

Numerical Hydrodynamics from Gas-Kinetic Theory

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We present a new hydrodynamics code, based on the solution of the Bhatnagar–Gross–Krook model of the Boltzmann equation. The basic idea is to construct an approximate, locally valid solution of a set of non-linear integral equations for the equilibrium Maxwell–Boltzmann distribution, and use this solution to solve the BGK equation for the velocity distribution function at cell walls. Once this is known it is possible to compute time-dependent fluxes of mass, momentum, and energy between cells. All steps are carried out explicitly for the case of a perfect gas; the details of the distribution functions disappear in the final code. In common with other “Boltzmann-type” codes employing distribution functions, the Riemann problem does not arise. The novelty of the present code consists in solving for the distribution function, taking account of collisions, rather than assuming a convenient form for it. Results are presented for a number of standard test cases, with features ranging from cavitation (Sjögreen test) to the collision of strong shocks (Woodward–Colella test). All cases are run with precisely the same code, and all cells are treated in the same way. Our code appears to behave as well as current high-order difference schemes at shocks and to give better results for rarefaction waves. It is competitive with current codes that do not employ special means of diagnosing and treating contact discontinuities—the inclusion of such devices in our scheme remains an option. © 1993 Academic Press, Inc.

I. INTRODUCTION

In an important and influential paper, Harten, Lax, and van Leer [7] drew a distinction between two numerical approaches to the solution of the Euler equation, namely, Godunov and Boltzmann schemes. Broadly speaking, a Godunov scheme relies on solving a Riemann problem, and the characteristics are the curves given by $dx/dt = U$ and $dx/dt = U \pm c$ in x, t space (i.e., the characteristics of the Euler equation); Boltzmann schemes employ a distribution function of particle velocities, and the characteristics are the lines of constant values of $x - ut$ and u in phase space. In physical terms, Godunov schemes use sound waves and streamlines to propagate information, and Boltzmann schemes use trajectories of individual particles of the gas. The prototypical Godunov scheme is, of course, Godunov’s scheme, which is first-order, and therefore of comparatively low accuracy. There exists a rich literature of high-order schemes incorporating some of the devices in Godunov’s

scheme, particularly the use of solutions of the Riemann problem, either exact or approximate; these include ENO schemes [8] and the PPM method of Woodward and Colella [20].

The earliest scheme of the Boltzmann type appears to be the beam scheme (Sanders and Prendergast [17]); another example is the Steger–Warming [18] scheme. The beam scheme evolved from a lattice gas treatment of the collisionless Boltzmann equation used by Miller, Prendergast, and Quirk [11] for the gravitational N -body problem. In its simplest version one supposes that the mass, momentum, and energy densities are uniform within cells, and the values of these quantities are used to construct (unique) Maxwellian distribution functions within each cell. The collisionless Boltzmann equation is used to find the time evolution of the distribution function, which continually departs from its Maxwellian form. The connection with hydrodynamics is furnished by the observation that the Euler equations are moments of the Boltzmann equation and describe the flow correctly if the true distribution function is everywhere nearly Maxwellian; the mechanism for keeping the distribution function nearly Maxwellian being the collisions suffered by the molecules of the gas. In the beam scheme one supposes that the collisions operate instantaneously after some short time interval has elapsed and the result is a new uniform Maxwellian in each cell, from which new mass, momentum, and energy densities are computed. In practice the time interval is governed by a Courant–Lewy–Friedrichs condition. The scheme is conservative, first-order, and flux-split; it is highly stable and very dissipative. In a sense, the “beams” in the beam scheme are an accident—they were introduced to avoid evaluating the error functions required to compute fluxes for an exact Maxwellian. (Actually, error functions are almost as easily computed as square roots. The first use of error functions to compute fluxes appears to be by Pullin [14]; cf. also Macrossan [10].) The introduction of beams replaces the Maxwellian with a set of Dirac delta-functions, and, as has often been noted, this replacement is not unique (cf. Harten *et al.*)—for example, a parabolic distribution function can be used instead of beams or Gaussians (cf. Chudnovsky

et al. [4]). In the present paper we will be concerned with higher-order schemes based on considerations of gas-kinetic theory, but the resemblance to the beam scheme is slight. A second-order scheme was constructed by van Albada, van Leer, and Roberts [19], but without attempting to go back to the physical origin of the scheme. Reitz [16], Deshpande [5] and Perthame [13] have also worked on the problem of improving the performance of codes inspired by gas-kinetic considerations.

Our starting point in this paper is the well-known fact that the coefficients of heat conduction and viscosity are proportional to the mean time between collisions. The original beam scheme has an effective collision time equal to the CFL time and a mean free path equal to the cell size. For an economical computation intended to describe the motion of a real gas these quantities are much too big—therefore, we seek a mechanism for embodying the continuing effect of collisions during a time step. To make the presentation self-contained and to indicate possible directions for generalization we summarize in Section II some results of gas-kinetic theory. The main point of this section is to arrive at a set of coupled nonlinear integral equations for the mass, momentum, and energy densities in the gas based on the Bhatnagar–Gross–Krook (BGK) model of the Boltzmann equation [1]. In the BGK model the classical two-body Boltzmann collision integral is replaced by the difference between the true distribution function and a Maxwellian, divided by a relaxation time τ . The solutions are not identical, but the BGK model often gives surprisingly good results, even for problems of rarefied gas dynamics. Discussions of the connection between gas dynamics and hydrodynamics may be found in a number of standard sources. Derivations of the Navier–Stokes equations from the Boltzmann have been given by Kogan [9] and Chapman and Cowling [3], and from the BGK equation by Cercignani [2] for the case of a perfect monatomic gas. These derivations also furnish explicit expressions for the viscosity and heat conduction coefficients in terms of molecular quantities. For the BGK model of a perfect gas it can be shown that the dynamic viscosity and second viscosity coefficients are $\eta = \tau p$ and $\zeta = \frac{2}{3}(K/(K+3)) \tau p$ respectively, and the thermal conductivity is $\kappa = ((K+5)/2)(k/m) \tau p$, where $K = (5-3\gamma)/(\gamma-1)$, k is the Boltzmann constant, m is the mass of a molecule, and p is the pressure. (The ratio η/κ given above is 50% larger than the “true” value from the Boltzmann collision integral.)

In Section III we derive an approximate local solution of the BGK equation, linear in space and time. This solution, together with the formal solution of the BGK equation, is used to find an approximation for the distribution function at a cell wall from which time-dependent fluxes are found explicitly. Details of a numerical code are given in Section IV, and results are presented for a number of standard test cases.

II. KINETIC THEORY PRELIMINARIES

Our numerical code is based on the dynamical theory of gases, rather than the Euler or Navier–Stokes equations. As is well known these equations can be derived from gas dynamics, so that a solution of a problem in gas dynamics is automatically a solution of a problem in hydrodynamics if the mean free path is small enough. In the interest of making the presentation self-contained and of indicating possible directions in which to generalize results we review here some elements of the kinetic theory of gases.

Consider a classical molecule of mass m , with N degrees of freedom, whose motion (in the absence of other molecules) is governed by the Hamiltonian $\mathcal{H}(p_i, q_i)$. Let the one particle distribution function f be such that $f(p_i, q_i, t) \prod_{i=1}^N dp_i dq_i$ is the probability of finding a molecule in the element of phase space $\prod_{i=1}^N dp_i dq_i$ at time t . The evolution of f is given by

$$f_{,t} + \mathcal{H}_{,p_i} f_{,q_i} - \mathcal{H}_{,q_i} f_{,p_i} = \left(\frac{df}{dt} \right)_{\text{coll}}, \quad (2.1)$$

where the right side of the equation is the rate of change of f due to collisions. If two-body collisions are dominant this term is the Boltzmann collision integral $Q(f, f)$, which is both nonlinear and non-local. The notorious difficulty of solving the Boltzmann equation has motivated the search for simpler “model” equations—perhaps the most useful of these is the Bhatnagar–Gross–Krook (BGK) model, obtained by replacing $Q(f, f)$ by the difference between f and the equilibrium distribution g , divided by a relaxation time τ . According to classical statistical mechanics, g is the Maxwell–Boltzmann distribution

$$g = \exp[\alpha - \mathcal{H}(\hat{p}_i, \hat{q}_i)/kT], \quad (2.2)$$

where T is the temperature, k is Boltzmann’s constant, and the coordinates \hat{q}_i and momenta \hat{p}_i are measured in a frame moving with the mean velocity of the fluid. The BGK equation is

$$f_{,t} + \mathcal{H}_{,p_i} f_{,q_i} - \mathcal{H}_{,q_i} f_{,p_i} = \frac{(g-f)}{\tau}, \quad (2.3)$$

which is linear in f . If g and τ are known we can find f by the method of characteristics. Hamilton’s equations for the motion of a single particle are

$$\frac{dq_i}{dt} = \mathcal{H}_{,p_i}, \quad \frac{dp_i}{dt} = -\mathcal{H}_{,q_i}; \quad (2.4)$$

suppose that the solution is given in the form

$$p_i = P_i(t; p'_i, q'_i, t'), \quad q_i = Q_i(t; p'_i, q'_i, t'); \quad (2.5)$$

i.e., the particle having momenta p_i and coordinates q_i at time t had momenta and coordinates p'_i, q'_i at time t' . Using Hamilton's equations we can rewrite the left side of the BGK equation as df/dt , where it is understood that f is differentiated along the trajectory (characteristic) given by Eq. (2.5) for a particular p'_i, q'_i . The problem of solving the BGK equation is now reduced to solving the ordinary differential equation

$$\frac{df}{dt} + \frac{f}{\tau} = \frac{g}{\tau} \quad (2.6)$$

for each trajectory. As there is a unique trajectory through each point in phase space, any trajectory can be labelled by giving definite values to p'_i and q'_i . In solving Eq. (2.6), g and τ are regarded as functions of t once a particular trajectory has been selected—that is, p_i and q_i in the arguments of g and τ are replaced by $P_i(t; p'_i, q'_i, t')$ and $Q_i(t; p'_i, q'_i, t')$. The physical meaning of the BGK equation is made clear by this construction: along any trajectory in phase space particles are destroyed at a rate given by τ and regenerated from the equilibrium distribution g .

The solution of Eq. (2.6) is

$$f(t) = \int_{t_0}^t e^{-[\eta(t) - \eta(t')]} \frac{g(t')}{\tau(t')} dt' + f_0 e^{-\eta(t)}, \quad (2.7)$$

where

$$\eta(s) = \int_{t_0}^s \frac{ds'}{\tau(s')}. \quad (2.8)$$

The constant of integration has been chosen to make $f(t) = f_0$ at $t = t_0$. This solution is valid along any trajectory in phase space characterized by a particular choice of p'_i and q'_i ; the initial value t_0 and the value of f at this point (denoted by f_0) are arbitrary functions of p'_i, q'_i . The complete formal solution of the BGK equation can now be obtained by considering the inverse of Eq. (2.5); let

$$p'_i(t') = P'_i(t'; p_i, q_i, t), \quad q'_i(t') = Q'_i(t'; p_i, q_i, t). \quad (2.9)$$

(In effect, we fix the "final" position of a particle at time t and ask where it was at an earlier time t' .) Then

$$f(p_i, q_i, t) = \int_{t_0}^t e^{-[\eta(t) - \eta(t')]} g(p'_i, q'_i, t') \frac{dt'}{\tau(p'_i, q'_i, t')} + e^{-\eta(t)} f_0 [p'_i(t_0), q'_i(t_0)], \quad (2.10)$$

where

$$\eta(s) = \int_{t_0}^s \frac{ds'}{\tau[p'_i(s'), q'_i(s'), s']}. \quad (2.11)$$

In the two preceding equations p'_i and q'_i are understood to be defined by Eq. (2.9) and are therefore dependent on p_i, q_i , and t ; $p'_i(t_0)$ and $q'_i(t_0)$ are the values of these quantities at $t' = t_0$, and f_0 is an arbitrary function of its arguments. Again, the value of f at $t = t_0$ is f_0 . Note that t_0 can be chosen differently on each trajectory, and this freedom can be used to meet boundary conditions. For the mixed initial and boundary value problem, $t_0 = 0$ for characteristics which extend backwards from p_i, q_i, t all the way to $t = 0$ without intersecting the boundary, and f_0 is the initial value of f on these characteristics. For trajectories which intersect the boundary for some $t_0 > 0$, the value of t_0 must be determined as a function of p_i, q_i, t , and appropriate boundary conditions must be supplied for f .

The formal solution of the BGK equation is quite general, but somewhat misleading, because there is another connection between f and g —the equilibrium distribution must have the same mass, momentum, and energy densities as f itself. To elucidate this point it is convenient to consider a model Hamiltonian of the form

$$\mathcal{H}(p_i, q_i) = \frac{m}{2} (u_i^2 + \xi^2), \quad (2.12)$$

where u_i are the Cartesian velocity components of the particle and the internal energy has been written as $\frac{1}{2}m\xi^2$. The quantity ξ may be considered as the length of a K -dimensional vector of (Cartesian) velocities associated with internal degrees of freedom of a molecule. (This parameterization of the internal energy is particularly useful for perfect gases with constant ratio of specific heats, which corresponds to constant K .) We can also suppose that f and g have been multiplied by m to give the mass per unit volume in phase space. As we do not need the distribution over the coordinates associated with internal degrees of freedom, we can suppose that they have been integrated out. Also, since we need only the total internal energy of a molecule and not the energy associated with any particular internal degree of freedom, we can suppose that an integral has been taken over angles in ξ . With these changes, then, we can redefine f to be such that

$$f(u_i, \xi, x_i, t) \xi^{K-1} d\xi du_i dx_i \quad (2.13)$$

is the total mass in the indicated volume element in the reduced phase space of u_i, ξ, x_i at time t . In the absence of external forces the BGK equation for f now reads

$$f_{,t} + u_i f_{,i} = \frac{(g-f)}{\tau}, \quad (2.14)$$

and the formal solution for f becomes

$$f(u_i, \xi, x_i, t) = \int_{t_0}^t e^{-[\eta(t) - \eta(t')]} g[u_i, \xi, x_i - u_i(t - t'), t'] \times \frac{dt'}{\tau[x_i - u_i(t - t'), t']} + e^{-\eta(t)} f_0(u_i, \xi, x_i - u_i t), \quad (2.15)$$

where

$$\eta(s) = \int_{t_0}^s \frac{ds'}{\tau[x_i - u_i(s - s'), s']}. \quad (2.16)$$

The Maxwell-Boltzmann distribution can be written as

$$g(u_i, \xi, x_i, t) = A e^{-\lambda((u_i - U_i)^2 + \xi^2)}, \quad (2.17)$$

where the parameters A , U_i , and λ are functions of x_i and t and are related to the macroscopic mass (ρ), momentum (P_i), and energy (ε) densities by

$$\begin{pmatrix} \rho \\ P_i \\ \varepsilon \end{pmatrix} = \int \begin{pmatrix} 1 \\ u_i \\ \frac{1}{2}(u_i^2 + \xi^2) \end{pmatrix} g d\Xi, \quad (2.18)$$

where $d\Xi = \xi^{K-1} d\xi du_i$. There are five parameters in g and five macroscopic quantities—the preceding equations for the moments of g define a one-to-one correspondence between these two sets of variables:

$$\begin{pmatrix} \rho \\ P_i \\ \varepsilon \end{pmatrix} = \begin{pmatrix} A\pi^{(K+3)/2} \lambda^{-(K+3)/2} \\ \rho U_i \\ \frac{1}{2} \rho \left(U_i^2 + \frac{K+3}{2\lambda} \right) \end{pmatrix}. \quad (2.19)$$

It is convenient to introduce an abbreviated notation for the moments and parameters of g . Let

$$\psi_\alpha = \{1, u_1, u_2, u_3, \frac{1}{2}(u_k^2 + \xi^2)\} \quad (2.20)$$

and

$$\Psi_\alpha = \{\rho, P_1, P_2, P_3, E\}. \quad (2.21)$$

We can also define five functions $\chi_\alpha(x_i, t)$ such that

$$g = e^{-\chi_\alpha \psi_\alpha}, \quad (2.22)$$

where $\chi_\alpha = (-\ln(A), -2\lambda U_1, -2\lambda U_2, -2\lambda U_3, 2\lambda)$. Equa-

tion (2.18) for the mass ($\alpha = 1$), momentum ($\alpha = 2, 3, 4$), and energy ($\alpha = 5$) densities in this notation are

$$\Psi_\alpha(x_i, t) = \int \psi_\alpha e^{-\chi_\alpha(x_i, t) \psi_\alpha} d\Xi. \quad (2.23)$$

The fundamental hypothesis of the BGK model is that the true distribution function f tends to relax to a local equilibrium distribution g having the same mass, momentum, and energy densities as f itself. This implies that

$$\int \psi_\alpha (f - g) d\Xi = 0, \quad (\alpha = 1, 2, \dots, 5) \quad (2.24)$$

for all x_i and t . As there are only five functions of x_i and t in g , the preceding equations uniquely determine g if f is given. On the other hand, we have the formal solution for f given g , the initial conditions for f and τ . So far as τ is concerned we take it to be the mean time between collisions and therefore a function of the macroscopic quantities—these in turn are moments of g .

By introducing the formal solution of the BGK equation (cf. Eqs. (2.15) and (2.16)) into the compatibility condition (Eq. (2.24)), we can find the set of coupled nonlinear integral equations for the parameters of g ,

$$\begin{aligned} \int \psi_\alpha e^{-\psi_\alpha \chi_\alpha(x_i, t)} d\Xi &= \int \psi_\alpha \int_{t_0}^t e^{-\psi_\beta \chi_\beta(x_i', t') - \eta(x_i, t) + \eta(x_i', t')} \\ &\times \frac{dt'}{\tau(x_i', t')} d\Xi \\ &+ e^{-\eta(x_i, t)} \int \psi_\alpha f_0(u_j, \xi, x_i') d\Xi, \end{aligned} \quad (2.25)$$

where $x_i' = x_i - u_i(t - t')$ in the first integral and $x_i'' = x_i - u_i t$ in the second. Equation (2.25), when supplemented with appropriate boundary conditions, is valid all the way from the Euler regime (in the limit $\tau = 0$) through the Navier-Stokes regime (small, non-zero τ) to free molecular flow at $\tau = \infty$. This particular formulation of gas flow problems does not seem to have received much attention in the literature, perhaps because it is so obviously and strongly nonlinear.

If we can find a solution of Eq. (2.25) for g the formal solution of the BGK equation gives f (cf. Eqs. (2.15) and (2.16)). Oddly enough, it seems that the parameters of g , or the equivalent set of mass, momentum, and energy densities, are all that is needed to solve a gas-dynamic problem in the BGK formulation; these are precisely the quantities that appear in the hydrodynamic equations. It is not true, however, that a solution of the hydrodynamic equations leads automatically to a solution of a problem in rarefied

gas dynamics, for two reasons: the first is that g is determined by the fundamental integral equations, not by the hydrodynamic equations, which give only an approximation to g in the limit of small mean free path. This assumption breaks down near surfaces treated as discontinuities in the Euler equations, e.g. boundary layers, shock fronts and contact discontinuities. Second, the integral equation calls for information not usually furnished when posing a hydrodynamic problem. To be quite correct, we must give the initial value of the distribution function f and its value at the boundaries in order to solve for g . The circumstance that makes hydrodynamics possible is that the regions where f and g are very different are of the order of a mean free path thick and these regions may occupy only a small part of the volume of the gas.

Successful application of the BGK equation depends on being able to find the five parameters of g as functions of the four variables x_i and t , and in one sense it is easier than solving the Boltzmann equation for the real distribution function f , which depends on the seven variables x_i , u_i and t . On the other hand, the set of coupled integral equations for the parameters of g look formidable enough to discourage one from believing that they can be used except in the simplest cases. This pessimism is unwarranted, at least for numerical hydrodynamics, as we shall see in the next section.

Note. The notation in this section facilitates the passage between parameters and moments of a Maxwellian. Here we record a number of elementary results for the case of constant K , i.e., for perfect gases with constant γ . Let

$$\Psi = \int g d\Xi, \quad (2.26)$$

where

$$g = e^{-\chi_\alpha \psi_\alpha}. \quad (2.27)$$

It is obvious that Ψ depends on χ_α only, as these are the only parameters appearing in g , and that the variables in χ_α have been integrated out. Now define

$$\Psi_\alpha \equiv \int \psi_\alpha g d\Xi = -\frac{\partial \Psi}{\partial \chi_\alpha} \quad (2.28)$$

and

$$\Psi_{\alpha \dots \mu} \equiv \int \psi_\alpha \dots \psi_\mu g d\Xi = (-1)^n \frac{\partial^n \Psi}{\partial \chi_\alpha \dots \partial \chi_\mu} \quad (2.29)$$

for n indices $\alpha \dots \mu$. The $\Psi_{\alpha \dots \mu}$ are symmetric in all indices and are functions of χ_β which can clearly be written in explicit form, since Ψ is known explicitly as a function of χ_α .

For the case of constant K the equations for $\Psi_\alpha(\chi_\beta)$ can be inverted explicitly to give

$$\chi_\beta \equiv X_\beta(\Psi_\alpha) \quad (2.30)$$

and

$$d\chi_\beta = \frac{\partial X_\beta}{\partial \Psi_\alpha} d\Psi_\alpha \equiv X_{\beta\alpha} d\Psi_\alpha. \quad (2.31)$$

On the other hand, from (2.29) we have

$$d\Psi_\alpha = \frac{\partial \Psi_\alpha}{\partial \chi_\beta} d\chi_\beta = \Psi_{\alpha\beta} d\chi_\beta, \quad (2.32)$$

or

$$X_{\beta\alpha} \Psi_{\alpha\gamma} = \delta_{\beta\gamma},$$

and all quantities can be written as explicit functions either of χ_α or Ψ_β . For the expansion of g as a function of x_i and t about the point $x_i = 0$, $t = 0$, which we will need in the next section, we have

$$g_{,i} = -\psi_\alpha \chi_{\alpha,i} g = -\psi_\alpha \frac{\partial \chi_\alpha}{\partial \Psi_\beta} \Psi_{\beta,i} g = -\psi_\alpha X_{\alpha\beta} \Psi_{\beta,i} g, \quad (2.33)$$

with a similar expression for $g_{,t}$. Since $X_{\alpha\beta}$ can be written explicitly as a function of Ψ_γ , this expression allows us to express space and time derivatives of g in terms of moments of g , i.e., the functions Ψ_γ and their space and time derivatives. Each space or time derivative of g has a characteristic dependence on ψ_α . An easy extension of these considerations shows that it is possible to construct an explicit solution of the initial value problem for f in the form of a Taylor series in t by repeated differentiation of the BGK equation (2.14) and the compatibility conditions (Eq. (2.24)). The series could be made the basis of a numerical method, but it presumes that the initial data are sufficiently smooth, and this is too restrictive a condition for high speed flow. In the next section we consider a numerical method which allows discontinuities in the initial conditions, but we will use the characteristic dependence of derivatives on velocities discussed above.

III. A HYDRODYNAMIC CODE

We consider one-dimensional flow of a perfect gas with constant ratio of specific heats. It will be convenient to treat the motion of the molecules in the direction perpendicular to the flow by adding two internal degrees of freedom to the

ones required to give the correct value of γ . For a real gas in three dimensions classical statistical mechanics gives $\gamma = (n+2)/n$, where n is the total number of "effective" degrees of freedom of the molecule: thus a monoatomic gas has $n=3$, $\gamma = \frac{5}{3}$, and a diatomic gas, with two rotational degrees of freedom excited at ordinary temperatures, has $n=5$, $\gamma = \frac{7}{5}$. For a flow in D dimensions we treat D of the n degrees of freedom explicitly, and $K = -D + 2/(\gamma - 1)$. Thus for air, for example, $\gamma \simeq \frac{7}{5}$, and for flow in one dimension $K = 4$. The expressions for g and the volume element $d\Xi$ in the reduced phase space do not require K to be an integer, or even a constant—this freedom could be exploited to accommodate imperfect gases.

For numerical purposes we divide the region occupied by the gas into a number of equal intervals (cells) of unit length along the x -axis and suppose that initial values of mass, momentum, and energy are given in each cell. The boundary conditions are assumed to be either periodic or reflecting. A solution of the fundamental integral equations would be a solution of the problem, but in the interest of deriving a conservative scheme we have found it useful to follow a somewhat less direct route. Our strategy for finding a numerical solution using Eq. (2.25) for g is the following:

(1) To update the solution from $t=0$ to $t=T$ in a conservative fashion we compute the flux of mass, momentum, and energy across each cell boundary for $0 < t < T$. These fluxes are given by

$$F_{\alpha i} = \int u_i \psi_\alpha f d\Xi, \quad (3.1)$$

and to find them we need to know f at each cell wall as a function of t during the time interval T . This information can be obtained from Eq. (2.15), provided that we know g in the neighborhood of each cell wall.

(2) To find g , we use a very crude solution of the fundamental integral Eq. (2.25), retaining only the linear terms in the Taylor series expansion of g as a function of x and t about the point $t=0$ and x corresponding to a cell wall; we can temporarily choose $x=0$ to correspond to a boundary between two adjacent cells.

Assume that the Maxwellian in the neighborhood of a cell wall can be approximated as

$$g(x, t) = g(0, 0)(1 + ax + At), \quad (3.2)$$

where $g(0, 0)$ is the distribution function at $t=0$ at the beginning of a time step and the origin of x is a cell wall. (We suppress the u and ξ dependence of f and g in this section.) According to the preceding section, the ψ_α dependence of a and A are given by

$$a = a_\alpha \psi_\alpha, \quad A = A_\alpha \psi_\alpha, \quad (3.3)$$

and, if the initial data were sufficiently smooth, we would have $a_x = -\Psi_{\alpha, x}(0, 0)$ and $A_x = -\Psi_{\alpha, t}(0, 0)$. The notation a_x and A_x is chosen to emphasize that these quantities will, in general, not be determined by fitting Ψ_x to the data and differentiating it. The procedure for estimating $g(0, 0)$ and a from the initial conditions is postponed to the next section; here we suppose that $g(0, 0)$ and a_x are known.

The integral equation is used to determine A_x . Recalling the steps that lead to Eq. (2.15), we start by finding f from the formal solution of the BGK equation, assuming for numerical purposes that τ is locally constant. In this case we have simply $\eta(s) = s/\tau$ and

$$f(x, t) = \frac{1}{\tau} \int_0^t g(0, 0)(1 + ax' + At') e^{-(t-t')/\tau} dt' + f_0(x - ut) e^{-t/\tau}, \quad (3.4)$$

where $x' = x - u(t - t')$. The integration is elementary and gives

$$f(x, t) = g(0, 0)((1 - e^{-t/\tau})(1 + ax - \tau ua - \tau A) + te^{-t/\tau} ua + tA) + f_0(x - ut) e^{-t/\tau}. \quad (3.5)$$

In this expression f_0 is an arbitrary initial distribution function and is not necessarily the same as g at $t=0$. Our numerical experience strongly indicates that the freedom to choose f_0 to be different from g at $t=0$ can be useful. In particular, we have found that a discontinuous f_0 of the form

$$f_0(x) = \begin{cases} g_l(0, 0)(1 + a_l x), & x < 0, \\ g_r(0, 0)(1 + a_r x), & x > 0, \end{cases} \quad (3.6)$$

with $a_l = a'_l \psi_\alpha$, $a_r = a'_r \psi_\alpha$, and g_l and g_r Maxwellian gives satisfactory results. The determination of g_l and g_r from the initial conditions will be covered in the next section. Note that we actually use the initial conditions in two different ways, one to compute a smooth $g(x, 0)$, the other to approximate a discontinuous f_0 . By way of excuse for this assumption (aside from the fact that it works) we offer the remark that g is the distribution function towards which f is continually trying to relax and that it is plausible that g is smoother than f . Also, if the discontinuity of $f_0(x)$ is substantial and if τ is large (as it will be at shocks; cf. Eq. (4.8)), then our choice of f_0 has the effect of using a bimodal velocity distribution in the flux computation. This is in qualitative agreement with the behavior of f at a shock given by a more exact treatment (Mott-Smith [12]).

To find fluxes we only need f as a function of t at $x=0$, i.e., on a cell wall. From Eq. (3.5) we have

$$f(0, t) = g(0, 0)\{(1 - e^{-t/\tau})(1 - \tau ua - \tau A) + t(e^{-t/\tau} ua + A)\} + e^{-t/\tau} f_0(-ut), \quad (3.7)$$

where

$$f_0(-ut) = \begin{cases} g_l(0, 0)(1 - a_l ut), & u > 0 \\ g_r(0, 0)(1 - a_r ut), & u < 0. \end{cases} \quad (3.8)$$

It remains to determine A . From the discussion leading to the integral equation (2.25) we recall that f and g should have the same moments for all x and t . We cannot achieve this with the present approximation, but we can insist that at $x=0$, and in the mean over the time interval $0 < t < T$, f and g have the same moments. That is, we impose the three conditions

$$\int_0^T \int \psi_\alpha [f(0, t) - g(0, t)] d\xi dt = 0 \quad (\alpha = 1, 2, 3) \quad (3.9)$$

which satisfies the time average of the integral equation at each cell wall. Equation (3.9) gives the three linear equations

$$\begin{aligned} A_x \int \psi_\alpha \psi_\beta g(0, 0) d\xi \\ = \frac{1}{\tau(s_1 - T)} \int \{ \psi_\beta(s_1 - [\tau(s_1 - T) + s_2] u a_\gamma \psi_\gamma) \\ \times g(0, 0) - \hat{f}_0 \} d\xi, \end{aligned} \quad (3.10)$$

where

$$\hat{f}_0 = \begin{cases} (s_1 - s_2 u a_l) g_l(0, 0), & u \geq 0, \\ (s_1 - s_2 u a_r) g_r(0, 0), & u \leq 0, \end{cases} \quad (3.11)$$

$$s_1 = \int_0^T e^{-t/\tau} dt = \tau(1 - e^{-T/\tau}), \quad (3.12)$$

and

$$s_2 = \int_0^T t e^{-t/\tau} dt = \tau^2(1 - e^{-T/\tau}) - \tau T e^{-T/\tau}. \quad (3.13)$$

The matrix multiplying A_x is precisely the $\Psi_{\alpha\beta}$ introduced in the preceding section, and it can be inverted in explicit form to give A_x . Once A_x is known, $f(0, t)$ follows from Eq. (3.7), and the time dependent fluxes $F_{\alpha i}$ are computed at $x=0$ from Eq. (3.1), again explicitly. Finally the total flux over the interval $0 \leq t \leq T$ is found by an elementary explicit integration and used to update the mass, momentum, and energy in each cell.

IV. NUMERICAL EXAMPLES

In Section III we passed over the question of computing $f_0(x)$ and $g(x, 0)$ at $t=0$ from the initial value of the total

mass, momentum, and energy in each cell. Let $i=0$ correspond to the cell wall at $x=0$ and number the cell walls with integer values of i and the cell with half-odd integers. Let $\Psi_{\alpha|i+1/2}$ ($\alpha = 1, 2, 3$) be the values of the mass, momentum, and energy in the cell $i + \frac{1}{2}$ at time $t=0$. First we use these data for $i = -2, -1, 0, 1$ to find $g(0, 0)$ and a_α . For each α , let $\tilde{\Psi}_\alpha(x)$ be a cubic in x whose coefficients are determined from the conditions

$$\Psi_{\alpha|i+1/2} = \int_i^{i+1} \tilde{\Psi}_\alpha(x) dx, \quad i = -2, \dots, +1. \quad (4.1)$$

It is really found that

$$\tilde{\Psi}_0(0) = \frac{7}{12}(\Psi_{\alpha|1/2} + \Psi_{\alpha|-1/2}) - \frac{1}{12}(\Psi_{\alpha|3/2} + \Psi_{\alpha|-3/2}), \quad (4.2)$$

and the derivative of $\tilde{\Psi}_\alpha(x)$ at $x=0$ is

$$\tilde{\Psi}_{\alpha,x}(0) = \frac{5}{4}(\Psi_{\alpha|1/2} - \Psi_{\alpha|-1/2}) - \frac{1}{12}(\Psi_{\alpha|3/2} - \Psi_{\alpha|-3/2}). \quad (4.3)$$

Where the data are sufficiently smooth we can use Eq. (2.30) for $\chi_\beta(\Psi_\alpha)$ to find the parameters $\chi_\beta[\tilde{\Psi}_\alpha(0)]$ of the Maxwellian $g(0, 0)$, and from Eq. (2.33) for $g_{,\alpha}$ we can find the derivatives of these parameters at $x=0$. From Eq. (2.31) we have

$$X_{\lambda\beta} \Psi_{\beta,x} = \chi_{\lambda,x}, \quad (4.4)$$

and we can identify the derivative $\chi_{\lambda,x} = -a_\lambda$ or

$$a_\lambda = -X_{\lambda\beta} \tilde{\Psi}_{\beta,x}(0) \quad (4.5)$$

for the expansion of g about $(0, 0)$. However, we require that the interpolated values $\tilde{\Psi}_\alpha(0)$ satisfy some reasonable constraints:

1. if $\tilde{\Psi}_\alpha(0)$ falls outside the range $[\Psi_{\alpha|-1/2}, \Psi_{\alpha|1/2}]$, we replace $\tilde{\Psi}_\alpha(0)$ with the value of $\Psi_{\alpha|\pm 1/2}$ lying nearest to $\tilde{\Psi}_\alpha(0)$, independently for each α .
2. If $\tilde{\Psi}_{\alpha,x}(0)$ and $(\Psi_{\alpha|1/2} - \Psi_{\alpha|-1/2})$ have opposite signs for any α , we replace the values of $\tilde{\Psi}_\alpha(0)$ and $\tilde{\Psi}_{\alpha,x}(0)$ with $\frac{1}{2}(\Psi_{\alpha|1/2} + \Psi_{\alpha|-1/2})$ and $(\Psi_{\alpha|1/2} - \Psi_{\alpha|-1/2})$ respectively, for all α . In both cases the computation of a_λ is exactly the same as that given by Eq. (4.5) for $\tilde{\Psi}_\alpha(0)$ and $\tilde{\Psi}_{\alpha,x}(0)$, derived from cubic interpolation.

For the initial distribution $f_0(x)$ we need to determine the parameters of $\chi'_\alpha(0, 0)$ and $\chi''_\alpha(0, 0)$ of the Maxwellians $g^l(0, 0)$, $g^r(0, 0)$ and the quantities a'_α and a''_α . For the Maxwellian, we proceed in much the same way as above, but we use quadratic interpolation on $\Psi_{\alpha|i+1/2}$, with $i = (-2, -1, 0)$ for $\chi'_\alpha(0, 0)$ and $(-1, 0, 1)$ for $\chi''_\alpha(0, 0)$. If the

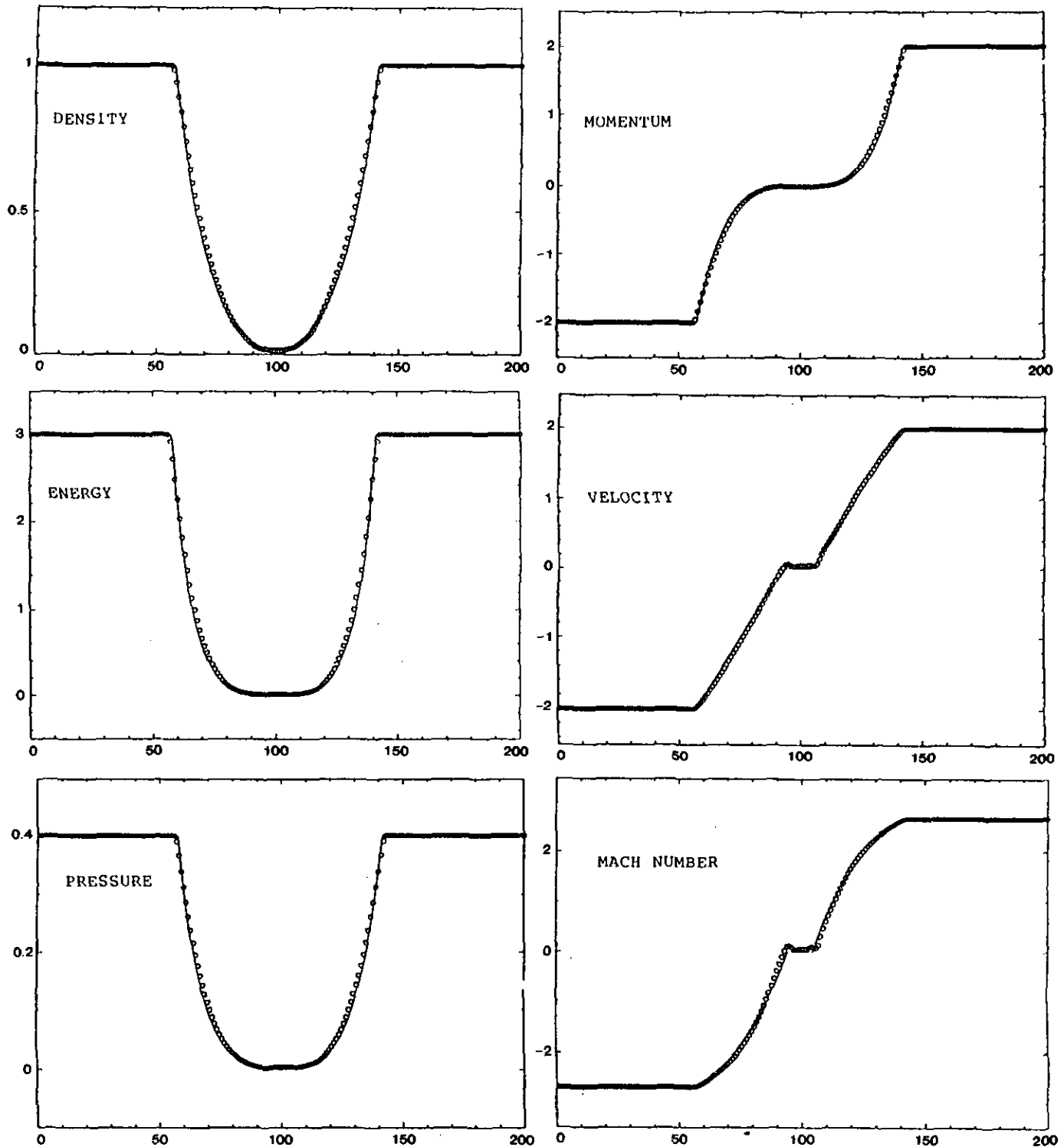


FIG. 1.1. First (supersonic) Sjögreen test case on a grid of two hundred points. The figures show density, momentum, energy, velocity, pressure, and Mach number; all of these quantities are zero at $x=0$. The solid line is the exact solution and is well reproduced by the code. The corners where the rarefaction wave meets the undisturbed gas are especially sharp. $\mathcal{C}_1 = 0.01$ and $\mathcal{C}_2 = 1.0$ (cf. Eq. (4.8)) for all test cases in this paper.

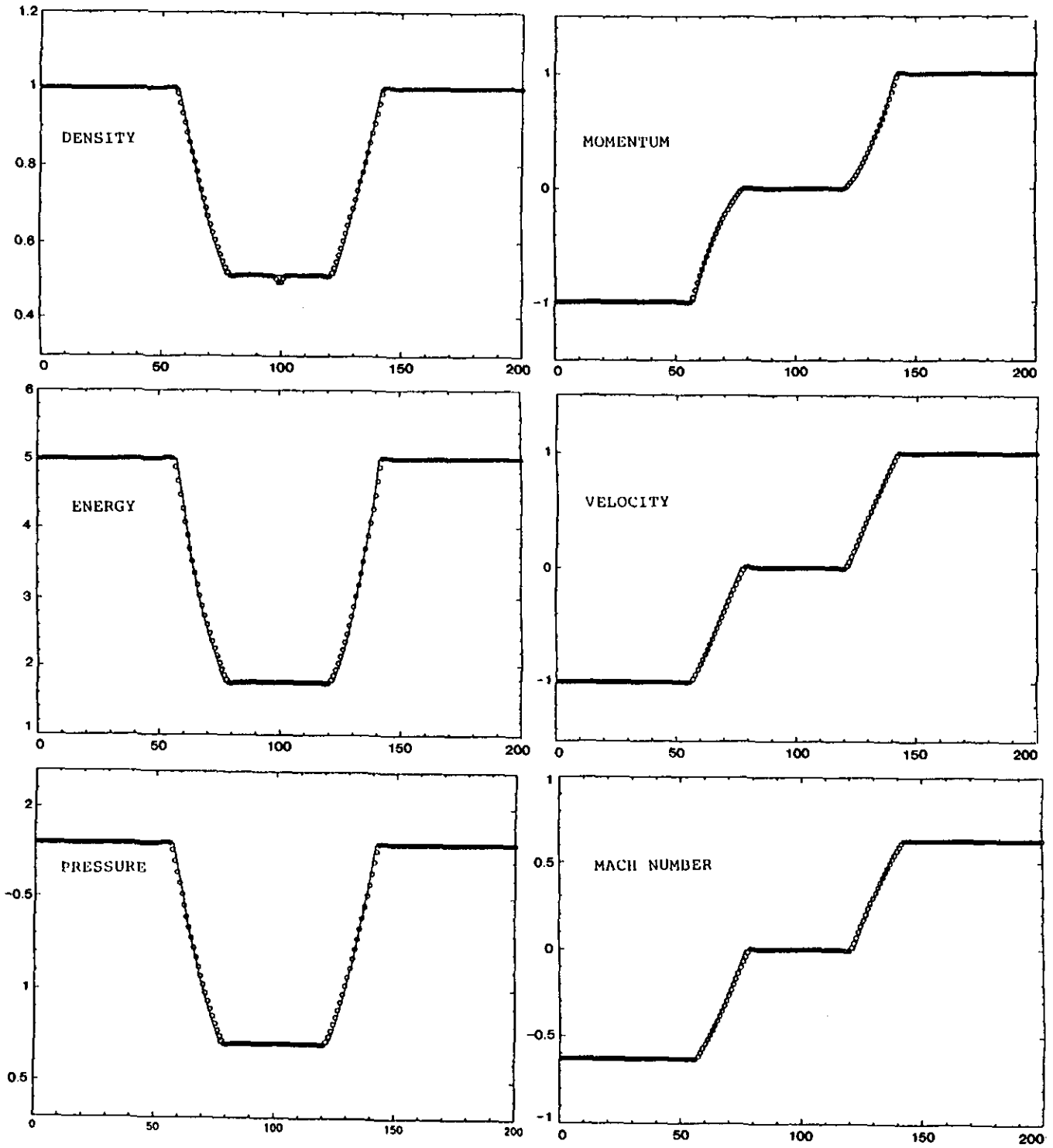


FIG. 1.2. Second (subsonic) Sjögreen test case. The graphs give the same quantities as shown in Fig. 1.1.

interpolated Ψ_x falls outside the range $[\Psi_{\alpha|-1/2}, \Psi_{\alpha|1/2}]$, we replace it with the closer value of the pair $\Psi_{\alpha|-1/2}$ and $\Psi_{\alpha|1/2}$. The determination of α'_x and a'_x is rather different from that of a_x , because we insist on conservation of $\Psi_{\alpha|-1/2}$ and $\Psi_{\alpha|1/2}$; that is,

$$\int_{-1}^0 \int \psi_x g'(0, 0)(1 + \psi_\beta a'_\beta x) d\Xi dx = \Psi_{\alpha|-1/2}, \quad (4.6)$$

with a similar expression for a'_x . These linear equations for the a'_x and a'_x are solved in exactly the same way as was Eq. (4.5) for a_x . We sometimes need to use a lower order interpolation scheme than the parabolic one. If

$$(\Psi_{\alpha|3/2} - \Psi_{\alpha|1/2})(\Psi_{\alpha|-1/2} - \Psi_{\alpha|-3/2}) \leq 0 \quad (4.7)$$

for any α , we find $g'(0, 0)$ and a' from conservative linear interpolation using the cells $-3/2$ and $-1/2$, and follow a similar rule for $g'(0, 0)$ and $a'(0, 0)$.

According to kinetic theory the mean collision time in a gas is proportional to $1/(\rho \mathcal{T}^{1/2})$, where \mathcal{T} is the temperature. From Eq. (2.22), \mathcal{T} is inversely proportional to χ_3 ($\alpha = 1, 2, 3$ for one-dimensional flow). We therefore have τ proportional to $(\chi_3)^{1/2}/\rho$, and our method seems to work well even for τ much less than a time step, except at shocks. We have found it useful to add a term to τ which is big at shocks and small elsewhere;

$$\tau = \mathcal{C}_1 \frac{\sqrt{\chi_3(0)}}{\rho(0)} + \mathcal{C}_2 \frac{|\sqrt{\chi_3^l/\rho_l} - \sqrt{\chi_3^r/\rho_r}| |p_l - p_r|}{\sqrt{\chi_3^l/\rho_l} + \sqrt{\chi_3^r/\rho_r} p_l + p_r}, \quad (4.8)$$

where p_l and p_r are the pressures on the left and right sides of $x=0$. This larger value of τ at a shock operates to increase the importance of the f_0 term in the Eq. (3.4) at the expense of the integral over g —it therefore lowers the order of the scheme. In extreme cases, with $\tau > T$ and f_0^l and f_0^r uniform, the current method reduces to the first-order beam

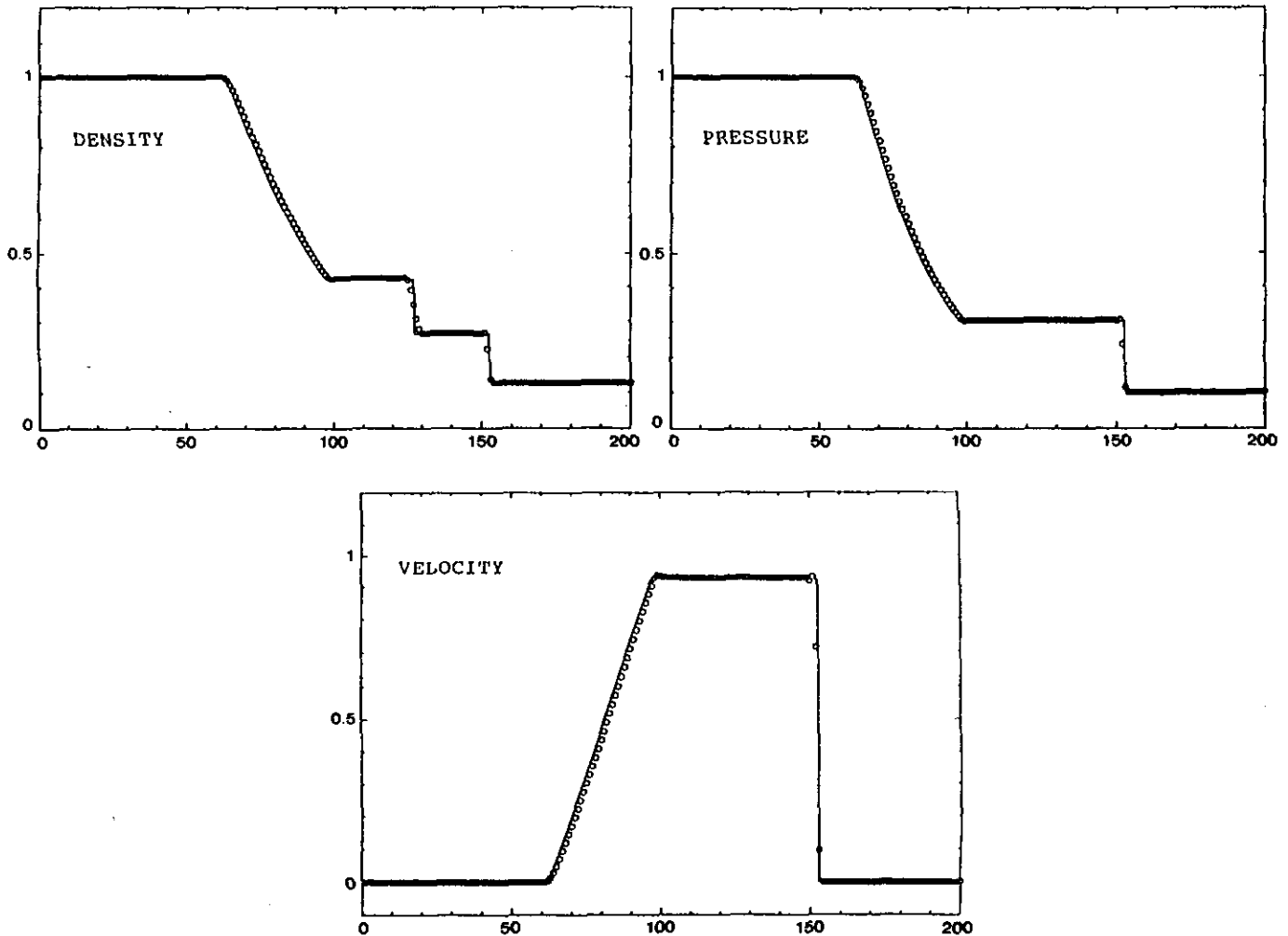


FIG. 2. Sod test case. Note the number of points in the shock and the reproduction of the rarefaction wave. The contact discontinuity has not been "sharpened" in any way. The solid line is the exact solution.

scheme with continuous fluxes. In smooth regions the current method is second order, as shown by a grid refinement experiment for a sound wave. Formally, at least, our scheme can be extended to any order by using higher order polynomial interpolation of the initial data and by taking t -moments of Eq. (3.9) over the interval T .

We have used our scheme on five well-known test cases—those of Sjögreen, Sod, Harten, Woodward and Colella, and Emery.

The two Sjögreen test cases are taken from a recently published paper by Einfeldt *et al.* [6]. In that paper, the authors analyzed the weakness of non-positive conservative schemes for the simulation of flows with large kinetic energy. They showed that no scheme whose interface flux derives from a linearized Riemann solution can be positively conservative. Fortunately, our scheme is very nonlinear. For all test cases, we use ρ , P , and ϵ to represent mass, momentum, and total energy in each cell, and we use 200

cells for the Sjögreen, Sod, and Harten tests and 400 cells for the Woodward-Colella test.

The initial data for the first Sjögreen test are $\rho_l = 1$, $P_l = -2$, $\epsilon_l = 3$ and $\rho_r = 1$, $P_r = 2$, $\epsilon_r = 3$, and for the second are $\rho_l = 1$, $P_l = -1$, $\epsilon_l = 5$ and $\rho_r = 1$, $P_r = 1$, $\epsilon_r = 5$. Our results are shown in Fig. 1.1 and Fig. 1.2. Conservative difference schemes may fail this test by producing non-physical states with negative density or internal energy, but we did not encounter the problem.

The classical Sod test case has the initial conditions $\rho_l = 1$, $P_l = 0$, $\epsilon_l = 2.5$ and $\rho_r = 0.125$, $P_r = 0$, $\epsilon_r = 0.25$. Our results are shown in Fig. 2. Note the number of points in the shock and the contact discontinuity, as well as the sharp corners of the rarefaction wave.

The Harten test case has initial conditions $\rho_l = 0.445$, $P_l = 0.311$, $\epsilon_l = 8.928$ and $\rho_r = 0.5$, $P_r = 0.0$, $\epsilon_r = 1.4275$. Our result is shown in Fig. 3. Note again the corners and the number of points in the contact discontinuity, which

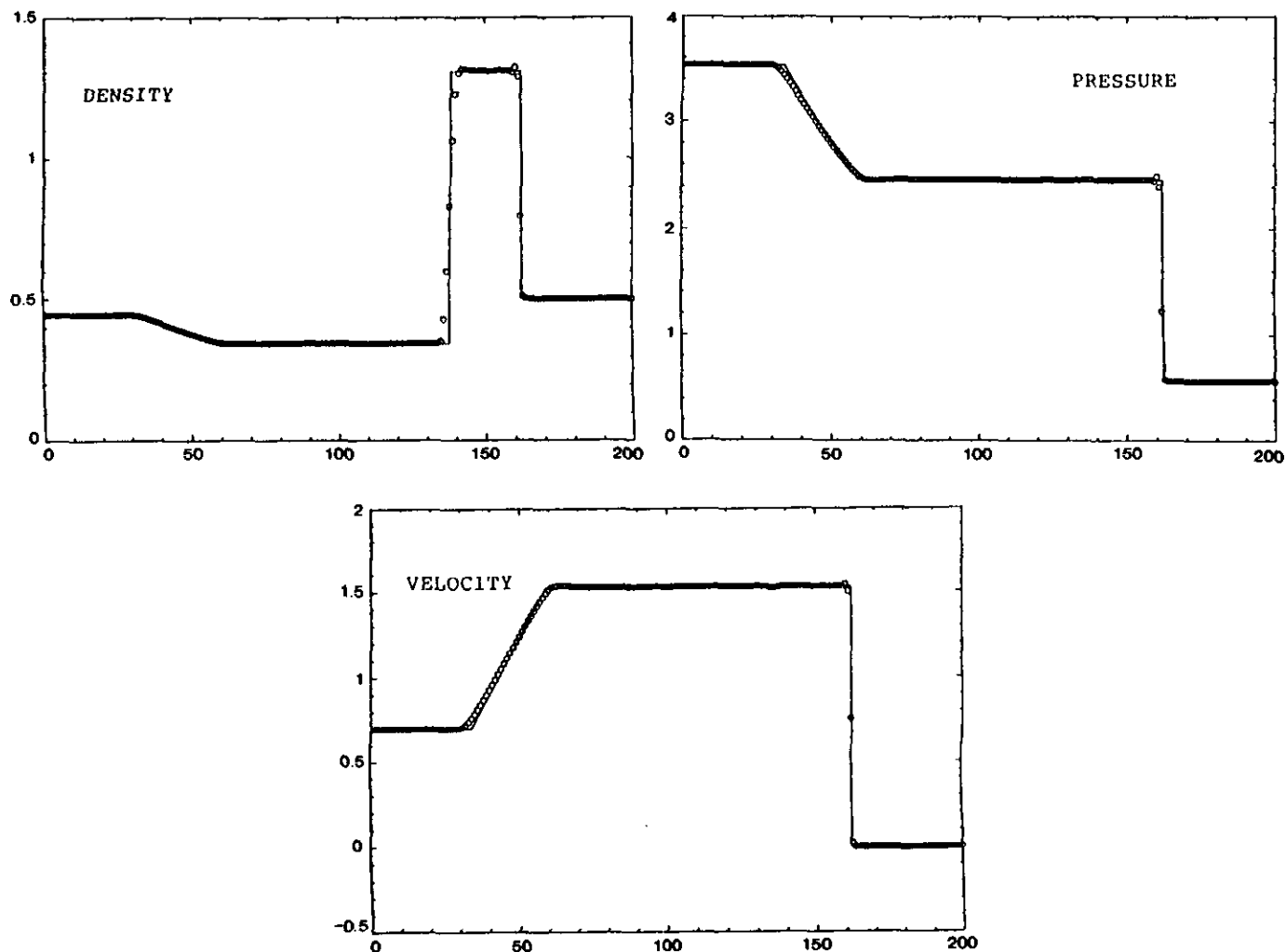


FIG. 3. Harten test case. There is a slight overshoot at the shock. Again, the contact discontinuity has not been sharpened. The solid line is the exact solution.

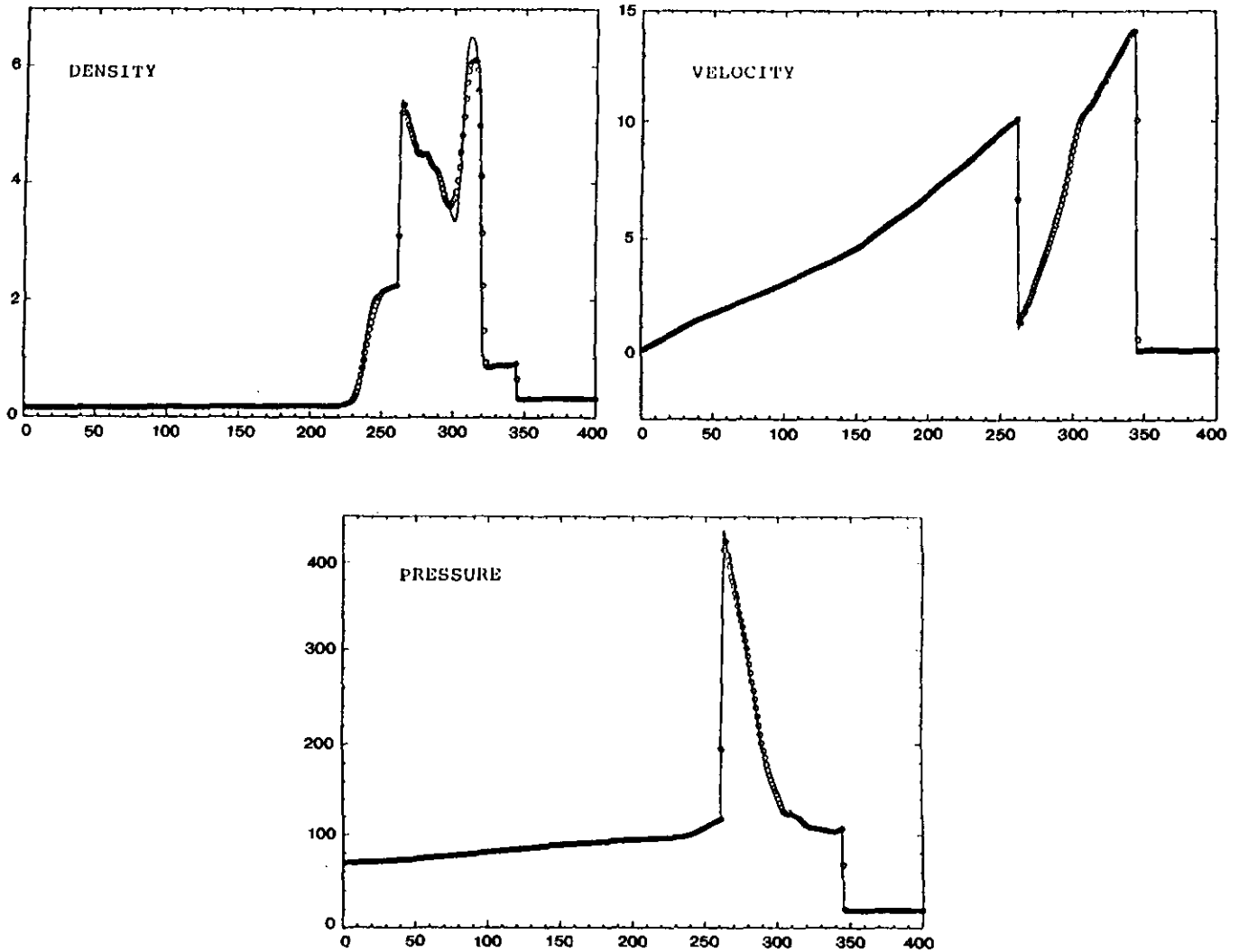


FIG. 4. Woodward-Colella test case, on a grid of 400 points. The solid line shows the solution from the same code using 800 points.

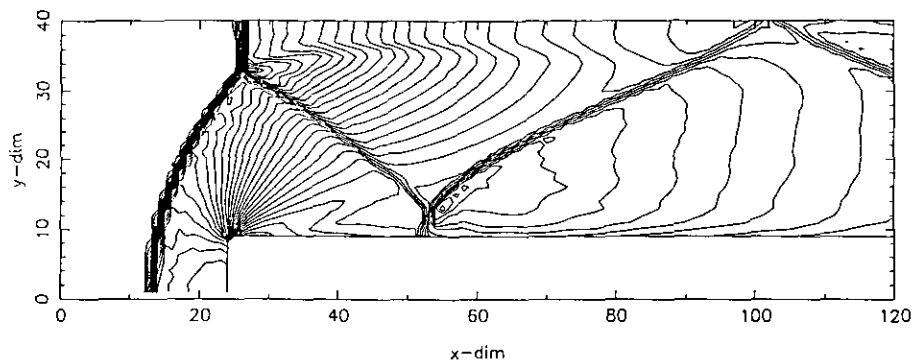


FIG. 5. Mach 3 flow in a wind tunnel with step, on a grid of 40×120 points using operator splitting. The code and parameter values are the same as those used in the one-dimensional test cases. No modifications were made to smooth the flow at the corner of the step, which may account for the Mach stem at $x \sim 52$.

are competitive with other high-resolution schemes not employing special treatment of contact discontinuities.

The fourth test case is that of Woodward and Colella [20], with the initial conditions $\rho_l = 1.0$, $P_l = 0$, $\varepsilon_l = 2500$ for $0 < x \leq 0.1$, $\rho_r = 1.0$, $P_r = 0.0$, $\varepsilon_r = 0.025$ for $0.2 < x \leq 0.9$ and $\rho_r = 1.0$, $P_r = 0.0$, $\varepsilon_r = 250$ for $0.9 < x \leq 1$. Our results are shown in Fig. 4. Note the number of points in the fronts, the heights of the maxima, and the contact discontinuities.

We have also used Strang's operator splitting method to calculate the two-dimensional Emery test case. The initial conditions can be found in Woodward and Colella's paper [20]. In Fig. 5 we present our result for a grid of 40×120 cells. In contrast to the boundary conditions used by Woodward and Colella, we did not alter our scheme in any way at or near the corner of the step.

In all cases we observe diffusion at the contact discontinuity. Physically, the thickness of a contact discontinuity should increase as \sqrt{t} , and it should be wider than the shock front. In all these test cases, we have used exactly the same code with different initial and boundary conditions, but we have not tried to identify and sharpen discontinuities in any way.

V. CONCLUSION

Our scheme is based on gas-kinetic theory and is of the "Boltzmann" type in that it uses a distribution function of particle velocities. It differs from other schemes of the Boltzmann type because it takes into account the particle collisions which occur during a time step. The machinery for doing this consists of combining an explicit solution of the BGK model of the Boltzmann equation with the compatibility conditions relating moments of the "real" distribution function to those of the equilibrium distribution towards which it continually tends to relax. The result is a set of nonlinear integral equations for the parameters of the local Maxwell-Boltzmann distribution, or, equivalently, for the moments of this distribution, which are the mass, momentum, and energy densities in the gas. The BGK model contains a relaxation time (or mean time between collisions) and is approximately valid for all values of this parameter. In particular, the Euler equations are recoverable from the BGK model in the limit of a vanishingly small relaxation time.

Some of the advantages of a numerical scheme based on the BGK model are the following:

(1) The scheme is based on a physical model, which can be exploited to indicate possible generalizations. For example, the characteristics for the BGK equation are the particle orbits in phase space, rather than the streamlines and Mach cones in space and time, and the integral equations which use these characteristics are valid in any coordinate system and for any problem with a known Hamiltonian. In principle, at least, a numerical method based on the integral

equations can be generalized by approximating the motion of a single particle in a particular coordinate system and moving in a particular force field. The numerical scheme we have constructed is for one-dimensional motion of a constant γ gas in Cartesian coordinates and without external forces. In this case we were able to carry through all steps explicitly—no numerical solutions of algebraic equations were needed. For an imperfect gas with an arbitrary equation of state this would no longer be the case, because we could not explicitly invert the transformation from moments of the Maxwellian to find the parameters of the Maxwellian. So far as we know, comparable difficulties occur in all other numerical schemes with a generic equation of state.

(2) Since the integral equations hold for all values of the relaxation time they offer the possibility of generalizing the scheme to treat the Navier-Stokes equations and even problems in rarefied gas dynamics, where the mean free path is comparable to the dimensions of the system. Of course, much more information about the true distribution function than its low-order moments must be carried in the latter case, and the boundary conditions are more complicated.

(3) For the Euler and Navier-Stokes equations the distribution functions completely disappear in the final code, which could therefore be written as a (highly nonlinear) difference scheme. In common with other Boltzmann-type codes effective upwind differencing is achieved by using the distribution function to weight the information carried by all characteristics through a given point in space. It has often been noted that conventional Boltzmann-type codes have a high degree of arbitrariness in the choice of the distribution function—we have effectively resolved this question by using the BGK model to solve for the evolution of the distribution function in time and subsequently finding time-dependent fluxes from this solution. The remaining arbitrary elements of the scheme have to do with the reconstruction of appropriate initial conditions from the initial data and the approximations made in solving the integral equations for the Maxwellian. There is plenty of room here for further development—we cannot claim to have found the most effective way of extracting information from the integral equations.

(4) Many current high-order schemes rely on solving the Riemann problem, either exactly or approximately. Our scheme, in common with other Boltzmann-type schemes, does not have an embedded Riemann problem—a fact which offers certain advantages. The first is that we do not have to use fluxes computed under the assumption of uniform states on both sides of a discontinuity; the second is that the Riemann problem is hard to generalise to include more complicated physics than the free flow of a perfect gas; and the third is that the Riemann problem does not generalise readily to two or more dimensions. While we

have not yet attempted it (so far we have used the customary operator splitting in two dimensions), there seems to be no obstacle in principle to using the integral equations to construct a true multidimensional code.

(5) Aside from a safety factor (usually 0.65) in the Courant condition, the only adjustable parameters in the scheme occur in the expression (4.8) for the collision time. One of these is physically necessary—it determines the shear and bulk viscosity coefficients, as well as the heat conduction coefficient. The other is numerically useful—it increases the mean free path at a shock and therefore effectively lowers the order of the scheme.

(6) All test cases reported in this paper were run with precisely the same code, and all cells were treated in exactly the same way. It is encouraging that we seem to be able to treat evaporation into a vacuum (Sjögreen test case) and the collision of strong shocks (Woodward–Colella test case) without modifying the code in any way. There are no discontinuity detection algorithms, with subsequent special treatment, for example, of contact discontinuities. Our results at contact discontinuities are not as good as those produced by codes employing such devices, but the option to insert them remains open. We seem to do at least as well as other codes in the treatment of shocks, and probably better in the treatment of rarefaction waves. We did not need to modify our code to treat the flow near the corner in the two-dimensional test case of flow in a wind tunnel with a step, nor did we need to take precautions to avoid an unphysical rarefaction shock above this corner; many of the published results for this test case do both.

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