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APPLICATION OF THE DISCRETE GENERALIZED MULTIGROUP METHOD TO ULTRA-FINE ENERGY MESH IN INFINITE MEDIUM CALCULATIONS

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ABSTRACT

The Discrete Generalized Multigroup (DGM) method uses discrete Legendre orthogonal polynomials to expand the energy dependence of the multigroup neutron transport equation. This allows a solution on a fine energy mesh to be approximated for a cost comparable to a solution on a coarse energy mesh. The DGM method is applied to an ultra-fine energy mesh (14,767 groups) to avoid using self-shielding methodologies without introducing the cost usually associated with such energy discretization. Results show DGM to converge to the reference ultra-fine solution after a small number of recondensation steps for multiple infinite medium compositions.

Key Words: discrete generalized multigroup, ultra-fine energy mesh, infinite medium

1. INTRODUCTION

The workhorse of modern reactor physics calculations is multigroup neutron transport. Current methods take evaluated nuclear data, process this data to create a very-fine energy grid, and simultaneously simplify the energy structure and increase the spatial complexity. At the lattice physics level, where 2-D representations of fuel assemblies are considered, self-shielding procedures are undertaken to ensure reaction rates are conserved as the energy structure is collapsed.

This approach leads to very accurate modeling of current nuclear systems, but its range of applicability is relatively small. As new designs continue to be developed, novel ideas and sweeping changes to existing technologies are becoming more and more popular. Changes as simple as increasing minor actinide content in fuels through MOX fuel assemblies or high-burnup assemblies, thus leading to significantly overlapping resonances, can cause some of the legacy self-shielding methodologies to break down. Different fuel types, other new reactor materials, spectrum changes, etc., require an increasingly robust macro cross-section generation process.

One possible solution is to use continuous energy cross-section data to bypass the need to use explicit self-shielding methodologies. This can be accomplished via Monte Carlo neutron transport codes, but these are far too expensive for detailed core design at the current time. A similar idea is to stay in the multigroup framework but use an ultra-fine energy mesh to closely replicate the continuous energy data [1] [2] [3]. As with Monte Carlo, this has been shown to be a viable option but is simply too expensive for detailed design applications.

The subject matter of this paper suggests a methodology that can provide the benefits of an ultra-fine energy mesh at a much lesser cost. The discrete generalized multigroup method allows a fine energy flux to be closely approximated for a cost comparable to a problem on a coarser energy grid. To evaluate the feasibility of this approach without excessive complexity, infinite homogeneous media are considered. This allows for energy dependence to be studied without coupling with spatial effects.

2. DISCRETE GENERALIZED MULTIGROUP (DGM) METHOD

2.1. Initial Development

In [4] and [5], a generalized multigroup procedure was introduced. Rather than assuming no energy dependence inside an energy group, this procedure assumed that energy dependence could be expanded in a set of orthogonal basis functions. Using Legendre polynomials as the basis, the zeroth order leads to the classical multigroup equations; higher modes provide additional information about the energy spectrum in each energy group.

This method struggles in the existing multigroup framework, where cross-sections are represented as step functions, as very high order polynomials are needed to approximate discontinuities. Furthermore, such high order polynomials introduce oscillations, causing some cross-section representations to fall below zero, without a remedy easily available. To combat these issues, a different set of basis functions, discrete Legendre orthogonal polynomials (DLOPs), were used [6]. These polynomials are described in the next section. With the DLOPs, the method was rebranded as the discrete generalized multigroup (DGM) method.

Once the DGM procedure was successfully demonstrated, a recondensation procedure was introduced [7]. This uses the fine-group solution obtained with the original DGM procedure as the guessed spectrum needed at the start of the procedure. Iteratively applied, the DGM solution will converge to the exact fine-group solution under certain conditions. For clarity, the DGM procedure will be derived for application in this paper in Section 2.3.

2.2. Discrete Legendre Orthogonal Polynomials (DLOPs)

Discrete Legendre orthogonal polynomials [8] are a set of basis functions in which the independent variable can only assume a finite number of values on a given interval. DLOPs are given by $P_m(K,N)$, where the discrete interval is given as $K = 0, 1, 2, \ldots, N$ and the order $m = 0, 1, 2, \ldots, N$ is the degree of the polynomial. The orthogonality relation is given as:

$$\sum_{K=0}^{N} P_m(K,N) P_l(K,N) = \frac{\delta_{ml}}{a_m} \tag{1}$$

where δ_{ml} is the Kronecker delta functional and the normalization factor a_m is given as:

$$a_m = (2m+1)\frac{N^{(m)}}{(N+m+1)^{(m+1)}} \tag{2}$$

where $N^{(m)}$ is the m^{th} fading factorial of N and is defined as:

$$N^{(m)} = \begin{cases} N(N-1)(N-2)\dots(N-m-1), & m > 0 \\ 1, & m = 0 \end{cases} \tag{3}$$

The normalization relation is:

$$P_m(0, N) = 1, \qquad \forall m \tag{4}$$

The first two DLOPs are:

$$\begin{aligned} P_0(K, N) &= 1 \\ P_1(K, N) &= (N - 2K)/N \end{aligned} \tag{5}$$

With these, a recurrence relation can be used to generate higher order DLOPs:

$$(m+1)(N-m)P_{m+1}(K, N) = (2m+1)(N-2K)P_m(K, N) - m(N+m+1)P_{m-1}(K, N) \tag{6}$$

A particularly important property of DLOPs can be derived using Equations 1 and 5:

$$\sum_{K=0}^{N} P_l(K, N) = \frac{\delta_{0l}}{a_0} = \begin{cases} N+1, & l = 0 \\ 0 & l \neq 0 \end{cases} \tag{7}$$

2.3. DGM in Infinite Medium

For a full derivation of the DGM method and recondensation procedure for the general transport equation, see [6] and [7]. For the case of infinite medium, the subject of this paper, the DGM equations are derived here.

The transport equation in infinite medium with the k-eigenvalue is given as:

$$\sigma_t(E)\phi(E) = \int_0^\infty \mathrm{d}E'\, \sigma_s(E' \to E)\phi(E') + \frac{\chi(E)}{k} \int_0^\infty \mathrm{d}E'\, \nu\sigma_f(E')\phi(E') \tag{8}$$

First, the energy structure is broken into G coarse groups. Inside each energy group, parameters are still allowed to vary continuously with energy; thus, this is simply a change of notation.

$$\sigma_t(E_g)\phi(E_g) = \sum_{g'=1}^{G} \int_{E_{g'}} \sigma_s(E_{g'} \to E_g)\phi(E_{g'}) + \frac{\chi(E_g)}{k} \sum_{g'=1}^{G} \nu\sigma_f(E_{g'})\phi(E_{g'}) \tag{9}$$

Inside each coarse group, the multigroup procedure is applied. To be consistent with DLOP notation, $K = 0, 1, 2, \ldots, N-1$ and $L = 0, 1, 2, \ldots M-1$ will be used to represent the N and M fine groups inside coarse group g and g', respectively. This yields the standard multigroup equations for the fine energy structure.

$$\sigma_t(K)\phi(K) = \sum_{g'=1}^{G} \sum_{L=0}^{M-1} \sigma_s(L \to K)\phi(L) + \frac{\chi(K)}{k} \sum_{g'=1}^{G} \sum_{L=0}^{M-1} \nu\sigma_f(L)\phi(L) \tag{10}$$

Next, the energy dependence inside each coarse group is expanded using DLOPs.

$$\begin{aligned} \phi(K) &= \sum_{i=0}^{N-1} a_i P_i(K, N-1)\phi_i \\ \phi_i &= \sum_{i=0}^{N-1} P_i(K, N-1)\phi(K) \end{aligned} \tag{11}$$

At this point, many of the details are left out of this derivation but are presented in full in [6]. To summarize, Equation 11 is inserted into Equation 10 and multiplied/summed by $\sum_{K=0}^{N-1} P_i(K, N-1)$. Then, the scattering and fission sources are similarly expanded. This leads to the DGM equations:

$$\sigma_{t,0,g}\phi_{i,g} + \delta_{i,g}\phi_{0,g} = \sum_{g'=1}^{G} \sigma_{s,i,g'\to g}\phi_{0,g'} + \frac{\chi_{i,g}}{k} \sum_{g'=1}^{G} \nu\sigma_{f,g'}\phi_{0,g'} \tag{12}$$

where the cross-sections and related moments are given by:

$$
\begin{aligned}
\sigma_{t,0,g} &= \frac{\sum_{K=0}^{N-1} \sigma_t(K)\phi(K)}{\phi_{0,g}} \\
\delta_g(K) &= \sigma_t(K) - \sigma_{t,0,g} \\
\delta_{i,g} &= \frac{\sum_{K=0}^{N-1} P_i(K, N-1)\delta_g(K)\phi(K)}{\phi_{0,g}} \\
\sigma_{s,i,g'\to g} &= \frac{\sum_{K=0}^{N-1} P_i(K, N-1) \sum_{L=0}^{M-1} \sigma_s(L \to K)\phi(L)}{\phi_{0,g'}} \\
\chi_{i,g} &= \sum_{K=0}^{N-1} P_i(K, N-1)\chi(K) \\
\nu\sigma_{f,g} &= \frac{\sum_{L=0}^{M-1} \nu\sigma_f(L)\phi(L)}{\phi_{0,g'}}
\end{aligned} \tag{13}
$$

Note that the total cross-section is expanded using its zeroth order moment and a correction term rather than the straightforward expansion, as this improves stability. Also note that χ is considered to be a combination of the fission spectra for each fissionable isotope present, weighted by the fission rate.

The DGM equations can be written in operator notation as:

$$
\begin{aligned}
\mathbb{T}_0\phi_0 &= \mathbb{S}_0\phi_0 + \frac{1}{k}\mathbb{F}_0\phi_0 \\
\mathbb{T}_i\phi_i &= \mathbb{S}_i\phi_0 + \frac{1}{k}\mathbb{F}_i\phi_0 \qquad i > 0
\end{aligned} \tag{14}
$$

Thus, the zeroth order is an eigenproblem, equivalent to a coarse group multigroup equation. The higher orders, however, are decoupled from each other and depend only on the zeroth order solution. Furthermore, they are fixed source equations, as the RHS depends only on the zeroth order. Thus, in this formulation, the eigenvalue is determined solely from the coarse group problem, but a more detailed description of the energy dependence is gained by solving the higher order equations. The cost of solving these equations is comparable to the cost of the coarse group eigenproblem, as fixed source calculations are very quick.

To obtain the fine group flux, the moments can be unfolded with Equation 11. This fine group flux will yield the exact fine group flux if the spectrum used to collapse into moments initially was taken to be the exact solution. However, if any other spectrum is used, the accuracy of the fine group flux is limited by this guessed spectrum. As the solution is not known *a priori*, another option is to use a recondensation procedure [7].

The unfolded fine group following a DGM calculation can be used as the guessed spectrum in a subsequent DGM calculation. This calculation will yield a better estimate of the actual spectrum.

This process can be applied in succession until the solution converges to the exact spectrum or until a desired level of accuracy is achieved.

It was found that this recondensation procedure is not sufficient to assure convergence. When applied to a group structure with hundreds to thousands of energy points, flux updates were needed at the end of each DGM calculation. These updates eliminate negative fluxes that may have arisen from the expansions and avoid instabilities arising from widely varying resonance cross sections. The flux updates are given by:

$$\phi^{update} = \mathbb{T}^{-1}\left(\mathbb{S}\phi^{DGM} + \frac{1}{k^{DGM}}\mathbb{F}\phi^{DGM}\right) \tag{15}$$

These updates are essentially source iterations. Three updates applied in succession after each DGM step assured convergence for all cases encountered at this time.

3. ULTRA-FINE ENERGY MESH

3.1. Existing Uses

Ultra-fine energy meshes have been used to bypass self-shielding methodologies with a reasonable degree of success in past applications. Westinghouse developed a 6,064-group library for use with the lattice physics code PARAGON [1]. The energy mesh started with the SHEM group structure [9] below 23 eV and constant lethargy intervals in the resonance range. Comparing to reaction rate tallies from MCNP5, the group boundaries were optimized to minimize deviation inside each energy mesh. The resulting cross-section library was used in a 2-D full core PWR calculation, and results agreed with MCNP within 80 pcm [10]. Westinghouse also developed a 30,069 group mesh for comparison and determined that no additional benefit was gained over the optimized 6,064 group structure.

Other ultra-fine energy meshes have been developed for use with the AEGIS and APOLLIO codes. The AEGIS code employs a 32,000-group structure, with the number of groups being determined from sensitivity calculations [3]. For the APOLLO code, CEA developed a 11,276 group structure, using a 525-group thermal block TRESFIN and several regions of equal lethargy intervals for higher energies [2].

In all cases, these ultra-fine group structures are very expensive to use, and have been developed for benchmarking purposes only. As the DGM method is applied to such structures, this could allow their use in more design-based applications.

3.2. Mesh Used For This Study

An ultra-fine energy mesh was developed for this study. The 11,276-group CEA structure was taken as the starting point. However, as this mesh was developed for use with ENDF/B-VI, it was necessary to increase the number of groups for the high end of the resonance range when used with ENDF/B-VII data. Also, as some energy self-shielding effects were still seen, some further

energy refinement was introduced. The resulting structure contains 14,767 groups, as described in Table I.

Table I. 14,767-group energy mesh

Energy Range	Mesh Structure	Number of Groups
$E \leq 5.04348\text{eV}$	TRESFIN	525
$5.04348 < E \leq 51\text{eV}$	$\Delta u = 1/960$	2220
$51 < E \leq 203\text{eV}$	$\Delta u = 1/960$	1326
$203 < E \leq 1434\text{eV}$	$\Delta u = 1/1920$	3754
$1.434 < E \leq 200\text{keV}$	$\Delta u = 1/960$	4740
$0.2 < E \leq 19.64\text{MeV}$	$\Delta u = 1/480$	2202

Infinite medium calculations were performed with this structure and compared to MCNP for various compositions. Group cross-sections were generated with NJOY 99.336 and ENDF/B-VII.0; for comparisons, the point-wise ENDF file used as input to the GROUPR module was used to create an MCNP library with the ACER module.

At 293.6 K, the multigroup calculation with this structure under-predicted the eigenvalue as calculated by continuous-energy Monte Carlo by approximately 200 pcm. At 600 K, this deviation was found to decrease to 150 pcm. This suggests that some self-shielding phenomenon is still influencing the multigroup calculation. It is expected that refinement of the structure and an optimization procedure similar to that done by Westinghouse could reduce this discrepancy and reduce the number of groups. However, the goal of this paper is not to develop an effective ultra-fine energy mesh; rather, it is to show the applicability of DGM to such a mesh.

4. RESULTS

4.1. Description of Problem

The slowing down equation in an infinite homogenous medium was studied. Two compositions were considered, one representing a UO_2 pin-cell and one representing a MOX pin-cell. The pin-cells were assumed to have the geometry from the Mosteller benchmark for the Doppler reactivity coefficient [11], summarized in Table II. This was converted to an infinite medium simply by volume weighting the number densities in each region. Densities were assumed to be 10.1 g/cc for the fuel, 6.55 g/cc for the clad, and 0.85 g/cc for the coolant regardless of composition. Temperature for all isotopes in the problem is taken to be 293.6 K. Uranium was assumed to be enriched to 3.9% for all cases; MOX fuel contained 80% uranium and 20% minor actinides (summarized in Table III); clad was assumed to be natural zirconium; and the coolant was assumed to be non-borated light water. Resulting number densities are given in Table IV.

The exact solution to these cases are taken to be the 14,767-group solutions. For the UO_2 case, the eigenvalue was found to be 1.35035; for the MOX case, 1.09824. Also used as comparisons to reference are the mean relative error (MRE) in flux, given in Equation 16, and two-group total reaction rates, defined in Equation 17.

Table II. Geometry specifications

Measurement	Value (cm)
Pitch	1.26209
Fuel OR	0.39306
Clad OR	0.45802

Table III. Minor actinide concentrations

Isotope	Relative Concentration
Np-237	0.05343
Pu-238	0.02636
Pu-239	0.48408
Pu-240	0.21778
Pu-241	0.10506
Pu-242	0.06222
Am-241	0.03368
Am-243	0.01740

Table IV. Number densities for test problems

Isotope	N_{UO_2}[a/b-cm]	N_{MOX}[a/b-cm]
H-H2O	0.0333426	0.0333426
O-16	0.0303996	0.0303996
Zr-0	0.0047264	0.0047264
U-235	0.0002677	0.0002142
U-238	0.0065964	0.0052771
Np-237	-	0.0000734
Pu-238	-	0.0000362
Pu-239	-	0.0006646
Pu-240	-	0.0002990
Pu-241	-	0.0001442
Pu-242	-	0.0000854
Am-241	-	0.0000462
Am-243	-	0.0000239

$$\bar{\phi} = \frac{\sum_{g=1}^{G}\sum_{K=0}^{N-1}\phi(K)}{\sum_{g=1}^{G}N}$$
$$MRE = \frac{\sum_{g=1}^{G}\sum_{K=0}^{N-1}|\phi(K)-\phi_{reference}(K)|}{\bar{\phi}\sum_{g=1}^{G}N} \quad (16)$$

$$RR_1 = \sum_{g=1}^{G} \sum_{E(K)>0.625\text{eV}} \sigma_t(K)\phi(K)$$
$$RR_2 = \sum_{g=1}^{G} \sum_{E(K)\leq 0.625\text{eV}} \sigma_t(K)\phi(K) \quad (17)$$

For all DGM results presented, the starting spectrum guess was taken to be the narrow resonance approximation flux ($\phi \sim {}^{1}/_{E\cdot\sigma_t(E)}$) in the resonance region, a Maxwellian in the thermal region, and the fission spectrum for the fast region.

4.2. DGM Results

Prior to this study, DGM had not been applied to more than 300 groups. However, as presented in the following results, this study shows that DGM will converge to the true solution when applied to an ultra-fine group structure in infinite medium.

One degree of freedom in implementing the DGM procedure is the mapping from a fine group structure (14,767 groups in this case) to a coarse group structure. Eigenvalue convergence was obtained with as high as 60^{th} order DLOPs. Error in the flux was seen to decrease more quickly with lower expansion orders with a constant number of fine groups in each coarse group.

The rate of convergence was found to be very sensitive to the mapping. Consider two example mappings used with the UO_2 case, summarized in Tables V. Mapping 1 uses a constant expansion order in each coarse group, representing a 14,767- to 493-group mapping. Mapping 2 uses a constant expansion order within each coarse group in a given energy range, but allows the order to change in different energy ranges, leading to a 14,767- to 366-group mapping.

Table V. Example coarse-to-fine group mappings

Energy Range	Fine Groups per Coarse Group	
	Mapping 1	Mapping 2
$E \leq 5.04348\text{eV}$	30	25
$5.04348 < E < 51\text{eV}$	30	25
$51 < E \leq 203\text{eV}$	30	30
$203 < E \leq 1434\text{eV}$	30	50
$1.434 < E \leq 200\text{keV}$	30	50
$0.2 < E \leq 19.64\text{MeV}$	30	50

Despite higher order expansions and thus fewer coarse groups, Mapping 2 is seen to far outperform Mapping 1 after the first iteration, as shown in Tables VI and VII.

Similar results were seen with the MOX case, shown in Tables VIII and IX.

Table VI. Convergence for UO2 case, Mapping 1

DGM Iteration	Eigenvalue Error (pcm)	Flux MRE	RR_1 Relative Error	RR_2 Relative Error
1	279.910	6.5969E-03	3.2147E-03	-1.1031E-02
2	49.492	5.6616E-04	3.6906E-04	-5.9286E-04
3	17.877	1.3616E-04	4.8322E-05	2.2975E-05
4	5.359	4.0390E-05	1.1468E-05	1.6003E-05

Table VII. Convergence for UO2 case, Mapping 2

DGM Iteration	Eigenvalue Error (pcm)	Flux MRE	RR_1 Relative Error	RR_2 Relative Error
1	198.184	5.6379E-03	2.5087E-03	-1.0344E-02
2	-3.342	3.2436E-04	2.0430E-04	-6.6638E-04
3	0.080	1.75801E-05	1.0306E-05	-3.1409E-05
4	0.029	1.0930E-06	5.7751E-07	-1.6392E-06

Table VIII. Convergence comparisons for MOX case, Mapping 1

DGM Iteration	Eigenvalue Error (pcm)	Flux MRE	RR_1 Relative Error	RR_2 Relative Error
1	70.455	5.0077E-03	1.3747E-03	-4.1587E-03
2	18.025	2.3345E-04	8.1386E-05	2.3909E-04
3	5.450	5.4569E-05	1.7576E-05	8.3621E-05
4	1.283	1.2992E-05	4.4187E-06	1.9910E-05

Table IX. Convergence comparisons for MOX case, Mapping 2

DGM Iteration	Eigenvalue Error (pcm)	Flux MRE	RR_1 Relative Error	RR_2 Relative Error
1	139.582	2.1709E-03	2.1143E-04	-1.7948E-04
2	-2.526	1.6147E-05	-9.0651E-07	-4.4138E-05
3	-0.023	4.4438E-07	-1.2296E-07	-3.0517E-07
4	-0.004	3.8579E-08	-1.2539E-08	-7.7328E-08

These results show that the DGM solution converges to the exact solution very quickly. One may deem an eigenvalue error on the order of 5 pcm to be acceptable for some applications; if so, no more than two DGM steps are needed to produce an accurate output flux spectrum.

4.3. Timing Considerations

For the infinite homogeneous medium problem discussed here, power iteration is an extremely efficient eigensolver. This is because, without spatial dependence, only one eigenmode exists, leading to a vanishing dominance ratio. A single step of power iteration leads to full convergence of the eigenvalue.

Thus, the method shown here did not outperform power iteration in terms of time, nor was it expected to. The fixed source calculations corresponding to the higher order DGM moments are not trivially inexpensive in this context; in fact, they are comparable to the eigenproblem. However, when spatial dependence is introduced, the eigenproblems will slow down significantly. A small number of DGM solutions is then expected to outperform power iteration significantly, as the much smaller DGM eigenproblem is much less expensive.

5. CONCLUSIONS AND FUTURE WORK

This study shows the applicability of DGM to arbitrarily large numbers of groups. For both a UO_2 and a MOX system, a coarse-to-fine group mapping was found to allow the DGM solution to converge within 10^{-8} in eigenvalue after only four iterations. Although this does not lead to cost savings in this study, this suggests that extending this work to 1-D and 2-D geometries could successfully lead to close approximations of an ultra-fine group flux without the currently associated expense.

Work is currently underway to apply DGM to a 1-D cylindrical discrete ordinates code. When results are obtained, accuracy and timing comparisons will be made between this DGM procedure and existing self-shielding methodologies. To make these comparisons, though, it may be necessary to optimize the ultra-fine mesh so as not to introduce outside error into the solution.

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