Preconditioned Krylov Subspace Methods for Transport Equations

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Abstract

Transport equations have many important applications. Because the equations are based on highly non-normal operators, they present difficulties in numerical computations. The iterative methods have been shown to be one of efficient numerical methods to solve transport equations. However, because of the nature of transport problems, convergence of iterative methods tends to slow for many important problems. In this paper, we focus on the development of algorithms to accelerate iterative methods. We investigate the applicability and performance of some Krylov subspace methods with preconditioners, particularly, the incomplete LU factorization and the multigrid algorithm. Three cases (isotropic equations without absorption, isotropic equations with absorption, and anisotropic equations) are considered. Our numerical experiments show that the use of an appropriate multilevel preconditioner can make much considerable improvement for Krylov subspace methods, such as GMRES and CGS.

§1 Introduction

Transport equations are mathematical models which describe the transport of particles, momentum, energy, or any transportable quantity [2]. They originally arose in the study of electron transport in solid, later were found in many other applications, such as neutron transport, gas kinetics, radiative transfer. Many mathematical theories and tools have been developed for the study of transport problems, including obtaining analytic and numerical solutions. It turns out that finding explicit solution is very difficult due to the complexity of equations and limits of analytical tools developed so far. Although researchers have successfully obtained closed form solutions to some particular problems, for most of the problems which are of practical interest their explicit solutions are impossible to obtain. Therefore, developing numerical methods has become an important aspect in understanding the nature of transport problems. There have been many discretization schemes and numerical methods designed for solving transport problems. Among them, iterative methods have been proved to be one of the most efficient numerical methods. However, for many important problems, the convergence of iterative methods tends to be very slow, for example, problems with strong scattering. Consequently, there has been a lot of interest recently in the development of acceleration techniques for iterative methods, such as for example multigrid methods.

In this paper, we consider an one–dimensional static model, whose physical domain is a semi-infinite slab of width b in the x-dimension (in what follows, without loss of generality we assume that $b = 1$). In general, such a model can be described by an integro-differential equation in one spatial variable and one angular variable as follows.

$$\mu \frac{\partial \psi}{\partial x}(x,\mu) + \sigma_t \psi(x,\mu) = S(x,\mu) + q(x,\mu), \quad x \in (0,1) \quad \mu \in [-1,1], \tag{1}$$

where $\psi(x,\mu)$ represents the flux of particles at position x traveling at an angle $\theta = \arccos(\mu)$ from the x-axis, $\sigma_t\, dx$ is the expected number of interactions (absorptive or scattering) that a particle will have in traveling a distance dx, $S(x,\mu)$ is a source due to rescattering, $q(x,\mu)$ is an external source. The boundary conditions prescribing the flux of particles entering the slab are

$$\begin{aligned} \psi(0,\mu) &= g_0(\mu), & (2)\\ \psi(1,-\mu) &= g_1(\mu), & (3) \end{aligned}$$

for $\mu \in (0,1)$. The source $S(x,\mu)$ is given by an integral operator with spherical harmonics as its singular kernel, called the scattering function, as follows:

$$S(x,\Omega) = \sigma_s \int_{-1}^{1} \Sigma_s(x,\mu' \to \mu)\psi(x,\mu')d\mu', \tag{4}$$

where Σ_s is the probability density that a particle will be scattered from direction μ' to μ, $\sigma_s\, dx$ is the expected number of scattering interactions. Thus, $(\sigma_t - \sigma_s)\, dx$ is the expected number of absorptive interactions.

If the probabilities of scattering of particles are the same for all directions (called the isotropic case), then Σ_s in above integral is constant in angle and $S(x,\mu)$ is simply expressed as

$$S(x,\mu) = \frac{1}{2}\sigma_s \int_{-1}^{1} \psi(x,\mu')d\mu', \tag{5}$$

which is independent of μ. It is noticed that as $\sigma_t \to \infty$ and $\gamma \equiv \sigma_s/\sigma_t \to 1$, the problem becomes singularly perturbed. Consequently, the conventional numerical methods for solving transport equations encounter difficulties in this thick limit.

In recent years, there have been a lot of efforts invested in the development of numerical methods for solving transport equations, especially in multigrid or multilevel algorithms. Morel and Manteuffel [10] presented angular multigrid techniques for anisotropic problems. Based on the modified linear discontinuous (MLD) scheme, Manteuffel, et al. [6] developed a fast multigrid algorithm for isotropic problems with pure scattering. Multigrid algorithms for two dimensional transport equations are investigated in Nowak [11, 12]. Parallel multigrid algorithms for solving either isotropic and anisotropic equations have also been developed, see Manteuffel, et al. [6, 7], and Oliveira [13, 14]. Multigrid methods have been successfully applied to transport equations. Here we shall use multigrid algorithms as preconditioners of Krylov subspace methods. It is noted that the discretization of transport equations in general will lead to nonsymmetric systems, which make Krylov subspace methods particularly attractive in numerical computations. In addition, Krylov methods allow the easy incorporation of preconditioners. Hence, it is expected that convergence can be improved if appropriate preconditioners are applied.

In this paper we investigate the applicability and performance of some Krylov subspace methods with preconditioners, particularly, the incomplete LU factorization (ILU) and the multigrid (MG) algorithm developed in [6], for solving transport equations in three cases: isotropic equations with no-absorption, isotropic equations with absorption, and anisotropic equations. It is worth remarking that multigrid methods developed in [6, 7, 13] have difficulties with isotropic scattering with small but significant absorption. We show that if multigrid methods are used as a preconditioner of some Krylov subspace methods, such as GMRES, the convergence rate can be significantly improved. The rest of this paper is organized as follows: In Section 2 we describe the discretization for transport equations. A summary of the Krylov space methods and preconditioners used is given in Section 3. The numerical results are shown in Section 4, where a comparison of these methods is also given. Finally, in Section 5 we outline a few conclusions.

§2 **Discretization**

The angular discretization is accomplished by expanding the angular dependence in Legendre polynomials (see [5]). That is, letting $p_\ell(\mu)$, $\ell = 0, 1, \cdots, N-1$, be the first N Legendre polynomials, we assume that $\psi(x, \mu)$ is discretized by the S_N approximation as follows:

$$\psi(x,\mu) = \sum_{\ell=0}^{N-1} (2\ell+1)\phi_\ell(x) p_\ell(\mu), \tag{6}$$

where $\phi_\ell(x)$, $\ell = 0, \cdots, N-1$, represent moments. It is easily seen that $\phi_\ell(x)$ can be obtained by

$$\phi_\ell(x) = \frac{1}{2}\int_{-1}^{1} p_\ell(\mu')\psi(x,\mu')d\mu' = \sum_{k=1}^{N} w_k p_\ell(\mu_k)\psi(x,\mu_k), \tag{7}$$

where μ_i and w_i, $i = 1, \cdots, N$, are the Gauss quadrature points and weights, respectively. It follows that scattering term $S(x, \mu)$ in (1) becomes

$$S(x, \mu) = \sum_{k=0}^{N-1} (2k+1)\sigma_k \phi_k(x)\ p_k(\mu), \tag{8}$$

where $\sigma_k = \frac{1}{2}((N-1)N - k(k+1))$. If we consider the isotropic case (see (5)), we readily see that

$$S(x, \mu) = \sigma_s \sum_{k=1}^{N} w_k \psi(x, \mu_k), \tag{9}$$

where σ_s is a constant.

Now let μ in equation (1) be μ_i, $i = 1, \cdots, N$. In view of (8) we see that one-dimensional anisotropic equation (1) is deduced to a system of semidiscrete equations that resemble collocation at N Gauss quadrature points, μ_j, $j = 1, \ldots, N$:

$$\mu_j \frac{\partial \psi}{\partial x}(x, \mu_j) + \sigma_t \psi(x, \mu_j) = \sum_{k=0}^{N-1} (2k+1)\sigma_k\ \phi_k(x)\ p_k(\mu_j) + q(x, \mu_j), \tag{10}$$

where $x \in [0, 1]$. Since the quadrature points and weights are symmetric about zero, that is,

$$w_k = w_{k+n} \qquad \text{and} \qquad \mu_k = -\mu_{k+n}, \qquad k = 1, \cdots, n,$$

where $n = N/2$, we can reformulate (10) in terms of the positive values, μ_j, $j = 1, \ldots, n$. To this end, we define

$$\psi_i^+(x) = \psi(x, \mu_i), \quad \psi_i^-(x) = \psi(x, -\mu_i), \quad i = 1, \cdots, n,$$

and

$$\begin{aligned} \underline{\psi}(x) &= (\psi_1^+(x), \cdots, \psi_n^+(x), \psi_1^-(x), \cdots, \psi_n^-(x))^T, \\ \underline{\phi}(x) &= (\phi_0(x), \phi_1(x), \cdots, \phi_{N-1}(x))^T. \end{aligned}$$

Let T and T^{-1} be $N \times N$ matrices with entries $t_{i,j}$ and $\bar{t}_{i,j}$ given by

$$t_{i,j} = w_j p_{i-1}(\mu_j), \qquad \text{and} \qquad \bar{t}_{i,j} = (2j-1)p_{j-1}(\mu_i),$$

respectively, and D be an $N \times N$ diagonal matrix given by

$$D = diag\{\sigma_0, \sigma_1, \cdots, \sigma_{N-1}\}.$$

Then, in view of (6) and (7), we can see that

$$\underline{\psi}(x) = T^{-1}\underline{\psi}(x), \qquad \text{and} \qquad \underline{\phi}(x) = T^{-1}\underline{\phi}(x),$$

which implies that

$$(S(x, \mu_1), \cdots, S(x, \mu_N))^T = T^{-1} D T \underline{\psi}(x).$$

Denote by $s_{i,j}$ entry (i,j) of an $N \times N$ matrix $S \equiv T^{-1}DT$. Then equation (10) can be rewritten as

$$\mu_j \frac{d\psi_j^+}{dx}(x) + \sigma_t \psi_j^+(x) = \sum_{k=1}^{n} s_{j,k}(\psi_k^+(x) + s_{j,k+n}\psi_k^-(x)) + q_j^+(x), \tag{11}$$

$$-\mu_j \frac{d\psi_j^-}{dx}(x) + \sigma_t \psi_j^-(x) = \sum_{k=1}^{n} s_{j+n,k}(\psi_k^+(x) + s_{j+n,k+n}\psi_k^-(x)) + q_j^-(x), \tag{12}$$

where $q_i^+(x) = q(x, \mu_i)$, $q_i^-(x) = q(x, -\mu_i)$, $i = 1, \cdots n$.

The spatial discretization is accomplished by the MLD scheme, which uses elements that are linear across each cell and discontinuous in the upwind direction, as described in [4] and [6]. In our grid representation, the variable $\psi_{ij}^{+(-)}$ denotes the flux of particles at position x_i in the direction μ_j $(-\mu_j)$. Proceeding as in [6], we can obtain the following discrete equations

$$\frac{\mu_j}{h_i}(\psi^+_{i+\frac{1}{2},j} - \psi^+_{i-\frac{1}{2},j}) + \sigma_t \psi^+_{i,j} = \sum_{k=1}^{n}(s_{j,k}\psi^+_{i,k} + s_{j,k+n}\psi^-_{i,k}) + q^+_{i,j}, \tag{13}$$

$$\frac{2\mu_j}{h_i}(\psi^+_{i+\frac{1}{2},j} - \psi^+_{i,j}) + \sigma_t \psi^+_{i+\frac{1}{2},j} = \sum_{k=1}^{n}\{s_{j,k}\psi^+_{i+\frac{1}{2},k} + s_{j,k+n}(2\psi^-_{i,k} - \psi^-_{i-\frac{1}{2},k})\} + q^+_{i+\frac{1}{2},j}, \tag{14}$$

$$\frac{\mu_j}{h_i}(\psi^-_{i-\frac{1}{2},j} - \psi^-_{i+\frac{1}{2},j}) + \sigma_t \psi^-_{i,j} = \sum_{k=1}^{n}(s_{j+n,k}\psi^+_{i,k} + s_{j+n,k+n}\psi^-_{i,k}) + q^-_{i,j}, \tag{15}$$

$$\frac{2\mu_j}{h_i}(\psi^-_{i-\frac{1}{2},j} - \psi^-_{i,j}) + \sigma_t \psi^-_{i-\frac{1}{2},j} = \sum_{k=1}^{n}\{s_{j+n,k}(2\psi^+_{i,k} - \psi^+_{i+\frac{1}{2},k}) + s_{j+n,k+n}\psi^-_{i-\frac{1}{2},k}\} + q^-_{i,j}, \tag{16}$$

$$i = 1, \ldots, m,$$

with boundary conditions

$$\psi^+_{\frac{1}{2},j} = g^+_{0,j}, \quad \text{and} \quad \psi^-_{m+\frac{1}{2},j} = g^-_{1,j}, \qquad j = 1, \ldots, n, \tag{17}$$

where $g^+_{0,j} = g_0(\mu_j)$ and $g^-_{1,j} = g_1(\mu_j)$. In our model, $x_{i+\frac{1}{2}}$ and $x_{i-\frac{1}{2}}$ are cell edges, $x_i = \frac{1}{2}(x_{i+\frac{1}{2}} + x_{i-\frac{1}{2}})$ is the cell center, and $h_i = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}$ is the cell width, $1 \le i \le m$. Equations (13) and (15) are called balance equations and (14) and (16) are called edge equations. We may rewrite equations (13)–(16) in a block matrix form:

$$B_i(\underline{\psi}^+_{i+\frac{1}{2}} - \underline{\psi}^+_{i-\frac{1}{2}}) + \underline{\psi}^+_i = S_{11}\underline{\psi}^+_i + S_{12}\underline{\psi}^-_i + \underline{q}^+_i \tag{18}$$

$$2B_i(\underline{\psi}^+_{i+\frac{1}{2}} - \underline{\psi}^+_i) + \underline{\psi}^+_{i+\frac{1}{2}} = S_{11}\underline{\psi}^+_{i+\frac{1}{2}} + S_{12}(2\underline{\psi}^-_i - \underline{\psi}^-_{i-\frac{1}{2}}) + \underline{q}^+_{i+\frac{1}{2}}, \tag{19}$$

$$B_i(\underline{\psi}^-_{i-\frac{1}{2}} - \underline{\psi}^-_{i+\frac{1}{2}}) + \underline{\psi}^-_i = S_{21}\underline{\psi}^+_i + S_{22}\underline{\psi}^-_i + \underline{q}^-_i, \tag{20}$$

$$2B_i(\underline{\psi}^-_{i-\frac{1}{2}} - \underline{\psi}^-_i) + \underline{\psi}^-_{i-\frac{1}{2}} = S_{21}(2\underline{\psi}^+_i - \underline{\psi}^-_{i+\frac{1}{2}}) + S_{22}\underline{\psi}^+_{i-\frac{1}{2}} + \underline{q}^-_{i-\frac{1}{2}}, \tag{21}$$

$$i = 1, \ldots, m,$$

where

$$B_i = \begin{bmatrix} \frac{\mu_1}{\sigma_t h_i} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \frac{\mu_n}{\sigma_t h_i} \end{bmatrix},$$

$S_{11}, S_{12}, S_{21}, S_{22}$ are submatrices of $\frac{1}{\sigma_t} S$ such that

$$\begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} = \frac{1}{\sigma_t} S,$$

and

$$\begin{aligned} &\underline{\psi}_k^+ = (\psi_{k,1}^+, \psi_{k,2}^+, \cdots, \psi_{k,n}^+)^T, \qquad \underline{\psi}_k^- = (\psi_{k,1}^-, \psi_{k,2}^-, \cdots, \psi_{k,n}^-)^T, \\ &\underline{q}_k^+ = \tfrac{1}{\sigma_t}(q_{k,1}^+, q_{k,2}^+, \cdots, q_{k,n}^+)^T, \qquad \underline{q}_k^- = \tfrac{1}{\sigma_t}(q_{k,1}^-, q_{k,2}^-, \cdots, q_{k,n}^-)^T, \\ &k = \tfrac{1}{2}, 1, \tfrac{3}{2}, \cdots, m, m + \tfrac{1}{2}. \end{aligned}$$

In the isotropic case, we have that

$$S_{11} = S_{12} = S_{21} = S_{22} = \gamma \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} \begin{bmatrix} \omega_1 & \cdots & \omega_n \end{bmatrix}.$$

Consequently, for cell i, $i = 1, \cdots, m$, we arrive at the following matrix equation:

$$A_i \underline{\Psi}_i = B_i \underline{\psi}_{i-\frac{1}{2}}^+ + B_i \underline{\psi}_{i+\frac{1}{2}}^- + Q_i, \tag{22}$$

where matrix A_i is given by

$$A_i = \begin{bmatrix} I + 2B_i - S_{22} & -2S_{21} & -2B_i & S_{21} \\ 0 & I - S_{11} & -S_{12} & B_i \\ B_i & -S_{21} & I - S_{22} & 0 \\ S_{12} & -2B_i & -2S_{12} & I + 2B_i - S_{11} \end{bmatrix},$$

and

$$\begin{aligned} \underline{\Psi}_i &= (\underline{\psi}_{i-\frac{1}{2}}^-, \underline{\psi}_i^+, \underline{\psi}_i^-, \underline{\psi}_{i+\frac{1}{2}}^+), \\ \underline{Q}_i &= (\underline{q}_{i-\frac{1}{2}}^-, \underline{q}_i^+, \underline{q}_i^-, \underline{q}_{i+\frac{1}{2}}^+). \end{aligned}$$

Figure 1 shows the computational domain with $2m+1$ spatial points and n angles. We see that for cell i, $\underline{\psi}_{i-\frac{1}{2}}^-$ and $\underline{\psi}_{i+\frac{1}{2}}^+$ in equation (22) represent the inflows from its left and right ends, respectively. Hence, if the inflows of the cell are assumed to be known, matrix equation (22) can be solved by performing a μ-line relaxation on the cell, that is, center variables $\underline{\psi}_i^+$ and $\underline{\psi}_i^-$, together with the outflow variables $\underline{\psi}_{i-\frac{1}{2}}^-$ and $\underline{\psi}_{i+\frac{1}{2}}^+$ are updated by using (22). It is noted that boundary conditions (17) represent, in the computational grid, the inflow for positive angles on the left and for negative angles on the right of the domain. To perform a μ-line relaxation on the entire domain, we

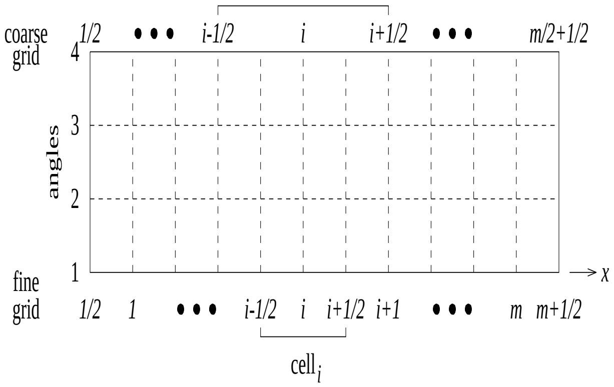

Figure 1: Computational grid.

consider all the cells coupled together. Hence, we derive the following linear system for the whole domain:

$$\begin{bmatrix} A_1 & -C_1 & & & \\ -D_2 & A_2 & -C_2 & & \\ & \ddots & \ddots & \ddots & \\ & & -D_{m-1} & A_{m-1} & -C_{m-1} \\ & & & -D_m & A_m \end{bmatrix} \begin{bmatrix} \underline{\Psi}_1 \\ \underline{\Psi}_2 \\ \vdots \\ \underline{\Psi}_{m-1} \\ \underline{\Psi}_m \end{bmatrix} = \begin{bmatrix} \underline{b_1} \\ 0 \\ \vdots \\ 0 \\ \underline{b_m} \end{bmatrix} + \begin{bmatrix} \underline{Q}_1 \\ \underline{Q}_2 \\ \vdots \\ \underline{Q}_{m-1} \\ \underline{Q}_m \end{bmatrix} \tag{23}$$

where

$$C_i = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ B_i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \qquad D_i = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & B_i \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},$$

and

$$\underline{b_1} = (0, B_1 \underline{\psi}^+_{1-\frac{1}{2}}, 0, 0)^T \quad \text{and} \quad \underline{b_m} = (0, 0, B_m \underline{\psi}^-_{m+\frac{1}{2}}, 0)^T,$$

which are known due to the boundary conditions (17). We now can solve the system for all the variables at each iterative step.

§3 Krylov Subspace Methods and Preconditioners

In Section 2 we have seen that the coefficient matrix for linear system (23), which is derived from discretization of either isotropic or anisotropic equations, is block tridiagonal. Such a matrix is sparse and, in general, nonsymmetric. We now intend to find efficient numerical methods for solving system (23).

There are many iterative methods for solving large sparse linear systems $Ax = b$, where A is a $d \times d$ nonsymmetric matrix and x, b are d-dimensional vectors. One class of iterative methods is Krylov subspace methods. Here we need nonsymmetric Krylov subspace methods, such as CGS (Conjugate Gradient Squared), GMRES (Generalized Minimal RESidual), CGNE (Conjugate Gradient for Normal Equation), and

LSQR (Least Squares/QR) methods. In these methods, iterative solutions are of the form $x^{(k+1)} = x^{(k)} + p^{(k)}$, where $p^{(k)}$ is in $K_k(A, r^0) \equiv span\{r^0, Ar^0, A^2r^0, \cdots, A^{k-1}r^0\}$, the Krylov space of dimension k with $k \leq d$. To obtain bases of Krylov subspaces, the methods employ either the symmetric or unsymmetric Lanczos methods or the Arnoldi method. For instance, CGS method uses unsymmetric Lanczos, GMRES method applies Arnoldi, and LSQR utilizes symmetric Lanczos. The symmetric Lanczos and Arnoldi algorithms generate (in exact arithmetic) an orthonormal base of space $K_k(A, r^0)$, while the unsymmetric Lanczos produces a pair of biorthonormal bases of spaces $K_k(A, r^0)$ and $K_k(A^T, r^0)$. In both cases the Lanczos method yields a tridiagonal matrix which represents the original matrix on the Krylov subspaces, while the Arnoldi method gives a Hessenberg matrix which represents the matrix on the Krylov subspace $K_k(A, r^0)$. The unsymmetric Lanczos process is fast, but may suffer from numerical instability, known as breakdown. However, there are variants of the unsymmetric Lanczos method, based on the look-ahead Lanczos algorithm, which are stable.

One advantage of Krylov subspace methods is to allow the easy incorporation of preconditioners. For system $Ax = b$, a preconditioner is a matrix B such that Bu can be easily computed for a given vector u and system $BAx = Bb$ is easier to solve than the original one. Usually, to this end one intends to find B such that matrix BA is well conditioned. Such an appropriate matrix B can obtained by a number of different approaches. One of the simplest preconditioners is the diagonal preconditioner, where B is simply taken as the inverse of the diagonal of A if A is "diagonally dominant". Another type of preconditioner is to utilize incomplete factorizations of sparse matrices, for example, ILU (Incomplete LU factorization). Some iterative methods can also be used as a preconditioner, such as multigrid methods. Here we shall investigate use of multigrid methods with respect to spatial variables as a preconditioner (refer to [6] for details on the multigrid method for the isotropic scattering case. It is noted that Krylov subspace methods only require three operations for their implementation: linear combinations, inner products, and matrix–vector products. Thus, for a preconditioner which is incorporated into a Krylov subspace method, it is convenient to use a routine to compute BAu for a given vector u by first computing $v = Au$, and then using a routine for computation of Bv.

§4 **Numerical Results**

In this section, we present some numerical results about convergence, when we solve linear systems derived from isotropic and anisotropic equations by using various Krylov subspace methods, such as GMRES, CGS, and CGNE, with ILU and MG (multigrid) preconditioners, respectively. The test problems were selected by randomly generating the right-hand side vectors of linear systems and the numerical experiments were all performed on a Sun Sparc workstation in the Department of Computer Science, Texas A&M University. We run our codes on problems with various sizes. However, as all the problems that we tested exhibited similar behavior, we only present results for a case where $N = 8$ (16 angles) and $m = 64$ (64 cells),

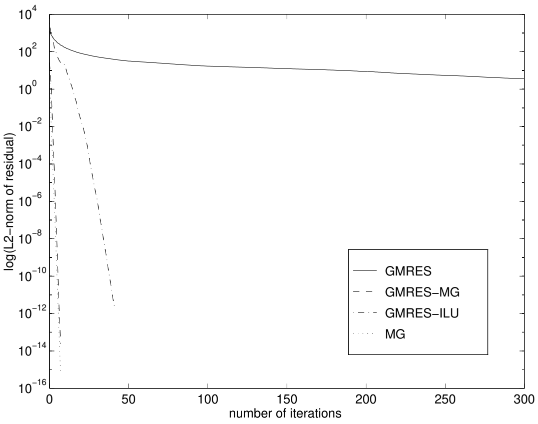

Figure 2: GMRES (case 1).

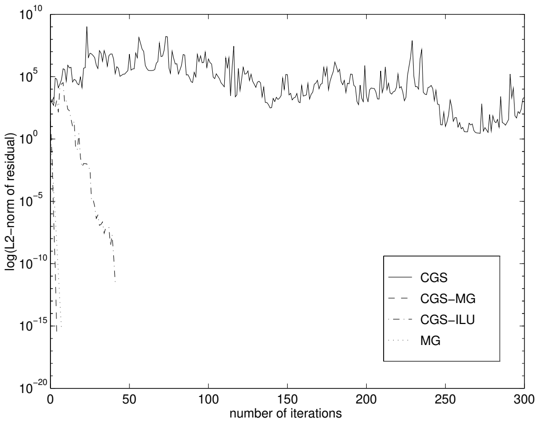

Figure 3: CGS (case 1).

which yields a discrete problem with dimension 2048. We will show residual behavior during an iteration process for each of the following three cases: (1) isotropic equations without absorption ($\gamma = 1$, where $\gamma = \frac{\sigma_s}{\sigma_t}$), (2) isotropic equations with absorption ($\gamma < 1$), and (3) anisotropic equations. In all cases, the iteration process is terminated as long as the Euclidean norm of the residual is reduced by a factor of 10^{-15} or the number of iterations exceeds 300.

1. isotropic equations without absorption. The nonabsorption case is the simplest of three cases considered. Residual reduction for each iterative methods is plotted, respectively, in Figures 2-4, where the x–axis is the number of iterations and the y–axis is the base 10 logarithm of the Euclidean norm of the residuals.

For GMRES(k) methods, we let k, the number of directions, be 50 in our computation. It is shown that GMRES(k) and CGS display very good convergence rate (Figures 2 and 3), whereas CGNE shows very poor performance with either ILU

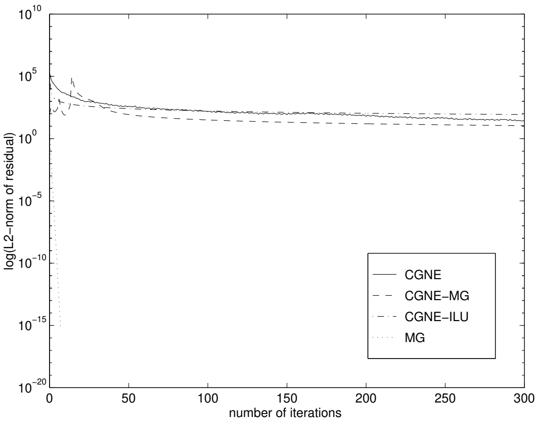

Figure 4: CGNE (case 1).

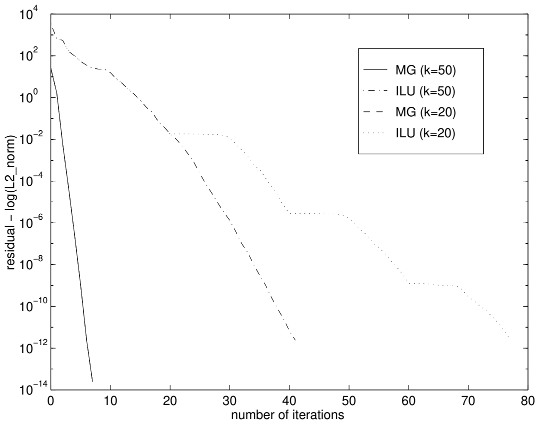

Figure 5: GMRES(k), k=20,50 (case 1).

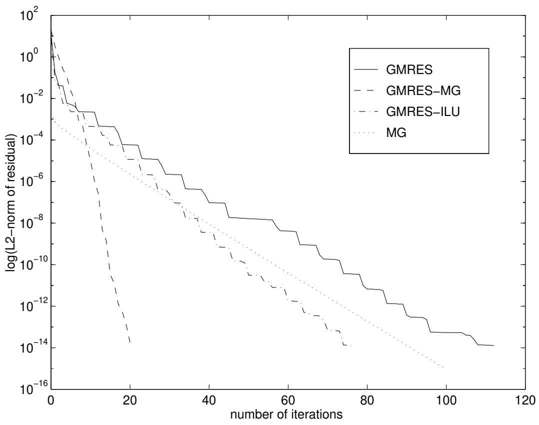

Figure 6: GMRES (case 2).

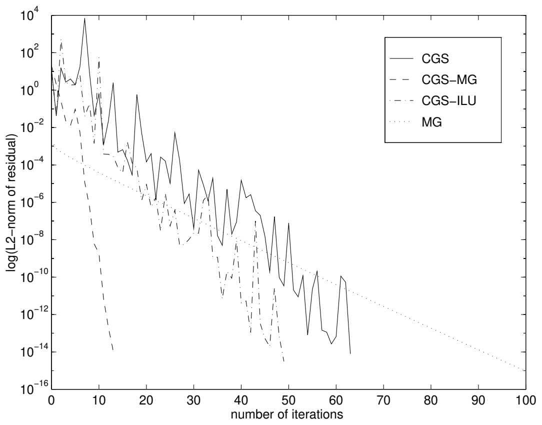

Figure 7: CGS (case 2).

or MG preconditioner (Figure 4). Comparing ILU and MG preconditioners, we see that the latter is significantly faster than the former when they are applied to either GMRES or CGS method. We computed average convergence factors for GMRES, as shown in Table 1, and we see that convergence factor for ILU preconditoner is 0.459, whereas convergence factor for MG preconditioner is 0.014. In addition, we note that convergence rate GMRES(k) is dependent on k. As shown in Figure 5, the number of directions in GMRES(k) can be considerablely reduced if MG preconditioner is applied, in comparison with ILU preconditioner. The multigrid method works very well with isotropic equations without absorption. From Figures 2–4 it is seen that in comparison with the multigrid solver, we actually did not get much gain from the multigrid used as a preconditioner. In contrast, we lost some convergence rate when we applied the MG preconditioner to the CGS method.

	ILU		MG	
case	#iterations	CF	#iterations	CF
1	41	0.459	7	0.014
2	76	0.765	20	0.234
3	300	0.896	96	0.724

Table 1. Convergence Factor (CF) using GMRES(50).

2. isotropic equations with absorption. The absorption case is harder to solve and present computional difficulties, nevertheless is an important practical case. Here the absorption regime we tested is $\gamma = 1 - \frac{1}{(\sigma_t\, h)^2}$. This regime corresponds to a situation in which the scattered particles undergo a large number of scatterings. In addition, the particles have a significant probability of being absorbed in or "escaping" from a cell. The numerical results are displayed in Figures 6–8.

From Figure 6 and Table 1, we see again that MG preconditioner improves the

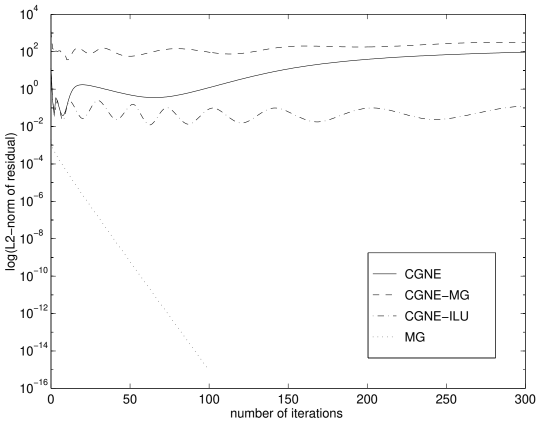

Figure 8: CGNE (case 2).

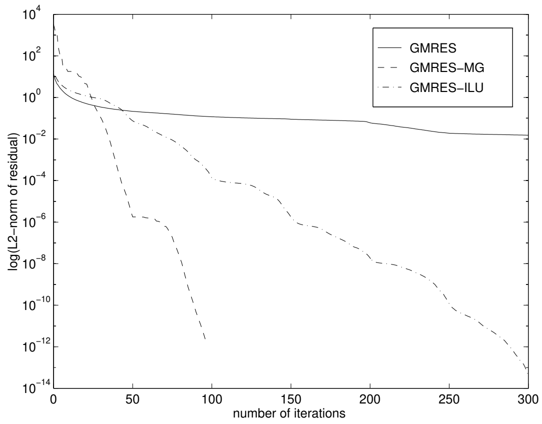

Figure 9: GMRES (case 3).

convergence of both GMRES and CGS, and this improvement is more than that when the ILU preconditioner is used. On the other hand, CGNE is not convergent at all.

3. Anisotropic cases. Figures 9–11 demonstrate the behavior of the residual for anisotropic equations, which is the most difficult case for numerical computations among the three cases considered. We see that convergence rates deteriorate for all the methods we tested.

In this case, the multigrid method for isotropic equations without absorption is used as a MG preconditioner. As we see, such an MG preconditioner still accelerates convergence much faster than ILU for the GMRES method. However, unlike the previous two cases, ILU preconditioner works better than MG preconditioner when they are applied to the CGS method. We think that this is probably because MG we used was specifically designed for isotropic equations. It is expected that if a MG preconditioner specifically designed for anisotropic equations, such as the angular multigrid

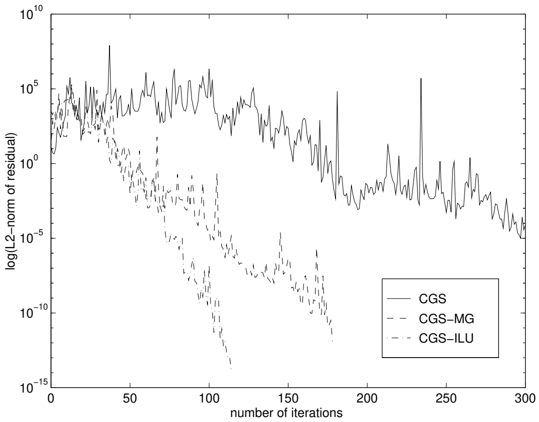

Figure 10: CGS (case 3).

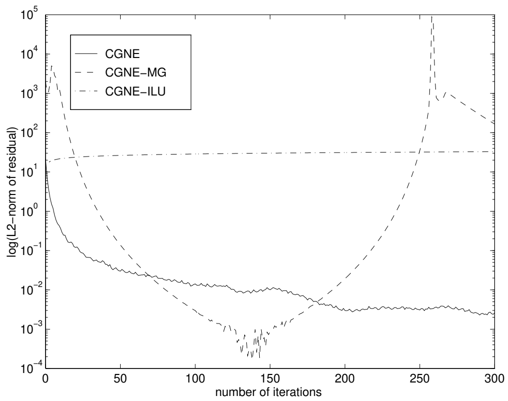

Figure 11: CGNE (case 3).

presented in [10], is used, convergence rate behaviour of GMRES and CGS will be improved even more. However, complexity of the algorithm will also be increased.

In summary, both GMRES and CGS with either ILU or MG preconditioner perform well on all three cases, although the convergence rate deteriorates from case 1 to case 3. In general, the use of the special multigrid preconditioner presented in [6] will make more considerable improvement than the use of ILU preconditioner for Krylov subspace methods, such as GMRES and CGS, except when CGS is being used for solving the anisotropic equations.

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