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Eliminating Flux Updates from the Discrete Generalized Multigroup Method

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INTRODUCTION

The discrete generalized multigroup (DGM) method, first presented in [1] and [2], expands the energy dependence of the angular flux in the multigroup transport equation with a discrete basis set. The resulting equations include a smaller eigenproblem for the 0^{th} order flux and higher order fixed-source equations that are very simple to solve. The smaller eigenproblem is equivalent to the transport equation with coarse-group cross sections, condensed with a guessed spectrum. In one spatial dimension with an isotropic scattering source, this is:

$$\mu\frac{d\psi_{ig}}{dx}+\sigma_{t,0g}\psi_{ig}+\delta_{ig}\psi_{0g}=\frac{1}{4\pi}\sum_{g'}\sigma_{s,i,g'\to g}\phi_{g'}+\frac{\chi_{ig}}{4\pi k}\sum_{g'}\nu\sigma_{f,g'}\phi_{g'} \quad (1)$$

where ψ_{ig} is the i^{th} energy moment of the angular flux in the g^{th} coarse group and ϕ_g is the scalar flux in the g^{th} coarse group. The collapsed group constants $\sigma_{t,0g}$, δ_{ig}, $\sigma_{s,i,g'\to g}$, χ_{ig}, and $\nu\sigma_{f,g'}$ are defined in [1] and are a function of the guessed flux. The fine group flux, with fine groups indicated by K, can then be unfolded using the discrete basis P_i and expansion coefficients a_i:

$$\psi(K)=\sum_{i=0}^{N-1}a_iP_i(K,N-1)\psi_{ig}. \quad (2)$$

This procedure can be applied in succession as a fixed point iteration which, under the right conditions, will converge to the same answer as a direct solve of the multigroup transport equation. Alternatively, the procedure can be used to provide more accuracy on the smaller problem with a limited number of iterations. Because the DGM iteration process condenses fine-group nuclear data to coarse-group data at each step, the process is commonly referred to as a re-condensation procedure.

In past work, it was found that flux updates were needed to ensure convergence of the re-condensation procedure for all cases. These flux updates are a simple fine-group transport sweep, holding both the fission and scattering sources fixed.

$$\mu\frac{d\psi^{update}(K)}{dx}+\sigma_t\psi^{update}(K)=\frac{1}{4\pi}\sum_{L}\sigma_s(L\to K)\phi(L)+\frac{\chi(K)}{4\pi k}\sum_{L}\nu\sigma_f(L)\phi(L) \quad (3)$$

For a small number of groups, a single flux update was shown to be successful, but with large numbers of groups (ranging from the 361-group SHEM library [3][4] through ultra-fine group libraries with as many as 20,000 groups), three to four flux updates applied in succession at each DGM iteration were needed.

The flux updates can be quite computationally expensive, especially for a large number of groups, consuming as much as 30% of the time per iteration. Furthermore, there is little advantage to using the DGM method over the traditional multigroup method when many fine-group sweeps are needed for convergence. This study investigates the stability of the DGM method and seeks to eliminate the flux update through changes to the iteration scheme.

FIXED POINT ITERATION

Fixed point iteration is the process of solving the equation $x=\mathbb{T}x$, where x is a vector and $\mathbb{T}$ is some operator that acts on x. For a more rigorous presentation of fixed points, see [5].

Picard Iteration

The most common solution technique is Picard iteration or the sequence of successive approximations [5]. From a starting guess $x^{(0)}$, subsequent iterates $x^{(n)}$ are obtained by applying the operator.

$$x^{(n+1)}=\mathbb{T}x^{(n)} \quad (4)$$

In practice, a solution is obtained when the difference between successive iterates, under some norm, is within a convergence criteria ε.

$$||x^{(n+1)}-x^{(n)}||<\varepsilon \quad (5)$$

The procedure of Equation 4, however, is not guaranteed to converge in general. Rather, it requires that the operator $\mathbb{T}$ be contractive. For two state points y_1 and y_2, that is:

$$||\mathbb{T}y_1-\mathbb{T}y_2||<||y_1-y_2|| \quad (6)$$

This is equivalent to saying that the distance between successive Picard iterates decreases. Also, this implies each successive iterate more closely approximates the solution x^* than the previous.

$$||x^* - \mathbb{T}x^{(n)}|| < ||x^* - x^{(n)}|| \quad (7)$$

Note that the commonly encountered power iteration method for computing an eigenvector and eigenvalue is an example of Picard iteration.

Krasnoselskij Iteration

If an operator does not satisfy the contractive condition in Equation 6, another iteration scheme is needed to solve the fixed point problem. The Krasnoselskij iteration [5][6] is one such iteration procedure. With $\lambda \in [0,1]$ as a fixed parameter, it is given by:

$$x^{(n+1)} = (1-\lambda)x^{(n)} + \lambda \mathbb{T}x^{(n)} \quad (8)$$

Note that this reduces to Picard iteration if $\lambda = 1$. This procedure requires a weaker condition on the operator: that it be Lipschitzian. That is, there exists a finite $L > 0$ such that:

$$||\mathbb{T}y_1 - \mathbb{T}y_2|| \leq L||y_1 - y_2|| \quad (9)$$

Other fixed point iteration schemes, including the Kirk, Mann, modified Mann, Ishikawa, Figueiredo, and Halpern iteration schemes [5][6], exist but have yet to be studied in this context.

PICARD DGM PROCEDURE

In past work, the DGM re-condensation procedure has been treated as a Picard iteration scheme. Starting from a guessed flux $\psi^{(0)}$ or a subsequent iterate flux $\psi^{(n)}$, the procedure shown in Equations 1 and 2 yields a new flux ψ^*. The next iterate flux is simply taken as this resultant flux.

$$\psi^{(n+1)} = \psi^* \quad (10)$$

This procedure has not been found to converge without a flux update, even when used with small numbers of groups. For some simple cases, Picard iteration without flux updates was successful; for instance, cases with smoothly varying cross sections were seen to stably converge. However, as complexity increases, such as by using realistic cross sections with larger numbers of groups, instabilities set in. This empirically suggests that largely disparate cross sections, such as those found in familiar reactor applications, cause the method to break down.

With this notion, stability analysis can be formalized. Consider a simple example, a two-group infinite medium problem. This problem has only one degree of freedom, the thermal to fast flux ratio. The standard DGM re-condensation procedure can then be cast as a univariate Picard iteration. The contractive requirement in Equation 6 is equivalent to requiring that the derivative of the operator output with respect to its input have a magnitude less than unity. Two illustrative cases are presented, with different values of the group 2 total cross section but holding all other nuclear data constant.

In Figure 1, the infinite medium problem with total cross section $\sigma = [1;2]$ cm^{-1} (notation: group 1 cross section is 1 cm^{-1}; group 2 cross section is 2 cm^{-1}) is shown. The solution to the fixed point problem exists where the curve of the output versus the input intersects the line $y = x$. The derivative of the curve is also shown, and its magnitude at the solution is clearly less than unity, meaning the operator is contractive in a neighborhood about the solution.

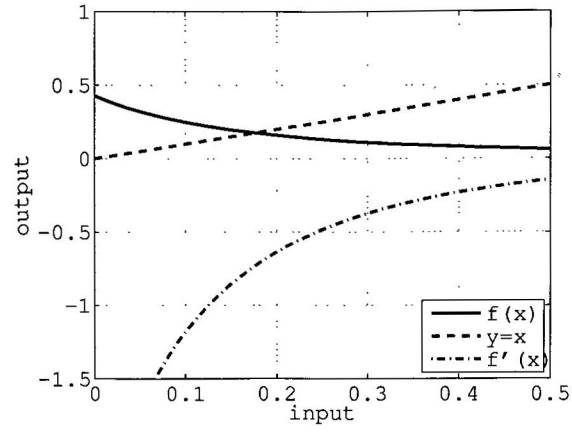

Fig. 1. Picard DGM with $\sigma = [1;2]$ cm^{-1}

In Figure 2, the total cross section is taken to be $\sigma = [1;3]$ cm^{-1}. In this case, the derivative at the solution has a magnitude greater than unity, and therefore the operator is non-contractive in a neighborhood about the solution.

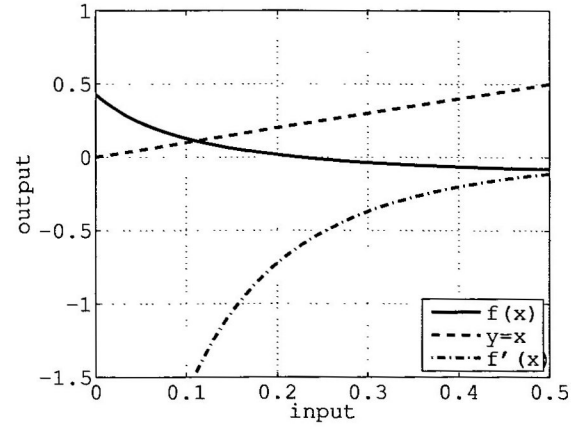

Fig. 2. Picard DGM with $\sigma = [1;3]$ cm^{-1}

Thus, a Picard iteration procedure for the first case is expected to converge but for the second case is expected to diverge. These expectations are confirmed in practice. Because

of the relatively small disparity in cross sections that leads to instability even in this simple case, Picard iteration used in the DGM procedure can be concluded to be unstable for any realistic problems.

KRASNOSELSKIJ DGM PROCEDURE

In past work, the instability of the standard recondensation procedure was addressed through the introduction of flux updates. However, recognizing these convergence issues stem from a non-contractive operator, a simple potential fix for DGM without turning to flux updates is the Krasnoselskij iteration, from Equation 8. As in the preceding section, an iterate flux $\psi^{(n)}$ is used with Equations 1 and 2 to yield a new flux ψ^*. The next iterate is then taken with the Krasnoselskij iteration.

$$\psi^{(n+1)} = (1-\lambda)\psi^{(n)} + \lambda\psi^* \tag{11}$$

As this is an initial study, formal analyses to confirm the operator is Lipschitzian and the existence of the fixed point are not presented. Rather, empirical results are discussed.

First, the infinite medium problem discussed in the preceding section is revisited. Whereas $\sigma = [1;3]$ cm^{-1} was found to be unstable with Picard iteration, choosing $\lambda = 0.8$ with a Krasnoselskij iteration circumvents this instability. If λ is reduced to 0.02, stable convergence was achieved with cross sections as disparate as $\sigma = [1;100]$ cm^{-1}. Of course, with this small value of lambda, convergence is achieved very slowly, requiring on the order of 350 iterations to converge the flux ratio to within 10^{-5}.

A more realistic problem was considered, that of a LWR pin-cell modeled as two slabs with reflective boundaries in 1-D discrete ordinates using the SHEM-361 cross section library. Convergence required that $\lambda \lesssim 0.02$, and thus convergence was again very slow, requiring on the order of 2000 iterations to converge the infinity norm of the flux within 10^{-5}. Note that in practice, the DGM procedure is expected to be used with relatively few iterations in order to improve the coarse group solution, as opposed to iterating to full convergence.

CONCLUSIONS AND FUTURE WORK

Implementing the Krasnoselskij iteration procedure with the discrete generalized multigroup method led to a convergent procedure without flux updates for all problems considered, including a 361-group 1-D problem. However, the value of λ was required to be very small, leading to a very large number of iterations being needed to obtain convergence. This large number of iterations precludes this process from being a viable solution technique for non-research applications, but it provides a starting point for future work.

Allowing the λ parameter to vary during the iteration process, as in the Mann iteration, could greatly reduce the number of iterations. Other schemes could improve results even more. Furthermore, alterations to the DGM procedure itself could reduce the cost of an iteration in these procedures enough to allow for a relatively large number of iterations.

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