\alpha, \beta)$ formulation. Updates will be made to the multigroup scattering kernel in the CSAPI multigroup library as well as the HFG scattering kernel to be used in the slowing down calculation for the EDC method. Note that the effective cross section of the resonance table method takes into account the up-scattering effect since the thermal up-scattering including the resonance up-scattering is accounted for in a Monte Carlo simulation [56, 57].

- Multigroup scattering kernel accounting for problem-dependent spectrum:

In the multigroup cross section libraries of most lattice physics codes, a multigroup scattering kernel of isotopes does not include a dependency on parameters other than temperature, even though a scattering cross section has a dependency on a background cross section as other reaction cross sections do. In the SCALE code system, a self-scattering has also a dependency on background cross section, and out-going scattering cross sections are determined based on a shielded scattering cross section and a shielded self-scattering cross section [58]. However, the accuracy of the multigroup scattering kernel is mainly determined by the overall slope of a within-group spectrum governed by a fuel-to-moderator ratio and lattice heterogeneity and weakly determined by energy self-shielding due to heavy isotopes in a group. This is very important for a major isotope in a moderator. A multigroup scattering cross section of such an isotope is smooth and does not depend on a within-group spectrum, whereas a pointwise scattering kernel has $1/E$ dependency over the incoming energy, which significantly affects the multigroup scattering kernel with the slope of the within-group spectrum. Unfortunately, the current CSAPI library does not consider this like most multigroup libraries of lattice physics codes. The need for improvements is demonstrated in the verification section and will be addressed in CSAPI as a future work.

- Angle-dependent multigroup cross section in pin-resolved heterogeneous calculation:

Most of the existing deterministic transport codes for the lattice physics calculation do not use angle-dependent multigroup total cross sections. For LWR applications, this approximation induces a significant bias in the lattice calculation when explicitly pin-resolved heterogeneous geometry is used. Unlike in the homogenized assembly problem, the angle dependency of multigroup total cross sections in the resonance energy range are large due to a strong variation in the within-group spectrum over angle at the periphery of a fuel rod, the neglect of which causes stronger streaming into the fuel rod and overestimates neutron fluxes in the fuel [59, 60]. This means that an accurate estimation of only the 0th Legendre moment of group cross section in the resonance energy range through the resonance treatment is not sufficient. Such a strong angle dependency of the within-group spectrum does exist in the thermal energy range, but cross sections in the thermal energy range are smooth in a typical energy group structure of lattice physics codes, and group cross sections themselves do not have notable variations over angle in the thermal energy range.

The error caused by only condensing pointwise cross sections with the scalar flux spectrum (the 0th

moment), not with the angular flux spectrum, is called the condensation error. The transport correction methods have been proposed a long time ago to handle this issue [61], but the target problem was not a pin-resolved heterogeneous transport calculation. Although the efficacy of the method for lattice physics calculations was shown in [59] for a 1D slab geometry, the authors' preliminary studies for a 2D pin-cell geometry revealed several issues in the transport correction method. First, the method requires higher Legendre order moments of the total cross section to obtain transport cross sections. Due to the opposite behavior of the higher order flux spectrum at the vicinity of resonances in the periphery of a fuel rod compared to the scalar flux spectrum, higher order cross sections are an order of magnitude larger than 0th order ones. This may induce instability in the transport solver. Second, there is no resonance treatment theory to estimate such higher order cross sections in pin-resolved heterogeneous geometry.

For these reasons, more simple approaches using equivalence parameters have been used for practicality [46, 60, 62–65]. The approach using the SPH factor is the most common and easiest to implement. This is often called the multigroup equivalence (between pointwise and multigroup calculations) in French and Japanese literature. As it turned out that the neighboring pin effect on the SPH factor of a target pin-cell is negligible, it is sufficient to generate the SPH factor at a pin-cell level [60]. Therefore, for the resonance table method in this work, SPH factors can be generated in the same pin-cell configurations used in generating the effective cross section table over the wide range of background cross sections. That is, SPH factors can be tallied together with effective cross sections from Serpent2. For the EDC method, SPH factors can be easily calculated on the fly after performing the slowing down calculation in an EDC. In this work, however, this SPH factor approach to resolve the condensation error has not yet been employed. In fact, this effect is dominant in a normal LWR fuel density, not in low fuel density applications like a graphite-moderated system. A simple test using MC²-3 for a VHTR pin-cell problem showed that the maximum eigenvalue error induced by the group condensation was at most 30 pcm due to low fuel density, whereas typical condensation errors in an LWR application can cause eigenvalue errors of 200–300 pcm [66] regardless of the energy group structure.

- Axial leakage effect on self-shielding:

Most lattice physics codes do not consider the axial leakage effect in the resonance treatment since

lattice physics calculations are usually performed on two-dimensional (2D) problems. The base theory of the self-shielding treatment is based on a 2D geometry. In a situation where neutrons can leak out of an axial segment of a fuel rod across its top or bottom plane, the fuel rod escape probability cannot be defined using the mean chord length of a fuel rod because the fuel rod is cut axially, and thus, the formulation in equivalence theory should be re-evaluated. For example, the definition of the Dancoff factor should be altered and the validity of the algorithm for the ENCM should be theoretically verified for such a 3D case. Nevertheless, the current implementation in the Griffin CSAPI uses the ENCM algorithm for a 3D geometry, producing seemingly reasonable Dancoff factors in different axial segments of a fuel rod. This would be from the fact that the axial neutron leakage in a fuel rod is negligible due to the black fuel assumption. Efforts are needed to verify this in the next fiscal year. This issue holds for the resonance table method as it should be checked whether the enforced equivalence works or not when using a 2D table for a 3D application.

- Core-wide spectral transition effect:

Since a direct pin-resolved heterogeneous whole-core calculation in the CSAPI library group structure (> 40 groups) is too demanding for the computing resources in general, an appropriate condensation scheme to a broad group level (≤ 10 groups) needs to be devised for practicality, as was done for heterogeneous assembly calculations in the CASMO code [67]. For example, only a local pin-cell calculation is performed with the CSAPI library group structure to obtain a local fine group spectrum. Then, pin/assembly-homogenized problems are solved in the intermediate/broad group structures to obtain the intermediate/broad group spectrum, which are fed back to the local spectrum to obtain the region-wise broad group cross sections and then perform the pin-resolved heterogeneous core calculation in the broad group structure. Appropriate equivalence parameters should be introduced at each condensation/homogenization stage. This should be investigated in future work.

3. Implementation of CSAPI in Griffin

This section focuses on implementation details in Griffin. The CSAPI module of PROTEUS [68], where only the resonance table method was available, was ported to Griffin in the last fiscal year [2]. The original Fortran routines in PROTEUS were kept, and the C++ interface was developed by introducing a new material type named *CSAPINeutronicsMaterial* in Griffin. In this fiscal year, the new resonance treatment methodology of the on-the-fly slowing down approach (the EDC method) and the double heterogeneity treatment capability (the ILSS method) were implemented in the Fortran routines. The first subsection explains the C++ interface part and the implementation schemes of the resonance table method and the EDC and ILSS methods are described in the second subsection.

3.1 C++ Interfaces

The CSAPI module was originally developed with Fortran for PROTEUS. Since it was designed and developed to be easily plugged into any heterogeneous transport solvers, the CSAPI module was integrated into Griffin starting from the last fiscal year by:

- Introducing *CSAPINeutronicsMaterial* to connect the region-wise cross sections computed from CSAPI to the Griffin material systems for transport calculations
- Implementing the Fortran/C++ interface routines to transfer material and region data and cross sections between CSAPI and Griffin
- Plugging the FSP solver (DFEM-SN) to incorporate the fixed source solver and CSAPI together in order to calculate escape cross sections in CSAPI.

In this fiscal year, further updates have been made in the interfaces and inputs for the CSAPI material type in order to improve its usability. The CSAPI interfaces in Griffin were updated to support the use of multiple CSAPI material blocks in the Griffin input system, as illustrated in Fig. 4, which allows the flexibility of input preparation for complicated material assignments. The FSP solver was also refactored to properly compute the region-wise fluxes based on the mappings of regions and compositions defined in the multiple material blocks. The interface was updated to fully support the parallel execution with distributed meshes for which each processor contains its own partitioned mesh data. Several test problems using CSAPI were added to the Griffin repository for software quality assurance and performance test purposes.

```

[Materials]
  [csapi_mat1]
    type = CSAPINeutronicsMaterial
    material_ids = '0'
    block = '0'
    isotope_names = 'U_235 U_238 O_16'
    isotope_atomic_densities = '7.18E-04 2.21E-02 4.57E-02'
    ...
  []
  [csapi_mat2]
    type = CSAPINeutronicsMaterial
    material_ids = '1'
    block = '1'
    isotope_names = 'O_16 H_001'
    isotope_atomic_densities = '2.48E-02 4.96E-02'
    ...
  []
[]

```

Figure 4: Sample input for *CSAPINeutronicsMaterial*.

The functionalities of CSAPI were elaborated to perform the robust heterogeneous transport calculations. First, the CSAPI interface to calculate the fission spectrum was updated to properly account for the isotopic data available in the CSAPI library. Previously, the fission spectrum was simply determined for each composition only once at the beginning of the code run by using a uniform spectrum and was not updated by taking into account the spectrum evolution during fission source convergence. This approximation works well without introducing noticeable errors for the thermal reactor case where the fission from U-235 is dominant. However, it can result in non-negligible errors on eigenvalue because fuels for many fission reactors are composed of multiple fissionable isotopes. *CSAPINeutronicsMaterial* was updated to compute the macroscopic fission spectrum through proper flux-weighting at each iteration to correctly reflect the up-to-date solution to the flux-weighting. Second, an interface to compute the fission power was added to the CSAPI material type, which is an essential feature in the reactor analysis. In addition, the CSAPI module was updated to compute a correct kappa-fission value with the spatial self-shielding. The performance of the FSP solver was also improved by removing inefficiencies in memory usage and with various improvements to the sweeper documented in Ref. [4]. The minor bugs in the integration were fixed in the detailed verification work. As shown in Table 1, the eigenvalues of Griffin and PROTEUS agreed very well within 17 pcm. Such a small difference could be caused by discrepancies in the spatial discretization and transport solvers between the two codes (DFEM-SN in Griffin and MOC in PROTEUS).

Table 1: Eigenvalue results of LWR pin cell problem for the CSAPI integration test.

Case	Δk_{eff} (Griffin - PROTEUS) in pcm
UO ₂ Pin	13
MOX Pin	12
UO ₂ /MOX Checkerboard	-17

3.2 Resonance Table Method

In order to calculate effective cross sections using Eqs. (3) and (9), escape cross sections need to be evaluated first. The flow diagram to compute escape cross sections of all resonant isotopes is shown in Fig. 5. An energy group is the outermost loop. For each energy group, effective group cross sections of all resonant isotopes are iteratively solved since they are all coupled together through Eqs. (3) and (9). Effective group cross sections are first evaluated at the infinite dilute condition. Then, background cross sections of all resonant isotopes with zero initial values of escape cross sections are calculated using Eq. (9), which are utilized to update effective total cross sections. Once effective total cross sections are determined, the procedure to reevaluate background cross sections starts by solving FSPs of each resonance category. In Fig. 5, C means category, which refers to a group of resonant isotopes of similar resonances in that energy group. Special care is needed in categorization, but just a one-to-one relation of isotope and category or element-wise categorization is used in the Griffin CSAPI at the moment. Note that the formulation of FSPs in Eqs. (10) and (11) is expressed per isotope. In the category loop, if any isotopes of the current category have resonances in the current energy group, FSPs for the category should be solved. Otherwise, FSP calculations are skipped for the next category. After solving FSPs, the escape cross sections of isotopes that belong to the category are updated using Eq. (12). Then, background and effective cross sections of all resonant isotopes are updated in the next outer iteration step and the convergence of cross sections is checked. This procedure is repeated until the convergence is satisfied or the maximum number of outer iterations is reached, whichever comes first. In the Griffin CSAPI, the convergence criterion is met when the maximum value of relative differences in total cross sections between successive iteration steps among all resonant isotopes becomes less than 10^{-3} . The maximum number of outer iterations is set to unity, which is effectively updating the effective cross section twice according to the algorithm of Fig. 5: once before the outer loop and the other with the updated escape cross section outside the outer loop, which is not shown in Fig. 5. It turned out that further updating escape cross sections does not bring practical benefits for the computational effort to solve FSPs.

Figure 5: Flowchart of calculating the isotopic background cross sections in the resonance table method.

3.3 EDC and ILSS Methods

This subsection explains the implementation details for the EDC and ILSS methods together. Fig. 6 shows the brief workflow. At the beginning, pin-cell geometry and composition are constructed using mesh information from an Exodus mesh as follows:

- To construct pins and internal geometry and compositions of each pin, an extra element integer ID that groups elements into a pin should be present in an Exodus mesh. A user can designate an ID name or *pin_id* is used. If no such an extra element integer ID is present, the code errors out.

- For each pin, the centroid point is determined using the centroid point information of each mesh that belongs to the pin. If the pin is cut by symmetry, a user should manually specify centroid points of such pins in an input. This case would be rare.
- For each unique combination of *subdomain_id*, *material_id*, and any additional user-specified extra element integer IDs, such as *region_id*, average distances of elements belonging to each ID set with respect to the centroid of the pin are compared among unique ID sets to determine the geometry and composition of a 1D cell. The ring radii are calculated by preserving the total volume of elements for each ID set and considering their orders from the center.
- Once pins are constructed, axial segments of pins are examined for whether a fuel region exists or not. Each pin segment that contains a fuel region is designated as an EDC, and EDCs in the whole domain are distributed to MPI (Message Passing Interface) processors.

Figure 6: Brief workflow of the EDC method to generate effective multigroup cross sections

Since the EDC and ILSS methods use the HFG slowing down algorithm of MC²-3, HFG cross sections are required. Thus, the MC²-3 library data and routines were employed to reconstruct HFG cross sections. In the process, the followings are accounted for:

- If HFG cross section files exist in a user-specified directory, data are just read from the files. If they do not exist, HFG cross sections are reconstructed using the MC²-3 library data and routines. The reconstruction task is distributed to MPI processors for parallel calculations.

- Since the MC²-3 library and HFG cross section data require a non-negligible amount of memory, possessing all the data for all MPI processors is not a viable option. Thus, each processor reads only the data of isotopes belonging to it to reconstruct HFG cross sections and perform the EDC and ILSS calculations.

A Dancoff factor for each pin segment that contains fuel is obtained by solving the FSP of Eq. (13) with the DFEM-SN solver and using the formula of Eq. (14). Note that the FSP can be solved only once regardless of the number of energy groups since Eq. (13) does not have a group dependency. Then, the outer radius of each fuel segment is determined by solving Eq. (15). For obtaining D_f^{1D} , the MC²-3 routines to perform the 1D CPM in a cylindrical geometry are used.

Once all EDCs are set up, each processor works on the EDCs assigned to it. Before performing the slowing down calculation, the code first checks whether a stochastic region exists in the EDC. If a stochastic region exists, stochastic region-averaged cross sections are prepared by performing the ILSS calculation, whose procedure is shown in Fig. 7. If a stochastic region does not exist in an EDC, the ILSS calculation is just skipped.

- The first step is to calculate stochastic region-averaged multigroup cross sections in the fast and thermal energy range and provide them to the DFEM-SN transport solver for the transport calculation. An eigenvalue problem is solved using the 1D CPM solver in a spherical geometry for a particle cell model of Fig. 3 to obtain multigroup DFs. In the particle cell model of Fig. 3, the outer radius of the moderator region is determined by preserving the fuel to moderator ratio of the EDC where the stochastic region belongs. Multigroup cross sections needed for the eigenvalue calculation are taken from the CSAPI multigroup library. Once multigroup DFs are obtained, stochastic region-averaged multigroup cross sections are calculated using Eq. (20) and passed to the DFEM-SN transport solver as well as the EDC solver. Note that stochastic region-averaged multigroup cross sections in the resonance energy range calculated in this way are just temporary values and will be updated in the next step. Those temporary values are just used in the EDC calculation initially for calculating fixed sources in the HFG slowing down calculation as explained later.
- The second step is to calculate stochastic region-averaged HFG cross sections in the resonance energy range and then provide them to the EDC solver for the lattice self-shielding. Since the slowing down

1) Eigenvalue Problem in Particle Cell of Fig. 3

For particle cell of each particle type
 Determine size of moderator region from EDC
 Prepare macroscopic multigroup cross sections in the homogenized composition region
 Solve eigenvalue problem
 Calculate multigroup DFs of all particle types and matrix
 Pass $\bar{\sigma}_g^i$ of Eq.(20) for fast and thermal energy groups to the EDC and DFEM-SN transport solver

2) Slowing-down Problem with DF Iteration in Particle Cell of Fig. 2

For particle cell of each particle type
 Prepare macroscopic pointwise cross sections in the homogenized composition region with DF=1
 Prepare fixed fission and nonelastic scattering sources
 For each energy point
 For DF iteration
 For particle cell of each particle type
 Update macroscopic pointwise cross sections in the homogenized composition region with the most recent DFs
 Update collision probabilities
 Calculate source
 Obtain flux solution and update pointwise DFs of the current particle and matrix
 Pass $\bar{\sigma}^i(E)$ of Eq.(19) for the resonance energy range to the EDC solver for lattice self-shielding

Figure 7: Procedure of the ILSS method.

calculation scheme is adopted from the MC²-3 formalism [13], the sources from fission and non-elastic (inelastic + (n,2n)) scattering reactions are assumed to be fixed, and only the elastic scattering sources are updated during the slowing down calculation. For each HFG, HFG cross sections in the homogenized composition of Fig. 2 for each particle cell problem of different particle types are updated with the latest HFG DFs of all particle types and matrix. Collision probabilities and sources are updated accordingly, and in turn, flux solutions and DFs are updated sequentially. This update procedure is iterated until DFs of all particle types and matrix converge. DFs are assumed to be converged when the maximum value of the relative differences between successive iterations among all particle types and matrix becomes less than 10^{-4} . Once the last energy group is reached, stochastic region-averaged HFG cross sections are computed using Eq. (19) and passed to the EDC solver.

Once stochastic region-averaged cross sections are prepared, the EDC method is performed as below:

- As is done in the ILSS method, the slowing down calculation requires fission and non-elastic scattering sources as fixed sources. For this, the eigenvalue problem is first solved in the EDC geometry. For an EDC with a stochastic region, multigroup cross sections for the eigenvalue problem should be stochastic region-averaged ones computed by the ILSS method. Using the spectrum solution of the eigenvalue problem and stochastic region-averaged fission, inelastic and (n,2n) scattering cross sections, fixed sources are prepared. Then, the slowing down calculation is performed using stochastic region-averaged HFG total and elastic scattering cross sections. A resulting spectrum is used as a weighting function for group condensation only for the CSAPI library energy groups within the resolved resonance energy range defined in the MC²-3 library. For the unresolved resonance energy range, multigroup cross sections obtained using the resonance table method in the EDC geometry are used. It means that the double heterogeneity treatment is not applied to the unresolved resonance energy range due to its negligible effect in such a high energy range.
- To properly simulate spatial self-shielding inside a fuel near a resonance peak in the EDC geometry, a large enough number of meshes should be used both in fuel and moderator regions. Otherwise, a non-negligible impact is expected on the spectrum solution due to an inaccurate spatial self-shielding. This is done automatically in the code by limiting the maximum optical thickness of each ring ($\Sigma_t \Delta R$) to 1 and 0.05 for fuel and non-fuel regions, respectively, in the whole slowing down energy range.

Currently, the EDC solver is unable to handle a non-fuel pin that contains resonant isotopes. Since the typical energy range of resonances for light and intermediate mass isotopes is different from that for heavy isotopes, the black optical thickness cannot be assigned to non-fuel regions simultaneously together with fuel regions when constructing EDCs. A Dancoff factor for such non-fuel pins could be obtained separately by performing the ENCM calculation one more time, and the average fission sources of fuel pins could be used in the slowing down calculation to obtain a weighting spectrum. The validity of this approach, however, has not been examined. Instead, just the resonance table method is used for resonant isotopes in non-fuel pins, which means that FSPs should be solved over the entire domain for resonant isotopes in non-fuel pins. The applicability of the EDC method to non-fuel pins will be examined in future work.

4. Verification Tests

The Griffin CSAPI was verified against the continuous energy Serpent2 [8] Monte Carlo solutions for graphite-moderated thermal reactor problems. First, the prismatic VHTR unit-cell problems over a wide range of pin-cell parameters were solved. Second, the EMPIRE unit-cell problem was solved to check the applicability to heat-pipe-cooled microreactor problems. Third, the HTTR assembly problems with and without B₄C burnable poison rods (BPs) were investigated. All problems discussed here are 2D problems, and 3D problems will be addressed in the next fiscal year. All Griffin calculations were performed using the DFEM-SN solver with the CMFD acceleration. The Gauss-Chebyshev angular quadrature of three polar and nine azimuthal angles per octant (108 angles for all directions) was used for all Griffin calculations. Coarser meshes for the CMFD calculation were chosen rather than those used for the transport calculation. The Executioner options used are shown in Fig. 8.

```
[Executioner]
  type = SweepUpdate
  richardson_rel_tol = 1e-4
  richardson_max_its = 500
  richardson_value = fission_source_integral
  inner_solve_type = GMRes
  max_inner_its = 2
  cmfd_acceleration = true
  coarse_element_id = coarse_element_id
  cmfd_solver_type = krylovshur
  prolongation_type = multiplicative
[]
```

Figure 8: Executioner block for all Griffin calculations.

The 68-group structure was determined to have the smallest eigenvalue errors over a wide range of spectra for a graphite-moderated system, which were used for all test problems discussed in this section. The lethargy widths of the 68-group structure are shown in Fig. 9 together with those of the WIMS-69 group structure [50] for comparison. It has almost uniform lethargy widths above 10 eV, and the energy range of the U-238 resonance at 6.67 eV is divided into several groups for the reason explained in Section 4.1. Note that this group structure is optimized for a fresh uranium fuel in the graphite-moderated system just for this work and will be further optimized for realistic applications to reactor types of interest in future work. The self-shielding treatment is applied to the resonance energy groups ranging from 1.05 eV to 100.52 keV, and only the temperature interpolation is involved for the other energy groups. The CSAPI multigroup

libraries for all problems were generated using the Serpent2 + NJOY path explained in Section 2.2. All Serpent2 reference solutions were generated using an explicit particle representation in Serpent2. Serpent2 calculations were performed multiple times using different random particle configurations, based on which averaged results were taken as reference solutions.

Figure 9: Comparison of lethargy widths of the 68-group structure and the WIMS-69 group structure.

4.1 VHTR Pin-Cell Problems

The performance of the Griffin CSAPI was first examined for the prismatic VHTR unit-cell problem, which is shown in Fig. 10 over a wide range of pin-cell design parameters, including double-heterogeneity. A total of 81 problems were constructed by combining different parameters as shown in Table 2. The particle radius and packing fraction are fuel particle (microscopic) design parameters, and the compact radius and compact-to-moderator volume ratio are fuel lattice (macroscopic) design parameters. The problems were constructed in a way that, while one parameter varied, the other three parameters were kept the same. For example, to achieve a desired packing fraction with different particle sizes, the number of particles was adjusted. As the number of particles should be an integer and the particle size is fixed, the resulting packing fractions deviate slightly from the targeted packing fraction within the first decimal point. The values of each parameter were chosen to cover most realistic designs. Nine cases of packing fractions and compact-to-moderator ratios in Table 3 were chosen to not overlap fuel(kernel)-to-moderator (outer layers of particles

+ matrix + graphite block) ratios for testing the problems in nine different spectra as shown in Fig. 11.

Temperature : 293.6 K				
	Region	Radius (cm)	Material	Density (g/cm ³)
Fuel Particle	Fuel Kernel	0.0175	10.36 wt.% UCO	10.5
	Buffer	0.0275	Graphite	1.00
	Inner PyC	0.0310	Graphite	1.90
	SiC	0.0345	SiC	3.20
	Outer PyC	0.0385	Graphite	1.90
	Fuel Compact	0.6225	Graphite	1.1995
	Coolant	0.6350	Helium	0.0032
	Graphite Block	-	Graphite	1.74

Figure 10: Compact design obtained from the NGNP design.

Table 2: Fuel particle and compact parameter values.

Scaling Type	Parameter	Abbreviation	Value
Microscopic Scaling	Particle Radius (cm)	PS ₁	0.0200
		PS ₂	0.0385
		PS ₃	0.0700
	Packing Fraction (%)	PF ₁	2.4
		PF ₂	11.2
		PF ₃	52.0
Macroscopic Scaling	Compact Radius (cm)	CS ₁	0.4
		CS ₂	0.8
		CS ₃	1.2
	Compact-to-Moderator Volume Ratio	CM ₁	0.606
		CM ₂	1.383
		CM ₃	2.992

For each problem, the homogeneous (single het.) and heterogeneous (double het.) compact configurations were solved. For the double heterogeneous problems, the Serpent2 results were generated by 25 independent runs with different random particle configurations for each case. Each Serpent2 simulation was performed with 10^5 particles/cycle, 100 active and 100 inactive cycles. For single heterogeneous problems, 10^5 particles/cycle, 1000 active and 100 inactive cycles were used. The mesh for the VHTR problem of the (CS₂, CM₂) case in the Griffin calculation is shown in Fig. 12. Different colors mean different cross section zones. Colors other than the red represent the fuel region with six rings of cross section zones with the equal area. Meshes for other problems were constructed in the same manner. A P₂ anisotropic scattering order

Table 3: Fuel to moderator volume ratios.

	CM ₁	CM ₂	CM ₃
PF ₁	8.55E-04	1.32E-03	1.70E-03
PF ₂	3.99E-03	6.14E-03	7.95E-03
PF ₃	1.88E-02	2.92E-02	3.80E-02

Figure 11: Serpent2 spectra at various fuel-to-moderator volume ratios (at fixed PS₂ and CS₂).

was used.

The CSAPI multigroup library was generated using the pin-cell configuration of the (PF₂, CS₂, CM₂) problem. That is, the baseline multigroup cross sections were generated using the weighting spectrum of the pink-colored one in Fig. 11, and those in the thermal and fast energy groups are used for all problems with a wide spectrum range in Fig. 11. Multigroup cross sections in the resonance energy range were obtained through the resonance treatment. One thing to note here is that the multigroup scattering kernel generated using the pink-colored spectrum was used for all problems in the current CSAPI scheme. As will be shown in the result, this causes a problem, especially for the under-moderated problems. This will be discussed further in this subsection.

Table 4 shows the Serpent2 eigenvalue results for the single and double heterogeneous problems in the first and second rows, respectively, and the TRISO heterogeneity effects in the third row for 81 different

Figure 12: Exodus mesh for the VHTR problem of the (CS₂, CM₂) case.

pin-cell configurations. The standard deviations of eigenvalues for the single heterogeneous problems range from 0.00002 to 0.00008, and the average values of 25 standard deviations of eigenvalues for the double heterogeneous problems range from 0.00007 to 0.00024. The standard deviations of 25 eigenvalues due to the random distribution of particles for the double heterogeneous problems range from 0.00010 (PS₃, PF₁, CS₁, CM₁) to 0.00069 (PS₃, PF₂, CS₁, CM₂), which indicates that a single run of a Monte Carlo code is not sufficient to provide an accurate solution for a stochastic medium even though the random distribution of particles is explicitly used in the run. Even though eigenvalue results of single heterogeneous problems at different particle size cases with other parameters fixed should be identical in principle, they are slightly different as shown in Table 4 since packing fractions vary within the first decimal point for each PF case as explained above.

For the same packing fraction, the reactivity increases with increasing particle size due to the increased spatial self-shielding in particles. Similarly, for the same compact-to-moderator volume ratio, the reactivity increases with increasing compact size due to the increased spatial self-shielding in compacts. When the fuel-to-moderator volume ratio increases, either at the same packing fraction of PF₂ or PF₃ (CM₁ to CM₃) or at the same compact-to-moderator volume ratio (PF₁ to PF₃), the reactivity decreases due to the reduced neutron moderation even though the relative amount of fuel increases. When the compact-to-moderator volume ratio increases for a very low packing fraction of PF₁, the reactivity increases due to the larger effect

Table 4: Serpent2 eigenvalues of homogeneous (single heterogeneous) and heterogeneous (double heterogeneous) compact problems and TRISO heterogeneity effects in pcm.

		CM ₁			CM ₂			CM ₃		
		CS ₁	CS ₂	CS ₃	CS ₁	CS ₂	CS ₃	CS ₁	CS ₂	CS ₃
PF ₁	PS ₁	1.57144	1.57383	1.57604	1.60943	1.61145	1.61324	1.60304	1.60417	1.60533
		1.60311	1.60375	1.60430	1.65661	1.65731	1.65795	1.65919	1.65965	1.66008
		(1257)	(1185)	(1118)	(1769)	(1717)	(1672)	(2111)	(2084)	(2054)
	PS ₂	1.57213	1.57403	1.57591	1.60952	1.61143	1.61322	1.60280	1.60412	1.60516
		1.61736	1.61670	1.61660	1.67993	1.67997	1.68004	1.68886	1.68909	1.68933
		(1779)	(1677)	(1597)	(2604)	(2532)	(2465)	(3179)	(3136)	(3104)
	PS ₃	1.56311	1.57173	1.57592	1.60787	1.61100	1.61326	1.60533	1.60484	1.60528
		1.61469	1.62342	1.62622	1.69612	1.70024	1.70165	1.71820	1.71951	1.71994
		(2044)	(2026)	(1963)	(3236)	(3258)	(3220)	(4092)	(4155)	(4153)
PF ₂	PS ₁	1.36726	1.39791	1.42110	1.21835	1.23313	1.24583	1.12940	1.13518	1.14021
		1.40391	1.42703	1.44574	1.25082	1.26235	1.27285	1.15633	1.16085	1.16518
		(1910)	(1460)	(1199)	(2131)	(1877)	(1704)	(2062)	(1948)	(1879)
	PS ₂	1.36747	1.39796	1.42087	1.21863	1.23342	1.24588	1.12946	1.13497	1.14011
		1.43799	1.45521	1.47002	1.28170	1.29049	1.29911	1.18258	1.18595	1.18956
		(3586)	(2814)	(2353)	(4038)	(3586)	(3289)	(3977)	(3788)	(3646)
	PS ₃	1.36742	1.39820	1.42074	1.21869	1.23366	1.24567	1.12967	1.13533	1.14002
		1.49348	1.50440	1.51356	1.33581	1.34205	1.34745	1.23079	1.23333	1.23553
		(6173)	(5049)	(4317)	(7194)	(6546)	(6064)	(7273)	(6999)	(6781)
PF ₃	PS ₁	1.23103	1.26680	1.29303	1.08222	1.09794	1.11106	1.00861	1.01409	1.01902
		1.25392	1.28474	1.30853	1.10096	1.11460	1.12647	1.02295	1.02783	1.03229
		(1483)	(1102)	(916)	(1573)	(1361)	(1231)	(1390)	(1318)	(1261)
	PS ₂	1.23115	1.26676	1.29311	1.08235	1.09799	1.11107	1.00874	1.01413	1.01898
		1.27717	1.30340	1.32453	1.11975	1.13165	1.14234	1.03766	1.04195	1.04601
		(2927)	(2219)	(1834)	(3086)	(2709)	(2464)	(2763)	(2633)	(2536)
	PS ₃	1.23057	1.26660	1.29301	1.08183	1.09780	1.11099	1.00821	1.01382	1.01902
		1.32036	1.34046	1.35710	1.15602	1.16598	1.17477	1.06669	1.07065	1.07425
		(5527)	(4350)	(3652)	(5932)	(5326)	(4886)	(5438)	(5235)	(5045)

of an increasing relative amount of fuel under sufficient moderation than the effect of decreasing moderation. The TRISO heterogeneity effect tends to be maximized at a proper range of fast-to-thermal flux ratios, and those at the 11.2% packing fraction are generally larger than those at the other packing fractions as the spectra at the 11.2% packing fraction have a moderate range of fast-to-thermal flux ratios.

Table 5 shows the eigenvalue errors of the EDC method for single heterogeneous problems. Using the multigroup library generated in the pin-cell configuration of the (PF₂, PS₂, CM₂, CS₂) case, the results of the EDC method deviate from reference solutions for problems with less moderation than the problem at which the multigroup library was generated (fuel-to-moderator volume ratio higher than 6.14E-3). The highest fuel-to-moderator ratio cases show about +1% error in reactivity. This error was not attributed to errors in

Table 5: Eigenvalue errors (pcm) of the EDC method for single heterogeneous problems.

		CM ₁			CM ₂			CM ₃		
		CS ₁	CS ₂	CS ₃	CS ₁	CS ₂	CS ₃	CS ₁	CS ₂	CS ₃
PF ₁	PS ₁	-8	-6	-8	-11	-10	-8	4	-1	-3
	PS ₂	-7	-10	-7	-10	-9	-8	5	-1	5
	PS ₃	-10	-7	-8	-10	-7	-9	5	-3	1
PF ₂	PS ₁	10	-5	-19	67	63	53	196	168	175
	PS ₂	6	-4	-13	71	62	55	202	171	180
	PS ₃	11	-4	-18	63	66	59	192	174	175
PF ₃	PS ₁	239	166	162	724	653	624	1132	1045	1047
	PS ₂	238	168	157	724	644	621	1126	1041	1050
	PS ₃	234	171	164	720	656	631	1134	1064	1048

effective cross sections evaluated from the EDC method, but to an overestimated multigroup down-scattering kernel of graphite from the epithermal energy range to the thermal energy range. That is, over-moderation led to a higher reactivity. Since erroneous cases are under-moderated ones, reactivity would be very sensitive to errors in the amount of moderation.

To be more specific, the reason for the overestimation of the multigroup down-scattering kernel can be explained from Fig. 13, which shows the spectrum of the (PF₃, CM₃) case and the spectrum used for generating the multigroup library. As noted in Section 2.3.4, it is often that a multigroup scattering kernel does not account for a problem-dependent spectrum, as illustrated in this example. For simplicity, the multigroup quantities for an s-wave scattering kernel are expressed as

$$\sigma_{g \rightarrow g} = \int_{E_g}^{E_{g-1}} \frac{\sigma_s(E)}{1 - \alpha} \left(1 - \frac{E_g}{E}\right) w(E) dE, \quad (21)$$

$$\sigma_{g \rightarrow g'} = \int_{E_g}^{E_{g-1}} \frac{\sigma_s(E)}{1 - \alpha} \frac{\Delta E_{g'}}{E} w(E) dE \text{ for } g \neq g', \quad (22)$$

where E_g and E_{g-1} are the lower and upper boundaries of energy group g , respectively, and $w(E)$ is a weighting function. Since $\sigma_s(E)$ is nearly constant for most major moderators, its accuracy mainly depends on the overall slope of the within-group spectrum. Using the black instead of the red spectrum in Fig. 13 results in an overestimated down-scattering kernel and an underestimated self-scattering kernel due to the higher weighting on the lower energy part within the group. Errors in self- and down-scattering kernels from energy groups G1–G4 in Fig. 13 are shown in Table 6. Down-scattering cross sections of graphite can easily produce errors up to about 7%. Its consequence on the spectrum result would be huge for the under-moderated system, as illustrated in Fig. 14, which shows the spectrum results for the (PF₃, CM₃) case. Due

to an overestimated multigroup down-scattering kernel and an underestimated multigroup self-scattering kernel shown in Table 6, the spectrum in the thermal and epithermal energy range has about +2.5% and -2.5 to -5% errors, respectively, resulting in a reactivity error of about +1%.

Figure 13: Comparison of base weighting spectrum used for the multigroup library generation and problem spectrum in the epithermal energy range.

Table 6: Errors of self- and down-scattering kernels of graphite from Group-1 to Group-4 in Fig. 13 due to the use of spectrum with overestimated moderation.

	G1	G2	G3	G4
Self	-0.57%	-0.81%	-1.83%	-2.14%
Down	+1.71%	+2.44%	+5.91%	+7.10%

To improve the results, multigroup scattering kernels for nine representative spectra of different fuel-to-moderator ratios were generated using NJOY with corresponding spectra, producing nine different multigroup libraries. Note that the only differences among the libraries are the multigroup scattering kernel. Table 7 shows the improved results. Errors of about 1% were reduced to less than 200 pcm, and all results agreed well with the Serpent2 results. Table 8 and Table 9 show errors in the eigenvalues and the TRISO heterogeneity effect of double heterogeneous problems solved using the nine CSAPI multigroup libraries and the EDC + ILSS methods. All results agreed very well without any noticeable dependency on double heterogeneity parameters. This indicates the strong need for introducing a parameter accounting for this problem-dependent spectrum in the multigroup scattering kernel for major moderators in the CSAPI

Figure 14: Comparison of spectrum for the (PF_3, CM_3) case obtained with the multigroup scattering kernel of (PF_2, CM_2) and (PF_3, CM_3) .

multigroup library.

Table 7: Eigenvalue errors (pcm) of the EDC method for single heterogeneous problems with update of multigroup scattering kernels.

		CM ₁			CM ₂			CM ₃		
		CS ₁	CS ₂	CS ₃	CS ₁	CS ₂	CS ₃	CS ₁	CS ₂	CS ₃
PF ₁	PS ₁	36	36	35	43	43	45	62	56	55
	PS ₂	38	33	36	43	45	45	63	57	62
	PS ₃	33	36	35	43	46	44	61	54	58
PF ₂	PS ₁	59	44	28	68	66	57	130	102	110
	PS ₂	56	44	35	71	65	59	134	106	115
	PS ₃	60	45	29	64	68	63	125	108	110
PF ₃	PS ₁	-1	-49	-36	78	27	18	182	105	117
	PS ₂	-3	-47	-41	75	23	17	176	101	121
	PS ₃	-6	-43	-33	71	30	25	185	123	119

Table 8: Eigenvalue errors (pcm) of the EDC + ILSS method for double heterogeneous problems with update of multigroup scattering kernels.

		CM ₁			CM ₂			CM ₃		
		CS ₁	CS ₂	CS ₃	CS ₁	CS ₂	CS ₃	CS ₁	CS ₂	CS ₃
PF ₁	PS ₁	24	23	24	30	30	30	39	37	38
	PS ₂	15	16	16	17	17	22	22	23	22
	PS ₃	18	19	16	15	17	15	16	15	14
PF ₂	PS ₁	44	48	48	43	59	59	94	83	93
	PS ₂	20	30	29	23	34	33	52	51	51
	PS ₃	9	13	20	3	16	14	16	19	26
PF ₃	PS ₁	17	11	-5	43	46	36	165	113	129
	PS ₂	-3	14	12	4	26	28	123	83	106
	PS ₃	-10	8	14	-28	-5	-8	83	58	74

Table 9: Errors (pcm) in TRISO heterogeneity effect of the ILSS method (Table 8 - Table 7).

		CM ₁			CM ₂			CM ₃		
		CS ₁	CS ₂	CS ₃	CS ₁	CS ₂	CS ₃	CS ₁	CS ₂	CS ₃
PF ₁	PS ₁	-12	-14	-11	-13	-13	-15	-23	-19	-17
	PS ₂	-22	-17	-19	-26	-27	-23	-40	-34	-40
	PS ₃	-15	-17	-19	-28	-29	-29	-45	-39	-44
PF ₂	PS ₁	-16	4	20	-25	-7	3	-35	-19	-17
	PS ₂	-36	-14	-6	-49	-30	-26	-83	-56	-64
	PS ₃	-51	-32	-9	-61	-53	-49	-109	-89	-85
PF ₃	PS ₁	18	60	32	-35	19	17	-17	8	13
	PS ₂	-1	61	53	-71	3	11	-53	-18	-15
	PS ₃	-4	51	47	-98	-35	-33	-102	-65	-45

Fig. 15 shows the relative errors of compact-averaged multigroup U-238 capture cross sections for all CS and CM cases of PF₂ and PF₃ cases at PS₂. In the fast and thermal energy range, cross sections match well among all cases. In the resonance energy groups at major U-238 resonances, cross section errors are all within $\pm 0.5\%$ for both the single and double heterogeneous problems. About +4.5% error in the energy range of 3–5 eV resulted from the neglect of up-scattering in the slowing down problem. This is illustrated in Fig. 16, which compares the Serpent2 spectrum and the slowing down spectrum solution of Griffin for the single energy group from 3 to 5 eV in the left figure and for an energy range of 5 to 16.5 eV in the right figure. As seen in the left figure, the higher weighting on the energy portion where cross sections are higher for the red line results in the higher multigroup cross section in that energy group. The spectrum difference caused by neglecting up-scattering is clearly seen in the right figure. Since Serpent2 considers thermal up-scattering up to $400 k_B T$, which is around 10 eV for the room temperature, the blue and red curves deviate starting from 10 eV. This difference motivated us to divide the energy range near the 6.67 eV resonance of U-238 into several groups. An effective cross section in a single group from 5 eV to 9 eV, as in the WIMS-69 group structure, has 3–4% error, which results in more than a -100 pcm bias on reactivity. This indicates the strong need for accounting for thermal up-scattering in the slowing down calculation. In addition, the resonance up-scattering from heavy isotopes needs to be considered in the slowing down calculation as well. These are particularly important for high temperature problems with graphite moderator, which will be investigated in future work.

Figure 15: Relative errors of compact-averaged U-238 multigroup capture cross sections for all CS and CM cases of PF₂ and PF₃ cases at PS₂.

Figure 16: Comparison of Serpent2 spectrum and slowing down spectrum solution of Griffin at 6.67 eV U-238 resonance.

4.2 EMPIRE Unit-Cell Problem

The Griffin CSAPI was also verified for the microreactor unit-cell problem inspired from the EMPIRE benchmark concept initially developed at Los Alamos National Laboratory (LANL) [69]. The unit-cell problem solved in this work is shown in Fig. 17, which was imported from a modeling exercise for a microreactor concept in Reference [70]. For simplicity, the problem in Reference [70] was modified to a 2D problem. A traditional TRISO particle with 20.15 wt.% UCO fuel was adopted in a hexagonal graphite matrix with a packing fraction of 37.5%. Room temperature was assumed.

For the double heterogeneous problem, Serpent2 results were generated by 15 independent runs with different random particle configurations for each case. For each run, the same random particle configuration was used in all fuel compacts. Each Serpent2 simulation was performed with 10^5 particles/cycle, 100 active and 100 inactive cycles. For the single heterogeneous problem, 10^5 particles/cycle, 1000 active and 100 inactive cycles were used. For Griffin calculations, an Exodus mesh shown in Fig. 17 was used. A P_3 anisotropic scattering order was used, as this problem has a strong anisotropic scattering effect due to the large amount of light- and intermediate-mass nuclides. One cross section zone was used for each material region.

Figure 17: Exodus mesh and material layout of the EMPIRE 2D unit-cell problem.

The EDC radius of the fuel compact was 1.787 cm, which is much larger than 1.129 cm, the size determined from the volume preservation of the fuel cell only. This is because only the fuel is assumed to

be black and other materials serve as potential scattering sources. The size of the EDC is determined by calculating the amount of graphite that produces the equivalent neutron source to the fuel region to which all the other materials in the actual lattice would contribute.

Table 10 shows the eigenvalue results of Serpent2 and Griffin. Two uncertainties of the Serpent2 eigenvalue for the double heterogeneous problem are the average of 15 eigenvalue standard deviations and the standard deviation of 15 eigenvalues, respectively. One thing to note is that the TRISO heterogeneity effect is negative, which is opposite to the case observed from the VHTR problems. This negative TRISO heterogeneity effect is caused by the fact that the thermal utilization factor of the double heterogeneous problem is smaller than that of the single heterogeneous problem. Table 11 shows two group reaction rates per fission neutron at each region with the energy boundary of 5.0 eV. In the “ $\Delta\text{het.}$ ” row, it is shown that there are fewer captures ($-6.686\text{E-}3$) in the resonance energy range of the fuel due to spatial self-shielding and more thermal captures from YH_2 ($+4.690\text{E-}3$), heat pipe ($+7.838\text{E-}3$), and stainless-steel cladding ($+1.316\text{E-}3$). These reaction rate differences are translated to the reactivity difference of -757 pcm, which is consistent with the TRISO heterogeneity effect of -767 pcm in Table 10. This occurs because, by using TRISO particles, fuel becomes more transparent to neutrons due to less capture in the resonance energy range, more down-scattering from the moderator, and more thermal captures in YH_2 , heat pipe, and stainless-steel cladding take place. Note that the thermal capture cross sections of those three regions are larger than that of fuel due to the low density of fuel (2.247 g/cc).

Table 10: Eigenvalue results of Griffin compared to Serpent2 for EMPIRE unit-cell problem.

Code		Single Het.		Double Het.		$\Delta\text{Het. (pcm)}$	$\Delta\Delta\text{Het. (pcm)}$
		K-eff	$\Delta\rho$ (pcm)	K-eff	$\Delta\rho$ (pcm)		
Serpent2		0.93845	± 5	0.93174	$\pm 14^{\text{a}}/\pm 33^{\text{b}}$	-767	-
Griffin	EDC	0.93919	+84	0.93325	+173	-678	+89

a: Average of 15 eigenvalue standard deviations, b: Standard deviation of 15 eigenvalues.

Table 12 shows the absolute errors of 2-group reaction rates per fission neutron obtained using the EDC + ILSS method. Reactivity errors of +39, +32 and +16 pcm are contributed from the fuel, YH_2 and stainless-steel cladding, respectively, for the single heterogeneous problem, and those errors of +73, +53, +26, and +21 pcm are contributed from the fuel, YH_2 , heat pipe and stainless-steel cladding, respectively, for the double heterogeneous problem. Note that, unlike in the VHTR pin-cell problem, a small error of the resonance capture rate in the fuel region can cause non-negligible sequential errors in non-fuel regions due

Table 11: Two-group reaction rates per fission neutron of Serpent2 for each region.

Prob.	Energy Group	Capture					Fission
		Fuel	YH ₂	Heat Pipe	Graphite	S.S. Clad	Fuel
Single Het.	Fast	8.914E-2	9.038E-3	2.532E-2	4.929E-4	4.160E-3	4.304E-2
	Thermal	7.504E-2	1.655E-1	2.428E-1	1.568E-3	4.253E-2	3.670E-1
	Sum	1.642E-1	1.746E-1	2.681E-1	2.060E-3	4.669E-2	4.100E-1
Double Het.	Fast	8.245E-2	9.136E-3	2.559E-2	4.951E-4	4.203E-3	4.324E-2
	Thermal	7.511E-2	1.702E-1	2.506E-1	1.619E-3	4.384E-2	3.667E-1
	Sum	1.576E-1	1.794E-1	2.762E-1	2.114E-3	4.805E-2	4.100E-1
Δ Het.	Fast	-6.686E-3	9.835E-5	2.704E-4	2.252E-6	4.278E-5	1.941E-4
	Thermal	6.811E-5	4.690E-3	7.838E-3	5.160E-5	1.316E-3	-2.182E-4
	Sum	-6.618E-3	4.788E-3	8.108E-3	5.385E-5	1.359E-3	-2.403E-5

to a large streaming effect, which makes the problem more challenging to solve.

Table 12: Absolute errors of 2-group reaction rates per fission neutron obtained by the EDC + ILSS method of Griffin for each region.

Prob.	Energy Group	Capture					Fission
		Fuel	YH ₂	Heat Pipe	Graphite	S.S. Clad	Fuel
Single Het.	Fast	-1.491E-3	-4.206E-4	-8.786E-4	1.561E-6	-2.195E-4	-2.178E-4
	Thermal	1.099E-3	9.585E-5	9.206E-4	4.489E-6	6.381E-5	2.172E-4
	Sum	-3.922E-4	-3.247E-4	4.205E-5	6.051E-6	-1.557E-4	-6.094E-7
Double Het.	Fast	-1.871E-3	-4.412E-4	-9.099E-4	2.186E-6	-2.253E-4	-3.645E-4
	Thermal	1.146E-3	-8.720E-5	6.517E-4	2.095E-6	1.700E-5	3.701E-4
	Sum	-7.252E-4	-5.284E-4	-2.582E-4	4.282E-6	-2.083E-4	5.655E-6

Fig. 18 and 19 show relative errors of spectrum and compact-averaged multigroup capture cross sections of Griffin for the fuel compact. Notable spectrum errors are observed in the high energy range above 1 MeV and the energy groups around 1 eV. Multigroup cross sections agree well within 2% relative errors, but the consistent underestimation of capture cross sections in the major U-238 resonance groups is one of the main contributors for the slightly overestimated reactivity error. The causes of these errors need to be investigated in future work.

Figure 18: Serpent2 spectrum of the fuel compact and the relative error (%) of Griffin spectrum.

Figure 19: Relative errors of compact-averaged multigroup capture cross sections of U-238 in the fuel compact.

4.3 HTTR Assembly Problems

The Griffin CSAPI was verified using the 2D assembly problems derived from the HTTR configuration [71]. The assembly configuration selected for verification is shown in Fig. 20 with the meshes used in the DFEM-SN calculation. It is a 31-pin 6.3 wt.% UO_2 fuel assembly located in Zone 4 at the periphery of the core with two 2.5 wt.% B_4C BP rods inserted in two out of three BP insertion holes and a fuel handling hole at the center. In the verification tests, two problems were solved: one with two BP rods inserted and another with BP rods fully withdrawn. The fuel rod is the A-type fuel with a 30.0% packing fraction of TRISO particles (13,000 particles with a radius of 0.046 cm in a 3.9-cm-high annular compact with an inner radius of 0.5 cm and outer radius of 1.3 cm). A room temperature of 293.6 K was assumed for all problems.

Figure 20: Exodus mesh for the HTTR 2D assembly problem of B_4C rodded case.

For Serpent2 reference solutions, 31 different random particle locations were used in each fuel compact and randomly shuffled 10 times for 10 independent runs of Serpent2, and the averaged value for 10 results was taken as the reference solution. For each run of the double heterogeneous problems, 10^5 particles/cycle, 100 active and 100 inactive cycles were used, and for the single heterogeneous problems, 10^5 particles/cycle, 1000 active and 100 inactive cycles, were used. For Griffin calculations, each annular fuel compact and each B_4C rod were divided into 3 and 9 radial meshes of the equal area with a single cross section zone, respectively, while the graphite sheath and block were divided into the enough number of meshes as shown

in Fig. 20. A Dancoff factor and an EDC size of each fuel compact calculated in the Griffin CSAPI are shown in Fig. 21. A Dancoff factor and an EDC size are larger for compacts in the assembly periphery than for those around the assembly center, due to a larger amount of graphite, but it is noted that the amount of graphite in EDCs of compacts in the assembly periphery is much smaller than that of the graphite adjacent to those compacts.

Figure 21: Dancoff factors and radii of EDCs of fuel compacts for 2D HTTR assembly problem.

Eigenvalue results for the single and double heterogeneous problems of B_4C unrodded and rodded cases are compared in Table 13. In the Serpent2 results for the double heterogeneous problems, there are two uncertainties: the first indicates the average value of 10 standard deviations and the second indicates the standard deviation of 10 quantities. For the power result, RMS (root mean square) and maximum values show statistics of those values among the 31 pins. For the single heterogeneous problems, the resonance table method shows eigenvalue errors of about +240 pcm for both cases, while the EDC method shows eigenvalue errors of +76 and +39 pcm for unrodded and rodded cases, respectively. Power distribution results of the both methods agree very well with those of Serpent2: the RMS error is about 0.12 ~ 0.14% and the maximum error is about 0.18 ~ 0.21%. The EDC + ILSS method for the double heterogeneous problems shows the similar accuracy to the EDC results for the single heterogeneous problems: +30 ~ +40 pcm higher eigenvalue errors and less than a 0.1% difference in pin power error statistics.

Table 13: Comparison of eigenvalue results for single and double heterogeneous problems of 2D HTTR assembly problems with and without B₄C BP rods.

Problem w/o B ₄ C		Single Het.				Double Het.			
Code/Scheme		K-eff	$\Delta\rho$ (pcm)	ΔP_{pin} (%)		K-eff	$\Delta\rho$ (pcm)	ΔP_{pin} (%)	
				RMS	Max			RMS	Max
Serpent2		1.50820	± 4	± 0.04	± 0.05	1.53375	$\pm 13^a$ $\pm 21^b$	$\pm 0.18^c$ $\pm 0.19^d$	$\pm 0.19^c$ $\pm 0.33^d$
Griffin	R.T.	1.51369	+241	0.14	0.21	-	-	-	-
	EDC	1.50993	+76	0.14	0.21	1.53630	+108	0.14	0.23
Problem w/ B ₄ C		Single Het.				Double Het.			
Code/Scheme		K-eff	$\Delta\rho$ (pcm)	ΔP_{pin} (%)		K-eff	$\Delta\rho$ (pcm)	ΔP_{pin} (%)	
				RMS	Max			RMS	Max
Serpent2		1.25001	± 7	± 0.04	± 0.04	1.26976	$\pm 19^a$ $\pm 27^b$	$\pm 0.18^c$ $\pm 0.19^d$	$\pm 0.19^c$ $\pm 0.33^d$
Griffin	R.T.	1.25375	+238	0.12	0.18	-	-	-	-
	EDC	1.25062	+39	0.12	0.17	1.27103	+78	0.15	0.25

- a) Average of 10 eigenvalue standard deviations, b) Standard deviation of 10 eigenvalues
c) RMS and Max for averages of 10 standard deviations of each pin power
d) RMS and Max for standard deviations of 10 pin power values

Fig. 22 shows U-238 capture rates per fission neutron in all pins for the B₄C rodded case. That is, the flux normalization was done to produce one fission neutron in the whole problem. In this normalization, an absolute difference in capture reaction rates is approximately the reactivity error induced by the capture rate error. As shown in the values of the single heterogeneous and double heterogeneous problems, U-238 capture rates are reduced by spatial self-shielding inside particles when particles are taken into account. For the single heterogeneous problem, 8.7 and 2.8 more neutrons out of 10^5 fission neutrons are captured by U-238 in each pin on average, resulting in 269 and 86 more neutrons out of the 10^5 fission neutrons being captured in total for the resonance table method and the EDC method, respectively. For the double heterogeneous problem, 3.9 more neutrons out of 10^5 fission neutrons are captured by U-238 in each pin on average, resulting in 121 more neutrons out of 10^5 fission neutrons being captured in total for the EDC + ILSS method. These results are consistent with the eigenvalue error results. For the U-235 fission rate, the sum of their errors over all pins is very small since the total number of fission neutrons is fixed for the normalization. Fig. 23 shows the pin power distribution and relative errors (%) for the B₄C rodded case. All results agree very well to a similar extent. Fig. 24 shows the relative errors of compact-averaged multigroup U-238 capture cross sections at 11 pins of Fig. 20. For the single heterogeneous problem, cross section errors are all within $\pm 1\%$ except for the energy group of 3–5 eV, where the cause of the error was analyzed

Figure 22: Comparison of U-238 capture rates per fission neutron and absolute errors for B₄C rodged case (pin numbers in Fig. 20).

in Section 4.1. For the double heterogeneous problem, cross section errors are at a similar magnitude with those for the single heterogeneous problem, but slightly negative in a consistent manner (about -0.5%) between 10 and 100 eV. Large errors are shown at the 6.67 eV resonance peak. These errors will be revisited after implementing the up-scattering scheme in the slowing down calculation in future work.

Figure 23: Comparison of pin power distribution and relative errors (%) for B₄C rodged case (pin numbers in Fig. 20).

Figure 24: Relative errors of compact-averaged multigroup capture cross sections of U-238 at the selected pins in Fig. 20.

Lastly, the computational time is a concern for the online cross section generation capability. Table 14 lists the computational time of each task to solve the 2D HTTR assembly problem using 40 processors. The resonance table method took the least amount of time (~ 5 minutes) since the performance of the DFEM-SN solver for FSPs has been much improved [4]. For the EDC + ILSS method, 31 EDCs of 31 fuel compacts are distributed to 31 processors (nine idle processors) and the 1D CPM slowing down problem is solved by each of the 31 processors, which took about a minute. For the double heterogeneous problem, additional time is required to calculate DFs, which takes more time (~ 1.5 minutes) than the 1D CPM slowing down calculation for the EDC method since DF iterations are involved during the slowing down calculation. The slowing down calculation scheme will be optimized in future work. In the test problem, reading the MC²-3 library took about 6 seconds, and the Dancoff factor calculation and the binary search for the EDC geometry took negligible time. Note that you may add time to reconstruct pointwise cross sections if they have to be generated on the fly. As a result, the final computational times for the single heterogeneous (using the EDC method) and the double heterogeneous problems (using the EDC + ILSS method) are about ~ 5.5 minutes and ~ 7.5 minutes, respectively. These computational times are acceptable for a pin-resolved heterogeneous assembly calculation with the 68 energy group structure. There is ample room to further reduce the computation time, which will be addressed in future work.

Table 14: Computation time (seconds) of each task for 2D HTTR assembly problem with 68 energy groups using 40 processors.

Tasks	R.T.	EDC	EDC+ILSS
Fixed Source Problems	23	-	-
Read MC ² -3 Library	-		$\leq \sim 6$
HFG Cross Section Reconstruction	-		(if any) $\leq \sim 60$
Dancoff Factor Calculation + Binary Search for EDC	-		~ 1
DF Calculation	-	-	96
Slowing Down for DF	-		58
Transport Calculation (DFEM-SN + CMFD)			132 (14.66 $\times$ 9)
Others	139	141	164
Total	294	338	457
			(+ ~ 60 if any HFG XS Recon.)

4.4 Pebble Fuel Problems

The ILSS method was tested for pebble fuel problems with helium coolant. Since a significant effort is required to test pebble fuel problems using the Griffin CSAPI, preliminary tests were conducted for unit pebble cell problems using the 1D CPM of MC²-3 with spherical geometry to evaluate the performance of the ILSS method for pebble problems. Unit pebble cell problems were derived from the HTR-10 design [72], as shown in Fig. 25. The HTR-10 design uses TRISO particles of a 17 wt.% UO₂ fuel kernel surrounded by graphite and SiC layers. The pebble is composed of a fuel zone with a 2.5cm radius that has fuel particles dispersed in a graphite matrix and an outer 0.5-cm-thick graphite layer. Eight test cases were made by changing fuel particle packing fractions from 2.4% up to 57.9%.

For the Serpent2 reference calculation, since the code can neither use a spherical surface as the outer boundary nor apply the white boundary condition, the rectangular array model with a pebble shown in Fig. 25 was constructed with the reflective boundary condition at the cube surfaces. Then, this model was converted to the 1D spherical model for MC²-3 by preserving the coolant volume and applying the white boundary condition. To calculate the TRISO heterogeneity effect of the models, only the fuel zone (not a whole pebble) was homogenized.

Serpent2 calculations were performed using 10^5 particles/cycle, 1000 active and 100 inactive cycles, for the single heterogeneous problem. For the double heterogeneous problem, the reference Serpent2 solution was determined by the average of 25 Serpent2 results obtained with different random distributions of particles in the fuel zone. Each simulation was performed using 10^5 particles/cycle, 100 active and 100 inactive

Temperature : 293.6 K

	Region	Radius (cm)	Material	Density (g/cm ³)
Fuel Particle	Fuel Kernel	0.0250	17 wt.% UO ₂	10.4
	Buffer	0.0340	Graphite	1.10
	Inner PyC	0.0380	Graphite	1.90
	SiC	0.0415	SiC	3.18
	Outer PyC	0.0455	Graphite	1.90
	Fuel Zone	2.5	Graphite	1.73
	Graphite Layer	3.0	Graphite	1.84
	Coolant	-	Helium	0.0032

Figure 25: Pebble design obtained from HTR-10 design .

cycles. Table 15 shows the Serpent2 results obtained for helium-cooled pebble cell problems.

MC²-3 calculations were performed using the 1D spherical-geometry-based CPM solver. In addition to the ILSS method, the different methods, including the Williams method [10], the Hébert CPM method [73], and Sanchez-Pomraning (S-P) CPM method [74] implemented in MC²-3 were used, whose solutions were compared against Serpent2 solutions. A sufficient number of meshes were used in the fuel zone by using a 0.1 cm radial thickness, and one cross section set was assigned to the entire fuel zone. The use of a larger number of cross section sets inside the fuel zone produced marginally different solutions within 20 ~ 30

Table 15: Serpent2 results for helium-cooled pebble cell problems with different fuel particle packing fractions

Packing Fraction (%)	Single Het.		Double Het.		Δ Het. (pcm)
	K-eff	Std.	K-eff	Std.	
2.4	1.68165	± 2	1.77111	$\pm 7^a/\pm 15^b$	3004
4.8	1.60023	± 3	1.70900	$\pm 10/\pm 19$	3977
9.6	1.46652	± 5	1.56664	$\pm 13/\pm 21$	4358
19.3	1.30984	± 6	1.37811	$\pm 17/\pm 30$	3782
28.9	1.22425	± 6	1.27137	$\pm 18/\pm 22$	3028
38.6	1.17461	± 6	1.20728	$\pm 18/\pm 25$	2304
48.2	1.14615	± 6	1.16993	$\pm 18/\pm 24$	1773
57.9	1.13050	± 5	1.14869	$\pm 18/\pm 14$	1401

a) Average of 25 eigenvalue standard deviations, b) Standard deviation of 25 eigenvalues

pcm. The exception is the S-P CPM that has limitations on the mesh size and magnitude of cross sections. Since even one mesh for the entire fuel zone resulted in a negative collision probability for some HFGs where cross sections are too large, only one mesh for the fuel zone was used in the S-P CPM.

Table 16 compares the MC²-3 results obtained with the four methods (Williams, ILSS, Hébert, and S-P methods) with reference Serpent2 solutions for the helium-cooled problems. As shown in the table, the single heterogeneous problem results agree well with Serpent2 results within 41 pcm. The TRISO heterogeneity effect errors of the ILSS method are within 117 pcm of the corresponding Serpent2 solutions. It was shown that all other methods (Williams, Hébert, and S-P methods) yielded negative biases in the TRISO heterogeneity effect. The results indicate that the ILSS method works well for pebble fuel problems.

Table 16: Differences (pcm) in eigenvalue and TRISO heterogeneity effect between MC²-3 and Serpent2 solutions for helium-cooled pebble cell problems.

Packing Fraction (%)	Single Het.	Double Het.							
		Methods in MC ² -3							
		Williams		ILSS		Hébert		S-P ^a	
		$\Delta\rho$	$\Delta\text{Het.}$	$\Delta\rho$	$\Delta\text{Het.}$	$\Delta\rho$	$\Delta\text{Het.}$	$\Delta\rho$	$\Delta\text{Het.}$
2.4	3	-19	-22	10	7	-28	-31	-35	-39
4.8	2	-56	-58	18	17	-49	-50	-74	-75
9.6	-14	-131	-116	25	39	-88	-73	-156	-141
19.3	-12	-219	-208	23	35	-145	-133	-283	-271
28.9	-27	-239	-211	24	52	-167	-140	-341	-313
38.6	-30	-162	-132	86	117	-106	-75	-282	-252
48.2	-41	-160	-119	61	102	-119	-78	-270	-229
57.9	-38	-164	-127	25	62	-136	-98	-231	-194

a) Only one mesh for the fuel zone was used.

In the next fiscal year, pebble-bed problems as well as these unit pebble cell problems will be simulated using the Griffin CSAPI, which will be coupled with the Pebble Tracking Transport (PTT) module [75] in Griffin. The Dancoff factor of a fuel zone of each pebble will be obtained by using the EDC method coupled with the PTT method, and an EDC of each fuel zone will be constructed. For each EDC, the EDC + ILSS method calculations will be performed to obtain fuel-zone averaged cross sections which will be provided to the PTT solver for the transport calculation.

5. Conclusions

In this fiscal year, significant efforts were made to improve the capability of multigroup cross section generation in Griffin. Previously, multigroup cross sections were provided from an ISOXML-format external file that was generated from deterministic or Monte Carlo cross section generation codes for fast and thermal reactor problems. Last year, the implementation of the cross section generation capability in Griffin was initiated by plugging in CSAPI and reviewing the methodologies for treating particulate fuels.

The focus this year was on completing the CSAPI modules and implementing advanced self-shielding methods for applications to reactor problems with TRISO fuel. First, the process for cross section library generation was updated to accurately and rigorously produce isotopic cross section data. Second, the on-the-fly slowing down method (the EDC method) for the resonance treatment was implemented in CSAPI to improve the accuracy of effective multigroup cross sections in the resonance energy range. Third, the ILSS method was implemented under the calculation framework of the EDC method to accurately treat the double heterogeneity effect of particulate fuel.

The updated CSAPI with the advanced self-shielding methods, together with the improved cross section libraries, were verified against Serpent2 for graphite-moderated reactor problems including a heat-pipe-cooled microreactor problem. For comparison with accurate reference solutions, the stochastic dispersion of particles for double heterogeneous problems was taken into account in Serpent2 results. Eigenvalue results for all tested problems, including the VHTR pin-cell problems with a wide range of fuel particle and compact parameters, the HTTR assembly problems with and without BP rods, and the Empire unit-cell problem, agreed well with Serpent2 results within 200 pcm. Detailed multigroup cross sections also agreed well within 0.5% for the VHTR problems, 1% for all fuel pins in the HTTR assembly problem, and 2% for the EMPIRE problem in the energy groups above 10 eV. Relatively larger errors were observed for the thermal energy groups below 10 eV mainly because of the neglect of thermal up-scattering in the slowing down calculation, which will be addressed and resolved in the next fiscal year. Pin power results of the HTTR problem agreed well within 0.3%. As a preliminary work, the double heterogeneity treatment methodology of the Griffin CSAPI was also verified for the helium-cooled unit-pebble cell problem from HTR-10, using the MC²-3 code, demonstrating that the ILSS method works well for pebble fuel problems. Further improvements and verification tests will be performed next year, which are summarized in the next section.

6. Future Work

The initial implementation of CSAPI in Griffin was successful. However, there are many remaining tasks in order to deal with various advanced reactor problems. The recommended future work entails:

- Application of the EDC + ILSS method for pebble fuel problems to the PTT solver.
- Thermal up-scattering up to $400 k_B T$ (~ 10.36 eV at 300 K) and resonance up-scattering both in the slowing down calculation for the EDC method and the multigroup scattering matrix in the CSAPI multigroup library.
- Multigroup scattering matrix that accounts for problem-dependent spectrum, which requires to update the CSAPI multigroup library with additional parameters.
- Extension of the EDC method to non-fuel pins to eliminate the need for solving the FSPs for non-fuel pins with resonant isotopes.
- Equivalence parameters to reduce condensation error arising from pointwise to multigroup calculations.
- Investigation of the underestimation of capture cross sections in U-238 resonances for the Empire benchmark.
- Investigation of the validity of the Dancoff factor calculation scheme for 3D problems.
- Reduction in the computation time and optimization of the 1D CPM slowing down calculation schemes.
- Rewriting the CSAPI multigroup library in the ISOXML format.
- Integration of the Shift Monte Carlo code [28] into the CSAPI multigroup library generation process.
- Investigation of the validity of the particle cell model to compute DFs in the thermal range in the presence of low-lying resonances.
- Projection and prolongation methods for homogenization and condensation in spatial and energy domains for full core calculations coupled to self-shielding methods.

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