FINAL REPORT

Project Title: Continuous Energy, Multi-Dimensional Transport Calculations for Problem Dependent Resonance Self-Shielding

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Project Objective: The overall objective of the work here has been to eliminate the approximations used in current resonance treatments by developing continuous energy multi-dimensional transport calculations for problem dependent self-shielding calculations. The work here builds on the existing resonance treatment capabilities in the ORNL SCALE code system. Specifically, the methods here utilize the existing continuous energy SCALE5 module, CENTRM, and the multi-dimensional discrete ordinates solver, NEWT to develop a new code, CENTRM_NEWT. The work here addresses specific theoretical limitations in existing CENTRM resonance treatment, as well as investigates advanced numerical and parallel computing algorithms for CENTRM and NEWT in order to reduce the computational burden. The result of the work here will be a new computer code capable of performing problem dependent self-shielding analysis for both existing and proposed GENIV fuel designs. The objective of the work was to have an immediate impact on the safety analysis of existing reactors through improvements in the calculation of fuel temperature effects, as well as on the analysis of more sophisticated GENIV/NGNP systems through improvements in the depletion/transmutation of actinides for Advanced Fuel Cycle Initiatives.

Status: This project was completed in 2008. **The no cost extension period 6/30/08 to 12/31/08 was used to complete code documentation for ORNL and to prepare the final reports.** This project was a successful collaboration between Purdue and Oak Ridge National Laboratory as evidenced by two archival journal publications (Nuclear Science and Engineering) and the development of a computer code that is now in use at Oak Ridge National Laboratory. The following report will summarize the work.

Introduction

In the research performed here methods were developed to perform continuous energy self-shielding in multi-dimensional geometry. This work was a significant and original advance in reactor physics and was published in Nuclear Science and Engineering after the second year of the research (see **Appendix A**). A new computer code, GEMINEWTRN (Group and Energy Point-wise Methodology Implemented in NEWT for Resonance Neutronics) was developed at ORNL and a second publication (see **Appendix B**) describing the research performed and methods implemented in GEMINEWTRN to reduce the computational time for practical reactor applications was published this past year. As evidenced by the publication of two significant journal articles and the development of a computer code which is currently in use at ORNL, the objectives of the project were successfully accomplished.

Project Year 1 (07/1/2005 – 06/30/2006)

1. Coupling of CENTRM and NEWT (Purdue)
2. Verification/Benchmark Validation of CENTRM_NEWT(Purdue/ORNL)
3. Implementation of CENTRM_NEWT in SCALE5 (ORNL)
4. Advanced Numerical Methods for CENTRM_NEWT..... (Purdue)

Status: All Year 1 tasks were successfully completed.

Project Year 2 (07/1/2006 – 06/30/2007)

5. Parallel Computing Methods for CENTRM_NEWT (Purdue/ORNL)
6. Implementation/Verification of Tasks 4/5 in CENTRM_NEWT..... (ORNL)
7. Improvements in Submoment Expansion Method..... (Purdue)
8. Extensions of s-wave Scattering Assumption in Source Evaluation (Purdue)

Status: All Year 2 tasks were successfully completed.

Project Year 3 (07/1/2007 – 06/30/2008)

9. Development of Space Dependent Quadratures (Purdue)
10. Implementation/Verification of Tasks 7/8/9 in CENTRM_NEWT/SCALE5..... (ORNL)
11. Investigation of PW Lattice Physics for Time-Dependent Problems(Purdue/ORNL)
12. Preparation of Final Documentation/Report.....(Purdue/ORNL)

Status: All Year 3 tasks were successfully completed.

Appendix A

Publication #1:

“Continuous Energy Multi-Dimensional S_N Transport Problem Dependent Resonance Self-Shielding Calculations,” Z.Zhong, T. Downar, M. Williams, M. DeHart, *Nuclear Science and Engineering*, Vol. 152, No. 4, April, 2006.

Continuous Energy Multi-Dimensional S_N Transport for Problem Dependent Resonance Self-Shielding Calculations

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Abstract – A method is presented to obtain a continuous-energy representation of the neutron spectrum using two-dimensional discrete ordinates calculations with a combination of multigroup (MG) and pointwise (PW) nuclear data. This provides the capability of determining the fine-structure energy distribution of the angular flux and flux moments within the resonance range as well as the smoother spectrum in the high- and thermal-energy ranges. The continuous-energy flux spectra can be utilized as problem-dependent weighting functions within the whole two-dimensional domain to process self-shielded MG cross sections for reactor physics and/or criticality safety analysis, so that the two-dimensional heterogeneous effect in the resonance calculation can be fully considered. This calculation method has been implemented in a new PW transport code called GEMINEWTRN that may be executed as a module in the SCALE computer code system. Example applications using ENDF/B cross-section data are presented to study two-dimensional heterogeneous effect in the resonance calculations.

I. INTRODUCTION

In the past twenty 20 years considerable progress has been made in developing more accurate and efficient methods to solve the multi-dimensional transport problem for nuclear engineering applications. However, much less progress has been made in enhancing resonance-shielding techniques for generating problem-dependent multigroup cross sections for the multi-dimensional transport calculation. Most current lattice physics codes use some variation of the Bondarenko background cross section method with an approximate method to incorporate multi-dimensional effects during resonance self-shielding. For LWR applications, the most popular technique to treat multi-dimensionality is the subgroup method or group band method (ref.1), which works well if the flux spectrum within each band can be parameterized versus a “ background cross section” parameter defined by lattice equivalence theory. Codes using subgroup methods such as CASMO (ref.2), APOLLO2 (ref.3), and HELIOS (ref.4)) have worked well for most LWR applications. However, the fuel lattice has become increasingly heterogeneous for advanced LWR and GEN-IV fuel designs, as well as for applications in the Advanced Fuel Cycle Initiative (AFCI) (ref.5) in which lattice designs contain mixtures of higher actinides (e.g. U/Pu/Np/Am/Cm) that will introduce more resonance interference effects. With the development of advanced nuclear fuel designs and a wider range of fuel pin enrichments, heterogeneities within the lattice are more pronounced than in the past. This is particularly true of several of the new BWR lattices in which there are larger water holes and increased burnable absorber concentrations. Additionally, some of the advanced reactor designs such as the ACR-700 have lattices which are inherently multi-dimensional in design and resonance interference effects from adjacent fuel pins become increasingly important. The error introduced by self-shielding methods in these cases may exceed that due to uncertainties in the basic nuclear data, and may become the limiting factor in the accuracy of final results. The work here reported is to improve the accuracy of the resonance self-shielding calculation by developing continuous energy multi-dimensional transport calculations for problem dependent self-shielding calculations.

CENTRM (ref.6) is one of the resonance self-shielding modules in the SCALE 5 (ref.7) package and solves the discrete ordinates equation in 1-D (cylindrical, slab and spherical) geometry using pointwise (continuous-energy) neutron cross section libraries, which makes it possible to calculate problem-specific continuous-energy spectra. CENTRM is the most rigorous method currently available to compute space-dependent, high-resolution energy spectra within a unit cell of uniform lattices. However, because of its limitation to 1-D geometries, CENTRM can have difficulty in dealing with lattice non-uniformities. A specific objective of the work here was to eliminate this limitation and to develop a continuous energy multi-dimensional transport method for problem dependent self-shielding calculations. A new code was developed within the framework of the SCALE 5 package by utilizing the continuous energy resonance treatment (ref. 8) in the existing module, CENTRM, and the multi-dimensional discrete ordinates solver, NEWT (ref.9) . A new code, GEMINEWTRN (Group and Energy-pointwise Methodology Implemented in NEWT for Resonance Neutronics), was developed based on these codes to perform continuous energy, multi-dimensional resonance self-shielding calculations.

II. RESONANCE SELF-SHIELDING METHOD

Most criticality safety and reactor physics analyses performed today use multigroup (MG) methods, in which the energy dependence of the cross-sections has been discretized by dividing the energy of interest into

a number of broad groups. The exception to this would be some Monte Carlo methods which are capable of sampling directly from continuous energy cross section libraries. Multigroup cross-sections are typically generated by a processing code that reads information such as resonance parameters, secondary neutron distributions, and various other tabulated values from an evaluated nuclear data file (ENDF) and produces pointwise (PW) cross-section values versus energy for various types of reactions. The PW data can be interpolated with a specified interpolation (often linear) to obtain values at all energies within some error tolerance so that the set of PW data and the specified interpolation scheme define cross-sections with a continuous-energy variation. The processing code then averages the PW cross sections over desired energy intervals with a specified weight function to obtain MG data for computation of MG fluxes. The weight function should correspond to the actual flux spectrum to conserve the reaction rates.. However, the true flux spectrum is a function of space as well as energy and is not generally known during the data processing, therefore an approximate weight function must be used to average the group cross sections. The true flux distribution depends on the problem geometry and composition, especially within the resolved resonance range where the flux spectrum is very sensitive to the concentration of resonance nuclides. The fine structure in the flux spectrum has a significant impact on resonance reactions due to self-shielding effects and must be included in the MG weight function. The methods used to incorporate self-shielding effects into the MG weight function will have a considerable impact on the accuracy of MG analyses.

In the continuous energy resonance treatment of CENTRM, the neutron spectra is calculated using deterministic solutions to the Boltzmann transport equation, but doing so in one-dimensional geometry. The continuous energy representation for a specific problem makes it possible to compute highly accurate angular fluxes for applications that require a detailed description of the fine-structure variation in the neutron energy spectrum. A distinguishing feature of a CENTRM calculation is that a combination of multigroup and pointwise solution techniques allows a continuous spectrum to be computed over the full energy range of interest. CENTRM solves the fixed-source (inhomogeneous) form of the transport equation with a user-specified source such that the problem is simply a sequence of linear system slowing-down solutions. In CENTRM, the scattering source in the point-wise range is calculated analytically, without requiring point-to-point scattering matrix as in the multigroup method. A submoment method (ref.10) was introduced in CENTRM to improve the efficiency of the scattering source calculation in the pointwise range.

The two-dimensional discrete ordinates method used in GEMINEWTRN was taken from the ORNL code NEWT, a two-dimensional (2D) discrete ordinates (S_N) transport code based on the Extended Step Characteristic (ESC) approach (ref.11) for spatial discretization on an arbitrary mesh structure. The extended step characteristic approach was developed to obtain a discrete-ordinates solution in complicated geometries for which other methods provide less satisfactory solutions. Using the ESC approach, a more flexible and somewhat arbitrary problem grid may be defined in terms of general polygons; no limit is placed on the number of sides in a given polygon. Side-averaged fluxes for each polygon in the problem domain are computed and are used to calculate a cell-averaged flux. This process is repeated for each cell in the problem domain, and as with the traditional approach iterations are performed until convergence is achieved.

GEMINEWTRN combines the PW solution of CENTRM with the power and flexibility of NEWT's general-geometry 2D solver. Development of the hybrid code has introduced additional issues to be solved - the coupling of 4 boundary conditions in 2D is much more complicated than that of the 2 boundaries in CENTRM. Because boundary conditions affect the number of inner iterations required for convergence, special relationships have been developed to minimize this computational effort. Additionally, the memory requirements of many thousands of pointwise energy regions combined with the memory required for angular fluxes and flux moments for a large number of cells and cell boundaries requires an efficient memory

management strategy. The following sections will describe the methods developed in GEMINEWTRN to address those issues.

III. CONTINUOUS-ENERGY SPECTRA CALCULATION

The continuous energy representation (ref.10) for a specific problem makes it possible to compute highly accurate angular fluxes for applications that require a detailed description of the fine-structure variation in the neutron energy spectrum. In the continuous energy method, the steady-state Boltzmann transport equation is solved directly over the entire energy range that typically varies from ~0 to 20 MeV. GEMINEWTRN employs a combined multigroup (MG) and continuous, point-wise (PW) energy calculation which allows the neutron spectrum to be computed over the full energy range of interest for reactor physics and criticality safety analysis. As shown in Fig.1, the energy range of interest is divided into three intervals called upper MG (UMG), PW, and lower MG (LMG) ranges. The flux in the two MG ranges is computed by conventional MG transport discrete ordinates approximations with a fine-group energy structure. Fine-group fluxes are converted into a pseudo-PW form by dividing by the group lethargy width to obtain the average flux per lethargy and then assigning this flux value to the midpoint lethargy of the group. In this manner, a PW flux spectrum is obtained over the full energy range defined by the UMG and LMG intervals as well as the PW range.

Fig. 1 Definition of energy ranges and type of scattering in GEMINEWTRN

The steady-state neutron transport equation shown in Eq.(1) represents a particle per unit phase-space at an arbitrary point in phase-space.

$$\begin{aligned} \Omega \cdot \nabla \psi(r, u, \Omega) + \Sigma_t(r, u) \psi(r, u, \Omega) \\ = \int_0^\infty \int_0^{4\pi} \Sigma(r, u' \rightarrow u; \mu_0) \psi(r, u', \Omega') d\Omega' du' + Q_{ext}(r, u, \Omega) \end{aligned} \quad (1)$$

where

$\psi(r, u, \Omega)$ = angular flux (per lethargy) at special position $r = (x, y, z)$ and
phase space (u, Ω)

$u = \ln(E_{ref}/E)$ = lethargy at energy E relative to an origin ($u=0$) at E_{ref}

$\Omega = (\mu, \zeta)$ = Neutron direction defined by polar angle cosine μ and
azimuthal angle sine ζ .

$\Sigma_t(r, u)$ = macroscopic total cross section

$\Sigma(r, u' \rightarrow u; \mu_0)$ = double-differential scattering cross section per lethargy.

$\mu_0 = \Omega \cdot \Omega'$ cosine of scatter angle, measured in the laboratory coordinate
System.

$Q_{ext}(r, u, \Omega)$ = external source term.

The left and the right sides of Eqs. (1) are the neutron loss and production rates, respectively, per unit volume-direction-lethargy. In this research, the fission source is assumed to be known (at least approximately) and is contained in the external source term Q_{ext} ; hence a fixed source rather than an eigenvalue calculation is solved since the objective is not to compute the effective multiplication factor but rather to produce the detailed energy spectra for generating MG cross section which can then be utilized in a subsequent eigenvalue calculation.

The angular dependence of the differential macroscopic scattering cross section of some arbitrary nuclide j is represented by a finite Legendre expansion of arbitrary order L :

$$\Sigma^{(j)}(r, u' \rightarrow u, \mu_0) = \sum_{l=0}^L \frac{2l+1}{2} \Sigma_l^{(j)}(r, u' \rightarrow u) P_l(\mu_0) \quad (2)$$

where

$P_l(\mu_0)$ = Legendre polynomial evaluated at the laboratory scattering cosine

$\Sigma_l^{(j)}(r, u' \rightarrow u)$ = l -th cross-section moments of nuclide j , which can be defined by the
expression

$$= \int_{-1}^1 \Sigma^{(j)}(r, u' \rightarrow u, \mu_0) P_l(\mu_0) d\mu_0 \quad (3)$$

After substitution of the Legendre expansions for the scattering data of each nuclide composing the macroscopic cross section and after application of the spherical harmonic addition theorem in the usual manner, the scattering source becomes:

$$S(r, u, \Omega) = \int_0^\infty \int_0^{4\pi} \Sigma^{(j)}(r, u' \rightarrow u, \mu_0) \psi(r, u', \Omega') d\Omega' du'$$

$$= \sum_{l=0}^L \sum_{k=0}^l \frac{2l+1}{2} Y_{lk}(\Omega) S_{lk}(r, u) \quad (4)$$

The transport equation can be reduced to the form that is most often solved by standard multi-dimensional discrete ordinates codes:

$$\begin{aligned} \Omega \cdot \nabla \psi(r, u, \Omega) + \Sigma_t(r, u) \psi(r, u, \Omega) \\ = \sum_{l=0}^L \sum_{k=0}^l \frac{2l+1}{2} Y_{lk}(\Omega) S_{lk}(r, u) + Q_{ext}(r, u, \Omega) \end{aligned} \quad (5)$$

In Eq. (4), $Y_{lk}(\Omega)$ is the real part of the spherical harmonic function evaluated at direction Ω , and $S_{lk}(r, u)$ is the spherical harmonic moment of the scattering source per unit lethargy.

The S_{lk} moments in Eq.(4) correspond to the expansion coefficients in a spherical harmonic expansion of the scatter source, and if only s -wave elastic scattering is considered, it can be expressed in terms of the cross section and flux moments as:

$$\begin{aligned} S_{lk}(r, u) &= \sum_j \int_{u-\varepsilon^{(j)}}^u S_{lk}^{(j)}(r, u' \rightarrow u) du' \\ &= \sum_j \int_{u-\varepsilon^{(j)}}^u \Sigma_l^{(j)}(r, u' \rightarrow u) \psi_{lk}(r, u') du' \end{aligned} \quad (6)$$

where

$$\begin{aligned} \psi_{lk}(r, u') &= \text{spherical harmonic moments of the angular flux} \\ &= \int_0^{4\pi} Y_{lk}(\Omega) \psi(r, \Omega, u') d\Omega \end{aligned} \quad (7)$$

$$\begin{aligned} S_{lk}^{(j)}(r, u' \rightarrow u) &= \text{moments of the differential scatter rate from lethargy } u' \text{ to } u \text{ for} \\ &\quad \text{nuclide } j. \\ &= \Sigma_l^{(j)}(r, u' \rightarrow u) \psi_{lk}(u') \end{aligned} \quad (8)$$

and

$$\varepsilon^{(j)} = \ln \frac{1}{\alpha^{(j)}}, \quad \alpha^{(j)} = \left(\frac{A_j - 1}{A_j + 1} \right)^2, \quad A_j \text{ is the atomic mass of nuclide } j$$

The double-differential scattering kernel of nuclide j (per unit lethargy and solid angle) for s -wave elastic scatter of neutrons from stationary nuclei is equal to

$$\Sigma^{(j)}(u' \rightarrow u; \mu_0) = \frac{E \Sigma^{(j)}(u')}{E' [1 - \alpha^{(j)}]} \delta[\mu_0 - G^{(j)}(E', E)], \quad \text{for } u' \leq u \leq u' + \varepsilon^{(j)}$$

$$= 0 \quad \text{for } u < u' \text{ or } u > u' + \varepsilon^{(j)} \quad (9)$$

The cosine of the scattering angle $G^{(j)}(E', E)$ is uniquely determined by the initial and final energy E' and E . Substituting the double-differential cross-section expression from Eq. (9) into Eq. (3) gives the single differential Legendre moments of the cross section

$$\begin{aligned} \Sigma^{(j)}(u' \rightarrow u) &= \frac{E \Sigma^{(j)}(u') P_l[G^{(j)}]}{E' [1 - \alpha^{(j)}]}, \quad \text{for } u' \leq u \leq u' + \varepsilon^{(j)} \\ &= 0 \quad u < u' \text{ or } u > u' + \varepsilon^{(j)} \end{aligned} \quad (10)$$

With the forgoing expression substituted into Eq. (6), the following is obtained for the lk moment of the for nuclide j at a lethargy mesh point u :

$$\begin{aligned} S_{lk}^{(j)}(u' \rightarrow u) &= \int_{u-\varepsilon^{(j)}}^u \Sigma_l^{(j)}(r, u' \rightarrow u) \psi_{lk}(u') du' \\ &= \int_{u-\varepsilon^{(j)}}^u \frac{E \Sigma^{(j)}(u') P_l[G^{(j)}(E', E)]}{E' [1 - \alpha^{(j)}]} \psi_{lk}(u') du' \end{aligned} \quad (11)$$

$$= E \int_{u-\varepsilon^{(j)}}^u f_{lk}^{(j)}(u', u) du' \quad (12)$$

In Eq. (12) we can see that the integrand function $f_{lk}^{(j)}(u', u)$ is a function of both initial lethargy u' and final lethargy u , due to the factor $G^{(j)}$, this integrand is difficult to calculate because at each new lethargy point, the integrand function $f_{lk}^{(j)}(u', u)$ changes so that it requires that the u' integral be recomputed over all lower lethargy points for every moment. An efficient algorithm, based on submoment expansion method (ref. 10) is used here, so that the integrand function $f_{lk}^{(j)}(u', u)$ can be factored into a product of a function of u multiplied by the sum of a series of function of u' , as follows:

$$\begin{aligned} f_{lk}^{(j)}(u', u) &= h_{lk}^{(j)}(u) \sum_K g_{lk,K}^{(j)}(u') \\ S_{lk}^{(j)}(u' \rightarrow u) &= E h_{lk}^{(j)}(u) \sum_K \int_{u-\varepsilon^{(j)}}^u g_{lk,K}^{(j)}(u') du' \end{aligned} \quad (13)$$

The function of u can be factored out of the integral so that the new integrand can be calculated cumulatively.

IV. TWO-DIMENSIONAL DISCRETE ORDINATES SOLVER

Evaluating Eq. (5) at each energy mesh point n in the PW range gives a system of integro-differential equations that can be solved from low to high lethargy. In this case, the PW transport equation at energy point n is

$$\Omega \cdot \nabla \psi_n(r, \Omega) + \Sigma_{t,n}(r) \psi_n(r, \Omega) = \sum_{l=0}^L \sum_{k=0}^l \frac{2l+1}{2} Y_{lk}(\Omega) S_{lk,n}(r) + Q_n(r, \Omega) \quad (14)$$

where

$$\psi_n(r, \Omega) = \psi(r, u_n, \Omega)$$

$$\Sigma_{t,n}(r) = \Sigma_t(r, u_n)$$

$$S_{lk,n}(r) = S_{lk}(r, u_n)$$

Integrating Eq. (5) over the over the MG intervals, the ordinary MG form of the transport equation can be obtained.

$$\Omega \cdot \nabla \psi_g(r, \Omega) + \Sigma_{t,g}(r) \psi_g(r, \Omega) = \sum_{l=0}^L \sum_{k=0}^l \frac{2l+1}{2} Y_{lk}(\Omega) S_{lk,g}(r) + Q_g(r, \Omega) \quad (15)$$

where

$$\psi_g = \text{MG angular flux}$$

$$\Sigma_{t,g} = \text{MG cross section}$$

$$Q_g = \text{external source}$$

$$S_{lk,g} = \text{scatter source moments}$$

The MG external source and angular flux are given by

$$Q_g(r, \Omega) = \int_g Q(r, u, \Omega) du, \quad \psi_g(r, \Omega) = \int_g \psi(r, u, \Omega) du$$

The MG flux moments $\psi_{lk,g}(r)$ are computed from the following expression Eq. (16),

$$\psi_{lk,g}(r) = \int_0^{4\pi} Y_{lk}(\Omega) \psi_g(r, \Omega) d\Omega \quad (16)$$

The MG scatter source moment in Eq. (15) can be expressed in Eq. (17).

$$S_{lk,g} = \sum_{g'=1}^G \Sigma_{l,g' \rightarrow g} \psi_{lk,g'} \quad (17)$$

Aside from the definition of the cross-section data, the PW transport equation in Eq. (14) is identical in form to the MG transport equation in Eq. (15), and therefore once the scattering source term is determined it can be solved with virtually the same discrete ordinates algorithm as the MG solution. In fact, the same computer routines in GEMINEWTRN calculate both the MG and PW fluxes. However, a major difference between the PW and MG transport equations is that the PW equation describes a neutron balance per unit

lethargy (or energy) at an energy point while the MG flux represents an integral balance over an interval of lethargy (or energy) points.

The two-dimensional discrete ordinates solver used in GEMINEWTRN is taken from the ORNL code NEWT . (**NEW** Transport algorithm), which is a two-dimensional discrete ordinates (S_N) transport code based on the Extended Step Characteristic (ESC) approach (ref.11) for spatial discretization on an arbitrary mesh structure. This discretization scheme provides versatility for deterministic calculations in real-world non-orthogonal problem domains. Discrete-ordinates approaches are derived from the integro-differential form of the Boltzmann transport equation, while angular behavior is treated by considering a number of discrete directions in space. Because of the direct angular treatment of the discrete-ordinates approach, angularly dependent distribution functions can be computed; thus this approach is the preferred method of solution in many specific applications where angular anisotropy is important. However, the traditional discrete ordinates method is often limited in applicability due to the geometric constraints of the orthogonal grid system associated with the finite-difference numerical approximation.

Using the ESC approach, a more flexible and somewhat arbitrary problem grid may be defined in terms of convex polygons; no limit is placed on the number of sides in a given polygon. Side-averaged fluxes for each polygon in the problem domain are computed, and are used to calculate a cell-averaged flux. This process is repeated for each cell in the problem domain, and as with the traditional approach, iteration is performed for convergence.

V. SAMPLE CALCULATIONS

The GEMINEWTRN code was first verified by comparison with results obtained from CENTRM using a single pin cell model, in which the two-dimensional heterogeneous effect for the spectra calculation is trivial. Because a rigorous verification has been performed for CENTRM, CENTRM results could be used as a reference here for purposes of verification of GEMINEWTRN. In order to demonstrate the principal original contribution of this work which is the introduction of multi-dimensionality into the resonance self-shielding calculation, GEMINEWTRN was then applied to strongly heterogeneous advanced BWR and ACR-700 fuel designs.

V.A SINGLE PIN CELL MODEL

An approximately equivalent one-dimensional 3-zone cylindrical model (fuel-clad-water) was built for CENTRM as shown in Figure 2, in which there exists 40 flat source regions. Spectra calculations were performed using both CENTRM and GEMINEWTRN and comparisons were made for the spectrum in the fuel region. In the model used here, the PW range is from 3 eV to 17 keV, and there are a total 34,833 energy points within the PW range. The spectra comparisons were performed within that energy range as shown in Figures 3 and 4.

Fig.2 Single Pin Cell Model for Verification of GEMINEWTRN

Fig.3 Ratio of the flux calculated by CENTRM and GEMINEWTRN from 550 eV to 17 keV

Fig.4 Ratio of the flux calculated by CENTRM and GEMINEWTRN from 3 eV to 550 eV

From Figs. 3 and 4, it is apparent that the spectrum calculated by GEMINEWTRN agrees well with that calculated by CENTRM within the PW range, with the maximum difference about 6%, which is attributable primarily to differences in spatial and angular discretization. These results provide preliminary verification of the PW capability of GEMINEWTRN.

V.B ADVANCED BWR FUEL ASSEMBLY MODEL

CENTRM and GEMINEWTRN calculations were then performed on an advanced BWR lattice that is representative of the lattices proposed for advanced BWR cores. The lattice design used here is axially heterogeneous and includes two large central water holes, which provide increased moderation to the fuel. Figure 5 shows the design for the upper part of the assembly, which includes four gadolinium fuel pins, there exists about 7,300 flat source regions in the model. The PW range is from 1 eV to 25 keV, and there are totally about 36,000 energy points within the PW range. Calculations were also performed for the lower part of the assembly region (not shown), in which the water holes are replaced by fuel pins.

Fig.5 Advanced BWR Fuel Assembly Design

A 44-group NEWT calculation was performed with weighted cross sections prepared first by CENTRM and then by GEMINEWTRN. Since CENTRM is limited to one-dimensional geometry an equivalent 1-D concentric cylindrical model was built for each type of pin in the model. The value of k-effective calculated with NEWT using first CENTRM then GEMINEWTRN cross sections are shown in Table 1. These results show that there is good agreement in k-effective predicted for the bottom assembly; however, for the upper part of the assembly which is partially voided and much more heterogeneous, the difference in the value of k-effective predicted with CENTRM and GEMINEWTRN cross sections is more than 900 pcm.

Table 1 Comparison of k-effective for BWR Fuel Assembly Model

	<u>CENTRM</u> <u>resonance Scheme</u>	<u>GEMINEWTRN</u> <u>resonance Scheme</u>	<u>K_{eff} difference</u> <u>(pcm)</u> <u>(CENTRM –</u> <u>GEMINEWTRN)</u>
<u>Lower Assembly</u>	<u>1.08344</u>	<u>1.08305</u>	<u>40</u>
<u>Upper Assembly</u>	<u>1.20529</u>	<u>1.19608</u>	<u>920</u>

The ratio of the fluxes predicted with CENTRM and with GEMINEWTRN in a central pin in the upper part of the assembly is shown in Figure 6. The CENTRM cross-sections significantly over-predict the resonance self-shielding and lead to a substantial under prediction of the flux and consequently k_{eff} is significantly over-predicted. This result suggests that explicit consideration of the effect of the large internal water holes in the resonance self-shielding calculation for advanced BWR lattice designs is important. Additionally, CENTRM is also limited to a Wigner-Seitz cell approximation, with a cylindrical outer boundary in which moderator volume is conserved, and a white boundary condition is used. This results in a uniform-lattice approximation, resulting in over-shielding of cross sections.

Fig.6 Ratio of the Flux calculated by CENTRM and GEMINEWTRN

V.C ACR-700 FUEL BUNDLE MODEL

An ACR-700 fuel lattice model (Ref. 12) was also selected to study two-dimensional heterogeneous effects. Fig.7 shows the design of the fuel bundle in ACR-700 lattice and the spatial grid used in the NEWT calculation which contains about 10,200 flat source regions in the model. Four fuel rings, each with different kinds of fuel pins, are arranged in the fuel bundle, with coolant (light water) around inside the pressure tube; gas insulation (CO_2) is present between the pressure tube and calandria tube; outside the calandria tube is moderator (heavy water). In this design, the primary parameters of interest are the Doppler Coefficient and coolant void reactivity (CVR), which is defined as the reactivity change by the voiding of light water coolant inside the pressure tube. It can be seen that the inherent multi-dimensionality exists in the design for resonance self-shielding calculations, especially for the case in which the light water coolant inside the pressure tube is fully voided.

Fig.7 ACR-700 Fuel Lattice Design

For the CENTRM resonance calculation, four one-dimensional models were first constructed, with each corresponding to one type of fuel pin. To include resonance interference effects from adjacent fuel pins, an equivalent Monte Carlo calculation was performed to calculate the Dancoff factors, which were then be used in the CENTRM calculation to adjust the boundary conditions. In order to perform the resonance calculation for the moderator (heavy water) and calandria tubes, a second larger one-dimensional CENTRM model was also constructed, corresponding to the entire lattice, in which each fuel ring was homogenized into one mixture. Both 44-group and 238-group weighted cross sections were prepared by CENTRM and GEMINEWTRN using ENDF/B-V library, (approximately 33,000 energy points within the PW range for GEMINEWTRN model) transport calculations were then performed using NEWT. The k-effective calculated with NEWT using GEMINEWTRN and CENTRM then cross sections are shown in Table 2.

Table 2 Comparison of k-effective for ACR-700 Fuel Lattice Models

<u>Energy Group</u>	<u>COOLANT</u>	<u>GEMINEWTRN</u>	<u>Resonance Scheme</u>	
			<u>CENTRM with</u> <u>Dancoff</u> <u>(Difference : </u> <u>CENTRM-</u> <u>GEMINEWTRN)</u>	<u>CENTRM</u> <u>without Dancoff</u> <u>(Difference : </u> <u>CENTRM-</u> <u>GEMINEWTRN)</u>
<u>44</u>	<u>Cooled</u>	<u>1.24390</u>	<u>1.24283</u> <u>(-107 pcm)</u>	<u>1.24408</u> <u>(30 pcm)</u>
	<u>Full Voided</u>	<u>1.24420</u>	<u>1.24339</u> <u>(-81 pcm)</u>	<u>1.28109</u> <u>(3689 pcm)</u>
	<u>CVR</u>	<u>0.194</u>	<u>- 0.362</u>	<u>23.222</u>
<u>238</u>	<u>Cooled</u>	<u>1.24619</u>	<u>1.24553</u> <u>(-66 pcm)</u>	<u>1.24357</u> <u>(-22 pcm)</u>
	<u>Full Voided</u>	<u>1.24883</u>	<u>1.24876</u> <u>(-7 pcm)</u>	<u>1.25773</u> <u>(1143 pcm)</u>
	<u>CVR</u>	<u>1.696</u>	<u>2.077</u>	<u>9.053</u>

The CVR and change in reactivity calculations were computed using:

$$\Delta\rho = \left(\frac{1}{k_{cool}} - \frac{1}{k_{void}} \right) \times 1000mk \quad (18)$$

From the results shown in Table 2, it is first evident that for the case of fully voided coolant, the CENTRM calculation without Dancoff factor is in error for both 44-group and 238-group calculations. This shows that two-dimensional heterogeneity has a strong effect on the resonance self-shielding calculation. An independent Monte Carlo calculation has been performed on this model to calculate the Dancoff factor for CENTRM, so that the results of CENTRM calculation with Dancoff factor has been well adjusted and the correct k-effective can be achieved in the subsequent NEWT calculation. The same Monte Carlo calculation provided a reference and the results in Table 2 show that the value of k-effectives using GEMINEWTRN cross section are consistent with those of CENTRM cross sections with Dancoff factor.

A comparison of the flux predicted by GEMINEWTRN and by CENTRM with/without Dancoff factors in the fuel of the peripheral fuel ring for the fully voided coolant case is shown in Fig. 8. First it is apparent that the flux calculated by CENTRM without Dancoff factors is inaccurate, which also indicates that CENTRM can not deal with this problem without Dancoff factor. In the calculation with Dancoff factor included, there are apparent spectra differences between GEMINEWTRN and CENTRM, even though the values of k-effective are very close. This can be attributed to the fact that CENTRM solves a one-dimensional infinite medium problem and although DANCOFF factors are used to treat the contribution of adjacent pins and moderator regions, the two-dimensional heterogeneous effect on the spectra calculation still can not be accurately modeled. Conversely GEMINEWTRN performs the PW spectra calculation within the entire two-dimensional geometry domain so that it can predict accurately the spectra in any region.

Fig. 8 Comparison of the fuel averaged flux calculated by GEMINEWTRN and CENTRM

In order to further validate the GEMINEWTRN code, a direct comparison was performed for the ACR lattice model with NEWT/GEMINEWTRN and MCNP using the ENDF/B-VI library (for GEMINEWTRN model, the total number of energy points within the PW range is about 56,000). The k_{eff} calculated by NEWT with the cross sections calculated using GEMINEWTRN resonance scheme is compared to the k_{eff} calculated by MCNP in Table 3.

Table 3 Comparison of $k_{\text{effective}}$ between NEWT/GEMINEWTRN and MCNP

<u>Code/Resonance</u>	<u>Cooled</u>	<u>Void</u>	<u>CVR</u>
<u>NEWT/GEMINEWTRN</u>	<u>1.24781</u>	<u>1.25162</u>	<u>2.440</u>
<u>MCNP</u>	<u>1.24892</u>	<u>1.25229</u>	<u>2.155</u>

From Table 3, it is apparent that the k_{eff} calculated by NEWT/GEMINEWTRN and MCNP agree well for both the cooled and for the void cases. Pin-power comparison has also been performed between NEWT/GEMINEWTRN and MCNP for the void case and the result is shown in Fig.9. (Because the lattice is azimuthally symmetric and there exist 4 fuel rings in the lattice model, only the fuel ring-homogeneous pin power is compared to reduce the computation time of MCNP).

Fig.9 Comparison of Pin-Power Calculated by NEWT and MCNP

From the result shown in Fig.9, it can be seen that NEWT/GEMINEWTRN slightly over-predicts the pin power in the central fuel regions and under-predicts the pin power in the peripheral regions. The maximum pin power difference is about 1.3 % which is in the central pin. It should be noted that the calculation here was performed on a PC with an AMD 1.8GHZ CPU, and that the MCNP calculation for the ACR model required about 24 hours, whereas the NEWT/GEMINEWTRN calculation required about 6 hours, with 2 hours spent on GEMINEWTRN and 4 hours spent on NEWT. It should be noted that multiprocessing has already been implemented into GEMINEWTRN and NEWT, and linear speedups have been achieved on four processors of both a LINUX Cluster and an DEC ALPHA machine [ref 14]

VI. SUMMARY AND CONCLUSIONS

A new resonance self-shielding code was developed utilizing the continuous energy resonance treatment in the existing SCALE5 module CENTRM, and the multi-dimensional discrete ordinates solver NEWT. This new code, GEMINEWTRN, was developed to perform continuous energy, multi-dimensional resonance self-shielding calculations. Preliminary applications to advanced BWR and ACR fuel lattices indicate the problem-specific multi-dimensional calculation has a significant impact on the prediction of the lattice spectrum. The results reported in this paper show that it is possible to eliminate approximations used in current resonance treatments by developing continuous energy multi-dimensional transport methods for problem dependent self-shielding calculations.

GEMINEWTRN is one of the first in a new generation of resonance processing codes that will be developed without the computational limitations placed on earlier methods that utilized equivalence theory plus the narrow resonance approximation as in subgroup method, or that utilized one-dimensional continuous energy resonance methods. Freed from the burdens of limited computer resources, the lattices physics solution can be based on more fundamental techniques that will have a significant impact on the accuracy of the entire analysis sequence. The GEMINEWTRN code is useful for providing reference benchmark calculations to test more approximate resonance shielding methods currently used in lattice physics codes and can also be used to

examine difficult problems that have not been previously analyzed. Finally, because of the considerable improvements in computer resources and the anticipated continued developments in computer memory and speed combined with parallel computation technique, it is likely that the GEMINEWTRN approach will be practical in the near future as a production tool to process problem-dependent, MG cross sections within a comprehensive code package such as SCALE for reactor physics and criticality safety analysis.

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Appendix B:

Publication #2:

“Implementation of Two-Level Coarse-Mesh Finite Difference Acceleration in an Arbitrary Geometry Two-Dimensional Discrete-Ordinates Transport Method,” Z. Zhong, T. Downar, Y. Xu, Mark D. DeHart and Kevin T. Clarno *Nuclear Science and Engineering*, 158, 289–298 (2008).

Implementation of Two-Level Coarse-Mesh Finite-Difference Acceleration in an Arbitrary Geometry Two-Dimensional Discrete-Ordinates Transport Method

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Abstract – The coarse-mesh finite-difference (CMFD) formulation is applied as an efficient means of acceleration of the heterogeneous whole core transport calculation. The CMFD formulation enables dynamic homogenization of the cells during the iterative solution process such that the heterogeneous transport solution can be preserved. Dynamic group condensation is also possible with a two-level CMFD formulation involving alternate multigroup and two-group calculations. The two-dimensional discrete-ordinates (S_N) method is used as the kernel to generate the heterogeneous solution; the CMFD solution provides the S_N kernel with much faster convergence of fission and scattering source distributions. In this paper, the two-level CMFD acceleration has been tested using the VENUS-2 two-dimensional whole core model; it is shown that the number of the S_N transport sweeps can be reduced by a factor of about 10 while exactly reproducing the original transport solution. The second level of CMFD acceleration is also significant in reducing the computation time. The application of the CMFD formulation in arbitrary geometry demonstrates that CMFD also works well for irregular geometries.

1. INTRODUCTION

One of the fundamental approximations applied in modern reactor physics calculations is homogenization theory, which states that an equivalent homogenized problem can be constructed for a heterogeneous problem by introducing additional degrees of freedom. Smith proposed the most popular form of homogenization theory used today, and “discontinuity factors” (ref. 1) are routinely applied in light-water reactor (LWR) analysis. If discontinuity factors are calculated from a whole core heterogeneous problem, the homogenized problem will indeed have the same result as the original heterogeneous problem in terms of averaged reaction rates.

The concept of discontinuity factors, which were introduced for homogenization, was later extended to the coarse-mesh finite-difference (CMFD) formulation, in which an equivalent coarse -mesh problem is constructed to reproduce a fine-mesh or higher-order problem. However, in this case the discontinuity factor is determined dynamically for each coarse-mesh surface by employing a nonlinear iteration technique (ref. 2). In most CMFD applications, the discontinuity factor is replaced with a coupling correction factor or corrective nodal coupling coefficient.

The use of the CMFD method to accelerate a higher-order heterogeneous problem in reactor physics is a variation of the well-established multigrid methods (ref. 3), which have been used successfully for many years to accelerate generalized boundary value problems in computational physics. The essential idea is to use a coarse-grid solution to remove the low-frequency (long-range) components of the error which initially slows convergence of iterative methods on a fixed grid. The multigrid method is one of the most efficient general iterative methods known today (ref. 4).

The CMFD formulation has been particularly effective in recent years as a means to accelerate computationally expensive heterogeneous transport calculations, that is, CASMO-4E (ref. 5) and DeCART (ref. 6). CMFD utilizes a simplified representation of a complex problem (e.g., for a typical LWR problem a homogenized square pin-cell region is selected as the base coarse mesh to represent multiple intracell flat source regions representing fuel, clad, and coolant/moderator). The CMFD approach then utilizes coupling correction factors for each homogenized cell to dynamically homogenize the constituent cells during the iterative solution process such that the heterogeneous transport solution can be preserved. By extending the equivalence theory concept to energy and angle, it is possible to apply a consistent lower-order formulation in the form of a pin-cell homogenized, diffusion-like, finite-difference scheme. This simplified lower-order formulation is much less expensive to solve, and its solution can be used to accelerate the original higher-order solution just as the CMFD formulation does in conventional nodal methods.

However, in codes such as CASMO-4E, only one-level CMFD acceleration is adopted, in which the computation time spent on the multigroup finite-difference calculation remains nonnegligible, especially for large models. In CASMO-4E the coarse-mesh size is limited to square pin cells for Boiling Water Reactor (BWR) cores which contain different types of fuel assemblies (e.g., 8×8 , 9×9 , and 10×10 fuel lattices with water crosses, etc.); the surface current coupling schemes become much more complicated. For some fuel lattice advanced designs, that is, ACR CANFLEX fuel bundle (ref. 7), in which the pin pitch is not regular repeating geometry, it is even more difficult to apply CMFD.

In this work, dynamic group collapse is implemented within a two-level CMFD formulation in which alternating multigroup and two-group calculations are performed. The higher-order heterogeneous solution is

the two-dimensional discrete-ordinate method with the extended step characteristic (ESC) discretization of the NEWT transport code (ref. 8). By alternating between heterogeneous and coarse-mesh homogenized cells, the CMFD solution provides the transport solution kernel of NEWT with much faster convergence of the fission and scattering source distributions. To deal with the arbitrary geometry problem, ACR CANFLEX fuel lattice or BWR fuel assemblies in which the pin pitch is not rectangular, a flexible coarse-mesh structure is adapted using the current-based grid generation scheme of NEWT; thus, a rectangular coarse mesh can be still developed that is not limited by the pin pitch.

2. MULTIGROUP CMFD FORMULATION WITHIN THE MULTIGROUP ESC KERNEL

In multigroup NEWT transport calculations for heterogeneous configurations involving fuel/clad/moderator regions or cells, the computational mesh must be fine enough to capture the spatial variation of the angular flux within the cell. Thus such a cell will involve several (tens) of fine mesh cells and the pin cell itself can be regarded as *coarse* relative to the intracell discretization, as illustrated in Fig. 1. In this regard, the multi-component pin cell can be taken as the base coarse mesh in a CMFD calculation for ESC acceleration, differing substantially in size from the assembly-sized coarse meshes used in nodal diffusion calculations. In order to formulate a CMFD problem under this circumstance, one needs homogenized cell group constants (including diffusion coefficients) and cell- coupling coefficients that relate the cell interface current with adjacent cell-averaged fluxes. These CMFD parameters can be determined from a partially converged ESC solution that yields regional scalar fluxes as well as net interface average currents. The multigroup CMFD parameters can be further condensed to a two-group system which can be solved with even lower computational cost to further accelerate the fission source distribution and the eigenvalue of the problem.

Figure 1. Flat Source Regions within Heterogeneous Cells and Homogenized Cells.

Cell-averaged fluxes resulting from the partially converged CMFD solution can then be used to update the fission and scattering source distributions for the subsequent ESC calculation. In the reconstruction of the regional source, the spatial shape of the scalar flux within a cell determined in the previous ESC calculation is used. Only the amplitude of the scalar flux is adjusted according to the CMFD-determined cell average flux.

Similarly, the net current information obtained at the problem boundary by the CMFD solution is used to update the boundary incoming angular fluxes for the ESC calculation. The shape of the incoming angular flux determined from the outgoing current and the boundary condition in the previous ESC calculation is retained in the update of the boundary incoming current. The alternating execution of the homogeneous CMFD calculation and the heterogeneous ESC calculation continues until convergence is reached.

The remainder of this section provides specific details of the cell-based multigroup CMFD formulation, beginning with a brief description of the multigroup ESC kernel, which is the underlying higher-order solution for the NEWT transport calculation.

2.1. Multigroup ESC Kernel

A two-dimensional within-group discrete-ordinates solver with an ESC discretization scheme is implemented in the NEWT code. In each ESC update, an energy-group sweep is performed at the outermost level. For the given fission and scattering sources in each region and the incoming angular fluxes at the problem boundary, each within-group spatial transport problem during the sweep is solved by the ESC approach. The solution of the within-group ESC problem consists of determination of the scalar flux within each region, the surface angular flux at each cell surface, and the outgoing angular fluxes at the problem boundary. The scalar flux is used to update the scattering source of the subsequent group, while the fission source is updated only after the completion of the group sweep. The typical intracell regions defined in NEWT are as shown in Figure 1, which shows a nine-unit array of pin cells with 4 by 4 background grid with 2 cylinders (approximated by polygons) inlaid, such that in each pin cell there are 40 flat source regions. The solution accuracy can be enhanced by refining the intracell regions.

2.2. Equivalence by CMFD Formulation

If a converged multigroup ESC solution is available for a heterogeneous configuration, then according to homogenization theory it is possible to represent the original problem with a finite-difference formulation employing homogenized and condensed group constants, which can then be solved to generate the same solution in terms of spatial averages. The CMFD formulation imposes conservation of surface currents and volumetric reaction rates through consistent homogenization and group collapse.

For a heterogeneous cell such as the ones shown in Fig. 1, the homogenized group constants can be obtained through flux volume weighting to conserve the reaction rates as follows:

$$\bar{\Sigma}_{x,g}^i = \frac{\sum_{k \in i} V^k \Sigma_{x,g}^k \phi_g^k}{\sum_{k \in i} \phi_g^k V^k} = \frac{\sum_{k \in i} V^k \Sigma_{x,g}^k \phi_g^k}{\bar{\phi}_g^i V^i} \quad \text{and} \quad \bar{D}_g^i = \frac{\bar{\phi}_g^i V^i}{3 \sum_{k \in i} V^k \Sigma_{tr,g}^k \phi_g^k}, \quad (1)$$

where indices i , k , and g represent the homogenized cell, subcell region, and group numbers, respectively, and thus $\bar{\phi}_g^i$ is the cell average flux for a homogenized cell. Using these homogenized group constants only in the finite-differenced homogenized problem would not yield the same global average flux distribution as the heterogeneous problem. The equivalent finite-differenced problem can be established only when the interface

current of the transport reference solution is retrieved from the *coarse-mesh* finite-differenced interface current relation as follows:

$$\bar{J}_g^{i,s} = -\tilde{D}_g^{i,s} (\bar{\phi}_g^{i,s} - \bar{\phi}_g^i) - \hat{D}_g^{i,s} (\bar{\phi}_g^{i,s} + \bar{\phi}_g^i), \quad (2)$$

where index (i,s) indicates the s -th side of the i -th cell and thus is the cell average flux of the s -th side neighbor of cell i , and $\bar{J}_g^{i,s}$ is the surface average net current at the s -th side surface of cell i . Among the two coupling coefficients in Eq. (2), the first coefficient ($\tilde{D}$) is determined from the diffusion coefficients and cell width using a finite-difference relationship, and the second coefficient ($\hat{D}$) is determined from the reference solution in order to force the interface current obtained by Eq. (2) to be the same as the reference value:

$$\begin{aligned} \tilde{D}_g^{i,s} &= \frac{2\bar{D}_g^i \bar{D}_g^{i,s}}{\bar{D}_g^i h^{i,s} + \bar{D}_g^{i,s} h^i} \\ \hat{D}_g^{i,s} &= -\frac{\bar{J}_g^{i,s} + \tilde{D}_g^{i,s} (\bar{\phi}_g^{i,s} - \bar{\phi}_g^i)}{(\bar{\phi}_g^{i,s} + \bar{\phi}_g^i)}. \end{aligned} \quad (3)$$

Using the CMFD current relationship given by Eq. (2) together with the group constants defined in Eq. (1) and the correctional coupling coefficient of Eq. (3), the neutron balance in each cell can be guaranteed and thus the resulting solution of the CMFD problem will provide average fluxes and an eigenvalue which are identical to the higher-order ESC solution. In application, the reference solution used in Eqs. (1) and (3) is replaced by a partially converged heterogeneous ESC solution that is iteratively updated.

Because the equivalent CMFD problem involves significantly fewer unknowns and has a regular matrix structure, it can be solved much more rapidly than the original heterogeneous transport problem by using well-established linear system solution methods. The solution of the CMFD problem for a given set of the CMFD parameters (group constants and coupling coefficients) provides a new cell-average flux distribution, which can be used to update the regional source and boundary incoming angular fluxes for the heterogeneous problem. If the cell-averaged flux and eigenvalue of the CMFD problem are the same as the previous iteration, then the problem has converged.

2.2.1. Formulations of CMFD in NEWT

A two-dimensional CMFD module was implemented in NEWT using the methods discussed in the previous section. The coarse-mesh homogenized group constants can be calculated with Eq. (1); for example, the two surface-coupling coefficients for the right surface of a cell can be formulated as follows:

$$\begin{aligned}\tilde{D}_g^{i+\frac{1}{2}} &= \frac{2\bar{D}_g^{i+1}\bar{D}_g^i}{\bar{D}_g^{i+1}h_x^i + \bar{D}_g^i h_x^{i+1}}, \\ \bar{J}_g^{i+\frac{1}{2}} &= -\tilde{D}_g^{i+\frac{1}{2}}(\bar{\phi}_g^{i+1} - \bar{\phi}_g^i) - \hat{D}_g^{i+\frac{1}{2}}(\bar{\phi}_g^{i+1} + \bar{\phi}_g^i), \text{ and} \\ \hat{D}_g^{i+\frac{1}{2}} &= -\frac{\bar{J}_g^{i+\frac{1}{2}} + \tilde{D}_g^{i+\frac{1}{2}}(\bar{\phi}_g^{i+1} - \bar{\phi}_g^i)}{\bar{\phi}_g^{i+1} + \bar{\phi}_g^i},\end{aligned}\tag{4}$$

where cell i is in the interior part of the model, not at the boundary. Boundary surfaces must be treated in a special manner, which will be discussed later.

From Eq. (4), the first surface-coupling coefficient, $\tilde{D}$, is determined from the diffusion coefficients and the cell width using an ordinary finite-difference relationship, whereas the second surface-coupling coefficient, $\hat{D}$, is determined from the reference solution in order to preserve the net current at the right surface of cell i .

	Cell i,j+1	
Cell i-1,j	Cell i,j	Cell i+1,j
	Cell i,j-1	

Figure 2. Four side of cell (coarse mesh) i, j.

The coarse-mesh finite-difference form of the neutron balance equation for cell i, j (illustrated in Fig. 2) is as follows:

$$\begin{aligned}& \frac{1}{h_x^i} \left(-\tilde{D}_g^{i+\frac{1}{2},j} (\bar{\phi}_g^{i+1,j} - \bar{\phi}_g^{i,j}) - \hat{D}_g^{i+\frac{1}{2},j} (\bar{\phi}_g^{i+1,j} + \bar{\phi}_g^{i,j}) + \tilde{D}_g^{i-\frac{1}{2},j} (\bar{\phi}_g^{i,j} - \bar{\phi}_g^{i-1,j}) + \hat{D}_g^{i-\frac{1}{2},j} (\bar{\phi}_g^{i,j} + \bar{\phi}_g^{i-1,j}) \right) \\ & + \frac{1}{h_y^j} \left(-\tilde{D}_g^{i,j+\frac{1}{2}} (\bar{\phi}_g^{i,j+1} - \bar{\phi}_g^{i,j}) - \hat{D}_g^{i,j+\frac{1}{2}} (\bar{\phi}_g^{i,j+1} + \bar{\phi}_g^{i,j}) + \tilde{D}_g^{i,j-\frac{1}{2}} (\bar{\phi}_g^{i,j} - \bar{\phi}_g^{i,j-1}) + \hat{D}_g^{i,j-\frac{1}{2}} (\bar{\phi}_g^{i,j} + \bar{\phi}_g^{i,j-1}) \right) \\ & + \Sigma_{t,g}^{i,j} \bar{\phi}_g^{i,j} = S_g^{i,j},\end{aligned}\tag{5}$$

$$\text{where } S_g^{i,j} = \frac{1}{k_{eff}} \chi_g \sum_{g'=1}^G \nu \Sigma_{f,g'}^{i,j} \bar{\phi}_{g'}^{i,j} + \sum_{g'=1}^G \Sigma_{s,g' \rightarrow g}^{i,j} \bar{\phi}_{g'}^{i,j};\tag{6}$$

Reordering in terms of fluxes gives

$$\begin{aligned}
& \frac{1}{h_y^j} \left(\hat{D}_g^{i,j-\frac{1}{2}} - \tilde{D}_g^{i,j-\frac{1}{2}} \right) \bar{\phi}_g^{i,j-1} + \frac{1}{h_x^i} \left(\hat{D}_g^{i-\frac{1}{2},j} - \tilde{D}_g^{i-\frac{1}{2},j} \right) \bar{\phi}_g^{i-1,j} \\
& + \left(\Sigma_{i,g}^{i,j} + \frac{1}{h_x^i} \left(\tilde{D}_g^{i+\frac{1}{2},j} + \tilde{D}_g^{i-\frac{1}{2},j} + \hat{D}_g^{i-\frac{1}{2},j} - \hat{D}_g^{i+\frac{1}{2},j} \right) + \frac{1}{h_y^j} \left(\tilde{D}_g^{i,j+\frac{1}{2}} + \tilde{D}_g^{i,j-\frac{1}{2}} + \hat{D}_g^{i,j-\frac{1}{2}} - \hat{D}_g^{i,j+\frac{1}{2}} \right) \right) \bar{\phi}_g^{i,j} \\
& - \frac{1}{h_x^i} \left(\hat{D}_g^{i+\frac{1}{2},j} + \tilde{D}_g^{i+\frac{1}{2},j} \right) \bar{\phi}_g^{i+1,j} - \frac{1}{h_y^j} \left(\hat{D}_g^{i,j+\frac{1}{2}} + \tilde{D}_g^{i,j+\frac{1}{2}} \right) \bar{\phi}_g^{i,j+1} = S_g^{i,j};
\end{aligned} \tag{7}$$

From Eq. (7), it is apparent that for the two-dimensional CMFD formulation, the matrix system is in a pentadiagonal form, which can easily be solved using efficient iterative techniques such as preconditioned Krylov methods (ref . 9).

As mentioned earlier, the calculation scheme for surface-coupling coefficients at the boundary is different from that discussed above for interior cells. The concept of a surface scalar flux is introduced at the boundary by employing the relationship between the surface net current and cell- averaged scalar flux. At the boundary, (e.g., at the right boundary of the model), the surface-coupling coefficients are calculated as follows:

$$\begin{aligned}
\bar{J}_g^{i,S} &= -\frac{2\bar{D}_g^i}{h_x^i} (\phi_g^{i,S} - \bar{\phi}_g^i), \\
\bar{J}_g^{i,S} &= \alpha \phi_g^{i,S}
\end{aligned} \tag{8}$$

In Eq. (8), α is the radial albedo value, where $\alpha = 0$ for a reflective boundary condition and $\alpha = 0.5$ for a vacuum boundary condition.

Using Eqs. (8), the relationship between the surface scalar flux and the cell-averaged flux, as well as the relation between the surface net current and the cell-averaged flux, can be determined as follows:

$$\phi_g^{i,S} = \frac{2\bar{D}_g^i}{\alpha h_x^i + 2\bar{D}_g^i} \bar{\phi}_g^i \quad \text{and} \quad \bar{J}_g^{i,S} = \frac{2\alpha \bar{D}_g^i}{\alpha h_x^i + 2\bar{D}_g^i} \bar{\phi}_g^i;$$

To preserve the surface net current at the boundary, the surface-coupling factors are also modified in the current relationship as follows:

$$\bar{J}_g^{i,S} = -\tilde{D}_g^{i,R} \bar{\phi}_g^i - \hat{D}_g^{i,R} \bar{\phi}_g^i, \tag{9}$$

where $\tilde{D}_g^{i,R} = -\frac{2\alpha \bar{D}_g^i}{\alpha h_x^i + 2\bar{D}_g^i}$ and $\hat{D}_g^{i,R} = -\frac{J_g^{i,S} + \tilde{D}_g^{i,R} \bar{\phi}_g^i}{\bar{\phi}_g^i}$;

The surface-coupling coefficients can be calculated in a similar manner for the left, bottom, and top boundaries.

Some cases, that is, a large coarse-mesh size corresponding to the reflector region, with the coupling coefficients defined in Eq. (4), can result in the coefficient matrix of the linear system constructed from Eq. (7) not being positive definite (the diagonal term may be negative) and the numerical error can be substantial. In

this case some adjustments are made to the definition of the coupling coefficients to ensure that the diagonal terms of the coefficient matrix remain positive:

$$\tilde{D}_g^{i+\frac{1}{2}} = \hat{D}_g^{i+\frac{1}{2}} = -\frac{\bar{J}_g^{i+\frac{1}{2}}}{2\bar{\phi}_g^{i+1}} ; \quad (10)$$

2.3 Prolongation

In each ESC calculation, the regional source distribution and the incoming angular fluxes at the problem boundary are specified. Since only the cell-averaged values of the scalar flux and the surface-averaged net currents are available from the CMFD problem, *prolongation* operations are necessary to map the lower-dimensional space vector to the higher-dimensional space vector. This can be performed by using the spatial and angular *shapes* that were determined in the previous ESC calculation. Specifically, the regional scalar flux and the boundary outgoing angular fluxes are updated using Eqs. (11) and (12):

$$\phi_g^{k,l+\frac{1}{2}} = \frac{\phi_g^{k,l}}{\bar{\phi}_g^{i,l}} \bar{\phi}_g^{i,l+\frac{1}{2}} , \quad (11)$$

where $\phi_g^{k,l}$ is the scalar flux of group g and flat source region k (belonging to coarse-mesh cell i) after the l -th transport sweep; $\bar{\phi}_g^{i,l}$ is the averaged scalar flux of group g and cell i after the l -th transport sweep, which is determined using spatial homogenization of the heterogeneous solution;

$\bar{\phi}_g^{i,l+\frac{1}{2}}$ is the averaged scalar flux of group g and cell i after the CMFD calculation following the l -th transport sweep; $\phi_g^{k,l+\frac{1}{2}}$ is the scalar flux of group g and flat source region k (belonging to coarse mesh cell i) after the CMFD update following the l -th transport sweep.

$$\varphi_{g,m}^{p,l+\frac{1}{2}} = \frac{\varphi_{g,m}^{p,l}}{\bar{J}_g^{i,S,l}} \bar{J}_g^{i,S,l+\frac{1}{2}} = -\frac{\varphi_{g,m}^{p,l}}{\bar{J}_g^{i,S,l}} (\tilde{D}_g^l + \hat{D}_g^l) \bar{\phi}_g^{i,l+\frac{1}{2}} , \quad (12)$$

where $\varphi_{g,m}^{p,l}$ is the angular flux of group g and angle m at a point p on a boundary surface s of a boundary cell i after the l -th ESC transport calculation.

The incoming angular flux is then determined from the outgoing angular flux of Eq. (12) and the boundary condition. After each CMFD calculation that follows the ESC transport sweeps, the scalar flux of each flat source region can be updated; thus, both the fission source and the scattering source can be updated.

3. TWO-GROUP CMFD FORMULATIONS WITHIN THE MULTIGROUP CMFD

The multigroup CMFD problem formulated by using the CMFD parameters defined in Eqs. (1) and (3) and the interface current relation of Eq. (2) can be solved by the fission-source- iteration method, which involves the group sweep and within-group inner iterations. However, a pin-cell-based implementation of CMFD is in fact a fine-mesh problem (coarse relative to the base transport model).

Although the coarse-mesh geometry in the CMFD acceleration of NEWT is not limited to pin cell, it has been determined that as the coarse-mesh cell increases significantly beyond the size of a typical pin cell, the system can become unstable. Hence, the repeated multigroup CMFD solution by fission-source iteration still represents a substantial computational load, especially for large models. In order to further reduce the computational burden, an equivalent two-group CMFD formulation can be employed by extending the concept of the spatial CMFD formulation to energy (ref. 10). Another benefit of introducing the two-group CMFD formulation is that existing efficient two-group solvers developed for diffusion problems can be used.

Two-group constants can be obtained through energy condensation of the coarse-mesh multigroup constants (to conserve reaction rates) as follows:

$$\bar{\Sigma}_{x,G}^i = \frac{\sum_{g \in G} \bar{\Sigma}_{x,g}^i \bar{\phi}_g^i}{\sum_{g \in G} \bar{\phi}_g^i} = \frac{\sum_{g \in G} \bar{\Sigma}_{x,g}^i \bar{\phi}_g^i}{\bar{\phi}_G^i} \quad \text{and} \quad \bar{D}_G^i = \frac{\sum_{g \in G} \bar{\phi}_g^i}{\sum_{g \in G} \bar{\phi}_g^i / \bar{D}_g^i} = \frac{\bar{\phi}_G^i}{\sum_{g \in G} \bar{\phi}_g^i / \bar{D}_g^i}, \quad (13)$$

where indices i , g , and G represent the homogenized cell, multigroup numbers, and two-group numbers, respectively. Thus $\bar{\phi}_g^i$ and $\bar{\phi}_G^i$ are the multigroup and two-group cell-average flux for a homogenized cell. The equivalent two-group finite-differenced problem can be established in the same way as that shown in Eq. (2) and Eq. (3), with the exception of the group index, as follows:

$$\bar{J}_G^{i,s} = -\tilde{D}_G^{i,s} (\bar{\phi}_G^{i,s} - \bar{\phi}_G^i) - \hat{D}_G^{i,s} (\bar{\phi}_G^{i,s} + \bar{\phi}_G^i), \quad (14)$$

$$\begin{aligned} \tilde{D}_G^{i,s} &= \frac{2\bar{D}_G^i \bar{D}_G^{i,s}}{\bar{D}_G^i h^{i,s} + \bar{D}_G^{i,s} h^i}, \quad \text{and} \\ \hat{D}_G^{i,s} &= -\frac{\bar{J}_G^{i,s} + \tilde{D}_G^{i,s} (\bar{\phi}_G^{i,s} - \bar{\phi}_G^i)}{(\bar{\phi}_G^{i,s} + \bar{\phi}_G^i)}. \end{aligned} \quad (15)$$

The major difference is that the surface-averaged net currents $\bar{J}_G^{i,s}$ are calculated from the results of multigroup CMFD iterations instead of the solution of ESC transport sweeps, as shown in Eq. (16):

$$\bar{J}_G^{i,s} = \sum_{g \in G} \left(-\tilde{D}_g^{i,s} (\bar{\phi}_g^{i,s} - \bar{\phi}_g^i) - \hat{D}_g^{i,s} (\bar{\phi}_g^{i,s} + \bar{\phi}_g^i) \right). \quad (16)$$

The two-group coarse-mesh finite-difference formulations are the same as those for the multigroup case, shown in Eqs. (4–10). However, the key advantage of this approach is that the two-group system can be coupled and solved using existing and highly efficient two-group solvers developed for diffusion problems (ref. 11), instead of requiring iterative energy-group sweeps using a one-group solver for the multigroup case.

Once the two-group CMFD iterations converge, the prolongation process can be performed to update the solution of multigroup CMFD calculation, mapping the lower dimensional energy vector to the higher dimensional energy vector, as follows:

$$\bar{\phi}_g^{i,l+\frac{1}{2}} = \frac{\bar{\phi}_g^{i,l+\frac{1}{2}}}{\bar{\phi}_G^{i,l}} \bar{\phi}_G^{i,l+\frac{1}{2}} \text{ in which } g \in G, \quad (17)$$

where $\bar{\phi}_g^{i,l}$ is the multigroup flux of group g and coarse-mesh cell i after the l -th multigroup CMFD iteration; $\bar{\phi}_G^{i,l}$ is the condensed two-group flux of group G and cell i after the l -th multigroup CMFD iteration, which is determined using energy homogenization of the multigroup CMFD solution; $\bar{\phi}_G^{i,l+\frac{1}{2}}$ is the two-group flux of group G and cell i after the two-group CMFD calculation following the l -th multigroup CMFD iteration; and $\bar{\phi}_g^{i,l+\frac{1}{2}}$ is the updated multigroup flux of group g and to coarse-mesh cell i after the two-group CMFD calculation following the l -th multigroup CMFD iteration. The iterative solution scheme that alternates between the two-level homogeneous CMFD calculation and the heterogeneous ESC calculation is illustrated in Fig. 3.

Figure 3. Iterative CMFD and ESC Calculation Scheme.

4. COMPUTATIONAL PERFORMANCE OF THE TWO-LEVEL CMFD

The basic metric of effectiveness of CMFD acceleration is whether the number of outer iterations (transport sweeps) is reduced, assuming the extra computation time spent on the finite-difference diffusion calculation is negligible compared to a transport sweep. However, for large models, that is, multi-assembly calculations, this is not necessarily true and the computation spent on the finite-difference diffusion calculation is not negligible. However, the introduction of a two-level CMFD acceleration can considerably reduce the additional computational time.

Based on the OECD VENUS-2 MOX Benchmark (ref.12), a two-dimensional model was developed to test the performance of the two-level CMFD formulation. The configuration of the core is shown in Fig. 4, and consists of three 15×15 fuel assemblies, each with a 1.26-cm pin pitch, surrounded by baffle and reflector regions. The SCALE 238-group ENDF/B-VI library is used for this problem, and an S_6/P_2 calculation is performed in NEWT.

Figure 4. VENUS-2 2D Core Model.

The base NEWT grid scheme of this model is 45×45 , with each base grid cell 1.26 cm x 1.26 cm in size. Additional grid refinement is present within each fuel pin cell. The base grid was used to define the coarse grid for the CMFD solution, thereby forcing the CMFD mesh to be on the order of a pin cell. To test the performance of two-level CMFD, the two-group CMFD calculation was turned off, such that only multigroup CMFD was used. The unaccelerated case (without CMFD) is also analyzed as a basis and compared to the performance with one-level and two-level CMFD modes. The results are summarized in Table 1; the iteration history of the NEWT calculation for this model is shown in Fig. 5. In the results it is first apparent that for this model the unaccelerated NEWT requires a substantially larger number of outer iterations, primarily due to scattering in large reflector region, which reduces the rate of convergence. However, CMFD acceleration is still very efficient, reducing the total number of transport sweeps by a factor of about 9. It can also be seen from the results shown in Table 1 that the two-level CMFD reduces the time spent within CMFD calculations, although it does not further reduce the total number of transport sweeps. This would be expected, as the two-group CMFD solver is used only to accelerate the solution of the multigroup CMFD solver. The results show that the time required for the two CMFD solvers combined is one-third of that required using multigroup CMFD itself.

Table 1. Summary of the runtime and speedup for VENUS-2 whole core model

	# of transport sweeps	Total Run time (min)	CMFD run time (min)	<i>k-eff</i>	Speedup
Unaccelerated	145	2001.1	0.0	1.00102	
1-level CMFD¹⁾	16	382.2	89.7	1.00106	5.24
2-level CMFD²⁾	16	306.9	28.7	1.00106	6.52

1) Multigroup CMFD only

2) Both multigroup and two-group CMFD enabled.

Fig

ure 5. Iteration history of NEW/CMFD for VENUS-2 whole core model

5. CMFD FOR AN IRREGULAR GEOMETRY PROBLEM

In the CMFD formulation in NEWT, it is possible to take advantage of NEWT's grid generation scheme and flexible geometry capabilities. The NEWT grid-generation paradigm is built around a rectangular base grid, into which a more refined rectangular grid and polygonal elements are inlaid. The existence of a rectangular base grid enables the coarse mesh to be overlaid on an arbitrary geometry and is not limited to the pin cell. The ACR CANFLEX fuel lattice, as shown in Fig. 6 (ref. 7) was selected to test the CMFD performance for irregular geometry problem. It can be seen from Fig. 6 that the pin pitch is very irregular, and thus the coarse mesh is **not** related to the pin pitch. The base NEWT grid scheme of this model is 88×88 ($0.25 \text{ cm} \times 0.25 \text{ cm}$ cells), with each coarse mesh overlaid on 4×4 elements of the base grid (not shown in figure). For this model, a 238-group library is used and an S_8/P_3 calculation is performed with NEWT.

The iteration history of the NEWT calculation for this model is shown in Fig. 7. As indicated, the CMFD acceleration still significantly reduces the number of transport sweeps required for convergence, even though the geometry is irregular. A comparison of computational times is provided in Table 2. The differences in the values of k_{eff} predicted in the NEWT calculations are the same within convergence tolerance (1×10^{-5}).

Figure 6. ACR CANFLEX Fuel Lattice

Figure 7. Convergence history of NEWT calculation for ACR CANFLEX Fuel Lattice.

Table 2. Summary of the run time and speedup for ACR CANFLEX lattice

	# of	Total Run	CMFD run	k_{eff}	Speedup
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	transport sweeps	time (min)	time (min)		
Unaccelerated	39	1040.7	0.0	1.24850	
2-level CMFD	6	173.1	18.3	1.24851	6.52

6. CONCLUSION

The CMFD formulation enables dynamic homogenization of the cells in a heterogeneous transport calculation and provides an efficient means to accelerate convergence of heterogeneous calculations. As shown through the application of two-level CMFD acceleration to 2-D small core model, the heterogeneous transport solution is reproduced exactly, while the number of ESC transport sweeps is reduced significantly. Dynamic-group collapse is also possible with a two-level CMFD formulation involving alternate multigroup and two-group CMFD calculations. The work here has shown the two-group CMFD formulation to be a very efficient means of accelerating multigroup CMFD calculations and can provide a significant further reduction in the computational times for NEWT neutron transport calculations. It has also been shown that CMFD formulation can work well for irregular geometry and the coarse mesh is not limited to pin cell, although in most previous work with CMFD acceleration of transport calculations, square pin-cell-based coarse mesh is most commonly selected.

In principle CMFD formulations can be implemented into any 2-D or 3-D deterministic transport codes, if the codes can provide accurate net surface currents. In recent years, computer resources and parallel computing methods have matured very quickly. CMFD acceleration will play an important role in making it feasible to perform full core 2-D or even 3-D deterministic transport calculations for standard core analysis.

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