Chapter Three: The Euler Solutions from Gas-Kinetic Theory

3.1 Introduction

The system of Euler equations give a complete description of inviscid, non-heat-conducting flows and hence, they should describe physical flows in the limit of vanishing dissipation. Certainly, taking this limit is not a simple process, because the order of the equations and boundary conditions need also to be changed. A large number of methods have been developed to handle the complex, nonlinear system of advection-dominated conservation laws. One approach is to use the classical space-centered scheme and its basic concept is the application of Taylor expansions; the standard examples are Lax-Friedrichs and Lax-Wendroff schemes. Other discretization methods have been developed which relate to the propagation properties of solutions of the Euler equations. These "non-space-centered" schemes are classified as upwind schemes. Their common point is the relation between the characteristic propagation properties and the differencing, so as to apply directional space discretization in accordance with the physical behavior of inviscid flows. Flux-vector splitting and Godunov-type schemes are upwind schemes.

The gas-kinetic schemes we developed in the previous chapter use individual particles instead of characteristic waves to simulate gas flow, and this basic property is similar to upwind schemes. Since the Euler equations are the limit of the Navier-Stokes equations as the physical viscosity goes to zero, the transition to the Euler regime in this chapter is a natural extension of the Navier-Stokes solvers in the last chapter obtained by reconsidering the concept of physical and numerical viscosities. So, this chapter can be regarded as solving the Navier-Stokes equations in the limit of diminishing viscosity, rather than the Euler equations. To understand the dissipation dominated regions, such as shock fronts, in the limit of the advection-dominated Euler equations is one of the critical problems we have to face when
applying our gas-kinetic Euler solver. Results from our Euler solver 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 were 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.

3.2 The Euler Scheme and Numerical Examples

In the preceding chapter, we constructed one kind of Navier-Stokes solver by applying gas-kinetic theory. In several examples, such as the laminar boundary layer, the grid size is much smaller than the boundary layer thickness, so the Maxwellian expansion is generally correct in this smooth transition region. As a consequence, the boundary layer is numerically resolved and there is no need to add additional artificial viscosity to stabilize the scheme. However, as we increase the cell size adjacent to the flat plate to a value which is comparable with the size of the physical boundary layer thickness, oscillations emerge automatically near the boundary. To delete these oscillations, we have to increase the collision time $\tau$, which is equivalent to adding more physical viscosity $\nu$ and widening the boundary layer thickness to a scale larger than the grid size close to the boundary, where the boundary thickness $\delta \propto \sqrt{\nu}$.

The Euler equations are the limit of the Navier-Stokes equations when the real physical viscosity goes to zero, or, equivalently, the collision time $\tau$ goes to zero for the numerical BGK model (Eq.(2.15)). Hence, if we use an Euler solver to study a dissipation dominated boundary layer problem, the oscillations would certainly appear. Unfortunately, due to nonlinear interactions in the gas flow, even
for the Euler equations, dissipation dominated shock waves can emerge easily and frequently. In the past twenty years, stabilizing and accurately capturing the shock front has been one of the challenging problems for numerical Euler solvers, and many good schemes have been devised to cope with this problem. One of the common mechanisms used to suppress the post shock oscillations in shock capturing schemes is to include artificial viscosities in these regions. In this chapter, for the numerical gas kinetic scheme, we will meet the same problem of adding artificial viscosity to reduce oscillations. But the reason for this doesn’t seem too artificial; we can understand this procedure physically from the standpoint of the Navier-Stokes equations. Since, for the Navier-Stokes schemes, even with strong shocks, if the grid size is fine enough to be less than the thickness of the discontinuity, there is no reason to add any artificial viscosity.

The resolution limit for any numerical scheme is the grid size — we cannot resolve discontinuities of thickness less than one cell size. Instead, we usually use continuous functions to replace the unknown subcell structures. So, for shocks which arise in solving the Euler equations, the numerical mesh requires us to accept that the thickness of the shock front is at least as large as one cell size. Since the shock thickness is related to the physical viscosity and heat conduction, we need additional viscosity for an Euler solver to widen the zero-size shock structure to a size comparable with the grid size. Although we solve the Navier-Stokes equations in our gas kinetic schemes, in the application of our scheme to the Euler regime, the real physical viscosity will make the shock thickness too small to stabilize the simulation, as happens for the under-resolved boundary layer problem. As a result, we have to put an additional term in the expression for the collision time at strong shocks,

\[
\tau = C_1 \frac{\sqrt{\lambda}}{\rho(0,0,0)} + C_2 \sqrt{\lambda} \left[ \frac{\sqrt{\lambda^f/\rho_f(0,0,0) } - \sqrt{\lambda^r/\rho^r(0,0,0) } }{\sqrt{\lambda^f/\rho^f(0,0,0)} + \sqrt{\lambda^r/\rho^r(0,0,0)}} \frac{|p^f - p^r|}{p^f + p^r} \right], \quad (3.1)
\]
where the pressure ($p^l$ and $p^r$) and the temperature ($\lambda^l$ and $\lambda^r$) terms are obtained from $g^l(0,0,0)$ and $g^r(0,0,0)$ in the MET scheme. The formulation of the second term in the above equation is guided by the consideration that the discontinuity thickness $l$ should be comparable with the grid size $\Delta x$, e.g. $l = \Delta x$. It is true that we still have some small physical viscosity in our scheme represented by the first term in Eq.(3.1), because we believe that Navier-Stokes solvers can automatically give Euler solutions when the real physical viscosity is small enough and the dissipation dominated discontinuities are treated properly. Also this small physical viscosity helps the convergence of the numerical solution to the physical one; no entropy “fix” is needed in our gas-kinetic schemes to suppress rarefaction shocks.

An alternative explanation for the second term in Eq.(3.1) is this: in the neighborhood of a discontinuity, owing to the steep slopes for the mass, momentum and energy interpolations (cf. Eq.(2.20)), negative density or temperature can easily occur close to the cell boundary, and these would falsify the estimate of the distribution function $g$ (cf. Eq.(2.18)). We could look at this as numerical generation of “pseudo-particles” (with (perhaps) negative density or temperature). Since in our scheme, the whole slope is used to evaluate numerical fluxes, these “pseudo-particles” could propagate to the cell boundary and affect the numerical fluxes. The second term in the collision time $\tau$ is there to reduce these effects exponentially along the path to the cell boundary. In a smooth region, the second term is always small. For Godunov-type schemes, it is much easier to construct two constant and physically reasonable states, where an additional artificial viscosity is included implicitly in the preparation of the constant states. The reduction of oscillations in high-order central difference schemes can also be explained in this way, where putting $\frac{\partial u_i}{\partial x} \sim \frac{u_{i+1} - u_{i-1}}{2\Delta x}$ is equivalent to saying that physical quantities may be extrapolated to give indefinitely large values at large $|x|$, and this wrong
information in the far field would definitely affect the fluxes, so artificial dissipation is needed to suppress this effect.

Mathematically, in the MET scheme, our choice of increasing $\tau$ in Eq.(3.1) has the effect of increasing the weight of the bimodal velocity distribution $f_0(x, y, 0)$ in the final form of $f$ to get fluxes. This is in qualitative agreement with the behavior of $f$ at a shock given by a more exact treatment for shock structure calculations (Mott-Smith[23]). Also, if $\tau$ is really big, then $e^{-T/\tau} \approx 1$, and the MET scheme goes over to a second order beam scheme.

In the following, we will present several well-studied Euler test cases using our gas-kinetic MET scheme, with the collision time $\tau$ given by Eq.(3.1). Actually, this scheme is still a Navier-Stokes solver, but it doesn't hurt if we regard it as a relaxation scheme to the Euler equations if we take a small physical collision time (Jin and Xin [18]).

The MET scheme in the 2-D case is easily extended to a operator splitting code (Strang [41]) by ignoring the $b$ term in Eq.(2.18) and the $b^l, b^r$ terms in Eq.(2.42) in finding $f(0, 0, t)$. The final programming of this direction split code is much easier than the original MET scheme. In all simulations, we use $C_1 = 0.01$ and $C_2 = 1.0$ in Eq.(3.1), and $\gamma = 1.4$.

In one-dimension, we have used our scheme on four well-known test cases—those of Sjögreen, Sod, Lax-Harten and Woodward-Colella. In all these cases the solid lines in the figures can be regarded as the exact solution of the problem.

**Sjögreen Test Case**

The two Sjögreen test cases are taken from a recently published paper by Einfeldt et al [11] (1991). 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 derived from a linearized Riemann solution could be positively conservative. Fortunately, our scheme is very nonlinear.
For all test cases, we use $\rho$, $P$ and $\epsilon$ to represent mass, momentum and total energy in each cell. 200 points are used in this test case.

The initial data for the first case of subsonic expansion is $\rho_l = 1, P_l = -2, \epsilon_l = 3$ and $\rho_r = 1, P_r = 2, \epsilon_r = 3$, and for the second, supersonic, expansion case, $\rho_l = 1, P_l = -1, \epsilon_l = 5$ and $\rho_r = 1, P_r = 1, \epsilon_r = 5$. Our results are shown in Fig.(3.1a) and Fig.(3.1b). Especially for the second case, some well-known schemes may fail to reproduce correctly the strong expansion profiles, or they give badly rounded corners. To handle this kind of strong rarefaction wave is one of the advantages of our gas scheme.

**Sod Test Case**

The classical Sod test case has 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 from MET are shown in Fig.(3.2b) with 200 points. Note the number of points in the shock and the contact discontinuity, as well as the sharp corners of the rarefaction wave. The results from the METS-I scheme is shown in Fig.(3.2a), where the emergence of oscillations around discontinuity regions is consistent with the analysis in section(2.3.2).

**Lax-Harten Test Case**

The Lax-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.(3.3) with 200 points. Note again the corners and the number of points in the contact discontinuity, which are competitive with other high resolution schemes not employing special treatment of contact discontinuities.

**Woodward-Colella Test Case**

The fourth test case is that of Woodward and Colella with the initial conditions $\rho_l = 1.0, P_l = 0, \epsilon_l = 2500$ for $0 < x \leq 0.1$, $\rho_m = 1.0, P_m = 0.0, \epsilon_m = 0.025$ for $0.2 < x \leq 0.9$ and $\rho_r = 1.0, P_r = 0.0, \epsilon_r = 250$ for $0.9 < x \leq 1$. Our results are
Figure 3.1a: Sjögreen test case for subsonic expansion
Figure 3.1b: Sjögreen test case for supersonic expansion
Figure 3.2a: Sod test from METS-I scheme
Figure 3.2b: Sod test case from MET scheme
Figure 3.3: Lax-Harten test case
shown in Fig(3.4) with 400 points. Note the number of points in the fronts, the heights of the maxima and the contact discontinuities.

For the two dimensional case, we tried the Emery, double Mach reflection, and regular shock reflection test cases.

**Emery Test Case**

We first 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[44]. In Fig.(3.5a) we present our result for a grid of $120 \times 40$ 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.

The result from the MET scheme is given in Fig.(3.5b). The contours are almost identical to those obtained from an operator-splitting code. No special treatment of the cells near the step corner were employed in the calculation.

**Double Mach Reflection Test Case**

This is the case of the double Mach reflection of a strong shock, a problem presented in the paper by Woodward and Colella. The computational domain is $240 \times 60$, but here we give 30 contours in the region $180 \times 60$. The results from the splitting scheme are given in Fig.(3.6a); we see that the shock front is thinner than those produced by any of the codes tested in Woodward and Colella's paper, but the wall jet following the front shock is weak. The reason for this is still under investigation. The same result from the MET scheme is shown in Fig.(3.6b).

**Regular Shock Reflection Test Case**

The last test case is a regular shock reflection. The computational domain is a rectangle of length 4 and height 1 divided into a $60 \times 20$ rectangular grid with $\Delta x = 1/15, \Delta y = 1/20$. Dirichlet conditions are imposed on the left and upper boundaries as

$$(\rho, u, v, p)|_{(0,y,t)} = (1.0, 2.9, 0.0, 1/1.4),$$
Figure 3.4: Woodward-Colella test case
Figure 3.5a: Emery Test Case with operator-splitting scheme

Figure 3.5b: Emery test from the MET scheme
Figure 3.6a: Double Mach reflection case from splitting code

Figure 3.6b: Double Mach reflection from MET scheme
The bottom boundary is a reflecting wall and the supersonic outflow condition is applied along the right boundary. Initially, the solution in the entire domain is set to be that at the left boundary. We iterate for 500 time steps, by which time the solution has reached a steady state. Fig.(3.7a) shows the result using the operator splitting scheme. The solution from the MET scheme is shown in Fig.(3.7b). Numerical experience tells us that the central difference interpolation in the y-direction in Eq.(2.54) could generate some noise in some two-dimensional simulations. It seems that a non-linear limiter might also be needed in this direction.

In all cases we observe diffusion at contact discontinuities. Physically, the thickness of any contact discontinuity should increase as \( \sqrt{t} \) (\( t \) is the time), and it should be wider than the shock front. Actually, from numerical experience, we feel that the smearing of contact discontinuities is not caused by our way of evaluating fluxes, but is mainly due to the initial interpolation. The discontinuity is usually smeared inside each cell by some continuous interpolating function, and this process continues for hundreds or even thousands of time steps in a real numerical simulation.

In all these test cases we have used exactly the same codes (splitting or MET) with different initial and boundary conditions, but we have not tried to identify and sharpen discontinuities in any way.

3.3 Conclusion

In this chapter, we have presented a numerical scheme for solving the Euler equations, and given the results of several test cases. Our Euler scheme is a natural extension of our Navier-Stokes solver constructed by reducing the viscosity. Based on this relation with the Navier-Stokes solver, we believe that our scheme will never
Figure 3.7a: Regular shock reflection on a $60 \times 20$ grid from splitting code

Figure 3.7b: Regular shock reflection from the MET scheme
give rarefaction shocks (or other crazy unphysical features), although discontinuities could get smeared. In common with other high-resolution schemes, the "artificial" viscosity is also needed in our gas-kinetic scheme, but has some physical explanation. We also believe that in most cases the unavoidable numerical error in the reconstruction and evolution stages in our scheme is larger than the error caused by non-zero viscosities for the Euler solver, especially in the discontinuity region.

Several points need to be emphasized:

1). The BGK model provides a physical formulation for hydrodynamic problems which is distinct from, and in some ways superior to the pure Euler equations.

2). Aside from a safety factor (usually 0.65) in the Courant condition, the only adjustable parameters in the scheme occur in the Eq.(3.1) for the collision time. No additional "fix" for our scheme is needed.

3). All test cases reported in this chapter were run with precisely the same code (Splitting or MET), 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 we didn't need to modify our code to treat the flow near the corner in the Emery case, nor did we need to take precautions to avoid an unphysical rarefaction shock above this corner, since the solution of the BGK model definitely satisfies the second law of thermodynamics: The entropy of an adiabatically isolated system can never decrease.
4). Our code is logically simple but computationally intensive. Even so, it is by no means slow. The running time on a Sparc2 workstation for the Woodward-Colella case for roughly 1000 timesteps on a 400 point grid was 100 seconds.
Chapter Four: Conclusion and Future Work

Our scheme is based on gas-kinetic theory, and is of the "Boltzmann" type, in that it uses a distribution function of particle velocities and takes into account the particle collisions which occur during a time step to evaluate the final numerical fluxes. 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 and Navier-Stokes solutions are recoverable from the BGK model from the relation between viscosity and relaxation time.

The past several years have seen the development of many approximate multidimensional schemes for the Euler equations with improved shock-capturing properties (van Leer [43], Catalano et al [4]). These can be considered as falling into two classes: one method is based on the application of a rotated 1-D Riemann solver, and the other is a genuinely multidimensional approach to the fluid equations, separating them into an equivalent set of scalar wave equations with solution-dependent propagation directions. As pointed out by many authors [43] [32], the real extension of Godunov-type scheme to a multidimensional scheme needs to solve a multidimensional Riemann problem. But due to the intrinsic difficulties (there are 16 waves in two dimension) and the complicated geometry of real problems, a
truly multidimensional scheme based on a multidimensional Riemann solver seems unattainable.

As we pointed out in this thesis, there are two stages in a numerical scheme: reconstruction and evolution. In our gas-kinetic scheme, instead of using a set of scalar waves, we have used particle trajectories. As shown in Eq.(2.22b), each particle has a certain characteristic trajectory, and a particle can move in any direction in the two dimensional space at a rate given by its vector velocity \((u, v)\), which is not restricted to certain directions with respect to the numerical mesh. This property clearly demonstrates that our scheme is multidimensional, at least in the evolution stage, and this property separates this scheme from simple directional splitting codes, although we don't see much improvement in going from split to multidimension version of our code. In order to make it into a total multidimensional scheme, we would also have to use initial multidimensional interpolations for the mass, momentum and energy in the reconstruction stage, where the identification of the discontinuity orientation might be necessary.

Some comments and thoughts about future work for our gas-kinetic schemes follow:

1). One of the most important properties of our scheme is that the distribution function \(f\) combines the advective and dissipative effects. In the chapter we gave some Navier-Stokes test cases; in all three cases, the grid size is fine enough to resolve the shear layer structures. In most cases, actually, the mesh resolution is not fine enough to resolve the diffusive effects of the viscosity and heat conduction profiles in regions of severe gradients, such as shocks. Therefore, in these cases, artificial dissipation to widen the fronts to the scale of the mesh has to be introduced, even with the Navier-Stokes calculations, as we did in the Eq.(3.1). So, the concept of artificial dissipation introduced in the inviscid equations is generally applied also for viscous computations. Hence particular attention is required to control the
numerical dissipation in order not to influence, or even dominate, the physical effects and alter the viscous flow solutions. It seems that in our scheme, we have successfully treated the physical and numerical effects using the relation between the viscosity and collision time. Our schemes have some advantages over those which separate advection and dissipation terms, where the presence of the dissipation in the discretized Euler equations could interfere with the physical dissipation.

2). 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 these integral equations can be generalized by approximating the motion of a single particle in a particular coordinate system, moving in a particular force field. The numerical scheme we have constructed is for a constant $\gamma$ gas in Cartesian coordinates, and without external forces. In this particular 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.

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 generalize to include more complicated physics than the flow of a perfect gas, the third is that the Riemann problem does not generalize readily to two or more dimensions, and most importantly, it does not give Navier-Stokes solutions.

5). Once again, let's emphasize one point: for the BGK model, \( f_t + u f_x = (g - f) / \tau \), and the right hand side stiff source term usually determines the time step \( T < \tau \) in a simple numerical treatment. This condition could make the BGK model useless for hydrodynamical simulations. Fortunately enough, we can use the condition \( < f - g > = 0 \) implicitly to evaluate the time-dependent behavior of the equilibrium state \( g \), and allow \( T > \tau \). To the best of our knowledge, in all other gas-kinetic based hydrodynamic schemes, the condition \( < f - g > = 0 \) has never been used. Another way to relax the time step constraint of \( T < \tau \) is to use some implicit Runge-Kutta method.
6). In this thesis, a solution method for the Euler and Navier-Stokes equations are derived from the BGK model. However, the continuum assumption of the Navier-Stokes equations are no longer valid at high altitude where the density is very low. In such cases, it is necessary to solve the Boltzmann equation. But the direct numerical integration of the Boltzmann equation is still unapproachable; the complexity of the collision term not only generates numerical errors, but also makes the scheme computationally too costly. So far, most attempts to solve the Boltzmann equation use the Direct Simulation Monte Carlo (DSMC) method [3], which needs a large number of sample particles as well as large computer capability to obtain a sufficiently accurate solution, because of the inherent statistical noise. The BGK model avoids the complex Boltzmann collision term. Since the integral equations hold for all values of the relaxation time, they offer the possibility of generalizing the scheme to treat 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.

In this thesis, we have given a numerical treatment of the Navier-Stokes and Euler equations based on gas-kinetic theory. But we still need to distinguish these two descriptions (macroscopic vs. microscopic) of the gas flow. It is true that from the gas-kinetic theory, the Euler and Navier-Stokes equations can be derived, but this doesn't say that the numerical scheme presented in this thesis really solves the Euler and Navier-Stokes equations. In other words, if we really translate the kinetic numerical fluxes in terms of corresponding macroscopic quantities, the final equations will be much more complicated and include more terms than the standard fluxes in the Euler and Navier-Stokes equations. It is also true for other schemes: central difference and upwinding.
Numerical hydrodynamics based on gas-kinetic theory is just beginning. In the next several years, we believe that more accurate and efficient Boltzmann-type schemes will appear. We hope that this thesis will be helpful to people working on numerical hydrodynamics and gas kinetic theory.