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Solution of the particle transfer equation in a one-dimensional conservative potential

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Abstract. A numerical procedure for the solution of the single total energy group transfer equation is given. The acceleration of the iterative method which is employed is discussed and examples are given. For simplicity isotropic scattering is used.

The solution of the particle transfer equation, in the absence of external forces, has been discused by many authors (see, for example, Dudestadt and Martin 1979). Discrete ordinate methods have been widely used in neutron and radiation transfer calculations and have recently been applied to charged particle transfer problems (Wienki 1979, Antel and Lee 1976). This paper discusses the simplest possible application of the discrete ordinate method to charged particle motion in a conservative potential; one-dimensional slab geometry and isotropic scattering are assumed and only one total energy group is considered. The solution of this idealised problem does however present some interesting problems.

The time-independent transfer equation for particles moving under the influence of a potential field φ, being absorbed with characteristic length Σ_a^{-1} and scattered with characteristic length Σ_s^{-1} is

$$v_x \frac{\partial f}{\partial x} - \frac{\partial \varphi}{\partial x}\frac{\partial f}{\partial v_x} + v(\Sigma_s + \Sigma_a) f = \frac{v}{2}\Sigma_s \int_{-1}^{+1} f(v, \mu', x)\, \mathrm{d}\mu. \tag{1}$$

The characteristics of the collisionless version of equation (1) are the trajectories of the collisionless particles. Motion, including elastic scattering, in the potential will alter the kinetic energy but not the total energy, $\frac{1}{2}mv^2 + \varphi$, of the particles. These considerations suggest that a scheme for solving the transfer equation based on the total energy and a set of discrete directions which follow the motion of the collisionless particles may be adopted usefully. The motivation behind this is analogous to the use of the 'cylindrical approximation' for radiation transfer in a one-dimensional spherical atmosphere (Hummer and Rybicki 1970). It has been found convenient to solve not for the distribution function but for the particle flux per unit total energy in a given direction, ψ.

Figure 1 illustrates the angular mesh which is used. The potential is constant in each cell. In order to relate the flux to the flux per solid angle it is necessary to assign quadrature weights to each of the discrete angles which is used. This is done in the

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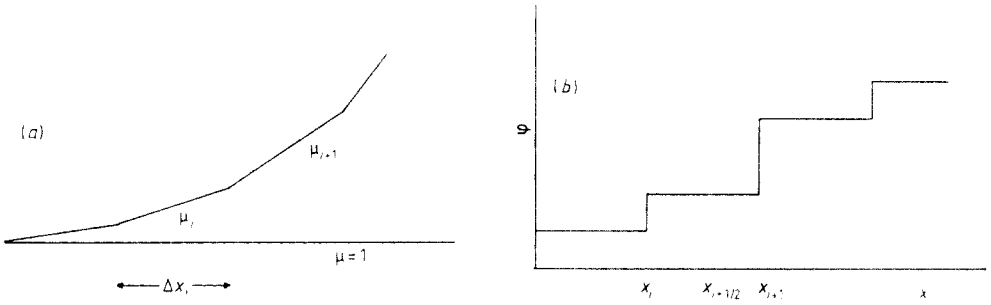

Figure 1. (*a*) The change of angle with position along a trajectory. (*b*) The potential as a function of position.

simplest possible manner by the prescription

$$\omega_i = \tfrac{1}{2}(\mu_{i+1}+\mu_i) - \tfrac{1}{2}(\mu_i + \mu_{i-1})$$
$$\omega_1 = 1 - \tfrac{1}{2}(\mu_1+\mu_2) \qquad \omega_N = \tfrac{1}{2}(\mu_{N-1}-\mu_N) \tag{2}$$

where N is the number of values of μ in the range 0–1. This number varies across the mesh. The choice of angles is somewhat arbitrary. That which has been adopted is to choose the set of angles in the first cell so that subsets of this set are distributed uniformly in direction cosine in a number of cells. Sufficient angles must be chosen so that the following approximations hold

$$\tfrac{1}{2} \simeq \sum \omega_i \mu_i \qquad \tfrac{1}{3} \simeq \sum \omega_i \mu_1^2. \tag{3}$$

In the computation results given below 50 angles were used.

The iteration strategy used to solve the tranfer equation is as follows. An initial guess is made at the source of particles from scattering for each group in each cell. The flux ψ is then calculated along the direction of motion of the collisionless particles one angle at a time. The fluxes are then used to obtain a new estimate of the source and the whole calculation is iterated. This is the usual inner-iteration strategy of neutron transport codes. The source is taken to be of the form

$$S(x) = S_{i+1/2} + T_{i+1/2}(x - x_{i+1/2}) \tag{4}$$

in the range x_i to x_{i+1}. This is the form used by (Alcouffe *et al* 1979, Lee and Vaidyanathan 1980) in one-dimensional neutron transport problems. The flux is integrated along the particle trajectories using (for $\mu > 0$)

$$\psi^*_{i+1} = \psi_i \exp(-\varepsilon_i) + S_i[1-\exp(-\varepsilon_i)] + (\Delta x_i T_i/\sigma_i)[1-(\tfrac{1}{2}+1/\varepsilon_i)(1-\exp(-\varepsilon_i))] \tag{5}$$

$$\psi_{i+1} = \psi^*_{i+1}\mu_i/\mu_{i+1} \tag{6}$$

where

$$\varepsilon_i = \sigma_{i+1/2}\Delta x_i/\mu_i \qquad \text{and} \qquad \sigma_{i+1/2} = (\Sigma_a + \Sigma_s)_{i-1/2}.$$

Equation (6) together with equation (2) and the relation $dE_T = mv\,dv$ ensure that for an infinitely fine mesh, f is a constant along the particle trajectories in the collisionless case. The value of S_i used for the next iteration is calculated from the cell average fluxes

$$\bar{\psi}_{i+1/2} = \frac{S_{i+1/2}}{\sigma_{i+1/2}} - \frac{1}{\varepsilon_i}(\psi_{i+1}-\psi_i) \tag{7}$$

T is calculated from the gradient of the sources calculated at the boundaries by

$$T_{i+1/2}=\frac{2(S_{i+1}-S_i)}{\Delta x(S_{i+1}+S_i)}. \tag{8}$$

Equations (5)–(8), together with appropriate boundary conditions, provide a basis for the solution of the one group transfer equation. However, the iteration procedure which is used, the Λ iteration of radiation transfer (Mihalas 1978), may be very slow to converge for systems which are many scattering distances across. A number of acceleration schemes exist (Miller 1978) of which the diffusion synthetic acceleration (Alcouffe 1977) has achieved considerable success. This method makes use of, but does not depend on the validity of, diffusion theory. The adoption of this method requires the use of the total energy group diffusion equation (Kershaw 1979, Bond 1980) which may be derived by transforming equation (1) so the independent variables are E_T, x and μ and expanding the distribution function in the $f(E_T, x, \mu)\simeq f_0(E_T, x)+\mu f_1(E_T, x)$. This yields

$$-\frac{\mathrm{d}}{\mathrm{d}x}\frac{\Sigma_s^{-1}v^2}{3}\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{N}{v}\right)+v\Sigma_a N=\text{source}. \tag{9}$$

This equation has been used as the basis of the following acceleration scheme

$$-\frac{\mathrm{d}}{\mathrm{d}x}\frac{\Sigma_s^{-1}v^2}{3}\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\tilde{N}}{v}\right)+\Sigma_a v^2\left(\frac{\tilde{N}}{v}\right)=\text{source}-\frac{\mathrm{d}}{\mathrm{d}x}\frac{\Sigma_s^{-1}v^2}{3}\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{N}{v}\right)-\frac{\mathrm{d}}{\mathrm{d}x}(J) \tag{10}$$

where

$$J=\int\psi\mu\,\mathrm{d}\mu \qquad \text{and} \qquad N=\frac{1}{v}\int\psi\,\mathrm{d}\mu.$$

This equation, subject to suitable boundary conditions, is solved to obtain $\tilde{N}/V$ at one side of the cell boundaries. The ratio of this to the unaccelerated value of N/V is used to multiply the fluxes.

Two problems arise in this approach. Firstly the approximations described by equation (3) result in the solution of the transfer equation not quite corresponding to diffusion theory. This may be partially overcome by using a large number of angular points. This may also be mitigated by, for instance, replacing $\frac{1}{3}$ in equation (10) by the approximation given in equation (3). No such approach is used in the numerical results presented here. Secondly (N/V) is discontinuous at the cell boundaries. This may lead, for example, to large jumps in N/V at boundaries, in the course of iteration, when the solution is well approximated by diffusion theory. For large E and scattering ratio $\Sigma_s/(\Sigma_s+\Sigma_a)$ close to unity this can lead to the iteration giving negative densities. This problem has been partially overcome by performing an unaccelerated iteration whenever the acceleration procedure gives rise to large changes in the densities. In the calculations used here, changes of greater than 10 or less than 0.5 resulted in the next iteration not being accelerated. This procedure has enabled mesh lengths of 10 mean free paths to be used with a scattering ratio of unity. This is more than adequate for most purposes.

A further problem associated with the use of equation (10) is that equation (7) does not hold for the accelerated fluxes. Indeed equation (5) must be used, together with the expression for T_i from equation (8) where the accelerated fluxes are used. This gives $S_{i+1/2}$ from which $\bar{\psi}_{i+1/2}$ may be calculated. In order that the converged

solution should be unaltered by the acceleration method it is necessary to use

$$(\Sigma_a v^2)_i = \tfrac{1}{2}(\Sigma_{a,-1/2} v\psi_{i-1/2}\Delta x_{i-1}\Sigma_{a,+1/2} v\psi_{i+1/2}\Delta x_i)(N/v)_i^{-1}. \quad (11)$$

Table 1 gives results on the number of iterations required for convergence to 10^{-3} in the densities for a variety of different values of ε and values of the scattering ratio. The source of particles is at one end of the mesh and either free flow or reflection boundary conditions are applied at the other end. This clearly demonstrates the value of the acceleration technique.

Table 1. The number of iterations required for convergence to 10^{-3} in the densities for a variety of different values of ε and values of the scattering ratio: A, no E field. Free flow at right hand boundary. $\Sigma_a = 0$. B, constant E field giving a potential of 0.6 of the total energy across the mesh. Free flow at right boundary. $\Sigma_a = 0$. C, as B but with reflection boundary condition. D, as C but with $\Sigma_a = \Sigma_s$. (* did not converge in 400 iterations.)

		Case			
Depth	Acceleration	a	b	c	d
1	Yes	9	7	11	7
1	No	14	15	16	7
2	Yes	10	9	4	8
2	No	23	23	43	9
10	Yes	14	10	12	9
10	No	140	111	231	15
25	Yes	16	14	9	12
25	No	*	*	*	22
50	Yes	21	23	11	21
50	No	*	*	*	31

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