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Application of the Chebyshev Method to Radiative Transfer Calculations for Laser Heated Targets

D. J. BOND

The Blackett Laboratory, Imperial College of Science and Technology, London SW7 2BZ, United Kingdom

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The Chebyshev semi-iterative method is used to accelerate the Λ iteration for solving the radiative transfer equation for a spectral line. For conditions typical of laser heated targets this method may be more efficient than those used in present calculations.

Recent simulations of X-ray line emission spectra from laser produced plasmas have employed sophisticated non-local thermodynamic equilibrium radiative transfer models [2, 4, 8, 11, 12, 17, 19]. These calculations involve a coupled solution of the radiative transfer equation and atomic rate equations. The hydrodynamic variables are assumed to be known; either from code calculations or experimental measurements.

In this paper one aspect of such a calculation is investigated; the efficient solution of the radiative transfer equation for a single spectral line. This is relevant to the simulation of laser produced plasmas since the equivalent two-level atom approach [13] has been found adequate for such applications [12]. Also the assumption of complete redistribution has been made. If the Eddington factor iteration method is employed (e.g. [12]) then the most time-consuming part of the calculation is the solution of

$$\frac{d}{d\tau}\frac{1}{\phi}\frac{d}{d\tau}fJ = \phi(J - S), \tag{1}$$

$$S = \frac{\langle J\rangle + \varepsilon^* B}{1 + \varepsilon^+}, \tag{2}$$

$$\langle J\rangle = \int_{-\infty}^{+\infty} \phi J_\nu \, d\nu$$

with appropriate boundary conditions.

The frequency-dependent Eddington factors, f_ν, are given by

$$f_\nu = \int_0^{+1} \mu^2 u_\nu \, d\mu \Big/ \int_0^{+1} u_\nu \, d\mu.$$

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The Eddington factors are found from the formal, frequency by frequency, solution of the radiative transfer equation. The computational cost of this is small. The notation used above is that found in the astrophysical literature (e.g. [5, 13]). For completeness we will give some definitions here. S, the line source function, is the ratio of emissivity to opacity within the spectral line. J_ν is the mean intensity at frequency ν. τ is the line centre optical depth and ϕ_ν is the line absorption profile. u is defined by

$$u_\nu = \tfrac{1}{2}(I_\nu(+\nu) + I_\nu(-\mu)),$$

where μ is the direction cosine with respect to the z axis and I_ν is the specific intensity of radiation.

B is the Planck function. ε^* and ε^+ describe the possible ways of collisionally "destroying" photons.

Present codes solve Eqs. (1) and (2) together. This involves solving a block tridiagonal system of $DN \times N$ blocks, where D is the number of depth points used and N is the number of frequency points. The computational effort involved in solving such a system scales as DN^3.

An alternative approach, the Λ iteration, is to solve Eq. (1) for an assumed value of S, recalculate S from Eq. (2) and iterate the whole process. The cost of such a calculation scales as $D \times N \times$ number of iterations. The convergence rate of the Λ iteration is poor; $\sim 1/\varepsilon^+$ iterations are needed in an infinite atmosphere. However in conditions typical of laser heated targets, $\varepsilon^+ \sim 0.1$–0.01, optical depths ~ 1–10^3, the Λ iteration technique has proved successful [8]. More recent work at the Naval Research Laboratory has used the core saturation technique [5] with considerable success [3].

A number of schemes have been developed in neutron transport to accelerate the Λ iteration [14]. One of these, the synthetic method relies on the existence of a good approximation to the Λ iteration matrix which may be efficiently inverted [1]. This method has had great success when applied to the single group equation in the inner iteration of neutron transport calculations. Cannon [6] has applied a variant of this method to multi-frequency line radiation transfer calculations. Because of the coupling between all frequencies within the line and the fact that photon transport may be dominated by photons in the wings of the spectral line the construction of a good approximation to the Λ iteration matrix presents considerable difficulties.

It should be noted, however, that recent work [16] has had considerable success in plane one-dimensional radiation transfer problems. A more rigorous application of the synthetic method to multi-frequency problems (cf. Alcouffe [1]) will avoid these problems. However the computing time required for this is of the same order as that required for the variable Eddington factor method.

An alternative acceleration tool is the Chebyshev semi-iterative method [18] which has been applied to neutron transport problems [9, 10]. This is applicable to solving the second order form of the transfer equation with angle averaged redistribution since the iteration matrix is self-adjoint. In fact one would not expect the non-self-

adjoint character to play a very significant role in these calculations [7]. It should be stressed that the Chebyshev method has been sucessfully applied to non-self-adjoint problems in neutron transport [10]. The author has found the method successful for accelerating the Λ iteration where the first order form of the radiation transfer equation was used.

If we are to use the Chebyshev semi-iterative method we require a knowledge of the spectral radius of the Λ iteration matrix. This may be obtained if we use the technique described by Reed [15]. To perform this analysis we must assume that the mesh spacing $\Delta\tau$, the Eddington factor, f, and the line profile ϕ_ν are all independent of position. The application of the scheme is not subject to these assumptions. It is straightforward to show that the eigenvalues of the iteration matrix are given by

$$g_k = (1 - \varepsilon^+) \int_{-\infty}^{+\infty} \frac{\phi_\nu \, d\nu}{1 + \lambda_k f/\phi_\nu^2 \Delta\tau^2},$$

where $\lambda_k = 2(1 - \cos \pi/k)$, $k = 1, 2, \ldots, D$. Clearly the spectral radius of the iteration matrix is less than $(1 - \varepsilon^+)$, its value in an infinite medium.

The Λ iteration may be represented by

$$Aw^{K+1} = Bw^K + v, \tag{3}$$

where u is a vector containing the depth and frequency variation of the radiation field; A is a matrix containing the difference representation of Eq. (1) and B is a matrix which contains information on the frequency quadrature which is used. If the vector, u, is grouped so as to consist of a number of sub-vectors each containing the position variation for a single frequency and three point differencing is used, then the matrix A is tridiagonal.

Equation (3) may be re-expressed as

$$w^{K+1} = Mw^K + A^{-1}v.$$

(Note that M need never be evaluated explicitly.)

The Chebyshev semi-iterative method is then given by

$$w^1 = Mw^0 + A^{-1}v,$$

$$w^{m+1} = \omega_{m+1}(Mw^m + A^{-1}v - w^{m-1}) + w^{m-1},$$

$$\omega_1 = 1,$$

$$\omega_m (m > 1) = 1 + \frac{C_{m-1}(1/\rho)}{C_{m+1}(1/\rho)},$$

where $1 > \rho > \|M\|$ for a stable convergent scheme. C_m are the Chebyshev polynomials. These may be calculated very easily by the relations

$$C_0(x) = 1,$$
$$C_1(x) = x,$$
$$C_{n+1}(x) = 2 \times C_n(x) - C_{n-1}(x).$$

After m iterations the size of the error associated with an eigenvector of M with eigenvalue λ_i will be reduced by

$$\frac{C_m(\lambda_i/\rho)}{C_m(1/\rho)}.$$

From this it can be seen that the error associated with a given eigenvector will not ncessarily be reduced from one iteration to the next. However, it is clear that the norm of the semi-iterative procedure after m steps is given by

$$\|\rho_m(M)\| = \max_{i=1,N} \frac{|C_m(\lambda_i/\rho)|}{|C_m(1/\rho)|}.$$

If ρ is equal to the spectral radius of M then we obtain

$$\|\rho_m(M)\| = 1/C_m(1/\rho), \qquad m \geqslant 0,$$

which is strictly decreasing for all $m \geqslant 0$. Clearly the convergence is improved as $1/\rho$ increases. Thus we want to choose ρ as close to the maximum eigenvector of M as possible. For the case of complete redistribution u^m need only represent a vector,

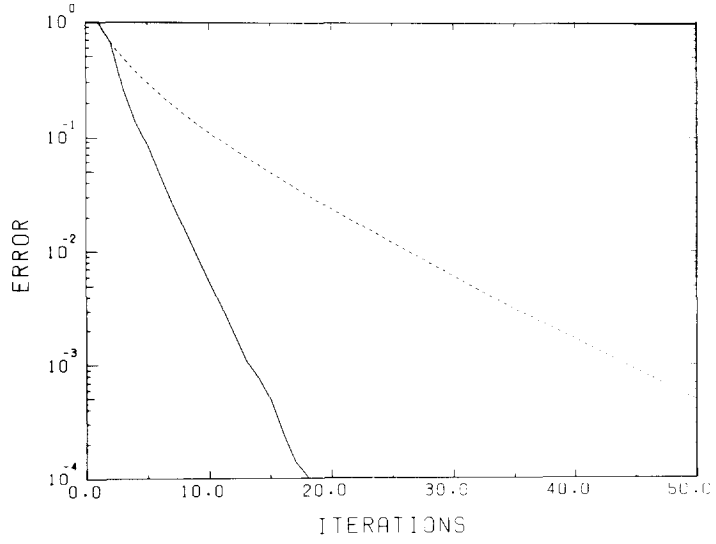

FIG. 1. Convergence of A iteration (– – –) and Chebyshev semi-iterative method (——). $\varepsilon = 10^{-4}$, Lorentz profile; $S = B$ as initial guess.

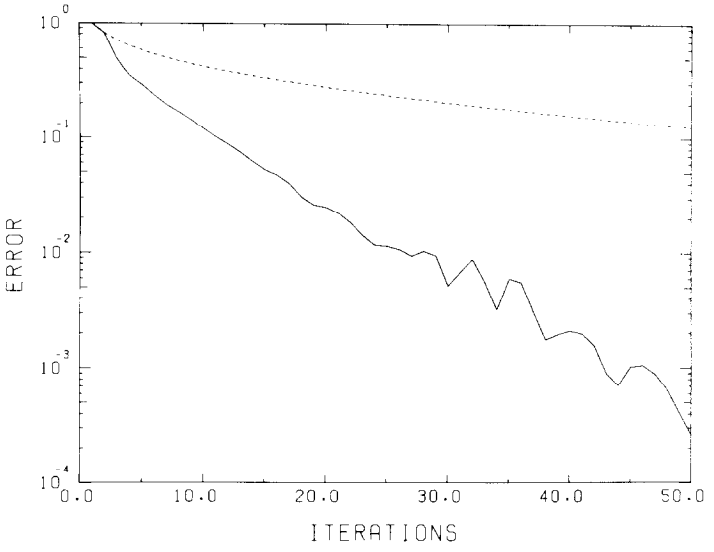

FIG. 2. As Fig. 1, but with $\varepsilon = 10^{-2}$.

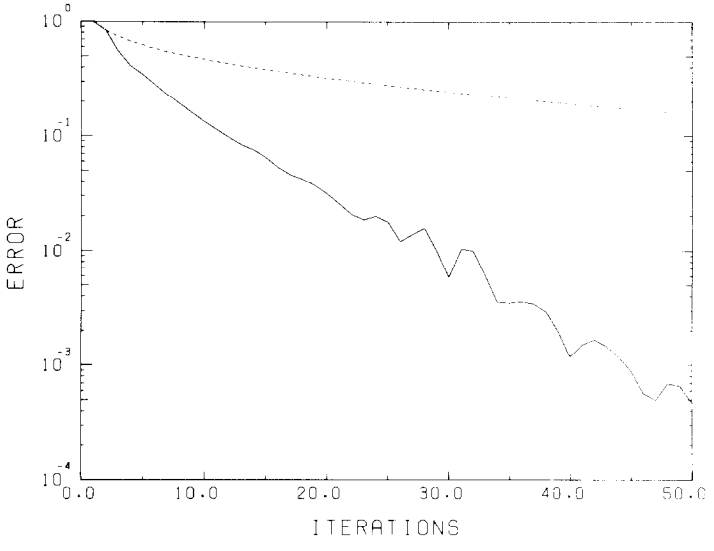

FIG. 3. As Fig. 1, but with $\varepsilon = 10^{-3}$.

length D, containing the values of $\langle J \rangle$. The extra storage needed for the semi-iterative method compared with the Λ iteration is minimal.

We have compared the Chebyshev method and unaccelerated Λ iteration on the following problem: a strict two-level atom and complete redistribution are assumed. The source function is of the form

$$S = (1 - \varepsilon)\langle J \rangle + \varepsilon B.$$

A value of $\rho = 1 - \varepsilon$ was used in the calculations.

The values of the Eddington factors were calculated from the formal solution of the radiation transfer equation with an initial estimate for the source function. It should be noted that similar convergence properties are found for all the stages of the Eddington factor iteration. The system which is modelled is a plane with total line centre optical depth of $\simeq 10^5$. The grid which is used starts at $\tau = 10^{-3}$ and used 5 points per decade. We have estimated the error by the quantity

$$\left(\sum_{\text{grid points}} (\langle J \rangle_{\text{iterated}} - \langle J \rangle_{\text{converged}})^2 \right)^{1/2}$$

Figures 1–3 show the convergence of the Λ iteration and the Chebyshev scheme for a line with a Lorentz profile and value of ε of 10^{-1}, 10^{-2} and 10^{-3}. The error has been normalised to its value after the first Λ iteration. In each case the initial guess for the source function was $S = B$. We see (Figs. 2 and 3) that the error is not a strictly decreasing function of the number of iterations. This possibility was noted above. In Fig. 4, $\varepsilon = 10^{-2}$ but an initial (and far worse) guess of $S = B\varepsilon$ was used. Here the

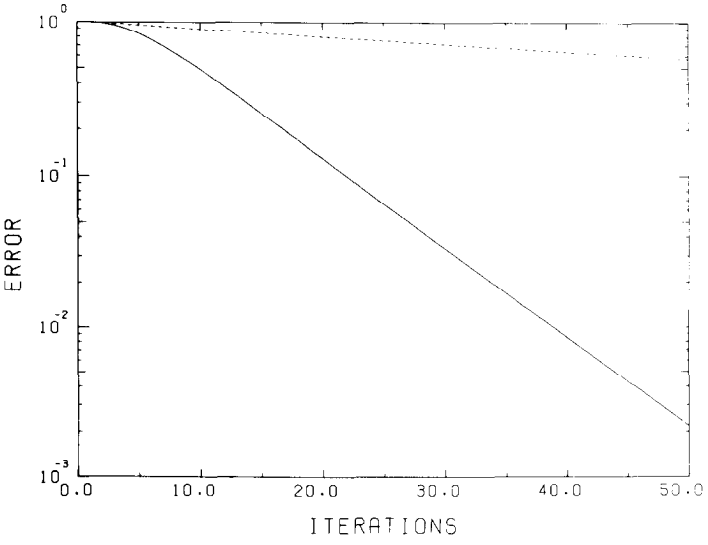

FIG. 4. As Fig. 2, but with $S = \varepsilon B$ as initial guess.

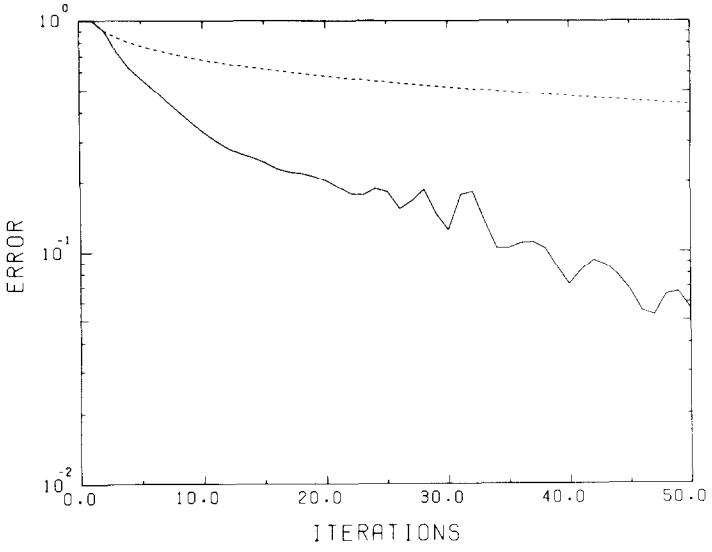

FIG. 5. As Fig. 2, but with Doppler profile.

error vector is dominated by the slowest decaying mode and the error decreases moothly with iteration. Fig. 5 shows results with a Doppler profile, $\varepsilon = 10^{-2}$ and $S = B$ initially. No marked differences to the behaviour with a Lorentz profile can be seen. The efficacy of the acceleration scheme has been found to be very insensitive to the frequency mesh which is used.

In conclusion, we have demonstrated the possibility of using the Chebyshev method to accelerate the Λ iteration in radiation transfer calculations. For all problems encountered in simulating laser produced plasmas we would expect the Chebyshev method to be computationally faster than those methods presently employed in radiation transfer codes.

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