

Available online at www.sciencedirect.com



Computer Physics Communications

Computer Physics Communications 175 (2006) 330-338

www.elsevier.com/locate/cpc

# On the performance of SPAI and ADI-like preconditioners for core collapse supernova simulations in one spatial dimension

Dennis C. Smolarski<sup>a,\*</sup>, Ramesh Balakrishnan<sup>b</sup>, Eduardo F. D'Azevedo<sup>c</sup>, John W. Fettig<sup>d</sup>, Bronson Messer<sup>c</sup>, Anthony Mezzacappa<sup>c</sup>, Faisal Saied<sup>e</sup>, Paul E. Saylor<sup>f</sup>, F. Douglas Swesty<sup>g</sup>

<sup>a</sup> Department of Mathematics and Computer Science, Santa Clara University, Santa Clara, CA 95053-0290, USA

<sup>b</sup> National Center for Supercomputing Applications, University of Illinois at Urbana–Champaign, Champaign, IL 61820, USA

<sup>c</sup> Oak Ridge National Laboratory, Oak Ridge, TN 37831-6354, USA

<sup>d</sup> Department of Mathematics, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA

<sup>e</sup> Rosen Center for Advanced Computing, Purdue University, West Lafayette, IN 47907, USA

<sup>f</sup> Department of Computer Science, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA

<sup>g</sup> Department of Physics and Astronomy, State University of New York at Stony Brook, NY 11794-3800, USA

Received 18 July 2005; received in revised form 28 April 2006; accepted 20 May 2006

Available online 7 July 2006

### Abstract

The simulation of core collapse supernovæ calls for the time accurate solution of the (Euler) equations for inviscid hydrodynamics coupled with the equations for neutrino transport. The time evolution is carried out by evolving the Euler equations explicitly and the neutrino transport equations implicitly. Neutrino transport is modeled by the multi-group Boltzmann transport (MGBT) and the multi-group flux limited diffusion (MGFLD) equations. An implicit time stepping scheme for the MGBT and MGFLD equations yields Jacobian systems that necessitate scaling and preconditioning. Two types of preconditioners, namely, a sparse approximate inverse (SPAI) preconditioner and a preconditioner based on the alternating direction implicit iteration (ADI-like) have been found to be effective for the MGFLD and MGBT formulations. This paper compares these two preconditioners. The ADI-like preconditioner performs well with both MGBT and MGFLD systems. For the MGBT system tested, the SPAI preconditioner did not give competitive results. However, since the MGBT system in our experiments had a high condition number before scaling and since we used a sequential platform, care must be taken in evaluating these results.

PACS: 02.60.Cb; 02.70.Bf; 95.30.Jx; 97.60.Bw

Keywords: Radiative transfer; Supernovæ; Numerical simulation; Solution of equations; Finite-difference methods; Multi-group Boltzmann equation; Multi-group flux limited diffusion; Preconditioners

\* Corresponding author. Department of Mathematics and Computer Science, Santa Clara University, 500 El Camino Real, Santa Clara, CA 95053-0290, USA. Tel.: +408 554 4174; fax: +408 554 2370.

*E-mail addresses:* dsmolarski@scu.edu (D.C. Smolarski), bramesh@ncsa.uiuc.edu (R. Balakrishnan), dazevedoef@ornl.gov (E.F. D'Azevedo), jfettig@uiuc.edu (J.W. Fettig), bronson@ornl.gov (B. Messer), mezzacappaa@ornl.gov (A. Mezzacappa), fsaied@purdue.edu (F. Saied), saylor@cs.uiuc.edu (P.E. Saylor), dswesty@blackhole.ess.sunysb.edu (F.D. Swesty).

0010-4655/\$ – see front matter @ 2006 Elsevier B.V. All rights reserved. doi:10.1016/j.cpc.2006.05.002

# 1. Introduction

The subject of our paper is the preconditioning of linear systems resulting from a specific physical problem, which happens to be a problem of the greatest interest in astrophysics, namely simulating core collapse supernovæ. The numerical simulation of this problem is beset with physical, mathematical, and computational challenges: a potpourri of nuclear and particle physics, hydrodynamics, radiation transport and general relativity; a mathematical formulation coupling the equations of inviscid hydrodynamics in three spatial dimensions with the neutrino transport equations in six-dimensional phase space; and the need for computational techniques that address efficiency and scalability on high performance platforms. (In this context, "scalable" roughly means that a method remains effective as the system size increase.) Of the two concerns of efficiency and scalability, it is efficiency that we stress here. Although scalability is of overriding importance, it is outside the scope of our paper even though we still comment on it from time to time.

A major bottleneck in most simulations is the numerical solution of linear systems. An efficient, scalable solution method becomes imperative. In the case that the solution method to solve a linear system is an iterative method, efficiency means that scaling and preconditioning are necessary. "Scaling" (not to be confused with "scalability") as used here means multiplication of the matrix rows by a scale factor, a form often called "row scaling". We note that "scaling" can also be in the form of column scaling, or both row and column scaling.

Appropriate preconditioning yields a linear system that is equivalent to the original, though with better numerical properties. The preconditioner one chooses is arrived at through a process partly scientific and partly a matter of personal taste and intuition.

In this report, we made use of two system matrices, one derived from the multigroup Boltzmann transport (MGBT) equation (see work by D'Azevedo et al. [1]) and the other from the multigroup flux limited diffusion (MGFLD) equation (see work by Swesty et al. [2]). The matrices resulted from discretizing the MGBT and MGFLD equations in one spatial dimension. We note that these two matrices result from linear algebraic systems whose variables are ordered differently. In the MGBT case, the variables are ordered according to the Mezzacappa scheme (see [3]) and, in the MGFLD case, according to the Swesty scheme (see [2]). We also note that the variables, in some cases, correspond to different physical realities. (Details regarding the equations from which the matrices are derived may be found, for the MGBT case, in [4,5], and [3], and, for the MGFLD case, in [2,6], and [7].)

In the iterative solution of systems using either of these matrices, two preconditioner types were employed and compared: a sparse approximate inverse (SPAI) preconditioner (used in Swesty et al. [2]) and a preconditioner based on the alternating direction implicit (iterative) method (used in D'Azevedo et al. [1]), hereafter referred to as an ADI-like preconditioner or even, more simply, an ADI preconditioner. We shall comment briefly on each of these preconditioners.

The ADI method originated in the 1950s, with strong connections to the solution of the discrete Poisson equation. The ADI method is an optimal solution method but only under specific conditions that the discrete Poisson matrix happens to satisfy (cf. [8, pp. 209–249]). For more general matrices, the ADI method has evolved into a preconditioning method. It is one of a number of well-known preconditioners, another of which is the incomplete LU decomposition (ILU).

Over time, hardware improvements have resulted in architectural designs unfriendly to those preconditioners that make use of triangular solves, which is characteristic of many of the classic preconditioners such as ILU and, in particular, ADI. These triangular solves are costly sequential operations that become a bottleneck on parallel platforms (cf. [1, p. 818]). This bottleneck opens up, to some extent, under pressure from ingenious users intent on parallelizing the solution of triangular systems. A discussion of issues involved in designing parallel solvers for triangular systems may be found in [9] and [10]. Certain successful solvers make use of selective inverses (see [11]) or partitioned inverses (see [12]).

An SPAI preconditioner (see [13]) is a matrix that approximates the inverse of the system matrix: no solutions of triangular systems are required, avoiding this major bottleneck. Other advantageous properties of the typical SPAI preconditioner are (1) computation in parallel of the elements of each row or column; and (2) sparsity. The field of SPAI preconditioners is undergoing lively development with many recent contributions for which references [14–18] are a sampling. A good, overall discussion may be found in [19].

This paper reports on tests comparing the performance of SPAI and ADI-like preconditioners applied to two matrices each representing a different class of equations. Studies on the use of the two preconditioners with a specific type of matrix have been reported independently, namely, the use of an ADI preconditioner with MGBT matrices in [1] and the use of SPAI preconditioners with MGFLD matrices in [2]. We studied the performance of the two preconditioners with a matrix of the type other than the one used in the published reports. The results of our experiments show that ADI performs remarkably well on a sequential platform with either type of matrix. Yet, we also believe that SPAI is a viable algorithm in the solution of large scale systems, especially on parallel platforms.

This paper is organized as follows: Section 2 contains an overview of the physics and also presents the structure of the matrices resulting from the discretization of the MGBT and MGFLD equations. Section 3 describes the SPAI and ADI-like preconditioners and the iterative methods used, and Section 4 describes the numerical experiments. Sections 5 and 6 describe the results and conclude that the SPAI and ADI-like preconditioners perform well for both types of matrices although in the MGBT case, careful analysis is required to interpret the results. The conclusion also outlines specific issues to address in future research.

We note that the MGBT system in our experiments was numerically singular. Scaling appears to improve the condition but does not replace a numerically singular system with a numerically nonsingular system.

## 2. Physics overview

Massive stars (with masses >  $10M_{\odot}$  where  $M_{\odot}$  denotes the mass of the sun) that have exhausted much of their nuclear fuel end their lives in a catastrophic gravitational collapse. The evolution of these stars may be explained, briefly, in the following way (Mezzacappa et al. [20]). One may envision a pre-collapse supernova progenitor star as an onion-like structure, in which the innermost iron core is surrounded by layers of silicon, oxygen, carbon, helium and, finally, hydrogen in the outermost layer. At any given instant, fusion reactions convert hydrogen

to helium, helium to carbon, and so on. As a result of these reactions, the mass of the iron core increases and this causes an increase in the gravitational force and consequently an increase in the density of the material in the iron core. Prior to collapse the core of the star approximately balances the inward pull of gravity by the outward pressure due to electron quantum mechanical degeneracy. As the density in the core slowly increases, the electrons and protons combine to form electron neutrinos and neutrons. This depletes the density of electrons, and thus reduces the electron pressure, until the gravitational field completely overwhelms the outward pressure gradient and the core collapses.

When the core collapses, material from the outer edges of the core begins to fall inwards, thereby increasing the core density at a rapid rate. Since the constituents of the core are nucleons, which are fermions, they cannot be squeezed into smaller volumes indefinitely. Doing so would violate the Pauli exclusion principle. At slightly beyond the point where the core density approaches nuclear density levels, the core bounces, thereby generating a shock wave which propagates from the inner regions of the core towards the outer regions. As matter is compressed to high densities, electrons combine with protons from the dissociated nuclei to create electron neutrinos that escape from the collapsing core. The escaping neutrinos carry away a large fraction (approximately 99%) of the energy released during the collapse of the iron core.

The propagating shock heats the matter and dissociates heavy nuclei into unbound neutrons and protons. In the process of doing so, the shock expends energy and weakens and eventually the shock stalls prior to reaching the edge of the collapsing iron core. The core of the star behind the stalled shock is made up of the proto-neutron star, consisting of the unshocked material inside the shock formation radius and the mantle of hot gases above the proto-neutron star and below the stalled shock front. As the mantle cools, three types of neutrinos, namely the electron, tau, and muon neutrinos and their antineutrino counterparts are produced by thermally induced pair-production reactions. It is conjectured (see [21]) that a tiny fraction of these released neutrinos and antineutrinos are re-absorbed by the mantle, thereby re-energizing the stalled shock. It is thought that the newly invigorated shock begins to move outward once again as a result of the neutrino heating. Once the shock wave reaches the edge of the silicon layer the shock can initiate explosive burning of lighter elements into heavier elements. These burning reactions are exothermic and provide the energy needed to propel the shock outward through the remaining layers of the star.

The time scales of the progenitor evolution prior to collapse are on the order of tens of billions of years during which all the hydrogen in the inner layers of the star is converted to heavier elements. In contrast, the collapse of the iron core of the progenitor and the cooling of the proto-neutron star via neutrino emission spans a time of about ten seconds. The goal of current computational research is to simulate this last ten seconds of the star's life.

Several computational challenges drive the simulation. The time and length scales required to capture the physics in the

final phase of the star span many orders of magnitude. The grid resolution, required to account for the length and time scales, and the coupling of the hydrodynamics and neutrino transport equations is affected by two major factors, namely, (1) the time scale for neutrino radiation transport being much smaller than the hydrodynamic time scale, and (2) the distribution of neutrinos being, in general, a function of three spatial, one spectral, and two directional coordinates. The solution of the radiation hydrodynamics (RHD) equations in three spatial dimensions will require the evolution of the MGBT equation for each energy (spectral) and angular (directional) location in the six-dimensional phase space. For the specific case of an isotropic radiation field, the neutrino distribution is not a function of the directional coordinates. This case also allows the representation of the radiation flux as a function of the gradient of the radiation energy density, leading to the MGFLD approximation. Accordingly, a RHD simulation in three spatial dimensions would require evolution of the MGFLD equations in a four-dimensional phase space. The time scales for hydrodynamics and radiation transport are of the order of the ratio of the time taken by sound to cross a computational cell to the time taken by light to cross the same computational cell. Since the speed of sound at these extremely high densities and temperatures is about a tenth of the speed of light, the time scale of the equations of hydrodynamics is about ten times the time scale of the radiation transport equations. Consequently, the system of RHD equations is evolved by the operator splitting technique where every step of the evolution process consists of an evolution of the equations of hydrodynamics by an explicit time stepping scheme followed by an implicit time evolution of either MGBT or MGFLD equations.

# 2.1. The structure of the matrices

As a first step in developing a working simulation, we consider the relatively simple case of a spherically symmetric star. The governing equations for hydrodynamic transport and neutrino transport involve one spatial dimension (see [2,20]) along the radial direction. For this case, the MGBT equations are in three-dimensional phase space and the MGFLD equations are in two-dimensional phase space, and storing the Jacobians does not exceed the memory available on present-day computers. This aspect helps focus attention on the performance of preconditioners per se by side-stepping the questions associated with storing the Jacobian versus generating the elements of the Jacobian on the fly, which is an issue that must be addressed in the simulation of the MGBT and MGFLD equations in higher spatial dimensions. In addition, as noted earlier, the performance of iterative methods with the preconditioners examined in this paper is based on sequential computation and application of the preconditioners.

The sparsity pattern of the MGFLD and MGBT matrices is shown in Fig. 1. (Because of differing sizes of the matrices, the sparsity patterns are not identical, but are close enough that a single pattern will suffice for our purposes. Details are given below.) In this pattern, the dense diagonal blocks represent coupling between the various energy groups of neutrinos in the



Fig. 1. The sparsity pattern of MGBT and MGFLD matrices. The dense diagonal blocks represent coupling between the various energy groups, angles, or  $v-\bar{v}$  pairs at the same spatial location. The two outlying diagonals denote coupling between neighboring spatial locations. The major difference between the two types of systems is in the size of the center blocks (34 × 34 for MGBT matrix and 20 × 20 for MGFLD matrix).

MGFLD case and coupling between angle and energy groups in the MGBT case at a given spatial location. The two outlying bands denote coupling between neighboring spatial grid points, where the number of bands, in general, depends on the spatial discretization stencil used. Spatial derivatives were approximated by the second-order central difference operator in both the MGFLD and MGBT cases.

## 2.2. Condition numbers and scaling

The condition numbers of the Jacobians resulting from both systems of equations range from approximately  $10^5$  for the MGFLD matrix to approximately  $10^{40}$  for the MGBT equations. We reduced the condition number of both types of matrices by row-scaling the elements, that is, by dividing all elements of a row by a preselected non-zero positive scalar.

Scaling is, in fact, a preconditioning, but we choose not to describe it that way because we do it one time only and then apply, within the iterative method, a general preconditioner to the scaled matrix. It is these general preconditioners that are the subject of this report.

In our experiments, we made use of one MGBT matrix (the 30-1 matrix in [1] consisting of  $102 \times 102$  blocks each of size  $34 \times 34$ ) and one MGFLD matrix (the 256 block matrix in [2] consisting of  $256 \times 256$  blocks each of size  $20 \times 20$ ) as samples representative of these two classes of matrices. These two matrices were chosen because they contain approximately the same number of non-zeroes. Table 1 shows the effect of row-scaling these two matrices by the magnitude of largest element in the row. The condition numbers were estimated via Matlab's condition number approximation function for sparse matrices. (In the case of the MGFLD matrix, since it was diagonally dominant, the largest element was on the main diagonal.)

Some comments on the algebraic properties of the MGBT matrix are appropriate. This "30-1" matrix corresponds to early

#### Table 1

	MGBT (30-1)	MGFLD (256 block)
cond(A <sub>original</sub> )	$2.05 \times 10^{40}$	$1.50 \times 10^{5}$
$cond(A_{scaled})$	$3.27 \times 10^{5}$	$1.78 \times 10^4$

core bounce with complex physics, specifically, to a typical timestep around the time of bounce of the inner core at supernuclear densities. Later timesteps would contain non-zero contributions from neutrino pair creation and annihilation, which are strongly suppressed (but calculated) in this earlier matrix. The maximum norm (also known as the  $\ell_{\infty}$  norm) of the first 32 rows of each  $34 \times 34$  diagonal dense block varies from approximately  $10^{-17}$  to  $10^{-8}$ . The maximum norm of the 33rd row is approximately  $10^{19}$ , however, and that of the last row is approximately 1. The large difference in magnitude between the first 32 row vectors and the last two row vectors is the reason for the large condition number of the MGBT matrix. Based on the way it was constructed, this "30-1" matrix is not analytically singular, although very ill-conditioned before row scaling, and could therefore be described as being numerically singular.

The large condition number of the MGBT matrix means, however, that care must be taken in interpreting the solution of the scaled system, which is nonsingular. For, let  $\hat{x}$  be the solution of the (nonsingular) scaled system. Then  $\hat{x}$  is also a solution of the original system, but there is no unique solution, due to numerical singularity. The correct solution cannot result from algebraic laws alone; any solution must also be validated by the physical principles and the physical constraints out of which the problem arose.

# 3. Preconditioners

The efficient iterative solution of a linear system, Ax = bwhere  $A \in \mathbb{R}^{n \times n}$  and  $x, b \in \mathbb{R}^n$ , usually requires preconditioning.

The preconditioned matrix equation, in its most general form, is

$$M_L^{-1} A M_R^{-1} M_R x = M_L^{-1} b \iff \tilde{A} \tilde{x} = \tilde{b}$$
(1)

where

$$\tilde{A} = M_L^{-1} A M_R^{-1}, \quad \tilde{x} = M_R x, \quad \tilde{b} = M_L^{-1} b$$

and  $M_L^{-1}, M_R^{-1} \in \mathbb{R}^{n \times n}$  denote left and right preconditioners respectively. The goal of using preconditioners is to obtain a preconditioned system  $\tilde{A}\tilde{x} = \tilde{b}$  that has better numerical properties. In general, the guiding principles for developing preconditioners are often based more on intuition than on mathematical rigor. Whatever the intuitive idea, a standard desideratum is that  $M_R^{-1}M_L^{-1} \approx A^{-1}$ . In the numerical experiments described below, preconditioners are limited to just the left preconditioner, i.e.,  $M_R^{-1} = I$ . Thus, subsequent discussion will focus only on  $M_I^{-1}$  which will be referred to as  $M^{-1}$ .

# 3.1. SPAI preconditioners

A sparse approximate inverse (SPAI) preconditioner (see [13,19]) is a sparse matrix  $M^{-1}$ , which approximates  $A^{-1}$  in some sense. The sparsity pattern of  $M^{-1}$  is chosen according to some algorithm. One commonly available algorithm to choose the sparsity pattern is that used in software developed by Grote et al. (see [22]). Another algorithm, employed in the numerical experiments reported here, is to predetermine the locations of non-zero elements of the preconditioner based on some heuristic, such as the one described further below.

Once the sparsity pattern of the SPAI preconditioner has been determined, the elements of the matrix  $M^{-1}$  are computed by minimizing  $||M^{-1}A - I||_F$ , where  $|| \cdot ||_F$  is the Frobenius norm (see [23, p. 55] or [24, p. 8]). Minimizing  $||M^{-1}A - I||_F$ is equivalent to minimizing  $||(M^{-1})_jA - e_j||_2$  for each row of the preconditioner, with j = 1, 2, ..., n and  $e_j$  the unit vector with 1 as the *j*th component. Minimizing the  $|| \cdot ||_2$  norm is a least squares problem. In practice, since least squares solvers assume the unknown to be a right vector of the system of linear equations, we obtain  $M^{-1}$  by minimizing  $||\hat{A}^T(M^{-1})_j^T - e_j||_2$ , where  $\hat{A}$  consists of those rows of A corresponding to the desired sparsity pattern in row j of  $M^{-1}$ .

The goal of SPAI is to obtain, in a cost-effective way, an approximate inverse that is sparse and also is an effective preconditioner. A sparse preconditioner would decrease the computation time per step, and an effective preconditioner would decrease the number of iterations needed for an iterative solver to achieve convergence.

In some cases, the true inverse is observed to possess a pattern of dominant values (as was determined in the MGFLD matrices studied in [2]), such as along diagonals equally spaced from the main diagonal. (We use the term dominant here to refer to any of several values in a row, each of whose magnitudes is greater than the sum of the magnitudes of the other, nondominant values in that row.) In a case such as this, it seems reasonable to force the SPAI sparsity pattern to reflect the pattern of the true inverse. For our numerical experiments, we used a predetermined sparsity pattern based on an examination of the actual inverses of the two matrices. We call such an SPAI preconditioner a "predetermined sparsity pattern" preconditioner. Computing the inverse is not, in general, practical, but tests in [2] have shown that a sparsity pattern coming from the inverse of a small matrix can be successfully applied to a larger matrix of the same class.

We also used the Barnard–Grote SPAI package<sup>1</sup> to obtain SPAI matrices for both the MGBT and MGFLD matrices. This package uses a heuristic to determine the optimal number of elements per row based on an input tolerance, and then computes a matrix with this sparsity pattern. Determining the sparsity pattern, however, incurs an overhead that is absent when a predetermined sparsity pattern algorithm was used with a very limited number of elements (e.g., 3 or 5) per row. In the case of the MGFLD matrix, the SPAI preconditioner from the Barnard– Grote package gave about the same convergence results as the SPAI preconditioner with the predetermined tridiagonal pattern mentioned below. In the case of the MGBT matrix, the Barnard–Grote SPAI preconditioner performed poorly after the first few iterations and even started to diverge. We attribute this poor performance to the numerical singularity of the original MGBT matrix as well as to the lack of a sharply defined sparsity pattern of dominant values in the actual inverse.

## 3.2. ADI-like preconditioners

The ADI-like preconditioning developed by D'Azevedo et al. [1], can be summarized in two steps: (1) solve a block diagonal system, neglecting the spatial coupling, and (2) solve the tridiagonal system, involving the spatial differencing terms, while neglecting the dense diagonal blocks (retaining only the main diagonal).

The system matrix A (see Fig. 1) can be decomposed in a particular way into the sum of matrices B, C, and  $D_{block}$ , as follows. Given a value for the center block size m, B is the matrix consisting of the mth diagonal below the main diagonal of A, C is the matrix consisting of the mth diagonal above the main diagonal of A,  $D_{block} = A - B - C$ , and T = diagonal(A) + B + C. The first step of this preconditioning consists of solving the system  $D_{block}z_1 = r_k$  where  $r_k$  is the residual  $r_k = b - Ax_k$  and the second step involves solving the system  $Tz_2 = p_k$  where  $p_k = r_k - Az_1$ . Together  $z_1$  and  $z_2$  form the correction to obtain a new value of  $x_k$ . (The Matlab code can be found in [1]. For a detailed discussion on ADI methods, see Chapter 7 of [8].)

# 4. Iterative solvers

In the numerical experiments described below, the systems of equations were solved by using three iterative methods: the fixed-point iteration (used in [1]), the generalized minimal residual method (GMRES), and the Biconjugate Gradient Stabilized (BiCGStab) method.

The fixed-point iteration is  $r_k = b - Ax_k$  where  $x_k = x_{k-1} + M^{-1}r_{k-1}$  and  $M^{-1}$  was the chosen preconditioner. This is also known as Richardson's method (see [25, p. 361]). Both GM-RES and BiCGStab are Krylov subspace methods. GMRES computes a new approximation at each step such that the norm of the residual is minimized. The BiCGStab algorithm is a variant of the Conjugate Gradient Squared (CGS) algorithm in which a residual vector is minimized over a different subspace than for GMRES. Details can be found in standard references, such as Saad [24] or Greenbaum [26]. Also see Press et al. [27] for a general introduction.

# 5. Numerical experiments

As noted earlier, in our experiments we made use of rowscaled versions of one MGBT matrix (the 30-1 matrix in [1]) and one MGFLD matrix (the 256 block in [2]) as representative samples of the two classes of matrices studied in [1] and in [2]. We report the results of these specific representative

<sup>&</sup>lt;sup>1</sup> See http://www.sam.math.ethz.ch/~grotc/spai/.



Fig. 2. The sparsity pattern of the dominant entries of a representative  $200 \times 200$  block along the diagonal of the inverse of the MGFLD matrix.

matrices and note, in particular, that the inversion of these matrices produces the solution of the linearized transport problem at a single time step taken from extended temporal evolution of MGBT and MGFLD systems coupled to hydrodynamics. The couplings exhibited in each of these matrices span a variety of thermodynamic conditions and are calculated from realistic physical models of the interactions of the neutrino radiation field with the stellar matter. Although the specific magnitude and structure of the coupling patterns will change if other time steps are chosen for examination, we expect that the results we obtain here are representative for a large portion of the coupled physics simulations.

An examination of the actual inverse of the MGFLD matrix showed that the dominant values were on diagonals spaced at 20 element intervals on either side of the main diagonal (Fig. 2). Various SPAI preconditioners, all with a predetermined sparsity pattern, were tested in [2] with different numbers of diagonals. The preconditioner that generally gave the best results in our tests was a tridiagonal matrix with a main diagonal and additional diagonals spaced 20 elements away on either side of the main diagonal. (Henceforth, we refer to this matrix as the tridiagonal SPAI matrix.) The tridiagonal SPAI matrix performed as well as a pentadiagonal and a 9-diagonal SPAI matrix (both with the same diagonal spacing), and the computational overhead was cheaper. As noted earlier, the convergence using the SPAI preconditioner from the Barnard-Grote package was quite similar to the convergence using the tridiagonal SPAI preconditioner.

The actual inverse of the MGBT matrix, in contrast, did not reveal a pronounced pattern that could be used to construct SPAI preconditioners (Fig. 3), unlike the case for the inverse of the MGFLD matrix. An SPAI preconditioner obtained from the Barnard–Grote package was applied to the MGBT matrix. With default values for the input tolerance, this preconditioner caused the convergence to stagnate after a few iterations. In contrast, using the predetermined sparsity pattern of a  $34 \times 34$  block diagonal matrix for our SPAI preconditioner led to convergence, although at a slower rate than the ADI-like preconditioner.

# 6. Results

Figs. 4(a)–4(d) compare the results of using tridiagonal SPAI and ADI-like preconditioning on the MGFLD matrix with GM-RES, BiCGStab, and Richardson's fixed-point iterative methods. For our numerical experiments, the GMRES restart parameter was 30 (the Matlab default). An ADI-like preconditioner for MGBT matrices, as described in [1], was effective. The same preconditioner, suitably modified, was also effective for the MGFLD matrix we investigated. In addition, we made use of the Barnard–Grote SPAI package to obtain an alternative SPAI matrix. It gave results comparable to those from the tridiagonal SPAI preconditioner at the cost of additional overhead to determine the sparsity pattern.

Since a flop count is dependent on the efficiency of an algorithm's implementation and CPU timing is dependent on a platform's user load, we decided to make use of two invariant measures: the number of matrix–vector products ("matvecs") and the number of iterations. Both matvecs and iterations are invariant across platforms and whether running an algorithm on a sequential platform or in parallel.

Figs. 5(a)–(5d) compare ADI-like and block diagonal SPAI preconditioning on the MGBT matrix also with GMRES, BiCGStab, and fixed-point iterations. The plots show the apparent superiority of ADI-like preconditioning. However, much of this apparent superiority derives from the tridiagonal solve as was noted in Swesty et al. [2] where similar results were obtained without the use of the costly block preconditioning step.

We note that the convergence behavior on display in Fig. 5 shows stagnation in the convergence of the SPAI preconditioned MGBT system. Stagnation could be related to numerical singularity, rather than the SPAI preconditioner per se.

Certain other features are important to note:

- For MGFLD matrices, SPAI is a tridiagonal matrix whereas for the ADI preconditioning matrix dense sub-blocks require a costly processing to implement.
- For the MGBT case, the SPAI preconditioner has, however, dense sub-blocks, but no preprocessing is required.



Fig. 3. The sparsity pattern of the dominant entries in the upper left corner, mid-matrix, and lower right corner of the inverse of the MGBT matrix.



Fig. 4. The performance of the SPAI and ADI-like preconditioners for the  $256 \times 256$  block Jacobian matrix from the MGFLD equations (labeled as nexp $256_{1.0e0}$ ). The plots compare the reduction in the residual versus the number of iterations and the number of matrix–vector products ("matvecs").

 SPAI parameters have to be computed prior to beginning any iterative solution process, whereas the ADI preconditioner requires no comparable parameters but does require an LU factorization.

## 7. Conclusions

Our primary objective was to compare, on a sequential platform, the use of two different preconditioners applied to linear systems involving two different matrices related to similar physical phenomena. As has already been noted, the original MGBT and MGFLD matrices, although similar in size and sparsity, were significantly different in conditioning, but the scaled matrices used in our tests were quite similar in their conditioning. We see our results as providing motivation for additional work addressing issues beyond the scope of this project, in particular, how an efficient implementation of the algorithms and the preconditioners on a parallel machine would vary the results.

Figs. 4 and 5 do not reflect the set-up and overhead time required to compute the SPAI preconditioner. But these set-up and overhead times are, in fact, quite minor since there is no cost associated with determining the sparsity pattern of a predetermined pattern SPAI preconditioner and only the relatively minor overhead of solving, for each row of the preconditioner,  $a k \times n$  least squares system where *n* is the number of non-zeros in that row of the preconditioner and *k* the number of values taken from the corresponding rows of the system matrix. Predetermined patterns, when they are identifiable, lead to lower set-up and overhead costs, in comparison with the work needed for the LU factorization of the dense diagonal blocks, which are necessary for the ADI-like preconditioning.

Our tests do show the apparent success of using ADI-like preconditioning for both MGBT and MGFLD matrices (using the schemes mentioned in Section 1 for ordering the variables). For the MGBT matrix, the use of the SPAI preconditioner results in a stagnation or very slow convergence, in comparison to the use of the ADI-like preconditioner. For the MGFLD matrix, however, the SPAI preconditioner did not stagnate, but converged steadily, yet at a somewhat slower rate than with the ADI-like preconditioner, no matter which of the two measurements of matvecs or iterations was used.

The steady convergence leads us, therefore, to suggest that, for an MGFLD matrix, the definite superiority of ADI-like preconditioning over SPAI is still inconclusive. One of the reasons for this statement is the inherent advantage on parallel plat-



Fig. 5. The performance of the SPAI and ADI-like preconditioners for the  $34 \times 34$  block Jacobian matrix from the MGBT equations (labeled as 30-1). The plots compare the reduction in the residual versus the number of iterations and the number of matrix-vector products ("matvecs").

forms in the multiplication of matrices, a feature of SPAI preconditioning, as compared to the backward and forward solves needed to implement ADI-like preconditioners, even with improved parallel implementations. This potential savings is not apparent in Figs. 4 and 5 and, we suggest, is one topic for future investigation.

We also believe our results encourage further studies with matrices of different sizes to address questions related to the scalability of the two preconditioners with either type of matrix. Some scalability tests were reported in [2, pp. 380–383] for SPAI preconditioners and three sizes of MGFLD matrices, and these tests show essentially the same number of iterations needed for convergence for all three sizes of matrices. Further studies are needed with ADI-like preconditioners on MGFLD matrices and with the use of both preconditioners on similarly-sized MGBT matrices.

# Credits and acknowledgements

The basic work on ADI-like preconditioners and MGBT matrices was done by Eduardo D'Azevedo, Bronson Messer and others from Oak Ridge National Laboratory. The basic work on SPAI preconditioners and MGFLD matrices by Doug Swesty from SUNY Stony Brook in collaboration with Paul Saylor (University of Illinois at Urbana–Champaign [UIUC]) and Dennis Smolarski (Santa Clara University [SCU], while on leave at UIUC). Anthony Mezzacappa from Oak Ridge National Laboratory suggested a comparison between the two different preconditioners on both MGBT and MGFLD matrices. The comparison of the two preconditioners was done by Ramesh Balakrishnan, John Fettig, Faisal Saied, Paul Saylor (all from UIUC) and Dennis Smolarski (from SCU).

We also would like to thank Victor Eijkhout from the Texas Advanced Computer Center at the University of Texas at Austin for discussions regarding the ADI-like preconditioner for the MGBT matrices.

This work is supported by the Department of Energy SciDAC cooperative agreement DE-FC02-01ER41185, http: //www.phy.ornl.gov/tsi/. This research work used the computational resources at the National Center for Supercomputing Applications, http://www.ncsa.uiuc.edu.

## References

 E.F. D'Azevedo, B. Messer, A. Mezzacappa, M. Liebendoerfer, An Adilike preconditioner for Boltzmann transport, SIAM J. Sci. Comput. 26 (2005) 810–820.

- [2] F.D. Swesty, D.C. Smolarski, P.E. Saylor, A comparison of algorithms for the efficient solution of the linear systems arising from multi-group fluxlimited diffusion problems, Astrophys. J. Suppl. Ser. 153 (2004) 369–387.
- [3] A. Mezzacappa, S.W. Bruenn, A numerical method for solving the neutrino Boltzmann equation coupled to spherically symmetric stellar core collapse, Astrophys. J. 405 (1993) 669–684.
- [4] M. Liebendörfer, Consistent modelling of core-collapse supernovæ in spherically symmetric relativistic space-time, Ph.D. Thesis, The University of Basel, 2000.
- [5] O.E.B. Messer, Questing for the grail: Spherically symmetric supernova simulations with Boltzmann neutrino transport, Ph.D. Thesis, The University of Tennessee, 2000.
- [6] D. Mihalas, B.W. Mihalas, Foundations of Radiation Hydrodynamics, Dover, Mineola, 1984.
- [7] N.J. Turner, J.M. Stone, A module for radiation hydrodynamic calculations with ZEUS-2D using flux-limited diffusion, Astrophys. J. Suppl. Ser. 135 (2001) 95–107.
- [8] R.S. Varga, Matrix Iterative Analysis, Prentice-Hall, Englewood Cliffs, 1962.
- [9] F.L. Alvarado, R. Schreiber, Optimal parallel solution of sparse triangular systems, SIAM J. Sci. Stat. Comput. 14 (1993) 446–460.
- [10] E.E. Santos, On designing optimal parallel triangular solvers, Inform. Comput. 161 (2000) 172–210.
- [11] P. Raghavan, Efficient parallel triangular solution with selective inversion, Parallel Process. Lett. 8 (1998) 29–40.
- [12] N.J. Higham, A. Pothen, The stability of partitioned inverse approach to triangular solution, SIAM J. Sci. Stat. Comput. 15 (1994) 139–148.
- [13] H.I.M. Gould, J.A. Scott, On approximate-inverse preconditioners, Technical Report RAL 95-026, Computing and Information Systems Department, Rutherford Appleton Laboratory, Oxfordshire, England, 1995.

- [14] M. Benzi, D. Bertaccini, Approximate inverse preconditioning for shifted linear systems, BIT 43 (2003) 231–244.
- [15] M. Bollhöfer, V. Mehrmann, Algebraic multilevel methods and sparse approximate inverses, SIAM J. Matrix Anal. Appl. 24 (2002) 191–218.
- [16] M. Bollhöfer, Y. Saad, A factored approximate inverse preconditioner with pivoting, SIAM J. Matrix Anal. Appl. 23 (2002) 692–705.
- [17] M. Bollhöfer, Y. Saad, On the relations between ILUs and factored approximate inverses, SIAM J. Matrix Anal. Appl. 24 (2002) 219–237.
- [18] K. Chen, An analysis of sparse approximate inverse preconditioners for boundary integral equations, SIAM J. Matrix Anal. Appl. 22 (2001) 1058– 1078.
- [19] E.T.-F. Chow, Robust preconditioning for sparse linear systems, Ph.D. Thesis, The University of Minnesota, 1997.
- [20] A. Mezzacappa, O.E.B. Messer, Neutrino transport in core collapse supernovae, J. Comput. Appl. Math. 109 (1999) 281–319.
- [21] H. Bethe, J.R. Wilson, Revival of a stalled supernova shock by neutrino heating, Astrophys. J. 295 (1985) 14–23.
- [22] M.J. Grote, T. Huckle, Parallel preconditioning with sparse approximate inverses, SIAM J. Sci. Comput. 18 (1997) 838–853.
- [23] G.H. Golub, C.F. van Loan, Matrix Computations, third ed., Johns Hopkins University Press, Baltimore, 1996.
- [24] Y. Saad, Iterative Methods for Sparse Linear Systems, second ed., SIAM, Philadelphia, 2003.
- [25] D.M. Young, Iterative Solution of Large Linear Systems, Academic Press, New York, 1971.
- [26] A. Greenbaum, Iterative Methods for Solving Linear Systems, SIAM, Philadelphia, 1997.
- [27] W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, Numerical Recipes in Fortran 77, Cambridge University Press, Cambridge, 1992.

-