FY18 Progress on Improvements and V&V of MC²-3 and PROTEUS

Nuclear Science and Engineering Division

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EXECUTIVE ABSTRACT

The PROTEUS code is a high-fidelity capable deterministic neutron transport code based on unstructured finite element meshes, which solves the steady-state and transient neutron transport problem using the 2nd-order discrete ordinate method (SN2ND), the method of characteristics (MOC), and the advanced nodal transport method (NODAL). The PROTEUS system in a broader sense consists of cross section generation tools, mesh generation tools, and output post processing tools as well as neutron transport solvers.

The main accomplishments in the FY18 NEAMS neutronics tasks are that the computational performance and the simplified thermal feedback of PROTEUS-MOC were significantly improved, that the transient simulation capability as well as the molten salt reactor (MSR) simulation capabilities were successfully implemented to PROTEUS-NODAL, that the MC²-3 versions with the updated thermal cross section capability and three-dimensional MOC capability were integrated, and that further verification and validation tests were performed with the updated PROTEUS demonstrating the applicability and accuracy of the code.

The computational performance of PROTEUS-MOC was upgraded by implementing the partial-current based coarse mesh finite difference (CMFD) option, the conventional transport sweeping option, and the preconditioner to the steady-state CMFD solution scheme. In addition, the multigroup CMFD option was added to the transient solution scheme, showing significant improvements in the computational performance.

The thermal feedback capability was completed for PROTEUS-MOC and has been tested using simple 3D benchmark problems as well as the 3D C5G7 benchmark problem, showing reasonable fuel and moderator temperatures and moderator density distributions in the axial direction.

The transient simulation capability was implemented to PROTEUS-NODAL this year, and the transient simulation capability implemented to PROTEUS-MOC last year was tested using the 3D C5G7-TD OECD/NEA benchmark problems, demonstrating very good agreement with the MPACT solutions in the power changes with time.

For PROTEUS-NODAL, in addition to the transient simulation capability, the MSR simulation capability was implemented by adding the delayed neutron precursor drift model, demonstrating a reasonable behavior of eigenvalue with the change of flowing fuel speed inside and outside the core.

The MC²-3 versions with thermal cross section, 2D/3D MOC, and updated gamma heating capabilities were successfully integrated, and further updates were made using the CMFD approach to improve the performance of the 2D/3D MOC calculation. Since the 3D MOC methodology of MC²-3 is based on that of PROTEUS-MOC, the pseudo cross section

approach was added to make the neutron balances between MOC and CMFD match in the axial direction.

In order to support code verification and validation, the cross section library generation procedure was updated using the combination of OpenMC and MC²-3. Code verification and validation activities continued using the updated capabilities of PROTEUS, demonstrating accurate steady-state solutions for the MSR problem and the RCF core compared to Monte Carlo solutions, showing very good agreement in eigenvalue and power with time with the MPACT solutions for the 3D C5G7-TD benchmark problems, and producing a reasonable power behavior with time for the M8CAL core transient problem of TREAT.

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1. Introduction

As a key component of the NEAMS SHARP high-fidelity multi-physics simulation package [1], the PROTEUS code is a high-fidelity deterministic neutron transport code based on unstructured finite element meshes, which solves the steady-state and transient neutron transport problem using the 2nd-order discrete ordinate (SN) method [2] or the method of characteristics (MOC) [3] as high-fidelity neutron transport solvers. Recently, the advanced nodal transport method (NODAL) option [4] has been added to provide a fast running solution option within the same framework so that a user can choose a level of solution fidelity and computational resource requirements depending on a user's need.

In a large sense, the PROTEUS system consists of cross section generation tools, mesh generation tools, and output post processing tools as well as neutron transport solvers, as illustrated in Figure 1-1. Neutron cross sections are provided in a file form using MC²-3 [5] or Monte Carlo codes such as Serpent [6] and OpenMC [7], or in a cross section library form with which multigroup cross sections are generated on the fly using the cross section API [8]. The system provides a tool that converts the Monte Carlo output to the format that PROTEUS can read. Meshes can be generated using CUBIT [9] for arbitrary geometry problems or the in-house mesh toolkit [10] for Cartesian and hexagonal geometry problems. Using the post processing tool, the code output is converted to a VTK format file for visualization using VisIt [11].

(The purple-colored boxes denote the codes developed by the Argonne neutronics team)

Figure 1-1. Overview of the NEAMS Neutronics Code Suite

Last year, an advanced nodal solver was implemented to PROTEUS for use in routine nuclear reactor design and analysis. [12] A simplified thermal-hydraulic (T/H) module was added to the NODAL and MOC solvers of PROTEUS to perform the thermal feedback calculation in a time efficient manner, compared to the coupled simulation with external T/H codes such as Nek5000. Significant performance improvements were made to PROTEUS-MOC using the coarse mesh finite difference (CMFD) numerical acceleration and code optimization. The thermal cross section capability of MC²-3 was improved with many thermal group data. Verification and validation tests were performed for PROTEUS-MOC using several benchmark problems.

The main objectives of the FY18 NEAMS neutronics tasks are 1) to continue to improve the computational performance and the simplified thermal feedback of PROTEUS-MOC, 2) to implement the transient simulation capability as well as the molten salt reactor (MSR) simulation capabilities to PROTEUS-NODAL, 3) to integrate versions of MC²-3 with the updated thermal cross section capability and three-dimensional (3D) MOC capability, and 4) to continue to verify and validate PROTEUS using benchmark problems and experiments. The last tasks includes updates of the cross section generation necessary for code verification and validation.

The computational performance of PROTEUS-MOC was upgraded by implementing the partial-current based CMFD option (compared to the current-based CMFD approach), the conventional transport sweeping option (compared to the Krylov transport sweeping approach), and the preconditioner to the steady-state CMFD solution scheme. In addition, the multigroup CMFD option (compared to the within-group CMFD approach) was added to the transient solution scheme, which has been found to be very efficient in solving the transient problem.

In the previous year, the simplified thermal feedback module were completed for PROTEUS-NODAL but was preliminary for PROTEUS-MOC. This year, the thermal feedback capability was completed for PROTEUS-MOC and has been tested using simple 3D benchmark problems as well as the 3D C5G7 benchmark problem [13].

The transient simulation capability was implemented to PROTEUS-NODAL this year, and that implemented to PROTEUS-MOC by the NEUP team last year was tested using the 3D C5G7-TD OECD/NEA benchmark problems [14].

For PROTEUS-NODAL, in addition to the transient simulation capability, the MSR simulation capability was implemented, which was initially planned as the workscope of U. Michigan but was later included in the regular workscope at a higher priority due to the urgent needs from industry users. With the MSR capability of PROTEUS-NODAL the delayed neutron precursor drifting can explicitly be modelled and simulated, which was demonstrated using each of thermal-spectrum and fast-spectrum MSR benchmark problems.

To support the code verification and validation, the cross section library generation procedure was updated using the combination of OpenMC and MC²-3. In the updated procedure, the base cross sections with temperatures were generated from OpenMC based on a pin cell geometry with

a representative composition of the reactor core of interest and the corresponding background cross sections are calculated from MC²-3 using its 2D MOC capability.

In addition to the version integration of MC²-3, further updates were made using the CMFD approach to improve the performance of the 2D/3D MOC calculation. Since the 3D MOC methodology of MC²-3 is based on that of PROTEUS-MOC, the pseudo cross section approach was added to make the neutron balances between MOC and CMFD match in the axial direction.

This year, code verification and validation activities continued using the updated capabilities of PROTEUS. With the updated transient capability of PROTEUS-MOC, the transient experiment of the M8CAL core of TREAT [15] were simulated, and the 3D C5G7-TD benchmark problems were solved and compared with MPACT [16] solutions. As a code validation effort, the modeling and simulation of the RCF core was updated based on the experiment configurations, whose power solutions were compared with the measurements. In addition to the aforementioned MSR benchmark problems, the industry design-based MSR core was simulated using PROTEUS-MOC and PROTEUS-NODAL whose eigenvalue and integrated flux solutions were compared with the OpenMC Monte Carlo solutions.

Sections 2 and 3 present updates made to PROTEUS and MC²-3, respectively. Section 4 shows verification and validation test results from the updated PROTEUS. Conclusions are discussed in Section 5.

2. Updates in PROTEUS

This year, the MOC and NODAL solvers of PROTEUS have been updated to improve the computational performance. Additionally, for PROTEUS-MOC the simplified thermal feedback capability was completed and for PROTEUS-NODAL the transient simulation capability was implemented. This section provides details of the updates.

2.1 PROTEUS-MOC Solver

2.1.1 Improvements in Steady-State Capability

Work continued to improve the computational performance in the steady-state simulation. As the first step, the conventional iterative solution scheme for the within-group transport calculation were added to PROTEUS-MOC because it could be more efficient in conjunction with the CMFD acceleration. With the conventional iterative scheme, the stability and performance of the CMFD solver were also improved through the stable partial current based CMFD (pCMFD) formulation and the new efficient preconditioning technique.

2.1.1.1 Iterative Solution Scheme for Within-group Transport Calculation

In the steady-state criticality calculation, PROTEUS-MOC by default adopts the conventional power method in conjunction with the group-by-group sweeping scheme to determine fission and scattering sources for the within-group (WG) transport problem for each energy group. For each within-group transport problem whose convergence is strongly dependent upon the scattering ratio, the Krylov subspace iterative method is employed to ensure the solution convergence in the parallel computation with the massive spatial domain decomposition. In FY2017, the CMFD acceleration scheme was successfully implemented, substantially reducing the number of fission source iterations with small additional computational burden. The CMFD implementation resulted in overall computational time reductions by a factor of about 4 to 5 for the C5G7 and TREAT benchmark problems, respectively. It is noted that the CMFD acceleration not only improves fission source convergence but also affects the within group (WG) calculations by providing a better flux distribution as the initial guess. Thus, the performance improvement for the WG calculation could be made by adopting a simple solution scheme instead of using the Krylov subspace method. The conventional solution scheme for the WG calculation that performs a couples of transport operations in the within-group scattering source update was revisited this year [17].

Conventional Iteration Scheme for Within-group Problem

The within-group transport problem in PROTEUS-MOC can be written in an operator as:

$$T\psi + W\psi = Q, \quad (2.1)$$

where T and W are the transport and within-group scattering operators, respectively. In the conventional iterative scheme, the transport operator is split as:

$$T = T_{LD} + T_U, \quad (2.2)$$

where T_{LD} is the diagonal and lower-diagonal part of T and T_U is the upper-diagonal part. For the transport operator for the 2D/3D MOC formulation implemented in PROTEUS-MOC, T_U is attributed from boundary conditions and spatial domain decompositions. Then, the following equation is actually solved in each WG iteration:

$$T_{LD} \psi^{(i+1)} = Q - (W + T_U) \psi^{(i)}, \quad (2.3)$$

where $\psi^{(i)}$ and $\psi^{(i+1)}$ are the flux solutions of previous and current iterations, respectively. With the CMFD acceleration, the global flux variation can be practically captured. The updated flux solution using the CMFD calculation can be a good initial guess for computing the right hand side of Eq. (2.3). With the assistance of CMFD acceleration, the within-group solution can be effectively obtained with a small number of WG iterations at each fission source iteration. Therefore, this iteration scheme can reduce the overall computational time because the computation expense of this scheme is substantially cheaper than the sophisticated Krylov iteration scheme involving multiple transport operations in a single iteration. However, note that the Krylov iteration scheme is more effective when the CMFD acceleration is not available.

Implementation in PROTEUS-MOC

In PROTEUS-MOC, the functionality required for Eq. (2.3) was already in place as the basic component of the Krylov solver and CMFD acceleration. It was not difficult to implement the conventional iteration scheme by properly coordinating the existing routines. The overall calculation procedure is illustrated in Figure 2-1.

Figure 2-1. Calculation Flow of PROTEUS-MOC with Conventional Transport Iteration Scheme

The number of transport iterations in the WG transport calculation is to be selected by a user but the default value is set to 5 iterations. When the spatial domain decomposition is applied, the performance might be deteriorated because the angular fluxes on the local domain boundaries formed by the domain partitioning are treated through the Jacobi iteration manner. This performance deterioration can be effectively alleviated in such a way that the corresponding angular fluxes are updated by making use of the P_1 approximation of angular flux in the CMFD acceleration [18].

2.1.1.2 CMFD Acceleration

The CMFD acceleration implemented in PROTEUS-MOC was updated to secure the convergence and enhance the performance. The CMFD acceleration method leads to construct and solve a low order system based upon the coarse mesh structure that yields the consistent solution with the original system. The stability of the CMFD acceleration is mainly subjected to the current relation formed by the surface currents produced from the transport calculation. It suffers a convergence problem when the WG iterations are not performed sufficiently or/and the coarse mesh size is significantly larger than a mean free path of neutron. Since the partial-current based CMFD (pCMFD) formulation is known to have the stable convergence in a wide range of conditions [19], the formulation was added to the CMFD module of PROTEUS-MOC as an additional option [18].

Currently, the CMFD acceleration uses the un-predconditioned GMRES algorithm. In the performance examination, we found that the overhead of the CMFD acceleration became non-negligible as the condition number of the CMFD linear system and the size of problem increase. This indicated that the preconditioning technique was needed to reduce the CMFD overhead to improve the computational performance. Thus, a new preconditioning technique was devised and implemented in the CMFD linear system solver.

Partial-current based CMFD Formulation

The CMFD formulation originally used in PROTEUS-MOC constructs coupling coefficients between two neighboring nodes based on the net current from the transport solution given as:

$$J_{i \rightarrow k} = \tilde{D}_{i \rightarrow k}(\phi_i - \phi_k) - \hat{D}_{i \rightarrow k}(\phi_i + \phi_k), \quad (2.4)$$

where i and k are indices for the coarse meshes connected through a common surface, $\tilde{D}$ is the coupling coefficient yielded from the finite difference method (FDM) formulation for diffusion equation. $\hat{D}$ is the current correction factor of the CMFD formulation. In the pCMFD formulation [19], the partial currents are used in constructing the coupling coefficient as:

$$J_{i \rightarrow k}^+ = \frac{1}{2} \tilde{D}_{i \rightarrow k}(\phi_i - \phi_k) - \hat{D}_{i \rightarrow k}^+ \phi_i, \quad (2.5)$$

$$J_{i \rightarrow k}^- = -\frac{1}{2} \tilde{D}_{i \rightarrow k}(\phi_i - \phi_k) - \hat{D}_{i \rightarrow k}^- \phi_k, \quad (2.6)$$

where J^+ and J^- are the outgoing and incoming partial currents, respectively, and $\hat{D}^+$ and $\hat{D}^-$ are the correction factors of the pCMFD formulation to preserve the partial currents obtained from the transport solutions. Using the partial current relations in Eqs. (2.5) and (2.6), the pCMFD scheme solves the discretized neutron balance equation below:

$$\sum_k (J_{i \rightarrow k}^+ - J_{i \rightarrow k}^-) + (\Sigma_r^i + \Sigma_p^i) \phi_i V_i = q_i V_i. \quad (2.7)$$

where Σ_p is the pseudo absorption cross section to enforce the neutron balance of coarse mesh solution with the 2D/3D MOC solution in PROTEUS-MOC [20]. The pCMFD scheme can alleviate a potential instability of the CMFD acceleration caused by the partially converged WG solutions. In particular, the pCMFD scheme would be beneficial when it was combined with the conventional WG iteration scheme.

The pCMFD acceleration capability was implemented in the framework of CMFD routines. In terms of implementation, the pCMFD calculation could be performed by modifying the existing linear system routines that are to be solved in the coarse mesh calculation. The routine for constructing the CMFD linear system was also updated to construct a matrix based upon Eqs. (2.5) to (2.7). In addition, a partial current tally function was added to the tally routine of the 2D/3D MOC operation that originally provided the net current. Now, the code offers a user to select the net current or partial current formulation used in the CMFD acceleration through the input keyword.

Krylov Solver with Preconditioner

To derive an efficient preconditioner, the CMFD linear system is converted into the equivalent form that yields the identical solution. In the Gauss-Seidel (GS) method, the iterative solution process can be expressed as:

$$Ax = b \rightarrow y^{(i+1)} = A_{LD}^{-1}b - A_{LD}^{-1}A_U y^{(i)}, \quad (2.8)$$

where A_{LD} is the diagonal and lower-diagonal part of A and A_U is the upper-diagonal part. If the solution is fully converged ($y^{(i)} = y^{(i+1)} = y$), it satisfies the following system:

$$(I + A_{LD}^{-1}A_U)y = A_{LD}^{-1}b. \quad (2.9)$$

Based on Eq. (2.9), one can define the equivalent linear system as:

$$(1-T)y = \tilde{b}, \quad (2.10)$$

$$T = -A_{LD}^{-1}A_U \text{ and } \tilde{b} = A_{LD}^{-1}b, \quad (2.11)$$

where T is commonly referred to the iteration matrix of the GS method. Thus, Eq. (2.10) can be alternatively solved to obtain the solution of the linear system. Under the assumption that the matrix norm of T is less than unity, a preconditioner can be simply derived for this modified system as:

$$y = (I - T)^{-1} \tilde{b} \rightarrow y \approx (I + \sum_{i=1}^n T^i) \tilde{b} . \quad (2.12)$$

The linear system solver for the CMFD acceleration was updated to employ this preconditioning technique. An additional function was prepared to perform an operation for the matrix T with a certain vector. Along with this, the CMFD solver was updated to handle the modified linear system shown in Eq. (2.10).

2.1.1.3 Performance Examinations

Conventional Iteration Scheme for Within-group Problems

The performance improvement was examined for the 3D C5G7 [13] and TREAT M8CAL core [15] problems by comparing the overall computing times of the newly implemented conventional iteration scheme and the Krylov iteration scheme. Hereafter, for brevity, the conventional and Krylov iteration schemes are denoted as the WG-sweeping and WG-Krylov scheme, respectively. These calculations were performed using 4,320 processors on the LCRC bebop clusters [21], whose results were summarized in Table 2-1. As shown in the table, the performances were improved by a factor of about 1.6 and 2.1 for the C5G7 and M8CAL problems, respectively. For both iteration schemes, Figure 2-2 compares the convergence of fission source errors for the M8CAL problem and Figure 2-3 shows the computing time of individual fission source iterations. The number of total outer iterations increased in the WG-sweeping scheme, while the computing time per a single outer iteration was considerably reduced, which resulted in the overall computing time reductions. The computing time of each iteration slightly varied in the WG-Krylov sweeping scheme because, as the termination criterion, the relative residual reduction was used in the WG scheme while the fixed number of iterations were used in the WG-sweeping scheme.

Table 2-1. Overall computing times of 3D C5G7 and M8CAL Problems Using PROTEUS-MOC

Problem	Computing Time, sec		Speed-up
	w/ WG-Krylov	w/ WG-Sweeping	
3D C5G7	60.1	36.1	1.66
TREAT M8CAL	735.3	349.4	2.10

Krylov Solver with Preconditioner

In order to measure the performance improvement of the CMFD linear solver, the 3D C5G7 and TREAT M8CAL problems were solved with and without the new preconditioner added to CMFD linear system solver. These calculations were performed using 4,320 processors on the LCRC bebop clusters [21] and the computing times of the CMFD portion are compared in Table 2-2. The CMFD computing time was reduced by a factor of 1.8 and 6.7 for the 3D C5G7 and M8CAL problems, respectively, by employing the new linear system solver with preconditioner.

Figure 2-2. Convergence of Fission Source Error for M8CAL Problem Calculation Using PROTEUS-MOC

Figure 2-3. Computing Time of Fission Source Iteration for M8CAL Problem Calculation Using PROTEUS-MOC

The new solver was especially effective for the M8CAL problem because of a large stiffness of the CMFD matrix yielded from the large voided regions associated with the hodoscope [15]. The existing solver suffered from the large stiffness with no preconditioner, resulting in a lot of iterations.

Table 2-2. Computing Time of PROTEUS-MOC CMFD Solver for 3D C5G7 and TREAT M8CAL Problems

Problem	Computing Time, sec		Speed-up
	w/o Preconditioner (Existing LS Solver)	w/ Preconditioner (New LS Solver)	
3D C5G7	17.3	9.5	1.8
M8CAL	144.4	21.7	6.7

The restart GMRES algorithm employed in the PROTEUS-MOC needs a sufficient number of back vectors to store the orthogonal basis vectors generated from the process of GMRES algorithm. Without preconditioner or with a crude preconditioner, a stable and quick convergence cannot be guaranteed unless a sufficient number of back vectors is used. With a robust and good preconditioner, the convergence would be insensitive to the number of back vectors. For the new preconditioner, the convergence sensitivity with respect to the number of back vectors was studied by solving the M8CAL problem with different numbers of back vectors ranging from 2 to 30. As shown in Table 2-3, without preconditioner, the CMFD computing time drastically increased as the number of back vectors were reduced. However, the CMFD computing time was almost insensitive to the number of back vectors when the preconditioner was applied to the linear system solver. These results indicate that the new CMFD solver with the preconditioner has stable and quick convergence characteristics. On the top of this, obviously, the computing memory can be saved by using the small number of back vectors.

Table 2-3. Computing Times of PROTEUS-MOC CMFD Solver with Different Number of Back Vectors for TREAT M8CAL Problem

Number of Back Vectors	Computing Time, sec*	
	w/o Preconditioner (Existing LS Solver)	w/ Preconditioner (New LS Solver)
30	144.4	21.7
15	206.6	22.0
5	518.8	20.2
2	Diverge	20.7

* w/ 4320 processors in LCRC bebop cluster

2.1.2 Improvements in Transient Capability

The transient capability of PROTEUS-MOC was implemented, employing the transient fixed source problem formation. For accelerating the transient calculation, the group sweeping CMFD

scheme used in the steady-state eigenvalue calculation was applied to the transient fixed source problem with the modification in solving the fixed source problem. Although the group sweeping CMFD method has proved to be effective, specifically for the C5G7-TD transient benchmark cases, as the number of outer iterations were reduced by one order of magnitude [22], the overall convergence rate of the fixed-source solver was still relatively slow. Since the existing group sweeping scheme is numerically very slow to converge the time-dependent transport equation, the multi-group system CMFD (MGS-CMFD) method could be more effective to accelerate the fixed-source solver [23]. In order to improve the computational performance of the transient calculation, the kinetics solver of PROTEUS-MOC was updated to incorporate the MGS-CMFD method which solves the entire multigroup equations directly without group iterations.

Multigroup System CMFD Scheme

In the group sweeping CMFD scheme, the fission sources of the current time step are treated through the fission source iterations, and the scattering sources are iteratively updated through the iteration over groups (namely, group sweeping). For each within-group calculation, the within-group CMFD problems are solved for the given fixed source without fission and scattering source updates. Hereafter, this scheme is referred to the within-group system CMFD (WGS-CMFD) scheme. The WGS-CMFD scheme is very effective for the steady-state eigenvalue calculations in which the convergence rate is dictated by the dominance ratio of the matrix. The WGS-CMFD scheme is not effective for the transient fixed source problem in which the convergence rate is governed by the spectral radius of the matrix. For most of transient cases, the spectral radius is almost unity for this scheme because the group associated values are closely coupled with each other through the prompt and delayed fission sources. Alternatively, the MGS-CMFD scheme explicitly treats the group couplings through the multigroup system which is directly solved with no group and fission source iterations. Therefore, the MGS-CMFD scheme can resolve the slow convergence rate issue, enhancing a computational efficiency of transient calculations.

In the MGS-CMFD scheme, the scattering source, the prompt fission source and the delayed neutron source contributed from the current time are moved to the left hand side of the CMFD equation. The only fixed source terms which are the previous time step contributions are in the right hand side of the CMFD equation. Then, the multi-group CMFD linear system is formed, yielding the linear system which is solved using the linear system solver in PROTEUS-MOC. In order to efficiently solve the MGS-CMFD linear system, its corresponding linear system matrix is arranged such a way that the entire group flux unknowns for each coarse mesh construct a single block. This yields a structured block matrix for the MGS-CMFD linear system as:

$$\begin{bmatrix} D^1 & U_2^1 & & \\ & \ddots & & \\ & L_{i-1}^i & D^i & U_{i+1}^i \\ & & & \ddots \\ & & L_{N-1}^N & D^N \end{bmatrix} \begin{bmatrix} \Phi_1 \\ \vdots \\ \Phi_i \\ \vdots \\ \Phi_N \end{bmatrix} = \begin{bmatrix} Q_1 \\ \vdots \\ Q_i \\ \vdots \\ Q_N \end{bmatrix}, \quad (2.13)$$

$$\Phi_i = [\phi_1^i \quad \cdots \quad \phi_g^i \quad \cdots \quad \phi_G^i]^T \text{ and } Q_i = [q_1^i \quad \cdots \quad q_g^i \quad \cdots \quad q_G^i]^T, \quad (2.14)$$

where i and g are indices for the coarse mesh and group, and D^i , L^i and U^i are the diagonal, lower-diagonal and upper-diagonal block matrices, respectively. A diagonal block is a full matrix while off-diagonal blocks have a diagonal matrix structure. The LU decomposition is applied to the individual diagonal block, and then the existing matrix solver can be applied based upon the block matrix operation. For example, the GS iteration scheme given in Eq. (2.8) can be explicitly performed based upon the block matrix. Note that the inverse operation for the diagonal block matrices can be performed using the LU decomposition (backward and forward substitutions). The inverse operation for the off-diagonal blocks are trivial because they are diagonal matrices. In the implementation, the linear system solver described in Section 2.1.1 was employed based on the block matrix operation.

Preliminary Performance Examinations

The updated transient capability of PROTEUS-MOC were tested for the TWIGL [24] and C5G7-TD1-1 [14] problems. In addition, calculations were performed using the WGS-CMFD scheme to examine a performance improvement.

Table 2-4. Computing Time of PROTEUS-MOC for TWIGL and C5G7-TD1-1 Problems

Problem	Computing Time, sec		Speed-up
	w/ WGS-CMFD	w/ MGS-CMFD	
TWIGL ¹⁾	472.0	58.0	8.1
C5G7 ²⁾ (TD 1-1)	106.6	24.0	4.4

¹⁾ w/ 16 processors in LCRC bebop cluster

²⁾ w/ 4320 processors in LCRC bebop cluster

Figure 2-4. Number of Transport Iterations at Each Time Step in PROTEUS-MOC for C5G7-TD1-1 Problem

Table 2-4 summarizes the computing times of PROTEUS-MOC for the two problems. As seen in the table, the MGS-CMFD scheme significantly reduced the overall computing time of the TWIGL and C5G7 problems by a factor of 4 and 8, respectively.

For the WGS-CMFD and MGS-CMFD schemes, the number of transport iterations performed at each time step in the C5G7-TD1-1 case are compared in Figure 2-4. The new CMFD scheme noticeably reduced the transport sweepings for the time steps between 0 to 2 sec where both power and flux shapes were drastically changed. These test results demonstrated that the MGS-CMFD scheme can enhance the computational efficiency of PROTEUS-MOC for kinetics calculations.

2.1.3 *T/H feedback Capability*

In this year, the capabilities of PROTEUS-MOC was extended to perform a T/H feedback inside the code. Currently, a T/H feedback capability is available for light water reactors (LWRs). Basically, the T/H capability can be applied to other reactor types if a relevant thermal feedback model fit to the reactor type of interest is plugged in.

2.1.3.1 *T/H feedback Framework*

The T/H feedback framework, developed this year, is constructed based on the channel and region-type concept. The channel is a base unit of the T/H calculation, and the feedback framework assumes that the T/H quantities are defined for each channel. The channel structure is provided by a user using the mesh file format. In the current implementation, the coarse mesh structure for the CMFD acceleration is re-used to specify the channel structure, which means that the coarse meshes aligned along the axial direction make a single channel. A single channel consists of multiple mesh blocks and thus we need to know a region type of each mesh in order to assign proper quantities. The region type is defined for each mesh block, which could be fuel, clad, coolant, or structure. It provides the essential information for a T/H solver to assign or map T/H quantities to neutronics meshes. For instance, if a certain mesh block is defined as a fuel region type, the fuel temperature among various quantities from the T/H calculation is assigned to this mesh block. Note that the region type information is provided to PROTEUS-MOC via the T/H assignment file which is a new input file created for the mapping purpose.

The role of this framework is to provide the interface to the T/H solver. When the channel-wise quantities are provided from a certain T/H solver, they could affect the subsequent PROTEUS-MOC calculation to account for the T/H feedback. It can also provide the neutronics data for channels, i.e. power, to the T/H solver. In order to update cross sections in accordance to temperature and density changes resulted from the feedback calculation, the feedback framework is linked to the CSAPI and ISOPAR [12] routines. Using this framework, PROTEUS-MOC can be coupled to the internal and external T/H solver such as a sub-channel code. Currently, it is only coupled to the internal T/H solver [12].

Figure 2-5. Relative Power, Fuel Temperature, and Coolant Temperature Distributions of C5G7 Obtained from PROTEUS-MOC with T/H Feedback

2.1.3.2 Coupling with Single Channel T/H Solver

The PROTEUS code suite contains the single channel T/H solver for a light water reactor application. This solver is coupled to PROTEUS-NODAL for thermal feedback modeling, providing assembly-average T/H parameters. [12] In this year, it was connected to PROTEUS-MOC using the feedback framework of PROTEUS-MOC. Now, the T/H feedback modeling for LWR application is available in PROTEUS-MOC via the single channel T/H solver. In the current version, the following feedback can be treated: temperature feedback for fuel, clad, coolant and other structure material, and density feedback for coolant. The T/H feedback results from PROTEUS-MOC for the 3D C5G7 problem is plotted in Figure 2-5, showing reasonable fuel and coolant temperature distributions in the radial and axial directions.

2.2 PROTEUS-NODAL Solver

In this year, work continued to extend the capabilities of PROTEUS-NODAL for various applications. The flowing fuel modeling capability for MSR applications and the transient simulation capability were implemented in PROTEUS-NODAL. Details are discussed in this section.

2.2.1 Transient Capability

The transient fixed source problem (TFSP) formation was implemented in PROTEUS-NODAL in the similar way to that of PROTEUS-MOC [12, 22]. In this formulation, a transient calculation is translated into the series of fixed source calculations at user-defined time steps,

which are solved sequentially. By referring to the transient implementation in PROTEUS-MOC, it was implemented in the PROTEUS-NODAL framework as shown in Figure 2-6.

Figure 2-6. Framework for Kinetics Solver of PROTEUS-NODAL

Transient Formulation

The time-dependent neutron diffusion equation for group g is written as follows:

$$\frac{1}{v_g} \frac{d}{dt} \phi_g(\mathbf{r}, t) - \nabla D(\mathbf{r}, t) \cdot \nabla \phi_g(\mathbf{r}, t) + \Sigma_g(\mathbf{r}, t) \phi_g(\mathbf{r}, t) = q_g(\mathbf{r}, t), \quad (2.15)$$

where $q_g(\mathbf{r})$ is the time-dependent neutron source term which consists of the scattering, prompt fission and delayed fission sources. For deriving the TFSP for each time step, the time derivative term is discretized using the implicit Euler method:

$$\frac{\phi_g^i(\mathbf{r}) - \phi_g^{i-1}(\mathbf{r})}{v_g \Delta t_i} - \nabla D_g^i(\mathbf{r}) \cdot \nabla \phi_g^i(\mathbf{r}, t) + \Sigma_g^i(\mathbf{r}) \phi_g^i(\mathbf{r}) = q_g^i(\mathbf{r}), \quad (2.16)$$

where i is an index for a time step and Δt is a time step size. Then, rearranging Eq. (2.16) to have a similar form of the steady-state equation, one can obtain the TFSP written as Eq. (2-17):

$$-\nabla D_g^i(\mathbf{r}) \cdot \nabla \phi_g^i(\mathbf{r}) + (\Sigma_g^i(\mathbf{r}) + \frac{1}{v_g \Delta t_i}) \phi_g^i(\mathbf{r}) = q_g^i(\mathbf{r}) + \frac{\phi_g^{i-1}(\mathbf{r})}{v_g \Delta t_i}. \quad (2.17)$$

The spatial discretization in PROTEUS-NODAL is applied to Eq. (2.17) and then the PROTEUS-NODAL steady-state solver can be used for a solver. For the SP₃ solver of PROTEUS-NODAL, the identical time discretization scheme is applied to the 2nd moment equation to form the TFSP.

The precursor integration technique [22, 25] used in PROTEUS-MOC was also adopted to deal with the delayed neutron precursor in the transient calculation without an additional time differencing for the precursor equations. In this technique, the quadratic variation of fission source during the current time interval is assumed so that the delayed neutron source for the current time step can be expressed in terms of fission sources of both the current and previous time steps and the precursor density of the previous time step. The contribution of precursor density of the current time step can be eliminated in the source term of TFSP. Consequently, the precursor equation does not need be solved explicitly in the transient calculation.

In this year, the transient capability based on the TFSP formulation was implemented on the SP₃ solver option of PROTEUS-NODAL. Thus, currently the transient calculation is only available for hexagonal geometries with the SP₃ equation. In future, it will be extended to the P_N solver option that can handle rectangular, triangular and hexagonal geometries.

CMFD Acceleration for Transient Calculation

In order to accelerate the transient PROTEUS-NODAL calculation, the multi-group system CMFD (MGS-CMFD) scheme was implemented as discussed in the previous section. The MGS-CMFD scheme implemented in PROTEUS-MOC was simply converted to the PROTEUS-NODAL solver. The details on the MGS-CMFD implementation can be found in Section 2.1.2. This solution scheme solves the entire MG form of the CMFD linear system directly, which is more efficient for transient cases. For thermal-spectrum test problems, the TFSP CMFD acceleration showed a remarkable improvement of performance.

Preliminary Verification Test

The transient capability of PROTEUS-NODAL has been verified using the modified TWIGL benchmark problem. In the modified TWIGL problem [24], the original Cartesian configuration was converted into the hexagonal configuration as shown in Figure 2-7.

Figure 2-7. Configuration of the Modified TWIGL Benchmark Problem

The transient calculation was performed using the SP₃ solver of PROTEUS-NODAL, and the reference solution was obtained using the transient solver of PROTEUS-MOC. Figure 2-8 compares the core power transients obtained from the two solvers, showing very good agreement between the two solutions within less than 1 % differences.

Figure 2-8. Comparison of Power Changes with Time between PROTEUS-MOC and PROTEUS-NODAL for the Modified TWIGL Benchmark Problem

2.2.2 MSR Capability

2.2.2.1 Precursor Drift Modeling

The transport equation of neutron flux and delayed neutron precursor concentration for a molten salt reactor (MSR) with flowing fuel can be written as:

$$\Omega \cdot \nabla \phi_g + \Sigma_{tg} \phi_g = \sum_{g'=1}^G \Sigma_{s,g' \rightarrow g} \phi_{g'} + \frac{1}{k_{eff}} \chi_{pg} \sum_{g'=1}^G v_{pg'} \Sigma_{fg'} \phi_{g'} + \sum_{k=1}^K \chi_{dkg} \lambda_k C_k, \quad (2.18)$$

$$\nabla \cdot [\mathbf{u} C_k] + \lambda_k C_k = Q_k, \quad (2.19)$$

where $Q_k = 1/k_{eff} \sum_{g'=1}^G v_{dkg'} \Sigma_{fg'} \phi_{g'}$, and the notations are standard, C_k is the precursor concentration for the precursor family k , and χ_{pg} and χ_{dkg} are the prompt neutron fraction and the delayed neutron fraction from the precursor family k , respectively.

Considering an axial velocity only, Eq. (2.19) can be re-written as:

$$u(r, z) \frac{\partial}{\partial z} C_k(r, z) + \lambda_k C_k(r, z) = \frac{1}{k_{eff}} \sum_{g'=1}^G v_{dkg'} \Sigma_{fg'}(r, z) \phi_{g'}(r, z), \quad (2.20)$$

which can be solved as:

$$C_k(r, z) = C_k(r, 0) \frac{u(r, 0)}{u(r, z)} \exp\left(-\lambda_k \int_0^z \frac{dz'}{u(r, z')}\right) + \frac{1}{u(r, z)} \int_0^z Q(r, z') \exp\left(-\lambda_k \int_{z'}^z \frac{dz''}{u(r, z'')}\right) dz', \quad (2.21)$$

$$C_k(r, 0) = \int_{A_{out}} u(r, H) C(r, H) e^{-\lambda_k t_{out}} dA / \int_{A_{in}} u(r, 0) dA, \quad (2.22)$$

where A_{in} and A_{out} are the areas of inlet and outlet, H is the height of active core, and t_{out} is the time spent outside the core. With the initial guess of the flux distribution, the delayed neutron source can be estimated, and the inlet precursor concentration are calculated and then the axial distribution of delayed neutron precursors are computed using Eq. (2.21). Then, Eq. (2.18) can be solved for new neutron fluxes and eigenvalue. An iteration is made until all of prompt neutron fluxes, delayed neutron fluxes, and eigenvalue are converged.

2.2.2.2 MSR Test Problems

As verification tests of the MSR simulation capability, the ABTR and Monju benchmark problems were solved with PROTEUS-NODAL and DIF3D-VARIANT using the 33 group cross sections generated from MC²-3. As shown in Table 2-5, the eigenvalues of NODAL and DIF3D-VARIANT are close to each other for the diffusion (P1-P0) option. The NODAL-SP3 solutions are in better agreement with DIF3D-VARIANT with P5-P3, compared to the NODAL-P1 solutions, indicating that the SP₃ equation can capture the majority of the transport effect in those benchmark problems. The detailed comparisons including assembly-wise power distributions can be found in Ref. [12].

In order to verify the flowing fuel capability of PROTEUS-NODAL, two benchmark problems were developed: one with a thermal spectrum and the other with a fast spectrum. The fast spectrum benchmark problem is based on a 2,050 MWt fast reactor with PuCl₃ fuel. The core size is approximately 370 cm × 370 cm with 480 cm high. The core is composed of three material regions: flowing PuCl₃ for the active core, flowing depleted UCl₃ with HT9 for the radial blanket, and a boron shielding region. There are five flowing channels, four channels in the fuel region and one channel in the blanket region, as shown in Figure 2-9, which are assumed to be completely isolated from each other. The flow time were varied in the core between 1 and 10 seconds, and the time spent outside the core between 0.3 to 5 seconds. A non-moving fuel calculation was performed as well to see the impact of the delay neutron loss from the systems.

Taking a 10 second flow time in the core and 5 second flow time external to the core, the eigenvalue solution is 1.01350. The non-moving fuel case yields 1.01458 indicating that the eigenvalue was reduced by 108 pcm due to the decay of delayed neutrons outside of the active core region. The change of the delayed neutron distributions due to flowing fuel vary with delayed neutron families because of different decay constants. As shown in Figure 2-11, the delayed neutron families 1 to 4 are the most impacted because of their large half-lives.

It should be quite apparent that as the flow speed is modified, each distribution of family precursors will be impacted in a similar direction (i.e. faster flow means more neutrons outside of the active core in all families) but not necessarily of the same magnitude (families 1 and 2 are impacted by the total time inside and outside of the core at the current flow speed). It is also very

important to note that the mixing of coolant outside of the reactor and long half-life of family 1 results in a flattened distribution over the core as opposed to a shape similar to the power distribution as would be typical of stationary fuel.

The thermal spectrum benchmark problem is a 32 MWt FLiBe core based partly on the specification discussed in Ref. [26]. The unit fuel block dimension is 10 cm × 10 cm containing 4 thin fuel channels (0.44 cm thick and 9 cm long each) surrounded by graphite, as shown in Figure 2-12. The reflector and shield blocks include flowing fuel regions thinner (0.14 cm thick and 9 cm long each) than in the fuel region. The core is composed of 1.2 m diameter fuel, 20 cm reflector and 20 cm shield. The core height is 6 m, including 4 m active core with 50 cm reflector and 50 cm shield at the top and bottom of the active core. In a quarter core model, there are 27 flowing channels, among which 25 channels are specified in the active core region and one channel is defined for each of reflector and shield regions, as shown in Figure 2-13.

The 13-group microscopic cross sections for each of fuel, reflector, and shield regions were generated using OpenMC/GenISOTXS [27]. The eigenvalue is 1.11177 for the case with no fuel flowing. With flowing fuel, as expected and shown in Table 2-7, eigenvalues become smaller due to the decay of the precursors external to the active core regions.

Table 2-5. Eigenvalues of ABTR and Monju Benchmark Problems

Problem	Code		k_{eff}	Δk , pcm
ABTR	DIF3D-VARIANT	P5-P3 ^{b)}	1.02452	Ref.
		P5-P0	1.02522	70
		P1-P0	1.01043	-1409
	NODAL	SP3-P0	1.02260	-192
		P1-P0	1.01077	-1375
MONJU ^{a)}	DIF3D-VARIANT	P5-P3	0.99576	Ref.
		P5-P0	0.99667	90
		P1-P0	0.98873	-704
	NODAL	SP3-P0	0.99632	55
		P1-P0	0.98914	-662

a) 200°C core configuration

b) Pm-Pn: mth-order transport approximation, nth-order anisotropic scattering

Pm-P0: isotropic scattering with transport approximation

Table 2-6. PROTEUS Eigenvalues of Fast Spectrum MSR Benchmark Problem with Elapsing Time of 10 sec inside Core and 5 sec outside Core

Model	Eigenvalue
w/o Flowing Fuel	1.01458
w/ Flowing Fuel	1.01350
Δk , pcm	-108

Figure 2-9. Flow Channels of Fast Spectrum MSR Benchmark Problem

Figure 2-10. Fuel Channel Map at the Middle of Fast Spectrum MSR Benchmark Problem

Figure 2-11. Delayed Neutron Precursor Distributions with (right) and without (left) Flowing Fuel Condition for Fast Spectrum MSR Benchmark Problem

Figure 2-12. Thermal Spectrum MSR Benchmark Problem

Figure 2-13. Core and Flow Channel Maps of Thermal Spectrum MSR Benchmark Problem

Three cases were tested by varying the elapsing times of flowing fuel in the inside and the outside of the core: i.e., 3 sec/8 sec for case 1, 3 sec/3 sec for case 2, and 6 sec/ 16 sec for case 3. The eigenvalue of case 1 was 501 pcm smaller than that of the non-moving fuel case. When reducing the flow time outside of the core from 8 sec to 3 sec (case 2), the eigenvalue difference is -472 pcm. This is due to the relatively smaller loss of neutrons from decay of precursors external to the domain. When the flow time across the core and external to the core is increased, the eigenvalue difference is -403 pcm. Increasing the flow time across the core reduces the number of precursor neutrons lost external to the active core in families 3 and 4, but increasing the time external to the core increases the loss of precursor neutrons from families 1 and 2 somewhat offsetting the gains in families 3 and 4. Because of the relative magnitude of family 4, the gain tends to dominate. Figure 2-15 shows the relative change in the neutron source derived from precursor family 4 for the three different cases.

Table 2-7. PROTEUS Eigenvalues of Thermal Spectrum MSR Benchmark Problem

Model	Eigenvalue	Δk , pcm
w/o Fuel Flowing	1.11177	0
w/ Fuel Flowing (Case 1)	1.10676	-501
w/ Fuel Flowing (Case 2)	1.10705	-472
w/ Fuel Flowing (Case 3)	1.10774	-403

Figure 2-14. Delayed Neutron Precursor Distributions with (right) and without (left) Flowing Fuel Condition for Thermal Spectrum MSR Benchmark Problem

Figure 2-15. Distributions of Delayed Neutron Precursor Family 4 for Different In-core/Out-core Elapsing Times in Thermal Spectrum MSR Benchmark Problem

2.3 Cross Section API

The cross section API (CSAPI) is a key component of PROTEUS which generates multigroup cross sections on the fly using the cross section library data based on the subgroup method or the resonance table method. This year, a new cross section library based on the resonance table method was developed and tested for LWR benchmark problems to more accurately generate multigroup cross sections. This section presents the details of the new cross section library generation procedure.

2.3.1 Library Generation for Cross Section API Using MC²-3 and OpenMC

The OpenMC Monte Carlo code provides a capability to perform both cross-section generation and flux calculations on a detailed 3D geometry in continuous energy. In the last few years, the code have provided more input flexibility, improved computing efficiency, and better capability for tallying cross sections that are to be used with deterministic neutronics codes. The OpenMC code was recently updated with the enhanced capability for cross-section generation, and the GenISOTXS code was updated at ANL to convert the OpenMC cross section output to the ISOTXS format for use in the ANL neutronics codes.

In order to generate the cross section library, the base isotopic cross sections with various background conditions for each isotope are generated from OpenMC Monte Carlo calculations using a heterogeneous unit pin cell with various number densities of the isotope of interest. In this calculation, it should be ensured that the number densities of the isotope of interest covers all possible background cross sections of the isotope in the reactor cores or problems of concern.

For LWR applications, for example, a typical pin cell is selected for calculating the base cross sections. An air gap between pellet and cladding can be removed for simplicity. For each isotope, its number densities are changed by multiplying 32 to 1/256 to its base number density in order to provide a wide range of background cross sections possible in the actual conditions. Currently, 14 cases are made with different number densities of the isotope of interest. OpenMC is then executed for those cases using 20 million particle histories, tallying all microscopic cross sections based on a given multigroup energy structure. Actinides and fission product isotopes are placed in the fuel region and other isotopes are put in the cladding or moderation region.

Conventionally, only resonances of the isotope of interest are considered in a pin cell calculation, using the potential cross sections for the other resonant isotopes, so that the effect of those resonances is separated out from that of the other resonance isotopes. In this procedure, the interference effect between resonant isotopes is simply ignored or additionally accounted for by introducing correlations between them. However, we do not account for the resonance interference effect explicitly, using all resonances of isotopes in the base cross section calculations.

Resonance Cross Section Table

Once the microscopic cross sections of the isotope of interest are produced from OpenMC, the background cross sections corresponding to those cross sections are calculated using MC²-3. The

recently updated version of the MC²-3 code includes a 2D and 3D MOC capabilities for Cartesian and hexagonal geometries. In this version, anisotropic scattering with up to P₃ can be handled with the 2D MOC calculation. The escape cross sections for heterogeneous problems are calculated by solving the fixed source problems. [28] With the cross sections provided from OpenMC, one-group fixed source problems are solved for all resonance energy groups of the isotope of interest. At every resonance energy group, data points (background cross sections) with the number of cases are generated, which would be all different between resonance energy groups.

Since a single set of background cross sections are needed for all resonance energy groups, a combined set of background cross section is generated by merging all background cross sections from all resonance energy groups, instead of using selected data points, in order to reduce the errors arising from interpolation. The cross section tables are made for absorption, nu-fission, and total scattering cross sections as

$$\sigma_x = f(\sigma_b, T), \quad (2.23)$$

where the subscript x represents absorption, nu-fission, and scattering and σ_b is the background cross section.

In this approach, it is necessary to check if the correlation of resonance cross sections and background cross sections prepared from pin cells with specific background cross section conditions can be applicable to other background cross section conditions. For the test, the cross section table generated with a pin cell was compared with those produced with three different 2×2 pin configurations: 1) 3 fuel pins + 1 guide tube (GT), 2) 2 fuel pins + 2 GTs, and 3) 1 fuel pin + 3 GTs. All cases have the same material background cross sections but very different escape cross sections due to different combinations of pins. As shown in Figure 2-16, comparisons indicated that the U-238 absorption cross sections at 4 - 9.9 eV from the three 2×2 pin calculations agreed well with those from a single pin cell. In fact, the three cases have very different neutron spectra due to the increased thermalization or absorption of neutrons in the different number of GT regions.

Figure 2-16. Four Different Combinations of Fuel Pins (Blue) and Guide Tubes (Yellow) for Calculating Self-shielded Cross Sections

Figure 2-17. Absorption Cross Section versus Background Cross Section of U-238 at 4 – 9.88 eV Obtained from 4 Different Pin Configurations.

Flux Correction Factors

The angular dependency of resonance multigroup cross sections [29] may become more significant as the number of energy groups is reduced. This means that even though the multigroup cross sections tallied from the reference code are used, its multigroup flux solutions may not be reproduced in other deterministic codes unless the angular dependency of cross sections of the reference solution is preserved. Figure 2-18 shows the comparison of fluxes produced from OpenMC and MC²-3 for the unit pin cell. Even though the 41-group cross sections tallied from OpenMC are used in MC²-3, the flux solutions are different from each other in the resonance and thermal energy range, which makes eigenvalue off by more than 200 pcm.

In order to reproduce reaction rates, we introduce the flux correction factor, based on Eq. (2.24), which is calculated from MC²-3 using the iterations until it is converged.

$$\mu_g(r) = \frac{\phi_g(r)}{\phi'_g(r)}, \quad (2.24)$$

where $\phi_g(r)$ and $\phi'_g(r)$ are the reference and calculated fluxes. The flux correction factors should vary with material and geometry conditions. However, we calculate the flux correction factors for the representative pin cell and apply them to the fuel region only, assuming that the fuel region is the most dominant contributor to determine neutron fluxes and eigenvalue. Verification tests that will be discussed in the next section indicated that the approximation works well for most of the benchmark problems.

Fuel Region

Cladding Region

Moderator Region

Figure 2-18. Neutron Flux Differences between OpenMC and MC²-3 for the Unit Pin Cell.

Figure 2-19. Energy Group Structures of the 41, 47, and 70-Group Cross Section Libraries.

Figure 2-20. 41, 47, and 70-group Flux Correction Factors for the Fuel Region.

Figure 2-19 illustrated the 41, 47, and 70-group structures tested. The 47-group and 70-group structures stem from the HELIOS and LANL group structures, respectively. Since the smaller number of groups is preferred for PROTEUS at the end and the 47-group structure was found to produce larger errors in eigenvalue estimation, the 41-group structure was proposed here maintaining almost the accuracy of the 70-group solutions. Figure 2-20 depicts the flux correction factors calculated from MC²-3, showing that relatively large corrections are needed in the resonance and thermal energy range. Interestingly, it was found that a relatively large correction is necessary for the group of 6.48 - 7.34 eV for the 47-group structure where the largest capture

resonance cross section of U-238 exists. The 47-group structure has finer groups in the range of 4 – 10 eV than the other two group structures.

Library Generation

Once the isotopic cross sections and background cross sections are calculated for each isotope with a wide range of background cross sections and temperature conditions, the resonance cross sections for absorption, nu-fission, and total scattering are tabulated with background cross sections and temperatures, and the cross sections in the non-resonance groups as well as scattering matrices are extracted from the representative pin cell.

The CSAPI reads the cross section library and solves the fixed source problems for each isotope and group to calculate the isotopic escape cross sections for all cross section regions. Varying with the background cross sections, the total cross sections used in the fixed source problems are iteratively determined but converged very quickly in 2 to 3 iterations. The final multigroup cross sections are determined by the total background cross sections composed of the escape cross sections and material background cross sections.

The contribution of the updated resonance cross sections to the background cross sections for other isotopes is accounted for by the Bondarenko iteration. The resonance interference effect is not explicitly considered in the procedure, but the most part of the effect is included at the generation of cross sections with a pin cell. This would be a source of inaccuracy when the composition of the actual problem is very different from that of the representative pin cell. Figure 2-21 digests the flow of the cross section library generation from the cross section generation to the PROTEUS calculation.

Figure 2-21. Generation of the Cross Section Library for PROTEUS.

2.3.2 Update of CSAPI for PROTEUS-MOC

In past years, PROTEUS-MOC was massively updated to improve performance and extend capabilities. Accordingly, CSAPI was revised to comply the up-to-date version of PROTEUS-MOC. First of all, the interface routine of CSAPI that invokes the transport solver of PROTEUS-MOC was updated so that it can perform the fixed source calculations to correctly yield background cross sections in self-shielding calculations.

The coupling of CSAPI and PROTEUS-MOC is fully compatible with parallel execution with spatial and angle decomposition. It was confirmed by running test cases with various parallel configurations. For the T/H feedback modeling, an additional interface routine was created to update the self-shielded cross sections when temperature and densities are perturbed. This interface is utilized in the T/H feedback framework described in Section 2.1.3.

2.3.3 Verification Tests

For verification of the cross section library generated based on ENDF/B-VII.0 data, multiple benchmark problems were selected including the Mosteller benchmark problems [30], the VERA fuel assembly benchmark problems [31], and the modified OECD/NEA C5 problems [32]. These benchmark problems were solved using PROTEUS-MOC (hereafter, PROTEUS for brevity) with the 41-group cross section libraries whose solutions were compared against the corresponding Monte Carlo solutions. Prior to testing the benchmark problems, a refinement study in terms of mesh, angle, and anisotropic scattering order was performed using a typical PWR pin cell to check a solution convergence. The in-house meshing tool [10] was used to create meshes for this study.

As verification tests, the Mosteller pin cell benchmark problems were used for verification tests, which include U or Pu enriched fuels with 0.71 to 5 wt.% U-235 (Cases 1 to 7) and 1 to 8 wt.% Pu-total (Cases 8 to 16). Among the MOX pins, Cases 8 to 12 contain reactor grade plutonium (60 wt.% Pu-fissile) while Cases 13 to 16 are composed of weapon grade plutonium (94 wt.% Pu-fissile). Eigenvalues from PROTEUS were compared with OpenMC solutions, indicating good agreement within 100 pcm Δk . No particular trend in eigenvalue differences between PROTEUS and OpenMC was observed with the change of enrichment.

The 2x2 pin problems were solved using PROTEUS with the 41-group cross section library, which were constructed by replacing one of the fuel pins with burnable poison, gadolinia pin, GT, control rod, and IFBA pin. The eigenvalue comparison showed that the PROTEUS results are maximum 173 pcm Δk off from the OpenMC solutions.

For verification tests of fuel assemblies, the selected VERA PWR benchmark problems developed by the DOE CASL program based on the Westinghouse fuel were used. For simplicity, the original benchmark problems were slightly modified by simplifying compositions and using a constant temperature of 300K for all regions, resulting in different eigenvalues from the original ones. Case 2A is a standard fuel assembly (FA) with 264 3.1 wt.% U-235 enriched fuel pins, 24 guide tubes (GTs) and 1 instrument thimble (IT). The other six FAs include pyrex-type or

WABA-type burnable poisons, AgInCd control rods, or IFBA. The calculation results indicated that the eigenvalues from PROTEUS agreed very well with MCNP6 solutions within 76 pcm Δk and the pin powers between the two codes had excellent agreement with 0.39%, except for Case 2P with 24 gadolinia (Gd) pins which showed a maximum difference of 2.05% at one of the Gd locations with 0.244 relative power. Excluding the Gd pins, the maximum and RMS differences of Case 2P are 0.43% and 0.17%, respectively, which are similar to the other cases. No particularly large differences were observed for Cases 2M and 2N with IFBA rods. The eigenvalue comparisons for Mosteller pins, 2x2 pins, and VERA fuel assembly problems are summarized in Figure 2-22.

Multi-assembly calculations were also performed for verification tests, which were created by modifying the original OECD/NEA C5G7 benchmark problems. In the modification, a pin is composed of fuel, gap, cladding, and moderator regions, and isotopic compositions are used for the fuel regions: standard UO₂ (3.1 wt.% U-235) and MOX (enrichment zoning with 3.8, 6.6, and 7.4 wt.% Pu-total).

Based on the modified C5 benchmark problem, the 2D core problems as well as the FA problems were solved using PROTEUS and MCNP6. As expected from the previous comparison for the VERA benchmark problems, FA eigenvalues and pin powers from PROTEUS agreed very well with MCNP6 solutions: eigenvalues within 52 pcm Δk , as shown in Table 2-8, and pin powers within 0.28% with RMS 0.16%, as illustrated in Figure 2-23.

For 2D core problems, a base C5 case without CR was first solved using the two codes. For more challenging flux shapes and relatively flatter power distributions, an additional case was created by inserting 24 AgInCd CRs in the four UO₂ FAs located at the core center where relative powers in the case without CRs are up to 2.23. Flux and power distributions of the two cases are illustrated in Figure 2-24.

Compared to MCNP6 solutions, eigenvalues from PROTEUS are in good agreement within 141 pcm Δk and the control rod worths from the two codes matched well within 0.1%. A pin power comparison indicated that for the case without CR, maximum and RMS differences are 2.28% and 0.48%, respectively. In fact, the maximum percent difference occurred at the low power location of 0.33. If excluding the pins with less than a relative power of 0.5, the maximum and RMS differences are reduced to 1.41% and 0.43%, respectively. For the case with CRs, the maximum and RMS differences in relative pin powers between the two codes are 1.45% and 0.53%, respectively. Its maximum difference is smaller than that of the case without CRs because the smallest relative power is as higher as 0.63 but the RMS of % differences is higher because of larger differences in the rodded UO₂ FAs.

Eigenvalue changes with temperature were tested using the selected VERA fuel assemblies: 2A, 2F, and 2G. Fuel temperatures were changed gradually from 300 to 1,200 K, maintaining the temperatures of the other regions with 300 K or 600 K, as shown in Table 2-9. Note that MCNP6 calculations were performed using 25 million particle histories.

As shown in Table 2-9 and Figure 2-25, the eigenvalue solutions between MCNP6 and PROTEUS agreed well for most cases except Case 2G in which eigenvalues were off by up to 321 pcm. It is noted that only Case 2G includes 24 AgInCd control rods. An investigation will be performed for Case 2G to identify error sources and make improvements.

Figure 2-22. Eigenvalue Comparison between PROTEUS-CSAPI and Monte Carlo

Table 2-8. Eigenvalue and Power Comparison for the Modified C5 Benchmark Problems.

Case	MCNP6 $\pm\sigma$, pcm	PROTEUS	
		Eigenvalue Δk , pcm	Pin Power Diff. Max/RMS, %
UO ₂ FA	1.39208 $\pm$ 17	-52	0.28 / 0.10
MOX FA	1.20450 $\pm$ 12	12	0.29 / 0.16
2D Core	1.19774 $\pm$ 2	121	2.28 / 0.48
2D Core w/ CR	1.04505 $\pm$ 2	141	1.45 / 0.53
CR worth	15,269 (pcm)	-20 (0.1%)

Figure 2-23. Pin Power Difference of the UO₂ (left) and MOX (right) Fuel Assemblies of the C5 Benchmark Problems.

Figure 2-24. Thermal Flux, Relative Pin Power, and % Pin Power Difference of the 2D C5 Benchmark Problems.

Table 2-9. Comparison of Eignvalues with Temperature Change between MCNP6 and PROTEUS for the Selected VERA Assemblies.

Case	Temperature Fuel / Other Regions (K)	MCNP6 $\pm \sigma$, pcm	PROTEUS Δk , pcm
2A	300 / 300	1.20546 $\pm$ 13	76
	600 / 600	1.19341 $\pm$ 13	198
	900 / 600	1.18467 $\pm$ 13	108
	1200 / 600	1.17693 $\pm$ 13	139
2F	300 / 300	1.00796 $\pm$ 13	-3
	600 / 600	0.98286 $\pm$ 13	52
	900 / 600	0.97565 $\pm$ 13	-52
	1200 / 600	0.96966 $\pm$ 13	13
2G	300 / 300	0.90467 $\pm$ 13	7
	600 / 600	0.87550 $\pm$ 13	-226
	900 / 600	0.86925 $\pm$ 13	-321
	1200 / 600	0.86410 $\pm$ 13	-259
2K	300 / 300	1.05108 $\pm$ 13	-5
	600 / 600	1.02748 $\pm$ 14	50
	900 / 600	1.02008 $\pm$ 13	-71
	1200 / 600	1.01356 $\pm$ 13	-69
2M	300 / 300	0.95933 $\pm$ 12	-67
	600 / 600	0.94709 $\pm$ 13	-23
	900 / 600	0.94051 $\pm$ 12	-109
	1200 / 600	0.93472 $\pm$ 12	-110
2N	300 / 300	0.89635 $\pm$ 13	40
	600 / 600	0.87664 $\pm$ 12	60
	900 / 600	0.87020 $\pm$ 12	-4
	1200 / 600	0.86512 $\pm$ 12	-49
2P	300 / 300	0.96792 $\pm$ 14	-39
	600 / 600	0.93559 $\pm$ 12	-37
	900 / 600	0.92899 $\pm$ 12	-135
	1200 / 600	0.92336 $\pm$ 12	-163

Figure 2-25. Eigenvalues with Temperature Change for the Selected VERA Assemblies

For the application to a MSR with FLiBe molten salt and graphite moderator, a cross section library was generated by performing base cross section calculations with OpenMC and corresponding background calculations with MC²-3, as discussed in Section 2.3.1. The 41-group structure was used for preliminary tests, so a group structure optimization study should be performed to determine a group structure appropriate for the MSR spectrum.

A pin cell used for the base cross section calculations using OpenMC is composed of two regions with fuel molten salt and graphite moderator. Using the cross section library, two verification problems shown in Figure 2-26 were solved, of which the graphite volume fraction is twice larger than that of the pin cell used for the cross section generation. The geometries and compositions are presented in Figure 2-26 as well. In the fuel, 3 wt.% enriched uranium was mixed with the FLiBe salt. The volumes of fuel and graphite are the same for both problems, but eigenvalues are very different from each other: 1.28513 for Case A and 1.21710 for Case B from OpenMC. Note the precursor drift from flowing fuel was not considered in this verification test.

For PROTEUS calculations, the meshes shown in Figure 2-26 were used to make solutions converged in terms of spatial discretization. Note that the mesh for Case A was generated using Ufmesh, while that for Case B was made using CUBIT. For angular discretization, a Legendre-Tchebychev angular cubature of L_9T_{15} (320 angles/ 4π) and $L_{15}T_{35}$ (1152 angles/ 4π) were used for Case A and Case B, respectively. A scattering order of P_3 was used in these calculations, but there were only minor differences (< 10 pcm) in eigenvalues between P_2 and P_3 . As listed in Table 2-10, PROTEUS solutions agreed well with OpenMC Monte Carlo solutions within 90 pcm.

Additionally, 2x2 unit cell problems were constructed with the different number of fuel unit cells to vary the background cross sections as well as neutron spectra, as shown in Figure 2-27. The directions of fuel salts are alternating with neighboring fuel unit cells. Eigenvalues between PROTEUS and OpenMC for the four cases were compared, resulting in good agreement within 98 pcm, as digested in Table 2-11. Note that, as expected, the neutron spectra of the 4 fuel unit cell case and the 1 fuel and 3 graphite unit cell case are very different from each other because of significant difference of the amount of graphite in the problems.

The 2D core problem with a single fuel unit cell type was created for additional verification tests. For the PROTEUS calculations, 29,335 elements and $L_{11}T_{25}$ (624 angles/ 4π) along with the 41-group cross section library were used. Figure 2-28 shows the thermal neutron flux distribution of the quarter portion of the 2D core with the vacuum boundary condition. Table 2-12 shows the eigenvalue comparison, indicating very good agreement between PROTEUS and MCNP within 37 pcm.

Figure 2-26. Fuel Blocks Composed of Fuel FLiBe Molten Salt (Blue) and Graphite (Red)

Table 2-10. Eigenvalues of MSR Fuel Blocks

Case	OpenMC	PROTEUS (Δk , pcm)
A	1.28513 ± 0.00012	-27
B	1.21710 ± 0.00012	-90

Figure 2-27. 2x2 MSR Block Benchmark Problems

Table 2-11. Eigenvalues of 2x2 MSR Fuel Block Benchmark Problems

Case	OpenMC	PROTEUS (Δk , pcm)
4 Fuels	1.21666 $\pm$ 0.00012	-53
3 Fuels	1.22771 $\pm$ 0.00016	-98
2 Fuels	1.20974 $\pm$ 0.00015	-94
1 Fuel	1.06955 $\pm$ 0.00014	-64

Figure 2-28. Thermal Flux Distributions for the 2D Core MSR Benchmark Problem

Table 2-12. Eigenvalues of 2D MSR Cores

2D Case	OpenMC	PROTEUS (Δk , pcm)
Reflective BC	1.20332 $\pm$ 0.00015	-37
Vacuum BC	0.77399 $\pm$ 0.00015	-12

3. Updates in MC²-3

3.1 CMFD Acceleration for 2D and 3D MOC Solvers

In MC²-3, a slowing-down calculation for a 3D problem is performed using the 2D/3D MOC solver. The 2D/3D MOC solver uses the same formulation used in PROTEUS-MOC. In FY 2016, the consistent CMFD formulation was devised for accelerating PROTEUS-MOC. This year, the CMFD acceleration scheme was implemented to the 2D/3D MOC solver of MC²-3 to accelerate the UFG slowing down calculations. The CMFD currently works for hexagonal geometries only. This section provide the details.

Review of Consistent CMFD Formulation

The 2D/3D MOC method does not satisfy the neutron balance equation because the non-conservative discretization is used for axial variable. In the consistent CMFD formulation a fictitious cross section, referred to a pseudo absorption cross section, is introduced to resolve the inconsistency of the neutron balance between CMFD and 2D/3D MOC solutions. With the pseudo absorption cross section, the neutron balance equation in CMFD scheme is written as:

$$\sum_k J_{i \rightarrow k} + (\Sigma_r^i + \Sigma_p^i) \bar{\phi}_i V_i = \bar{q}_i V_i, \quad (3.1)$$

where Σ_p is the pseudo absorption cross section. During the alternative calculation of CMFD and 2D/3D MOC schemes, the pseudo absorption cross section of each coarse mesh is iteratively determined using the 2D/3D MOC solution as:

$$\Sigma_p^i = \frac{\bar{q}_i V_i - \sum_k J_{i \rightarrow k}}{\bar{\phi}_i V_i} - \Sigma_r^i. \quad (3.2)$$

From the 2D/3D MOC solution, the homogenized group constants can be generated by the flux-volume weighting over the fine meshes that belong to the coarse mesh. The coupling coefficients can be determined using the following CMFD relation:

$$J_{i \rightarrow k} = -\tilde{D}_{i \rightarrow k} (\bar{\phi}_k - \bar{\phi}_i) - \hat{D}_{i \rightarrow k} (\bar{\phi}_k + \bar{\phi}_i). \quad (3.3)$$

By combining Eqs. (3.1) to (3.3), the CMFD linear system, can be formed in terms of averaged fluxes and neutron sources. The CMFD solution is obtained via the conventional fission source iteration and each group equation is solved using the Krylov subspace method. Based on a coarse mesh flux ratio of the previous MOC and newly obtained CMFD solutions, fine-mesh fluxes within the coarse mesh are updated. The updated fine-mesh solution together with the eigenvalue of CMFD result is put to the subsequent 2D/3D MOC calculation.

Implementation of CMFD Acceleration

In the implementation of CMFD acceleration, the most of functionalities developed for the proof-of-principle demonstration [33] were adopted and properly ported into the MC²-3 structure. This work includes the removal of geometry restrictions in the test version. In the test version, the entire assemblies should have the same number of pins and same pin pitch, which results in the

identical coarse mesh structure. The coarse mesh structure could not be configured for the assembly with inter-assembly gap and duct. The module for handling the coarse mesh geometry was extended to eliminate these limitations. Along with the coarse mesh geometry, the neutron current information at the coarse mesh interfaces is required to determinate the CMFD coupling coefficients. A surface current at the assembly or pin interfaces can be computed during the MOC calculation by using the following equation:

$$J_i^s = \sum_{k \in s} \sum_m \phi_{m,i}^{k,out} \sin \theta_m w_m \Delta_m - \sum_{k \in s} \sum_m \phi_{m,i}^{k,in} \sin \theta_m w_m \Delta_m, \quad (3.4)$$

where m , k , i and s are the indices for angle, ray, coarse mesh and surface respectively, w is the weight of angular cubature, and Δ is the ray spacing. The neutron current tally routines were added to the 2D and 3D MOC modules.

The group condensation procedure was implemented for efficient CMFD calculation. The CMFD calculation is performed with reduced group structure instead of UFG structure. In order to have the CMFD solution accelerate the MOC calculation, the following quantities are needed for each group and coarse mesh: the homogenized group constants for coarse meshes and the coupling coefficients that specify interface current relations between the two adjacent coarse meshes. The corresponding routines were updated to generate these quantities in the reduced group structure. The group structure for CMFD acceleration is selected by users and the default one is 200 groups.

The well-established iteration scheme used in various codes including PROTEUS-MOC was implemented for MOC calculations with CMFD acceleration. [12, 33] The three layers of nested iterations are performed: fission source, group and within-group iterations. At the end of each fission source iteration which is the outermost iteration, the CMFD calculation is performed and then the fine-mesh flux and fission source distributions are updated using the resulting CMFD solution. In the group iteration, the coarse mesh parameters required for constructing the CMFD problem are computed using the updated group solutions. In the innermost iteration which is a within-group iteration, the MOC calculation is performed repeatedly with the within-group scattering source update.

3.2 Version Integration and Updates

In the past few years, the following new features were added to MC²-3 codes: the 2D/3D MOC transport calculation, the improved thermal cross section calculation, and the improved gamma data generation based on the updated gamma library. These new features were developed and implemented in the individual SVN branches. In this year, these developmental branches were merged to a production version that is being prepared for release. This work also included code optimization with multiple calculation options. The input processing routine was modified in accordance with new calculation options and features. The benchmark test problems were added to verify the new capabilities. At the same time, the code manual was updated to include the methodologies and input usage of the new capabilities.

4. Verification and Validation Tests

As continued verification and validation efforts for PROTEUS, the following benchmark problems and experiments were simulated: the 3D C5G7-TD transient benchmarks [14], the TREAT M8CAL core experiment [34], the RCF core experiment [35], the MSR core benchmark [36]. All of them are thermal spectrum cores. This section describes the details of those benchmark problems and results.

4.1 3D C5G7-TD Transient Benchmark Problem

In FY2017, verification tests for the transient capability of PROTEUS-MOC were performed for the 2D C5G7-TD transient benchmark problem. This year, work continued to test the transient capability using the 3D C5G7-TD transient benchmark problems, which are more challenging in terms of control rod cross section treatment and computation performance and resources.

The 2D configuration of the fuel assemblies is shown in Figure 4-1. Each 17x17 fuel assembly consists of 264 fuel pins, 24 guide tubes for control rods and one fission chamber at the center. Each pin cell has a pin radius of 0.54cm and a pitch of 1.26cm. The 3D configuration of the problem is shown in Figure 4-2.

For MPACT [16], used are 0.05cm ray spacing, 273,972 elements for 2D mesh, 16 axial planes, Yamamoto-Chebyshev 2-8 cubature, whereas for PROTEUS-MOC, used are 0.05cm ray spacing, 52,020 elements for 2D mesh, 24 axial planes, and Legendre-Tchebychev cubature of L_3T_7 .

The 3D configuration for the C5G7-TD benchmark [14] was developed based on the 3D extension of the original C5G7 core [13]. The 2D configuration is extruded to a total height of 128.52 cm and two 21.42 cm thick water reflectors are added to the top and bottom of the core. Vacuum boundary condition is applied to the axial boundaries and control rods can be inserted through the guide tubes from the top.

Figure 4-1. Assembly Configuration and Pin Layout of the C5G7-TD Benchmark Problem

Figure 4-2. 3D Configuration of the C5G7-TD Benchmark Problem

For the initial steady state condition, referred to as the unrodded case, the control rod banks are inserted into the top reflector and the fission chambers are fully inserted into the active core through the top reflector. More details on the geometry specifications, 7-group cross section data and kinetics parameters for 6 delayed neutron groups can be found in Ref. [14].

For this study, 3D transient calculations were performed for 2 exercises, described briefly below, using MPACT and PROTEUS-MOC. Specifications for these exercises are listed in Ref. [14].

- Exercise 4 (TD4), 3D: Insertion/withdrawal of one or several control rod banks,
- Exercise 5 (TD5), 3D: Variation of moderator density in one or several fuel assemblies.

For PROTEUS-MOC, a 2D mesh file was created using the PROTEUS mesh tool. The mesh for each pin cell consists of 3 radial rings for the inner zone, 2 radial rings for the outer zone and one azimuthal mesh for each half-face (1/8 of the square cell). The mesh for each pin-cell-equivalent sub-region of the reflector is a 2x2 grid. In total, the 2D mesh for PROTEUS-MOC contains 52,020 first order elements. For the 3D configuration, the 2D mesh was extruded using 24 axial planes.

For MPACT, a similar structured but finer mesh with 273,972 elements was used: 5 radial rings for the inner zone, 3 radial rings for the outer zone of each pin cell, 3 azimuthal meshes for each half-face and each equivalent cell in the reflector region is divided into a 5x5 grid. The axial mesh for the 3D configuration consists of 16 planes.

Eigenvalue results from PROTEUS-MOC and MPACT are listed in Table 4-1. For the 2D configuration, the calculation with PROTEUS-MOC was performed using 0.05cm ray spacing

and the Legendre-Tchebychev cubature of L_3T_{15} (128 directions/ 4π); for MPACT the input options are 0.03cm ray spacing and the Yamamoto-Tchebychev cubature of Y_3T_{16} (96 directions/ 4π). For the 3D configuration, the same ray spacing values were used but the cubatures are L_3T_7 (64 directions/ 4π) and Y_2T_8 (32 directions/ 4π), respectively, for PROTEUS-MOC and MPACT. The MCNP5 reference result was given in Ref. [14].

Table 4-1. Eigenvalue Results for the C5G7-TD 2D and 3D Benchmarks

Code	2-D Eigenvalue	3-D Eigenvalue
MCNP5	$1.18646 \pm 0.07\%$	-
MPACT	1.18666	1.16351
PROTEUS-MOC	1.18651	1.16469

The 3D mesh for PROTEUS-MOC, and similarly for MPACT, consists of axial planes, or nodes, whose thicknesses are typically much larger than the travel distance of the control rods during each transient time step. It is therefore inevitable that for most of the transient duration, the tip of each control rod is partially inserted into a certain node. The macroscopic cross sections need to be properly homogenized for these partially rodded nodes. By definition, the homogenized macroscopic cross section of a heterogeneous region is the flux-volume-weighted average of the cross section values from each sub-region. Due to the high absorption cross section of the control rod material, the neutron flux varies drastically around the control rod tips and drops significantly for the rodded sub-region. Therefore, the simple volume-weighted homogenization would overestimate the contribution of the rodded sub-region and lead to the under-prediction of the core reactivity. This is often referred to as the control rod cusping effect.

To completely eliminate the cusping effect, the macroscopic cross sections need to be homogenized using the flux-volume weights which requires knowing the exact flux in each sub-region. For practical applications, the flux is not available before the code is run and therefore a decusping treatment must be employed to estimate the flux profile or flux-weighted volume. Several decusping methods have been studied and developed for MOC solvers, including the decusping scheme in Ref. [37] based on local CMFD calculation and the subplane-based method in Ref. [38]. These methods have proven to be effective but still require further development to be implemented directly to the PROTEUS-MOC.

Another method that has been applied successfully in MPACT for the C5G7-TD transient problem is polynomial decusping in which a pre-generated polynomial is used to estimate the effective rodded volume, i.e., the flux-weighted volume of the sub-region occupied by the control rod tip, in a partially rodded node [38, 39]. Specifically, for the C5G7 3D configuration, a series of 100 steady state cases were performed for a single UO₂ assembly with the control rod bank inserted from 0-100%. The polynomial was obtained by fitting the data of normalized reactivity for each inserted fraction value, using which the effective rodded volume for each case can be estimated. The result is plotted in Figure 4-3. The polynomial was approximately applied for both the UO₂ assemblies and MOC assemblies of the C5G7 3D core.

For our validation purpose, it is sufficient to use the same polynomial obtained in MPACT for the decusping treatment in PROTEUS-MOC. Using the decusping polynomial, the homogenized

macroscopic cross section for each partially rodded node can be calculated and provided as input for PROTEUS-MOC. Transient calculations were performed for 2 cases of Exercise 4, TD4-1 and TD4-5. In TD4-1, the control rod bank 1 was inserted at a constant speed into 1/3 of the active core in 2s and withdrawn in the next 2s by a reverse process. For TD4-5, in addition to the insertion and withdrawal of control rod bank 1 as in TD4-1, control rod bank 3 was also inserted starting at 2s to reach 1/3 of the core at 4s, remained at that position for the next 2s and was withdrawn within the next 2s. Results from PROTEUS-MOC and MPACT for these cases are shown in Figure 4-4 and Figure 4-5, respectively.

Overall, these results from MPACT and PROTEUS-MOC are in good agreement. A slight difference is expected and attributable to the different spatial and angular meshes used for the two codes and the fact that the decussing polynomial obtained in MPACT may not behave exactly the same in PROTEUS-MOC.

One case of Exercise 5, TD5-1, was also performed by PROTEUS-MOC and MPACT. The transient event in this case was driven by the variation of moderator density in assemblies 1 and 3. Detailed specifications can be found in Ref. [14]. For both MPACT and PROTEUS-MOC, the changes in moderator density can be modeled accurately by varying the macro cross sections of the moderator. The power changes with time for the TD5-1 transient are shown in Figure 4-6. The power results from PROTEUS-MOC and MPACT are nearly identical.

Figure 4-3. Effective Volume Fraction for a Partially Inserted Control Rod in C5G7-TD

Figure 4-4. Power Change with Time from PROTEUS-MOC and MPACT for TD4-1

Figure 4-5. Power Change with Time from PROTEUS-MOC and MPACT for TD4-5

Figure 4-6. Power Change with Time from PROTEUS-MOC and MPACT for TD5-1

4.2 TREAT M8CAL Transient Experiment

Previously, the minimum critical core (MinCC) and M8CAL core of TREAT in the steady-state condition were simulated using PROTEUS whose solutions were in very good agreement with Serpent Monte Carlo solutions in terms of eigenvalue and power distribution. [40] This year, an attempt was made to simulate the M8CAL core in the transient condition using the transient capability of PROTEUS updated this year.

First of all, the axial configuration of M8CAL was updated based on the experiment condition since previously the simplified axial structure was used for the steady-state calculation. Next, in the same as previous, the 11-group cross sections generated from Serpent were used based on the 3D M8CAL model. Serpent calculations were performed with different temperatures in order to formulate the cross sections with temperature. The temperature-dependent cross sections were generated in the ISOPAR format which is a group of ISOTXS files with the temperature parameter. In addition, the CMFD mesh was regenerated for the transient simulation as well as the numerical acceleration as temperature and density are updated based on the CMFD mesh.

PROTEUS-MOC was updated to include the heat capacity correlation of fuel-graphite specific for the TREAT experiment based on the adiabatic assumption. As control rods are withdrawn and thus the power is accumulated with time, the accumulated power is translated to temperature via the heat capacity correlation which is a function of temperature.

The transient scenario was set up based on the M8CAL transient experiment 2857 (3.9% reactivity), in which the transient control rods were completely withdrawn at the maximum speed (approximately 0.3 sec) [34]. The core was initially at the room temperature.

The PROTEUS calculation for the 3D M8CAL core was performed using 352,536 elements/plane, L_3T_3 (36 angles/ 4π), 11 energy groups, and 24 axial planes. The transient time step of 0.05 sec was used until 1 sec (i.e., 50 time steps) for the preliminary transient calculation, in which the transient control rods were withdrawn in about 0.3 sec at the beginning.

Figure 4-8 shows the power and energy changes with time and Figure 4-9 illustrates the thermal flux, power, and temperature distributions resulted from PROTEUS-MOC at the beginning and end time steps. Compared to the experiments, the results look reasonable but further refinement and investigation is necessary to make the PROTEUS solutions comparable to the experiments. In addition, the transient fuel conduction module will be implemented as well.

Figure 4-7. 3D Configuration of TREAT M8CAL

Figure 4-8. Power Changes with Time at the Rod Ejection Transient

Figure 4-9. Thermal Flux (top), Power (middle), and Temperature (bottom) Solutions from PROTEUS at the Beginning and End Time Steps

4.3 RCF Core

The Walthausen Reactor Critical Facility (RCF) is an open pool, low-power research nuclear reactor facility being operated by Rensselaer Polytechnic Institute (RPI). Standard reactor configurations include varying pin enumerations with the standard reactor setup ranging anywhere from 329 to 333 pin setups. For cases where larger experiments are inserted into the reactor, higher pin numbers may be used to over 400 pins in total. Figure 4-10 shows the actual experiment.

The preliminary steady-state core calculations using PROTEUS were performed last year [41], showing good agreement in eigenvalue and power distributions between PROTEUS and Serpent. This year, efforts were made to simulate the core with the actual experiment condition.

For the PROTEUS calculation, 3D meshes were generated again using CUBIT based on 333 fuel pins. Figure 4-10 shows the meshes and thermal flux solutions from PROTEUS. Note that the 11-group cross sections generated from Serpent were used for the PROTEUS calculation.

Figure 4-10. 3D Core Configuration of RCF

Table 4-2. Eigenvalue Results for the RCF core with 333 Fuel Pins

Code	MCNP	Serpent	PROTEUS-MOC
Eigenvalue	0.99922 ±0.00003	0.99982 ±0.00003	1.00270

Table 4-2 shows the eigenvalues from MCNP, Serpent, and PROTEUS-MOC, showing good agreement with the measurement which is in a critical condition. Radial and axial power distributions of the RCF core were calculated from PROTEUS for selected locations and were compared with the measurements, as shown in Figure 4-11 and Figure 4-12. For the radial power distributions, powers at the diagonal and vertical directions from the center were calculated and

compared with the measured, indicating very good agreement between them. For the axial power distributions, some power tilt to the bottom of the core was observed from the PROTEUS axial power distribution, while the measured shows a slight tilt rather to the top. The bottom tilt appears to be more reasonable, considering that the bottom reflector is thicker than the top. However, since the tilt would be more affected by the material difference between the bottom and top plenums, further investigation is necessary in terms of actual specification and measurement condition.

Figure 4-11. Predicted and Measured Radial Power Distributions of RCF

Figure 4-12. Predicted and Measured Axial Power Distributions of RCF

4.4 MSR Core

As a verification effort, a MSR core was constructed based on the ThorCon reactor core, which was simulated using PROTEUS. [36] The core is composed of fuel salt with 20% enriched uranium (Na-23, F-19, Be-9, Th-232, U-238, and U-235) moderated by graphite. The fuel salt density is 3 g/cc, the fuel salt volume ratio is about 11%, and the lattice pitch is 38 cm.

The OpenMC Monte Carlo code was used to provide a reference solution, producing 13-group cross sections as well based on a fuel assembly model, a graphite reflector model, and a center assembly model. For PROTEUS-MOC, cross sections were generated for heterogeneous geometry regions, while for PROTEUS-NODAL, those were generated for homogenized regions in terms of a fuel assembly, a graphite reflector, and a center assembly. For the cross sections of PROTEUS-NODAL, the assembly discontinuity factors, which are required for more accurate simulation, were not generated in this study. CUBIT [9] was used to generate meshes for components, which were merged using the in-house mesh toolkit to construct 2D or 3D cores.

Eigenvalue solutions from PROTEUS are listed in Table 4-3, which are in good agreement with the OpenMC solutions within 124 pcm for the 2D core and 204 pcm for the 3D core. Figure 4-13 illustrates a core configuration and a thermal flux distribution of the 2D core. Assembly fluxes between PROTEUS-MOC and OpenMC agree well within 2.3%, as shown in Figure 4-14. Due to a flux tilt that is typically observed in Monte Carlo solutions, differences are not 1/3

rotational symmetric. This study indicates that PROTEUS is able to accurately simulate the MSR core with an odd geometry.

Table 4-3. Eigenvalue Results for the 2D and 3D MSR Benchmark Problems

Cases	Eigenvalue	Δk from OpenMC, pcm
2D Core		
OpenMC	1.01282	-125
PROTEUS-MOC	1.01157	
3D core		
OpenMC	0.99196	207
PROTEUS-NODAL	0.99400

Figure 4-13. 2D Core Model and PROTEUS Thermal Flux Distribution of the MSR Benchmark Problem

Figure 4-14. % Difference of Assembly Fluxes of the 2D MSR Core between PROTEUS and OpenMC

5. Conclusions

The main accomplishments in the FY18 NEAMS neutronics tasks are 1) that the computational performance and the simplified thermal feedback of PROTEUS-MOC were significantly improved, 2) that the transient simulation capability as well as the molten salt reactor (MSR) simulation capabilities were successfully implemented to PROTEUS-NODAL, 3) that the MC²-3 versions with the updated thermal cross section capability and three-dimensional (3D) MOC capability were integrated, and 4) that further verification and validation tests were performed with the updated PROTEUS, demonstrating the good applicability and accuracy of the code.

The computational performance of PROTEUS-MOC was upgraded by implementing the partial-current based CMFD option (compared to the current-based CMFD approach), the conventional transport sweeping option (compared to the Krylov transport iteration approach), and the preconditioner to the steady-state CMFD solution scheme. In addition, the multigroup CMFD option (compared to the within-group CMFD approach) was added to the transient solution scheme. The conventional sweeping option improved double the computation performance than the Krylov iteration option, the use of preconditioner reduced the CMFD overhead by 2 to 7 times, and the use of the multigroup CMFD reduced the computation time by a factor of 5 to 8 than the within-group CMFD when solving transient problems.

This year, the thermal feedback capability was completed for PROTEUS-MOC and has been tested using simple 3D benchmark problems as well as the 3D C5G7 problem, showing reasonable fuel and moderator temperatures and moderator density distributions in the axial direction.

The transient simulation capability was implemented to PROTEUS-NODAL this year as well, and that implemented to PROTEUS-MOC by the NEUP team last year was tested using the 3D C5G7-TD OECD/NEA benchmark problems, demonstrating very good agreement with the MPACT solutions in the power changes with time.

For PROTEUS-NODAL, the MSR simulation capability was implemented. With the MSR capability of PROTEUS-NODAL the delayed neutron precursor drifting can explicitly be modelled and simulated, indicating that eigenvalue decreased with the increased speed of fuel flowing inside the core and that the precursor fluxes with small decay constants increased at the fuel flow inlet with the increased speed of fuel flowing outside the core.

To support the code verification and validation, the cross section library generation procedure was updated using the combination of OpenMC and MC²-3. In the updated procedure, the base cross sections with temperatures were generated from OpenMC based on a pin cell geometry with a representative composition of the reactor core of interest and the corresponding background cross sections are calculated from MC²-3 using its 2D MOC capability. Verification tests using the VERA benchmark problems and the modified C5 problem showed very good agreement in eigenvalue (within 200 pcm) and power distributions (within 2%) with the MCNP solutions.

Preliminary tests for a thermal-spectrum MSR problem indicated good agreement in eigenvalue with the Monte Carlo solutions.

The MC²-3 versions with thermal cross section, 2D/3D MOC, and updated gamma heating capabilities were successfully integrated. Further updates were made using the CMFD approach to improve the performance of the 2D/3D MOC calculation. Since the 3D MOC methodology of MC²-3 is based on that of PROTEUS-MOC, the pseudo cross section approach was added to make the neutron balances between MOC and CMFD match in the axial direction.

Code verification and validation activities continued using the updated capabilities of PROTEUS. As noted above, PROTEUS-MOC demonstrated accurate steady-state solutions for the MSR problem and the RCF core, compared with the OpenMC or Serpent Monte Carlo solutions, and showed very good agreement with the MPACT solutions for the 3D C5G7-TD transient benchmark problems. In addition, a reasonable power behavior with time was observed for the TREAT M8CAL core transient simulation. Further work is ongoing to refine the PROTEUS transient simulation for the M8CAL core transient as well as to simulate other transient experiments of TREAT.

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