Numerical schemes for kinetic equations in diffusive regimes

G. Naldi
Department of Mathematics, University of Pavia
via Abbiategrasso 215, I-27100 Pavia (Italy)
L. Pareschi
Department of Mathematics, University of Ferrara,
via Machiavelli 35, I-44100 Ferrara (Italy)

Abstract

The diffusive scaling of many finite-velocity kinetic models leads to a small-relaxation time behavior governed by reduced systems which are parabolic in nature. Here we demonstrate that standard numerical methods for hyperbolic conservation laws with stiff relaxation fail to capture the right asymptotic behavior. We show how to design numerical schemes for the study of the diffusive limit that possess the discrete analogue of the continuous asymptotic limit. Numerical results for a model of relaxing heat flow and for a model of nonlinear diffusion are presented.

1 Introduction

In the kinetic theory of rarefied gases, two-velocity models of the discrete Boltzmann equation describe the behavior of a fictitious gas of two kind of particles that move parallel to the $x-$axis with constant and equal speed. So we can consider at time t the particles with a density $u(x,t)$, which move in the positive $x-$direction, and the particles which move in the negative $x-$direction with a density $v(x,t)$. The most general two-speed gas, which is in local equilibrium when $u = v$, is described by the following hyperbolic system

$$\begin{aligned}
&\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = k(v-u) \\
&\frac{\partial v}{\partial t} - c\frac{\partial v}{\partial x} = k(u-v) \qquad (1) \\
&x \in \mathrm{R}, \quad t \geq 0,
\end{aligned}$$

where the collision kernel $k = k(u,\ v,\ x)$ is a nonnegative function which characterizes the binary interactions between particles.

In the *diffusive scaling* we consider the normalized system of equations (1) in the form

$$
\begin{aligned}
&\frac{\partial u}{\partial t} + \frac{1}{\epsilon}\frac{\partial u}{\partial x} = \frac{1}{\epsilon^2} k(v-u) \\
&\frac{\partial v}{\partial t} - \frac{1}{\epsilon}\frac{\partial v}{\partial x} = \frac{1}{\epsilon^2} k(u-v) \\
&x \in \mathrm{R}, \quad t \geq 0.
\end{aligned}
\tag{2}
$$

In (2) ϵ^2 is called the *relaxation time* and the limit problem for $\epsilon \to 0$ is called *diffusive limit*. When $\epsilon << 1$ both the collision terms and the spatial derivatives are called *stiff*.

In the sequel for simplicity we will restrict our analysis to collision kernels of the type $k(u, v, x) = k(u + v)$. The most famous example of this type of models was introduced by Carleman [3] and corresponds to the choice $k(u + v) = u + v$.

The macroscopic variables for the two-velocity kinetic model (2), are the mass density $\rho = u + v$, and the flux $J^\epsilon = (u - v)/\epsilon$. Then, the diffusive scaling problem (2) is equivalent to the following

$$
\begin{aligned}
&\frac{\partial \rho}{\partial t} + \frac{\partial J^\epsilon}{\partial x} = 0 \\
&\frac{\partial J^\epsilon}{\partial t} + \frac{1}{\epsilon^2}\frac{\partial \rho}{\partial x} = -\frac{1}{\epsilon^2} 2k(\rho) J^\epsilon.
\end{aligned}
\tag{3}
$$

As $\epsilon \to 0$, (3b) relaxes to the local equilibrium $J^0 = -(2k(\rho))^{-1}\partial\rho/\partial x$ and ρ formally satisfies the nonlinear diffusion equation

$$
\frac{\partial \rho}{\partial t} + A(\rho)\left(\frac{\partial \rho}{\partial x}\right)^2 = B(\rho)\frac{\partial^2 \rho}{\partial^2 x}
\tag{4}
$$

where $A(\rho) = (2k(\rho))^{-2} dk(\rho)/d\rho$ and $B(\rho) = (2k(\rho))^{-1}$.

Theoretical studies for these relaxation problems began with Kurz [5] and McKean [9] for the Carleman model. For more general collision kernels of the type $k(\rho) = \rho^{-\alpha}$ for $\alpha \geq -1$ the study of the diffusive limit were performed recently in [8]. From a numerical point of view semidiscrete numerical methods for similar problems have been studied by Jin and Levermore [6].

Here we would like to investigate the possibility of obtaining the macroscopic behavior described by the equilibrium system (4) by solving the original kinetic system (3) with coarse grids $\Delta t, \Delta x >> \epsilon^2$. Critical to this type of problems is that the underresolved numerical methods although stable may yield spurios numerical solutions totally unphysical [11].

As a first but crucial step we will concentrate on the stiff regime that is to say when $\epsilon << 1$. We will demonstrate that in the diffusive regime most of the popular methods for the solution to hyperbolic conservation laws with stiff relaxation present several limitations and fail to capture the right behavior of the limit equilibrium equation unless the small relaxation rate is resolved by a fine spatial grid. We show how to overcome this new difficulty and how to construct numerical schemes with the correct diffusive limit.

2 Numerical Approximation

The diffusive limit is more challenging for numerical methods than the corresponding fluid-dynamic limit [2, 4], because in addition to the stiff relaxation term the convection term is also stiff. Since the characteristic speed of the homogeneous hyperbolic system is of order $1/\epsilon$, the usual approach of keeping the convective part explicit and the collision part implicit leads to a stability constraint of the type $\Delta t \sim \epsilon \Delta x$. Clearly, this is too restrictive near the parabolic regime $\epsilon < \Delta x$ where a condition of the type $\Delta t \sim \Delta x^2$ is expected. For example, characteristic-based numerical schemes[12], because the characteristic mesh requires $\Delta t = \epsilon \Delta x$, do not allow to obtain a limit stability constraint independent of ϵ.

First we want to emphasize that this problem is not merely a numerical stability problem. In fact the popular splitting of the convection from the collision part, although solved with a stable method, does not provide the correct diffusive behavior as $\epsilon \to 0$. This operator splitting consists in solving separately the homogeneous hyperbolic problem and the ordinary differential equations associated to system (2). In the small relaxation limit, $\epsilon \to 0$, we obtain the equilibrium equations $\partial\rho/\partial t = 0$, $\partial\rho/\partial x = 0$, that clearly are unconsistent with the diffusive limit (4). The contruction of consistent operator splitting methods for this type of problems has been studied recently in [7, 10].

We will introduce the spatial grid points $x_{i+1/2}$, $i = \ldots, -1, 0, 1, \ldots$ with uniform mesh width $\Delta x = x_{i+1/2} - x_{i-1/2}$. The discrete time level t^n are also spaced uniformly with time step $\Delta t = t^{n+1} - t^n$ for $n = 0, 1, 2, \ldots$. As usual we denote by $U^n_{i+1/2} = U(x_{i+1/2}, t^n)$ the nodal values and by U^n_i the cell averages of U in the cell $[x_{i-1/2}, x_{i+1/2}]$ at time t^n

$$U^n_j = \frac{1}{\Delta x}\int_{x_{i-1/2}}^{x_{i+1/2}} U(x, t^n)\, dx.$$

In order to write a stable discretization to system (3) we should use implict temporal integrators on the stiff terms. Because the stiffness of the convection term depends on the size of the two eigenvalues $\pm 1/\epsilon$ of the Riemann invariant form (2) of system (3), both convection terms have to be implicit. However a fully implicit scheme causes global data dependencies, a severe disvantage if we consider second order nonlinear upwind schemes using slope limiters. Further, the gain of stability is partially offset by the loss of accuracy typical of implicit schemes in the context of wave-propagation phoenomena.

Thus we consider the following semi-implicit discretization in conservative form

$$\begin{aligned} &\frac{\rho_i^{n+1}-\rho_i^n}{\Delta t}+\frac{J_{i+1/2}^n-J_{i-1/2}^n}{\Delta x}=0 \\ &\frac{J_i^{n+1}-J_i^n}{\Delta t}+\frac{1}{\epsilon^2}\frac{\rho_{i+1/2}^{n+1}-\rho_{i-1/2}^{n+1}}{\Delta x}=-\frac{1}{\epsilon^2}2k(\rho_i^{n+1})J_i^{n+1}. \end{aligned} \tag{5}$$

With the aim to expose the basic ideas more clearly we will assume in the sequel $k(\rho)=1/2$, and hence $A=0$ and $B=1$ in (4). In this case the equilibrium equation is the heat equation. We will see how to remove this restriction at the end of the section.

To specify the scheme we need to relate the nodal flux values $\rho_{i\pm1/2}, J_{i\pm1/2}$ to the cell averaged values ρ_i, J_i. The most natural way to solve (5) is to use at the generic time t^n the standard upwind selection

$$\begin{aligned} \rho_{i\pm1/2}^n &= \frac{1}{2}(\rho_i^n+\rho_{i\pm1}^n)\pm\frac{\epsilon}{2}(j_i^n-j_{i\pm1}^n) \\ J_{i\pm1/2}^n &= \frac{1}{2}(J_i^n+J_{i\pm1}^n)\pm\frac{1}{2\epsilon}(\rho_i^n-\rho_{i\pm1}^n)\,. \end{aligned} \tag{6}$$

It is easy to verify that the use of (6) in the discrete equation (5) for small values of ϵ leads to the scheme

$$\frac{\rho_i^{n+1}-\rho_i^n}{\Delta t}-\frac{\rho_{i+2}^n+\rho_{i-2}^n-2\rho_i^n}{(2\Delta x)^2}-\frac{\Delta x}{2\epsilon}\frac{\rho_{i+1}^n+\rho_{i-1}^n-2\rho_i^n}{\Delta x^2}=0, \tag{7}$$

which corresponds to the modified equation [6, 10]

$$\frac{\partial\rho}{\partial t}=\frac{\partial^2\rho}{\partial^2 x}+\frac{\Delta x}{2\epsilon}\frac{\partial^2\rho}{\partial^2 x}. \tag{8}$$

Hence if $\Delta x\geq 2\epsilon$ the numerical dissipation rate will be comparable or dominate the physical dissipation and the numerical solution will dissipate faster then the physical one. We also have to solve temporally the stiffness of this numerical dissipation term and hence the CFL condition is once again of the type $\Delta t\sim\epsilon\Delta x$. In addition, second order extension of (6) using slope limiters give a system of nonlinear equations in J_i^{n+1} which has to be solved using iterative methods.

We propose two different way of constructing numerical schemes with the correct asymptotic behavior avoiding solving nonlinear algebraic equations. The main idea is to use modified explicit upwind schemes for equation (5a) combined with an implicit center difference scheme for equation (5b). The main motivation is given by the fact that, altough we have implicit relaxation terms, the new value ρ_i^{n+1} and J_i^{n+1} can be evaluated at the cost of an explicit scheme.

In fact using the center difference selection for $\rho^n_{i\pm1/2}$

$$\rho^n_{i\pm1/2} = \frac{1}{2}(\rho^n_i + \rho^n_{i\pm1}) \tag{9}$$

in the second equation (5b)

$$\frac{J^{n+1}_i - J^n_i}{\Delta t} + \frac{1}{\epsilon^2}\frac{\rho^{n+1}_{i+1} - \rho^{n+1}_{i-1}}{2\Delta x} = -\frac{1}{\epsilon^2} J^{n+1}_i, \tag{10}$$

we have an implicit scheme in time that can be solved explicitly, since the values of ρ^{n+1}_i can be easily computed from the first equation in (5a) and the term in J^{n+1}_i is linear. In addition as $\epsilon \to 0$ (10) projects over the correct local equilibrium

$$J^{n+1}_i = -\frac{\rho^{n+1}_{i+1} - \rho^{n+1}_{i-1}}{2\Delta x}. \tag{11}$$

A particular effective way to compute the fluxes $J^n_{i\pm1/2}$ has been introduced in [6]. The idea is to build into the numerical schemes the asymptotics that lead from the hyperbolic system to the parabolic equation in an implicit way. Applying this idea to (3) we obtain the upwind determination of the fluxes

$$J^n_{i\pm1/2} = \frac{\epsilon}{2\epsilon + \Delta x}(J^n_i + J^n_{i\pm1}) \pm \frac{1}{2\epsilon + \Delta x}(\rho^n_i - \rho^n_{i\pm1}). \tag{12}$$

Upon substituting (12) into the conservative form (5a) we obtain the scheme

$$\frac{\rho^{n+1}_i - \rho^n_i}{\Delta t} + \epsilon\frac{J^n_{i+1} - J^n_{i-1}}{2\epsilon\Delta x + \Delta x^2} - \frac{\rho^n_{i+1} + \rho^n_{i-1} - 2\rho^n_i}{2\epsilon\Delta x + \Delta x^2} = 0. \tag{13}$$

As $\epsilon \to 0$ (13) gives

$$\frac{\rho^{n+1}_i - \rho^n_i}{\Delta t} - \frac{\rho^n_{i+1} + \rho^n_{i-1} - 2\rho^n_i}{\Delta x^2} = 0, \tag{14}$$

which is a consistent and stable discretization of the heat equation under the parabolic CFL condition $\Delta t \leq \Delta x^2/2$.

The upwind selection (6) can be modified in another way so as to capture the proper parabolic behavior. The idea now is to apply the upwind selection on the variables $(\rho \pm J)/2$ instead of the characteristic variables $(\rho \pm \epsilon J)/2$. This can be better understood by rewriting system (3) in the form [7, 10]

$$\begin{aligned} &\frac{\partial \rho}{\partial t} + \frac{\partial J^\epsilon}{\partial x} = 0 \\ &\frac{\partial J^\epsilon}{\partial t} + \frac{\partial \rho}{\partial x} = -\frac{1}{\epsilon^2}\left(2k(\rho)J^\epsilon + (1-\epsilon^2)\frac{\partial \rho}{\partial x}\right). \end{aligned} \tag{15}$$

Thus $(\rho \pm J)/2$ are the characteristic variables of the non-stiff problem which lead to the modified fluxes

$$J^n_{i\pm 1/2} = \frac{1}{2}(J^n_i + J^n_{i\pm 1}) \pm \frac{1}{2}(\rho^n_i - \rho^n_{i\pm 1}). \tag{16}$$

With these fluxes the discrete equation (5a) leads to

$$\frac{\rho^{n+1}_i - \rho^n_i}{\Delta t} + \frac{J^n_{i+1} - J^n_{i-1}}{2\Delta x} = \frac{\rho^n_{i+1} + \rho^n_{i-1} - 2\rho^n_i}{2\Delta x}. \tag{17}$$

For small values of ϵ, applying (11) to (17) we have

$$\frac{\rho^{n+1}_i - \rho^n_i}{\Delta t} - \frac{\rho^n_{i+2} + \rho^n_{i-2} - 2\rho^n_i}{(2\Delta x)^2} - \frac{\Delta x}{2}\frac{\rho^n_{i+1} + \rho^n_{i-1} - 2\rho^n_i}{\Delta x^2} = 0, \tag{18}$$

which is an approximation of the equilibrium heat equation with an accuracy of $O(\Delta x/2)$ under a CFL condition of diffusive type $\Delta t \sim \Delta x^2$.

For general $k(\rho)$ it is easy to see that the discretization defined by (9) and (16) applies to the discrete equation (5) without any modification and has the correct diffusion limit. In fact the value of $k(\rho^{n+1}_i)$ can be computed directely from the first equation. On the contrary the upwind selection (12) depends on the equilibrium state. Instead of (12) we have to consider

$$J^n_{i\pm 1/2} = \frac{\epsilon}{2\epsilon + \Delta x k(\rho^n_{i\pm 1/2})}(J^n_i + J^n_{i\pm 1}) \pm \frac{1}{2\epsilon + \Delta x k(\rho^n_{i\pm 1/2})}(\rho^n_i - \rho^n_{i\pm 1}). \tag{19}$$

It is straightforward to show that also the scheme defined by (9) and (19) in the small relaxation limit provides a consistent discretization of (4) under a parabolic stability condition. We remark that the particular case $k(\rho) \equiv 0$ is not considered by our present approach.

Finally, we emphasize that because we use centered approximation in (5b) the development of second order schemes in space follows naturally simply considering high order extension of (12) and (16) in (5a).

3 Numerical results

In this section we apply the schemes in different situations. These include a model of relaxing heat flow and a model of nonlinear diffusion. First we consider the case $k(\rho) = 1/2$ in (3) which corresponds to the so called *hyperbolic heat equations* [12]. As $\epsilon \to 0$ the model relaxes towards the heat equation given by (4) for $A = 0$ and $B = 1$. We now test the methods for $\epsilon = 10^{-8}$ by solving a Riemann problem with the initial data

$$\begin{aligned} \rho_L &= 2.0, \quad j_L = 0, \qquad 0 < x < 0.5, \\ \rho_R &= 1.0, \quad j_R = 0, \qquad 0.5 < x < 1, \end{aligned} \tag{20}$$

on the interval $[0, 1]$. We take 100 spatial cells and $\Delta t = 0.005$. The boundary condition is numerical reflecting. We compare the numerical results with the 'exact' solution obtained

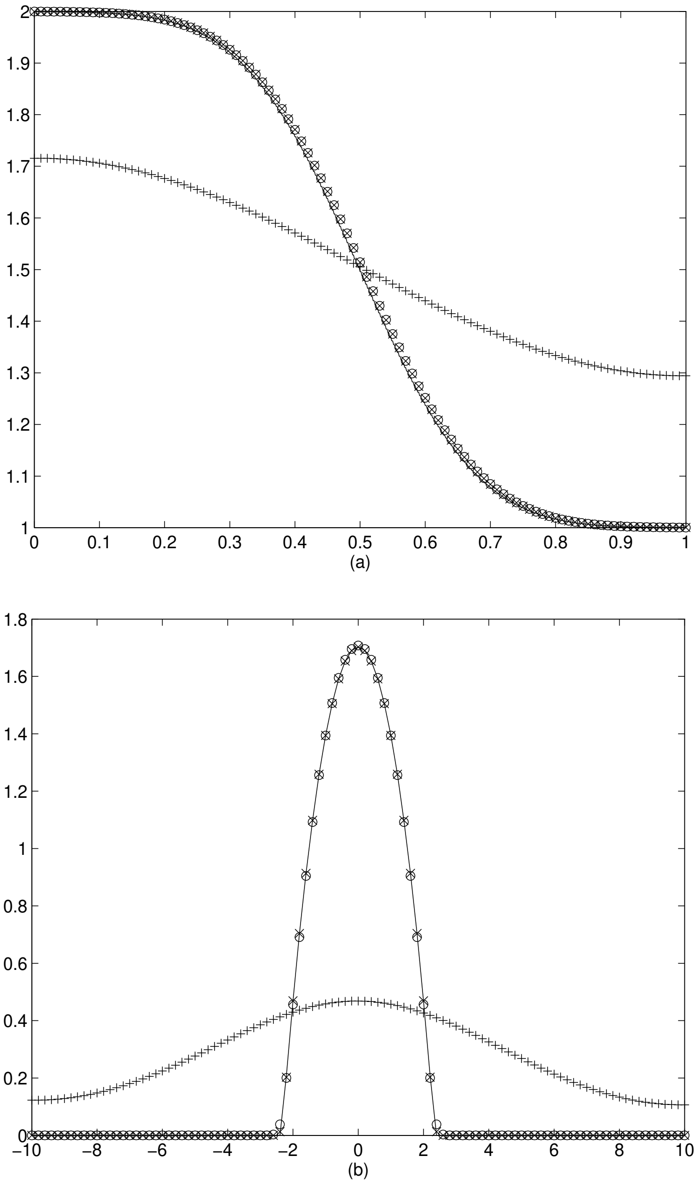

Figure 1: Numerical solutions for $\epsilon = 10^{-8}$ of the heat flow model (a) with initial data (20) and of the nonlinear porous media model(b) with initial data (21) for the different schemes. Scheme (12) ($\times$) and scheme (16) ($\circ$). The wrong behavior of the upwind scheme ($+$) for $\epsilon = 10^{-3}$ under the CFL condition $\Delta t \leq \epsilon \Delta x$ at the same time is also shown.

with a fine spatial grid of 5000 cells. The solution, output at $t = 0.04$ and depicted in Fig. 1a, contains a right moving viscous shock wave. As it can be seen, although the relaxation time is underresolved, both the numerical schemes we developed here capture the correct parabolic behavior given by the heat equation. On the contrary, the upwind scheme decays at unphysical rates.

Next we take a nonlinear case by choosing $k(\rho) = (2\rho)^{-1}$. In the small relaxation limit the model leads to the porous media equation given by (4) for $A = 2$ and $B = 2\rho$. We test the schemes by comparing the numerical solution with the solution of the porous medium equation given analytically by Barenblatt [1]

$$\rho(x,t) = \begin{cases} \dfrac{1}{r(t)}\left[1 - \left(\dfrac{x}{r(t)}\right)^2\right], & |x| \leq r(t), \\ 0, & |x| > r(t), \end{cases} \tag{21}$$

where $r(t) = [12(t+1)]^{1/3}$, $t \geq 0$ and $x \in [-10, 10]$.

The numerical solutions at time $t = 0.3$ are plotted in Fig. 1b for $\epsilon = 10^{-8}$, with 100 spatial cells and $\Delta t = 0.05$. Again, although the relaxation time is underresolved, the schemes describe well the dynamic of the two viscous shock fronts left-moving and right-moving. The wrong behavior of the upwind scheme is also shown.

4 Final Remarks

We have introduced a way of constructing underresolved numerical schemes for kinetic equations in diffusive regimes. We indicate that for this type of problems standard numerical methods for hyperbolic conservation laws present several limitations and fail to describe the right parabolic behavior unless the relaxation time is not spatially resolved. To designe schemes with the correct physical behavior they should have a discrete analogous of the asymptotic limit of the continuous system. Although we carry out our analysis for first order schemes and simple 2×2 systems the spirit of the analysis extends similarly to high order schemes and more complicated systems. Here we concentrate on developing the basic ideas. The development of fully second order schemes and of a numerical analysis theory will be presented elsewhere [10].

References

[1] G.I. Barenblatt *On some unsteady motion of a liquid or a gas in a porous medium*, Prikl. Math. Meh. **16**, p. 67 (1952).

[2] R.E. Caflish, S. Jin and G. Russo *Uniformly accurate schemes for hyperbolic systems with relaxation*, SIAM J. Num. Anal. **34**, 1, pp. 246-281, (1997).

[3] T. Carleman *Problémes mathèmatiques dans la thèorie cinètique des gas*, Publ. Scient. Inst. Mittag-Leffler (1957).

[4] E.Gabetta, L.Pareschi and G.Toscani *Relaxation schemes for nonlinear kinetic equations*, SIAM J. Num. Anal. **34**, pp. 2168-2194, (1997).

[5] T. G. Kurz *Convergence of sequence of semigroups of nonlinear operators with an applications to gas kinetics*, Trans. Amer. Math. Soc., **186**, pp. 259–272 (1973).

[6] S. Jin and D. Levermore *Numerical schemes for hyperbolic conservation laws with stiff relaxation,* J. Comp. Phys. **126**, pp. 449-467 (1996).

[7] S. Jin, L.Pareschi and G. Toscani *Diffusive relaxation schemes for discrete-velocity kinetic equations*, SIAM J. Num. Anal. to appear.

[8] P.L. Lions and G. Toscani *Diffusive limit for two-velocity Boltzmann kinetic models*, Rev. Math. Iberoamericana, 13, (1997).

[9] H.P. McKean *The central limit theorem for Carleman's equation*, Israel J. of Math., **21**, pp. 54–92 (1975).

[10] G. Naldi and L. Pareschi *Numerical schemes for hyperbolic systems of conservation laws with stiff diffusive relaxation*, preprint (1997).

[11] R. B. Pember *Numerical methods for hyperbolic conservation laws with stiff relaxation, I. Spurious solutions*, SIAM J. Appl. Math., **53**, pp. 1293-1330 (1993).

[12] P.L. Roe and M. Arora *Characteristic-based schemes for dispersive waves I. The method of characteristics for smooth solutions*, Numerical Meth. for PDE's, **9** pp.459-505 (1993)