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Solving the Linear Advection Equation for the BGK Method

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Abstract

The complexity of the collision term in the Boltzmann equation for rarefied flows is such that it is often replaced by a model equation such as the Bhatnagar-Gross-Krook (BGK) model [5]. To solve the BGK equation numerically a number of different advection equations - one for each molecular velocity range which is included in the numerical method - must be solved in parallel. For a fixed time step, the CFL numbers for these different advection equations can differ by an order of magnitude or more. For a feasible time-step, and a reasonable computational time, it becomes necessary to solve at least some of these linear advection equations with a CFL number much greater than 1. It is the purpose of this work to provide the groundwork for solving the BGK method by presenting a fast, accurate solution to the linear advection equation that is stable for CFL numbers greater than 1.

Introduction

The design of an atmospheric entry craft requires an accurate prediction of the local gas dynamic effects on the vehicle. For rarefied entry trajectories, the flow transit time past the vehicle is small with respect to the mean time between collisions; the gas molecules are not in thermal equilibrium and there is no single temperature that characterises the thermodynamic state. In these conditions the Navier-Stokes equations are not valid. Thus it becomes necessary to solve the Boltzmann equation which describes the flow at the molecular level by considering the effects of the free-flight and collisions on the distribution of molecular velocities, or to resort to particle simulations.

The standard simulation method is the Direct Simulation Monte Carlo (DSMC) method [6] which includes various collision models, chemical reactions and thermal radiation. DSMC does have its disadvantages, however. Simulations involve storing large numbers of molecules and data, and the statistical collision procedure introduces scatter into the solution.

The complexity of the collision term in the Boltzmann equation is such that even simple flows are difficult to solve. The Bhatnagar-Gross-Krook (BGK) model equation [5] (also proposed by Weylander [22]), replaces the collision term by a mathematically simpler source term which retains the important features of the original equation but is easier to solve numerically.

The effect of the free-flight (convection) terms in the model equation may be found by solving the linear advection equation for each molecular velocity to set up a new non-equilibrium distribution function throughout the computational domain at each time step. Then the model collision term in the BGK equation represents the effect of molecular collisions by a relaxation, at a finite rate, of the velocity distribution function to the local Boltzmann (equilibrium) distribution. It becomes necessary to solve the linear advection equations as accurately and as quickly as possible in order to ensure a reasonable computational time.

The range of the velocity distribution results in a large difference in CFL number between the smallest and largest velocity. If higher-order 'finite-volume' style solutions methods are used the time step must be based on a small CFL number for the largest molecular velocity in the solution. It is the purpose of this work to provide the groundwork for solving the BGK method by presenting a fast, accurate solution to the linear advection equation that is stable for CFL numbers greater than 1 in order to reduce computational time.

The BGK Model Equation

The BGK model equation is shown below in Equation 1, where ν_M is the collision frequency and f_M is the local Maxwellian velocity distribution function.

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} = \nu_M (f_M - f) \tag{1}$$

where the collision frequency is given by

$$\nu_M = \frac{\rho RT}{\mu}$$

The local Maxwellian velocity distribution function in three dimensions is given by

$$f_M = \frac{n}{(2\pi RT)^{\frac{3}{2}}} \exp\left(\frac{-c^2}{2RT}\right) \tag{2}$$

where $c^2 = (u-\overline{u})^2 + (v-\overline{v})^2 + (w-\overline{w})^2$.

The BGK method conserves mass, momentum and energy;

$$\int\int \nu_M (f_M - f)\, \psi_\alpha \, d\mathbf{v} = 0 \tag{3}$$

where $\psi_\alpha = \left\{1, u, v, w, \frac{1}{2}\mathbf{v}^2\right\}$ and $\mathbf{v} = u + v + w$.

The basic physical assumption underpinning the modified Boltzmann equation is that the collision frequency is independent of the relative speed of the colliding molecules [13]. This assumption is satisfied strictly only for Maxwellian particles.

In recent years, the development of the gas-kinetic BGK model equation method has been quite strong. Single and multidimensional BGK methods have been developed. Aoki *et al.* [3] used the model equation to solve for unsteady flow between two infinite parallel plates. Kim *et al.* [12] adapted a finite volume gas-kinetic BGK method to unstructured triangular grids with mesh adaption. Pieraccini *et al.* [18] developed a technique to construct BGK schemes of any order accuracy in space in time, while solving even very stiff problems quickly and easily.

One of the most significant drawbacks of the BGK method is that it does not result in the correct Prandtl number. Holway [9] introduced the 'ellipsoidal statistics' (ES-BGK) method in order to fix this issue. The ES-BGK model [9] was developed to adjust the BGK model to give the correct transport coefficients for the Navier-Stokes equation by relaxing towards a Gaussian equilibrium distribution rather than a Maxwellian and allowing for the addition of the Prandtl number to the collision term. Andries *et al.* [2] conducted some numerical comparisons between this method, the standard BGK method and DSMC

for transitional reentry flows that showed reasonable improvements in most flow aspects. Chae *et al.* [7] also improved the BGK method by correcting the Prandtl number. Li and Zhang [14, 15, 16] also modified the BGK method to correct for the Prandtl number and removed the continuous dependence of the distribution function on the velocity space through their discrete velocity ordinate method. This model is of particular interest in this work and will be described in detail in later sections.

Macrossan [17] developed the 'relaxation time simulation method' (RTSM) by extending the Equilibrium Particle Simulation Method (EPSM) of Pullin [19]. EPSM works in a similar way to the Direct Simulation Monte Carlo (DSMC) methods, but rather than simulating collisions, the momentum and energy of the particles in each cell are redistributed to establish local Maxwellian equilibrium at each time step. RTSM differs in that only a fraction of the particles are adjusted to equilibrium.

In order to include descriptions of thermal nonequilibrium, multi-temperature BGK methods have been developed in recent years [11, 24, 25, 26]. Xu *et al.* [27] also developed a diatomic gas BGK method with rotational and translational degrees of freedom included.

Gross and Krook [8] extended the original BGK method to allow for two component gas mixtures. One major drawback of their method is that when both species are defined identically, the one component method is not recovered. Bhatnagar [4] also continued development on this two component method, as did Xu [23] and Sirovich [20]. In the paper by Andries *et al.* [1], a two component method is presented which satisfies positivity and the entropy inequality, has the correct exchange coefficients and degenerates to the single component model.

Solver Details

Three solution methods have been used in this work. The first is a simple implementation of ray tracing, with linear interpolation. The second method, the 'large CFL advection method' was developed to provide stable results with more accuracy than the first order ray tracing method. The Riemann solution [10] is the third method, included to allow a comparison of the method results.

Linear ray tracing calculates the total distance that molecules with each particular velocity value will have travelled over the time step and locates the previous position of those particles. Linear interpolation is used to find the percentage of molecules from each of the two closest cells, and the distribution function of the current cell is created from these cells for each velocity.

The large CFL method modifies this simple method by locating the cell from which the molecule will have come and subtracting the time taken to travel from the closest interface of this cell from the total time step. The remaining time is then used to solve the limited anti-diffusion method for the originating cell. This provides more accuracy than the linear ray tracing method that is equivalent to solving the upwind [21] scheme locally.

Figure 1 shows a graphical outline of the large CFL method. This method insures that the local CFL number for the originating cell is always ≤ 1.0 for stability. If the original location is outside of the domain, it is given the boundary value.

The approximate (non-iterative) Riemann solver was developed by Jacobs [10] and works in three stages. In the first stage, the perfect gas relations are used to calculate the intermediate pressure and velocity assuming that the cells interact via isentropic compression or expansion waves. If the resulting pressure jump is large, the interface state guess is improved with the strong shock relations. The other flow properties are then calculated from the pressure and velocity states calculated in the first two steps.

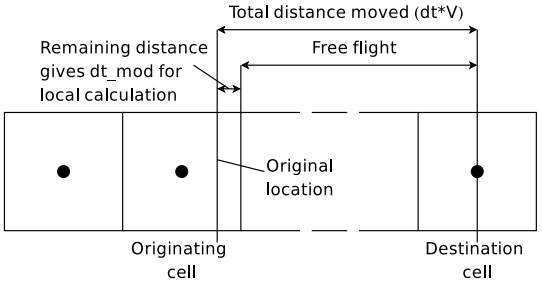

Figure 1: Graphical description of the large CFL number method. The local time step for the limited anti-diffusion method component is the difference between that used to cover the entire flight distance and that to cover the distance to the originating cell interface.

Results

Advection tests

A simple step function test was used to compare the accuracy of the large CFL method and simple ray tracing. The results are shown in Figure 2 (CFL number of 2.5) and Figure 3 (CFL number of 10.5) for two different velocity values. The length of which was set to 1.0 and it was discretized into 50 cells in the case of Figure 2 and 500 cells for the results in Figure 3. The final flow time was equal to $0.1 \times L/\mathrm{V_{max}}$. For this test, a step function was initiated in the leftmost cell and allowed to propagate to the right over time. Only two velocity values were used and these were both positive. A comparison is shown between the first order ray tracing and limited anti-diffusion methods and the exact step.

Modifying the method to solve the limited anti-diffusion method locally increases the accuracy of the result as expected. Unlike the standard limited anti-diffusion, however, this result is stable for any CFL number. Results are not shown for the negative velocity test case as they mirrored those from for the positive velocities.

One dimensional shock tube problem

Results were generated for the one dimensional shock tube problem with non-dimensional parameters. The BGK method used was the traditional BGK method with no correction for Prandtl number, but with two translational temperatures. On either side of the discontinuity the initial bulk velocity was set to zero and the temperatures (in equilibrium) were set to 1.0. A simple power law description of the viscosity was used, with the power being set to 0.75. A density decrease of 10 was initialised from left to right.

The length of the grid used was 100 times the maximum mean free path in the domain, coming to a value of 125.33 length units. This was then normalised for plotting purposes. The domain was then divided into 200 cells.

The velocity space was generated based on the mean thermal velocity in the initial state. The maximum velocity was six standard deviations above the maximum mean thermal velocity and the minimum velocity, six standard deviations below the minimum mean thermal velocity. This space was then divided into a number of discrete cells - either 100 or 200 in the results following.

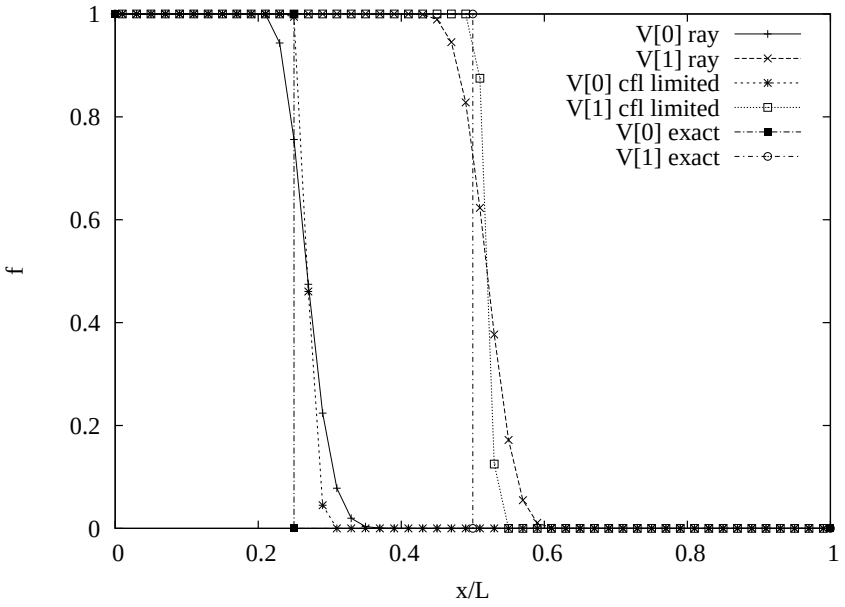

Figure 2: Comparison of the accuracy of the large CFL method with ray tracing for a step function. The CFL number for the larger velocity is set to 2.5 and the problem runs for 10 time steps. The step function is initiated by the left boundary cell value being set to 1.0. These results are for the positive velocity case.

Results were generated for a number of cases:

1. Linear ray tracing with 100% BGK relaxation.
2. Large CFL method with 100% BGK relaxation.
3. Riemann solution for comparison with the two BGK solutions.

The data was extracted after 100 time steps at a final solution time of 12.533 time units. This resulted in a CFL number of 1.52 for the ray tracing and large CFL methods. A CFL number of 1.0 was used for the Riemann solution and the number of time steps adjusted accordingly.

Figure 4 shows a comparison between the Riemann solution, the linear ray tracing method and the large CFL method for an infinite number of collisions and 100 discrete velocity cells. Figure 5 shows the same comparison with 200 velocity cells respectively. It can be seen that the results from the large CFL method correspond to those of the first order ray tracing and that no improvement on the first order method is achieved.

Following the successful test of the infinite collision case, the two advection methods were tested with the proper local BGK collision frequency as described previously. Again, Figure 6 shows no improvement in results due to the more accurate advection step.

Conclusions

The purpose of this work was to develop an accurate method of solving the linear advection step of the decoupled BGK model for large CFL numbers. A modified ray tracing method was developed which was more accurate than the first order linear ray tracing method but which required less computational time than standard solution methods for the linear advection equation. This reduction in computational time is simply due to the smaller number of time steps required to solve the flow problems.

Results were presented for the one dimensional shock tube test case with infinite collisions with a variety of physical and velocity space grid sizes and compared to the Riemann solution. Further data is shown for a simple BGK simulation of the one dimensional shock tube problem. Although the large CFL advection method did improve the accuracy of the advection step, the effect of the relaxation towards equilibrium negated the improvements in the one dimensional shock tube problem.

Acknowledgements

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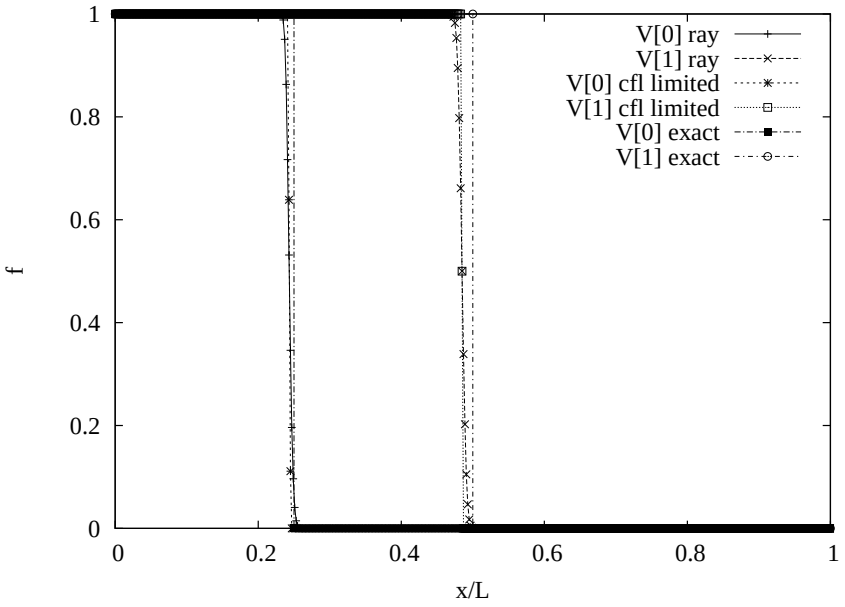

Figure 3: Comparison of the accuracy of the large CFL method with ray tracing for a step function. The CFL number for the larger velocity is set to 10.5 and the problem runs for 23 time steps. The step function is initiated by the left boundary cell value being set to 1.0. These results are for the positive velocity case.

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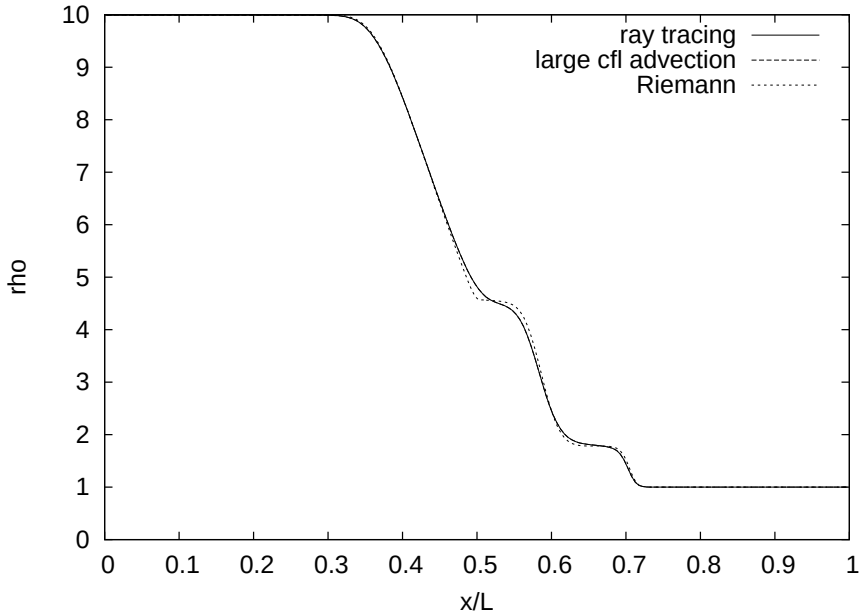

Figure 4: Comparison of the large CFL method with ray tracing and the Riemann solution for 100 velocity cells and infinite collisions. The solution final time is 12.533 time units over 100 time steps, resulting in a maximum CFL number of 1.52. For the Riemann solution, the number of time steps is modified to reduce the CFL to 1.0. The ray tracing and large CFL method results are identical to plotting accuracy.

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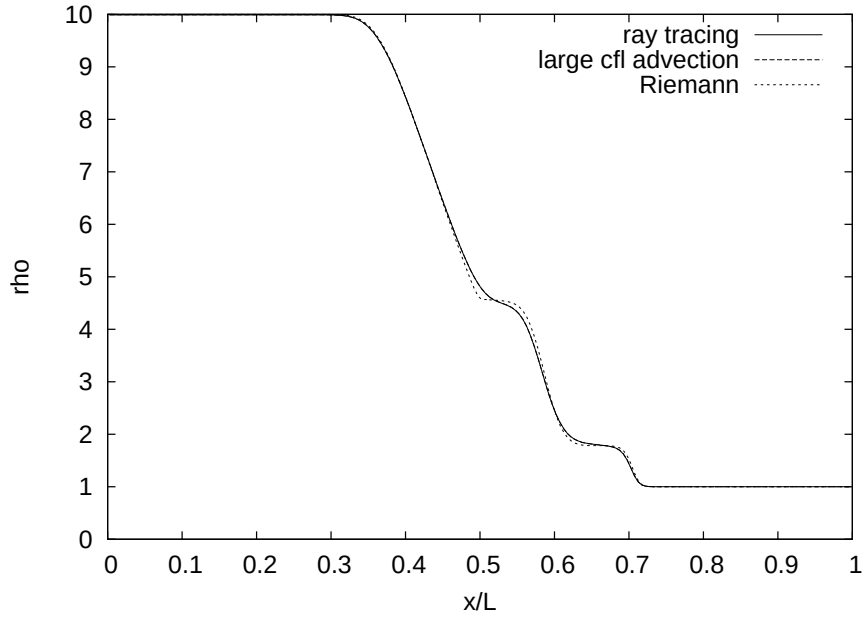

Figure 5: Comparison of the large CFL method with ray tracing and the Riemann solution for 200 velocity cells and infinite collisions. The solution final time is 12.533 time units over 100 time steps, resulting in a maximum CFL number of 1.52. For the Riemann solution, the number of time steps is modified to reduce the CFL to 1.0. The ray tracing and large CFL method results are identical to plotting accuracy.

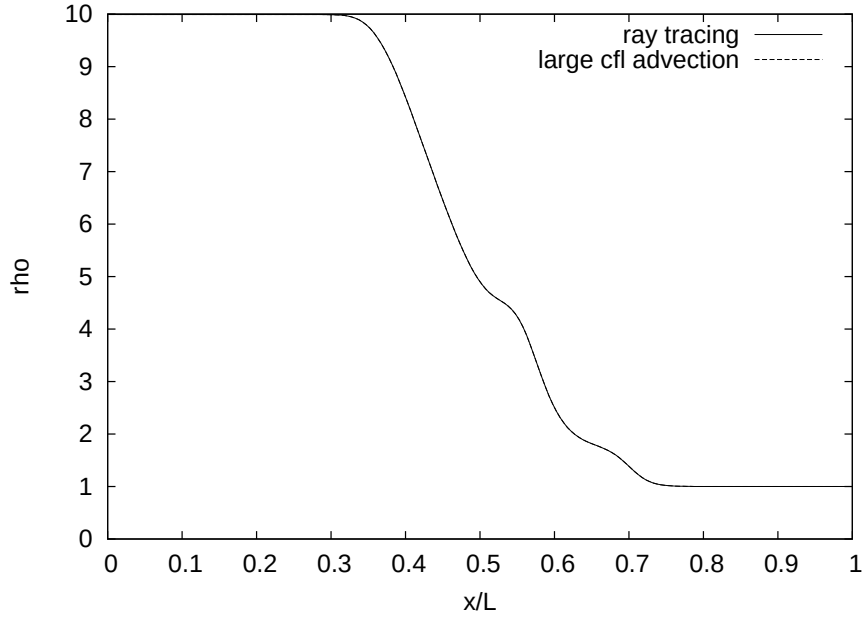

Figure 6: Comparison of the large CFL method with ray tracing and the Riemann solution for 100 velocity cells with the standard BGK method. The solution final time is 12.533 time units over 100 time steps, resulting in a maximum CFL number of 1.52. The ray tracing and large CFL method results are identical to plotting accuracy.