Mem. S.A.It. Vol. 80, 631

Memorie della

Projection methods for line radiative transfer in spherical media

L. S. Anusha and K. N. Nagendra

Indian Institute of Astrophysics, Koramangala 2nd Block, Bangalore 560 034, India
e-mail: anusha@iiap.res.in

Abstract. An efficient numerical method called the Preconditioned Bi-Conjugate Gradient (Pre-BiCG) method is presented for the solution of radiative transfer equation in spherical geometry. A variant of this method called Stabilized Preconditioned Bi-Conjugate Gradient (Pre-BiCG-STAB) is also presented. These methods are based on projections on the subspaces of the n dimensional Euclidean space $\mathbb{R}^n$ called Krylov subspaces. The methods are shown to be faster in terms of convergence rate compared to the contemporary iterative methods such as Jacobi, Gauss-Seidel and Successive Over Relaxation (SOR).

Key words. line: formation – numerical radiative transfer – methods: techniques

1. Introduction

The Krylov subspace methods are a class of projection methods which can solve large systems of equations rapidly (see, for e.g., Saad 2000). Such methods were introduced to radiative transfer by Klein et al. (1989). Recently Paletou & Anterrieu (2009) proposed Preconditioned Bi-Conjugate Gradient (Pre-BiCG) method to solve transfer in planar geometry. A slightly different method called GMRES was introduced to radiative transfer by Hubeny & Burrows (2007). Here we present the Pre-BiCG method as applied to the case of spherical radiative transfer with 2-level atom model and complete frequency redistribution. See Anusha et al. (2009) for more details. We also present a more advantageous, transpose free variant of it namely Pre-BiCG-STAB method.

Send offprint requests to: L. S. Anusha

2. Governing equations

The geometry of the problem is described in Anusha et al. (2009). The transfer equation is solved on a set of tangent rays.

For the outgoing (+) and incoming (−) rays respectively, the transfer equation can be written as

$$\pm\frac{\partial \boldsymbol{I}^{\pm}(z,p,x)}{\partial z} = [\chi_{\mathrm{L}}(r)\phi(x)+\chi_{\mathrm{C}}(r)] \times[\boldsymbol{S}(x,r)-\boldsymbol{I}^{\pm}(z,p,x)]. \quad (1)$$

Here r is the radial distance, z is the distance along the tangent rays and p is the distance from the center to those points on the vertical axis (the mid-line), where the tangent rays intersect it. The direction cosines μ $(0 \le \mu \le 1)$ and p are related by $\mu = \sqrt{1-(p/r)^2}$ for a shell of radius r. The optical depth scale along the tangent rays are computed using $\mathrm{d}\tau(z) =$

$d\tau(r)/\mu$. The line source function is given by

$$\boldsymbol{S}(r) = (1-\epsilon)\int_{-1}^{1}\frac{d\mu'}{2}\int_{-\infty}^{\infty}dx' \phi(x')\boldsymbol{I}(\tau,\mu',x') + \epsilon \boldsymbol{B}_\nu(r). \quad (2)$$

Substituting the formal solution expression for $\boldsymbol{I}$ in Eq. 2 we get an integral equation for $\boldsymbol{S}$, which can be written in an operator form as

$$[\hat{I} - (1-\epsilon)\hat{\Lambda}]\boldsymbol{S} = \epsilon \boldsymbol{B}_\nu. \quad (3)$$

We can re-write the above equation as

$$\hat{A}\boldsymbol{S} = \boldsymbol{b}; \quad \text{with} \quad \hat{A} = [\hat{I} - (1-\epsilon)\hat{\Lambda}], \quad \text{and} \quad \boldsymbol{b} = \epsilon \boldsymbol{B}_\nu. \quad (4)$$

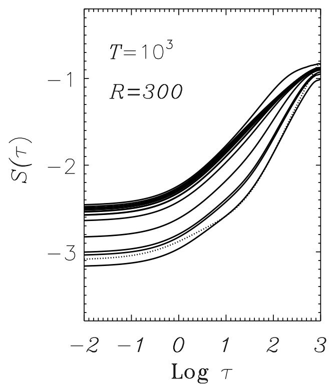

Fig. 1. Convergence history of the source function $\boldsymbol{S}(\tau)$ in the Pre-BiCG-STAB method.

3. Basics of the Preconditioned Bi-Conjugate Gradient method

Let $\mathbb{R}^n$ denote the n-dimensional Euclidean space of real numbers, and

$$\mathcal{K}_{\mathrm{m}} = \mathrm{span}\{\boldsymbol{v}_1, \hat{A}\boldsymbol{v}_1, \ldots, \hat{A}^{m-1}\boldsymbol{v}_1\}, \quad (5)$$

define an m-dimensional subspace of $\mathbb{R}^n$. We denote by $\mathcal{L}_{\mathrm{m}}$ another m-dimensional subspace of $\mathbb{R}^n$ orthogonal to $\mathcal{K}_{\mathrm{m}}$.

$$\mathcal{L}_{\mathrm{m}} = \mathrm{span}\{\boldsymbol{w}_1, \hat{A}^T\boldsymbol{w}_1, \ldots, \hat{A}^{T(m-1)}\boldsymbol{w}_1\}. \quad (6)$$

Here $\boldsymbol{v}_1$ is taken as the initial residual vector $\boldsymbol{r}_0 = \boldsymbol{b} - \hat{A}\boldsymbol{S}_0$ with $\boldsymbol{S}_0$ being the initial guess for the solution of Eq. (4). The vector $\boldsymbol{w}_1$ is taken arbitrarily such that the inner product $\langle \boldsymbol{v}_1, \boldsymbol{w}_1\rangle \neq 0$. The Pre-BiCG method recursively constructs a pair of bi-orthogonal bases $\{\boldsymbol{v}_{\mathrm{i}}; \mathrm{i} = 1, 2 \ldots, m\}$ and $\{\boldsymbol{w}_{\mathrm{i}}; \mathrm{i} = 1, 2 \ldots, m\}$ for $\mathcal{K}_{\mathrm{m}}$ and $\mathcal{L}_{\mathrm{m}}$ respectively, such that they satisfy the bi-orthogonality condition $\langle \boldsymbol{v}_{\mathrm{i}}, \boldsymbol{w}_{\mathrm{j}}\rangle = \delta_{\mathrm{ij}}$. We refer to Anusha et al. (2009) for the Pre-BiCG algorithm applied to the spherical transfer. We give below a transpose free variant of it namely Pre-BiCG-STAB.

4. Transpose free variant of the Pre-BiCG method (Pre-BiCG-STAB)

In spite of higher convergence rate, computation and storage of the $\hat{A}^T$ matrix is a main disadvantage of the Pre-BiCG method. To overcome this difficulty, the governing equations can be re-formulated to use only the 'action' of $\hat{A}$ matrix on an arbitrary vector. Re-defining the residual polynomial as a product of two polynomials and obtaining a recursive relation for the new residual polynomial constitutes the basis of the Pre-BiCG-STAB method. This product involves residual polynomial of the Pre-BiCG method and a new polynomial which 'smoothens' the iterative process. In this section we give the computing algorithm of the Pre-BiCG-STAB method as applied to a radiative transfer problem. As described below, we can avoid computing and storing of the $\hat{A}^T$ matrix. However we would now need to call the formal solver twice per iteration unlike the Pre-BiCG method, where it is called only once. This results in an increase in number of operations per iteration when compared to Pre-BiCG method, causing a slight increase in the CPU time per iteration. In spite of these the Pre-BiCG-STAB method turns out to be always faster than the regular Pre-BiCG method in terms of convergence rate (lesser number of iterations for convergence). The convergence behavior of this method is shown in Fig. 1. What is shown is the history of convergence of the line source function plotted as a function of optical depth τ in log scale. The $\boldsymbol{S}(\tau)$ in the first iteration is shown as the dotted line. The convergence rate shows a non-uniform behavior in the beginning. However, after the fourth iteration, the convergence rate is uniform.

4.1. The Pre-BiCG-STAB algorithm

Now we give the algorithm of Pre-BiCG-STAB method to solve the system $\hat{M}^{-1}\hat{A}\boldsymbol{S} = \hat{M}^{-1}\boldsymbol{b}$. Here $\hat{M}$ is a suitably chosen preconditioner matrix. The computing algorithm is organized as follows:

(a) The initial preconditioned residual vectors are defined through

$$z_0 = \hat{M}^{-1}\boldsymbol{b} - \hat{M}^{-1}\hat{A}\boldsymbol{S}, \quad z_0^* = z_0. \tag{7}$$

The initial conjugate direction vector $\boldsymbol{P}_0$ can be taken as z_0 itself.
(b) For j = 1, 2, ... the following steps ((c)-(k)) are carried out until convergence.

(c) Using $\boldsymbol{P}_{\rm j}$ instead of the source function a call to the formal solver is made, to compute $\hat{A}\boldsymbol{P}_{\rm j}$.

(d) The coefficient $\alpha_{\rm j}$ can now be evaluated as

$$\alpha_{\rm j} = \frac{\langle z_{\rm j}, z_0^*\rangle}{\langle \hat{M}^{-1}\hat{A}\boldsymbol{P}_{\rm j}, z_0^*\rangle}. \tag{8}$$

(e) Another vector $\boldsymbol{q}_{\rm j}$ is calculated as

$$\boldsymbol{q}_{\rm j} = z_{\rm j} - \alpha_{\rm j}\hat{M}^{-1}\hat{A}\boldsymbol{P}_{\rm j}. \tag{9}$$

(f) Using $\boldsymbol{q}_{\rm j}$ in place of the source function a call to the formal solver is made to obtain $\hat{A}\boldsymbol{q}_{\rm j}$.

(g) The coefficient $\omega_{\rm j}$ is estimated as

$$\omega_{\rm j} = \frac{\langle \hat{M}^{-1}\hat{A}\boldsymbol{q}_{\rm j}, \boldsymbol{q}_{\rm j}\rangle}{\langle \hat{M}^{-1}\hat{A}\boldsymbol{q}_{\rm j}, \hat{M}^{-1}\hat{A}\boldsymbol{q}_{\rm j}\rangle}. \tag{10}$$

(h) The updated new source function is calculated using

$$\boldsymbol{S}_{\rm j+1} = \boldsymbol{S}_{\rm j} + \alpha_{\rm j}\boldsymbol{P}_{\rm j} + \omega_{\rm j}\boldsymbol{q}_{\rm j}. \tag{11}$$

(i) Test for convergence is made as in the Pre-BiCG algorithm.

(j) Before going to the next iteration a set of recursive relations are used to compute residual vectors

$$z_{\rm j+1} = \boldsymbol{q}_{\rm j} - \omega_{\rm j}\hat{M}^{-1}\hat{A}\boldsymbol{q}_{\rm j}, \tag{12}$$

and the conjugate direction vectors

$$\boldsymbol{P}_{\rm j+1} = z_{\rm j+1} + \beta_{\rm j}(\boldsymbol{P}_{\rm j} - \omega_{\rm j}\hat{M}^{-1}\hat{A}\boldsymbol{P}_{\rm j}), \tag{13}$$

for the next iteration, where the coefficient $\beta_{\rm j}$ is

$$\beta_{\rm j} = \frac{\langle z_{\rm j+1}, z_0^*\rangle}{\langle z_{\rm j}, z_0^*\rangle}\frac{\alpha_{\rm j}}{\omega_{\rm j}}. \tag{14}$$

(k) The control is now transferred to the step (b).

5. Comparison of ALI and Pre-BiCG methods

In this section we compare the maximum relative change $R_{\rm c}$ for the Jacobi, Gauss-Seidel (GS), Successive Over Relaxation (SOR), Pre-BiCG and the Pre-BiCG-STAB methods. The SOR parameter used is 1.5. The maximum relative change is defined as

$$R_{\rm c} = \max_{\tau}\{\delta\boldsymbol{S}^n/\boldsymbol{S}^n\}, \tag{15}$$

where $\delta\boldsymbol{S}^n$ is the source function correction at nth iterate. It is worth noting that the overrates (the time taken to prepare the necessary set up, before initiating the iterative cycle) are expected to be different for different methods. For instance, in Jacobi and GS/SOR this is essentially the CPU time required to set up the $\hat{\Lambda}^*$ matrix. In the Pre-BiCG method this involves the time taken to construct the $\hat{A}^T$ matrix, which is a critical quantity of this method. For the Pre-BiCG-STAB method it is the time taken to construct the preconditioner matrix $\hat{M}$.

Fig. 2 shows a plot of $R_{\rm c}$ for different methods. We can take $R_{\rm c}$ as a measure of the convergence rate. In the case of spherical radiative transfer a spatial grid with a large number of points per decade becomes necessary to achieve reasonable accuracy. In the following we discuss how different methods respond to the grid refinement. It is a well known fact with the ALI methods, that the convergence rate is small when the resolution of the depth grid is very high. On the other hand the $R_{\rm c}$ of Pre-BiCG and Pre-BiCG-STAB methods have higher convergence rate even in a high resolution grid. Fig. 2(a) shows $R_{\rm c}$ for different methods when a low resolution spatial grid is used

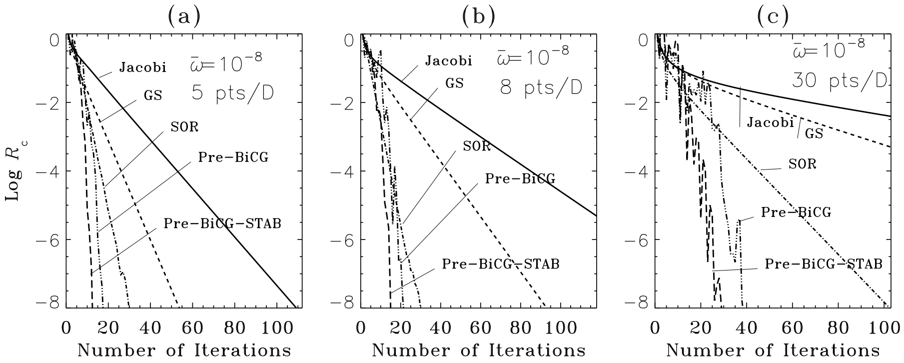

Fig. 2. Dependence of the Maximum Relative Change R_c on the iterative progress for different iterative methods. Panels (a), (b), and (c) represent models with low, medium and high spatial resolution respectively. The model parameters are ($\tilde{n}$, R, T, a, ϵ, β_c, B_ν)= (0, 10, 10^3, 10^{-3}, 10^{-4}, 0, 1) in standard notation (see Mihalas 1978). The convergence criteria is chosen arbitrarily as $\bar{\omega} = 10^{-8}$. The SOR parameter ω =1.5. The figures show clearly that Jacobi method has the smallest convergence rate, which progressively increases for GS and SOR methods. Pre-BiCG and Pre-BiCG-STAB methods have the largest convergence rate compared to the other three.

(5 points per decade, in short 5 pts/D, in the logarithmic scale for τ grid). Fig. 2(b) and 2(c) are shown for intermediate (8 pts/D) and very high (30 pts/D) grid resolutions. The essential point to note is that, as the grid resolution increases, the convergence rate decreases drastically and monotonically for the Jacobi and the GS methods. It is not so drastic for the SOR method. The Pre-BiCG and Pre-BiCG-STAB methods are relatively less sensitive to the grid resolution.

6. Conclusions

It is shown that the class of iterative methods called Pre-BiCG and Pre-BiCG-STAB which are derived from the idea of Krylov subspaces are quite efficient, when compared to the traditionally used iterative methods in radiative transfer theory.

Acknowledgements. K. N. Nagendra is grateful to the IAU for a grant, which enabled him to participate in the IAU General Assembly held in Rio de Janeiro, Brazil in 2009. The authors would like to thank Dr. M. Sampoorna from IAC, Tenerife for reading the paper, and suggesting useful changes.

References

Anusha, L. S., Nagendra, K. N., Paletou, F., & Léger, L. 2009, ApJ, (in press), arXiv:0906.2926)

Hubeny, I., & Burrows, A. 2007, ApJ, 659, 1458

Klein, R. I., Castor, J. I., Greenbaum, A., Taylor, D., & Dykema, P. G. 1989, JQSRT, 41, 199

Mihalas, D. 1978, Stellar Atmospheres (2nd ed.; San Francisco: Freeman)

Paletou, F., & Anterrieu. 2009, A&A, (accepted), (arXiv:0905.3258)

Saad, Y. 2000, Iterative methods for Sparse Linear Systems (2nd ed.)