GALERKIN METHODS FOR THE BOLTZMANN EQUATION USING VARIABLE COORDINATE SYSTEMS

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1. INTRODUCTION

In this paper we present a solution method for the Boltzmann transport equation based on a series expansion in a variable coordinate system. In an appropriately scaled form, the Boltzmann transport equation is given by

$$\varepsilon^2 \partial_t f + \varepsilon div_x(v(k)f) + \varepsilon div_k(Ff) = Qf, \tag{1}$$

Equation (1) is already given in a scaled and dimensionless form where the dimensionless parameter ε stands for the scaled mean free path. The term Qf on the right hand side of equation (1) denotes the collision operator. For the purpose of this paper we restrict ourselves to the collision operator resulting from the relaxation time approximation. This means, that the operator Q in (1) is given by

$$Qf(x,k,t) = a(\rho,u,t)M(x,k) - b(\rho,u,T)f, \tag{2}$$

where $M(x,k)$ is a given equilibrium distribution and a and b are functions of the density ρ , the group velocity u, and the scaled temperature T , given by

$$\rho(x,t) = \int_{R_k^3} f(x,k,t)dk, \quad \rho u(x,t) = \int_{R_k^3} v(k)f(x,k,t)dk, \quad \rho(3T+|u|^2) = \int_{R_k^3} |v|^2 f(x,k,t)dk. \tag{3}$$

The hydrodynamic model equations are usually obtained by by integrating equation (1) against the functions $1, v(k)$ and $|v(k)|^2$, assuming either a parabolic band structure or making an effective mass approximation, and assuming that the density function f has the shape of a drifted Maxwellian in the wave vector direction.

$$f(x,k,t) = \frac{\rho(x,t)}{\pi(2T)^{\frac{3}{2}}} exp[\frac{-|v-u(x,t)|^2}{2T}]. \tag{4}$$

For elastic scattering terms, which preserve momentum and energy, the hydrodynamic model can be justified via asymptotic analysis for small values of the scaled mean free path, the quotient of the mean free path and the length scale under consideration [BAR]. For inelastic collision processes, which are usually present for electron transport in solids, a similar asymptotic analysis exists, leading to slightly different model equations [POU]. However, the hydrodynamic model is frequently used in regimes where the scaled mean free path is actually quite large. An alternative approach is to expand the solution of the Boltzmann transport equation in a set of basis functions in velocity space (c.f. spherical harmonics) with coefficients which are dependent on position and time. After using a Galerkin approximation a set of macroscopic equations is obtained for these coefficients [VEN], [LIN]. However, the resulting expansion converges quite slowly in the presence of high velocities and strong forces. In this paper we present a series expansion method, also based on a Galerkin procedure which is better suited for high field regimes and a relatively large mean free path. The basic idea is to use a coordinate transformation in phase space which adapts locally to the shape of the distribution function f. This transformation is chosen such that the resulting expansion reduces to the hydrodynamic model if only a few terms are used.

2. GALERKIN APPROXIMATION

The method presented in this paper is a Galerkin approximation of the Boltzmann transport equation (1) in a weighted L^2 space, using a variable transformation in the velocity variable which is dependent on position and time. We employ the coordinate transformation $k \rightarrow w$, given in general by

$$w = G(x,k,t) \tag{5}$$

and expand the solution of the Boltzmann transport equation as

$$f(x,k,t) \approx \sum_{n \epsilon N} \hat{f}(x,n,t)\psi_n(x,k,t), \tag{6}$$

where the basis functions ψ_n are given by some suitable set of basis functions ϕ_n under the variable transformation G, which will be chosen such as to adapt locally to the shape of the distribution function f.

$$\psi_n(x,k,t) = \phi_n(w) \quad , \quad w = G(x,k,t) \tag{7}$$

holds. N in (6) denotes some suitable, finite index set. We introduce the weighted L^2 inner product for two scalar functions $f(x,k,t)$ and $g(x,k,t)$ and two vector valued functions $\mathbf{f}(x,k,t)$ and $\mathbf{g}(x,k,t)$ by

$$< f,g > (x,t) = \int_{R_k^3} \mu(G(x,k,t)) f(x,k,t) g(x,k,t) dk, \quad < \mathbf{f},\mathbf{g} > (x,t) = \int_{R_k^3} \mu \mathbf{f}^T \mathbf{g} dk. \tag{8}$$

The variable transformation G is assumed to be affine and the basis functions ϕ_n are assumed to be normalized. So

$$\int_{R_w^3} \mu(w)\phi_n(w)\phi_m(w)dw = \delta_{m,n} \tag{9}$$

holds. Taking the inner product $< .,. >$ of the Boltzmann transport equation with the test function $\psi_m, m \epsilon N$ yields the macroscopic equations for the coefficients $\hat{f}(x,n,t)$. Inserting the expansion (6) into the Boltzmann transport equation (1), taking the scalar product with the basis function $'\psi_m$, gives

$$\partial_t \hat{f}_m + \sum_{j=1}^{3} \sum_{n \epsilon N} \partial_{x_j} [A_{j,m,n} \hat{f}_n] - \sum_{n \epsilon N} B_{m,n} \hat{f}_n = C_m, \tag{10}$$

where the tensors A, B and C are given by

$$(a) \quad A_{j,m,n}(x,t) =< \psi_m, v_j \psi_n >, \quad (b) \quad C_m(x,t) = a < \psi_m, M > -b\hat{f}_m \tag{11}$$

$$B_{m,n}(x,t) =< \frac{1}{\mu}\psi_n, \partial_t(\mu\psi_m) + v \bullet \nabla_x(\mu\psi_m) + F \bullet \nabla_v(\mu\psi_m) > .$$

To this point the equations (10) represent a Galerkin approximation of the Boltzmann transport equation in a variable coordinate system, which will be convergent, provided the equations (10) are stable and the derivatives of the density function f stay bounded in the weighted L^2 space with the weight μ. We make the following choices for the basis functions ψ_m and Φ_m and the weight function μ, which lead to a generalization of the hydrodynamic model equations. We set

$$(a) \quad \mu(w) = exp(|w|^2), \quad (b) \quad \Phi_m(w) = exp(-|w|^2)P_m(w), \quad c) \quad \psi_m(x,k,t) = \Phi_m(G(x,k,t), \quad m \epsilon N \tag{12}$$

where the P_m are chosen as suitably orthogonalized polynomial functions. Furthermore, we choose the affine transformation G such that

$$|G(x,k,t)| = \frac{|v - \mathbf{p}(x,t)|}{\alpha(x,t)} \tag{13}$$

holds for some vector $\mathbf{p}$ and some scalar α. The basic idea behind these choices is that, because of (12), taking the scalar product of a given function with the basis function ψ_m corresponds to computing a certain linear combination of the moments of that function, and, because of (13), the zero order basis functions will have the shape of the drifted Maxwellian (4). This results in the hydrodynamic model being a special case of the above approximation procedure.

To this point we have not specified the choice of the functions $\alpha(x,t)$ and $p(x,t)$, which make up the variable transformation in velocity space. Indeed, any choice of $\alpha(x,t)$ and $p(x,t)$ would yield a convergent

Galerkin method for the Boltzmann transport equation, provided the density function $f(x,k,t)$ is sufficiently smooth. We now choose p and α dependent on the solution itself in order to minimize the number of terms needed in the expansion procedure. We choose $p(x,t)$ as the mean velocity u given by the solution of the Galerkin approximation. So we set

$$p(x,t) = \frac{1}{\rho(x,t)} \int_{R_k^3} v f(x,k,t) dk \quad . \tag{14}$$

The function α is chosen such that it matches the macroscopic temperature T in (3). So we set

$$\alpha(x,t) = \sqrt{\frac{2}{3}} \sqrt{\frac{1}{\rho(x,t)} \int_{R_k^3} |v|^2 f(x,k,t) dk - |p|^2} \quad with \quad \rho(x,t) = \int_{R_k^3} f(x,k,t) dk. \tag{15}$$

Of course, this choice of α and p transforms the linear problem (10) into a nonlinear one.

The hyperbolic system (10) can be discretized by any method suitable for systems of hyperbolic conservation laws. For the purpose of this paper the method of choice is the Lax - Wendroff scheme.

3. A NUMERICAL TEST EXAMPLE

To demonstrate the effect of the corrections to the hydrodynamic model resulting from the above approximation procedure, we present a one dimensional example of the reflection of an electron wave at a potential barrier. Assuming a parabolic band structure, the density function $f(x,k,t)$ remains cylindrically symmetric around the k_1- direction in the one dimensional case. So

$$f(x,k,t) = f(x_1, k_1, k_2^2 + k_3^2, t) \tag{16}$$

holds. The affine variable transformation G in (5) is given by

$$G(x,k,t) = \frac{k - p(x,t)\mathrm{e}}{\alpha(x,t)}, \quad \mathrm{e} = (1,0,0)^T, \tag{17}$$

and the polynomial basis functions P_m in (12) are given by the standard Laguerre polynomials. Calculations were performed for the scaled mean free path ϵ in (1) equal to 0.2, which corresponds to the regime where the hydrodynamic model is usually applied. Figure 1 shows the force F corresponding to the potential barrier. Figure 2 shows the currents at a given point in time resulting from three different calculations. The solid line has been obtained by using 10 terms in the expansion, 5 in the k_1- direction times 2 in the orthogonal $k_2^2+k_3^2-$ direction. The dotted line gives the current resulting from the corresponding hydrodynamic model, using only three terms in the expansion. Finally, the the dashed line represents the 'numerically exact' solution, obtained by using 32 times 8 modes. As observed in the past, the hydrodynamic solution exhibits artificial velocity overshoot phenomena. These phenomena are not present when 10 terms are used, and the current is essentially compute correctly. Figure 3 shows the L^2 norm of various modes as a function of time. It can be seen that the higher order modes produce a significant correction. In particular, a simple algebraic calculation shows that the (1,0) term is responsible for non - scalar temperatures. Finally, Figure 4 shows a snapshot of the distribution function f at the midpoint $x = 0.5$ and a certain point in time as a function of k_1 and $k_2^2 + k_3^2$. If the assumptions underlying the hydrodynamic model were correct, the distribution function would have to be a Maxwellian, shifted along the k_1- direction. The additional peak in the exact distribution function is responsible for the artificial velocity overshoot in the hydrodynamic model.

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FIGURE 1
Electric Field

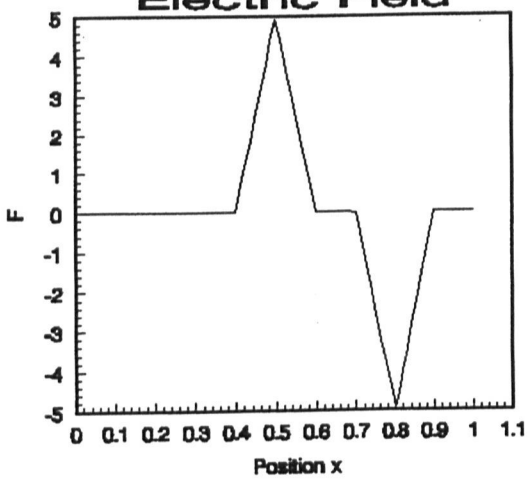

FIGURE 2
Currents at t=0.02

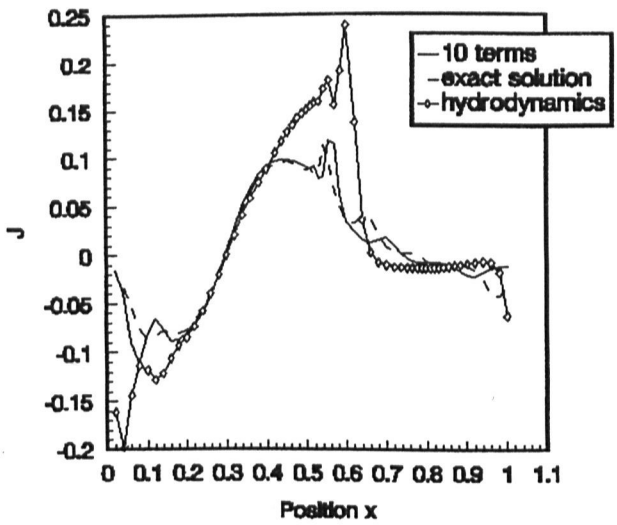

FIGURE 3
Expansion Coefficients

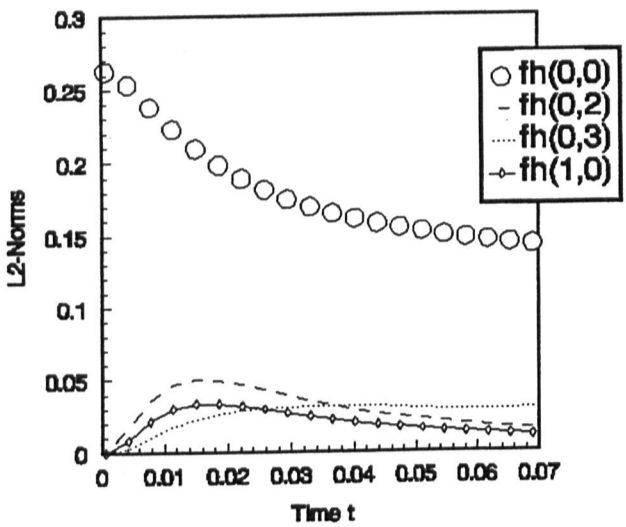

FIGURE 4
Distribution f for x=0.5 and t=0.02