

Validity and Inherent Viscosity of the Quiet Direct Simulation Method

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Abstract. The Quiet Direct Simulation (QDS) scheme is a numerical method for modelling gas flows, based on kinetic theory, with some similarities to the Lattice Boltzmann Method (LBM). It differs from LBM notably in that the discrete molecular velocities are not constant but are reset each timestep according to local values of bulk velocity and temperature. For this reason it performs well in highly compressible flows. Two features of the scheme limit its accuracy in low Mach number flows. QDS assumes a Maxwell distribution of molecular velocities. The validity of this assumption may be tested by calculating the gradient Knudsen number and average number of collisions per timestep. The separation of collision and streaming leads to excessive diffusion of momentum, leading to a very high effective viscosity of the modelled gas when the grid spacing is larger than the mean free path. This numerical dissipation is different in character from the dissipation due to the finite order of the spatial reconstruction, common to all finite volume methods, which is also present. The effective viscosity is quantified for simple shear flows and tested in models of a 2D channel flow. A crude model of intermolecular collision during streaming is implemented and shown to reduce the effective viscosity.

Keywords: CFD, QDS, KFVS, LBM, numerical viscosity, kinetic theory methods

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INTRODUCTION

Conventional computational fluid dynamics (CFD) methods, in which continuum governing equations such as the Euler or Navier-Stokes equations, have been very successful over the past 40 years. However some problems remain. The unstructured meshes used for most complex geometries are time consuming to set up and require prior knowledge of the flow. Computational cost remains high, particularly if time dependent turbulent flows are modelled. Methods based in kinetic theory differ from conventional methods in several interesting aspects, which may lead to better practical schemes for engineering flow modelling. Besides direct simulation Monte Carlo (DSMC), there is a class of schemes which discretise and store the molecular velocity distribution at each spatial node and evolve it in time explicitly. Most successful of these, to date, has been the Lattice Boltzmann Method (LBM) [1,2]. Attractive features of the scheme include simple structured meshes (although these are possible with conventional methods), reduced computational expense with good parallel speedup, and the ease with which mesoscopic physical processes can be modelled. However some problems remain with LBM. It is a weakly compressible method, with errors which grow with Mach number, limiting it to quasi incompressible flows. Methods exist to accommodate compressibility effects, at the cost of increased complexity. LBM is complex to understand and program. An alternative with some interesting features is the Quiet Direct Simulation method (QDS) [3-5]. This paper analyses some features of the scheme which bear on its potential for use in engineering flow modelling.

The QDS scheme

Space is discretised on a uniform Cartesian mesh. In each cell, the molecular velocity distribution is discretised into N (typically 3 or 4) molecular speeds in each spatial dimension, chosen according to the local bulk velocity and temperature. All molecules are assumed to be travelling with a velocity $\underline{v} = \hat{i}u_l + \hat{j}v_m + \hat{k}w_n$ where l, m, n are labels indicating the discrete speed in each direction. A weight is assigned to each combination of speeds, representing the fraction of the molecules lying in the cell which travel at that speed.

The discrete velocities u_l are calculated according to:

$$u_l = \bar{u} + \sqrt{\frac{2kT}{m}} q_l \quad (1)$$

Where \bar{u} is the local bulk velocity in the x-direction, k is Boltzmann's constant, T the local translational temperature, m the molecular mass and q_l the l^{th} abscissa of the quadrature chosen to numerically integrate the molecular velocity distribution. Where the Maxwell distribution is used the Gauss-Hermite quadrature is used:

$$\int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} f(\alpha) e^{-\alpha^2/2} d\alpha = \sum_{j=1}^J \frac{w_j}{\sqrt{\pi}} f(\sqrt{2}q_j) \quad (2)$$

Where w_j is the j^{th} weight of the quadrature, α is the molecular velocity and f is a moment of the molecular distribution function. The statistician's weights are used, which sum to $\sqrt{\pi}$.

The timestep is divided into streaming and collision phases. In the streaming phases, the fluxes of molecules from each cell to its nearest neighbours, and for each combination of molecular speeds, are calculated assuming collisionless flight. The fraction of molecules entering each neighbouring cell is calculated and stored. The remainder are retained in the source cell.

A global kinetic CFL criterion limits the timestep to prevent molecules streaming beyond neighbouring cells. The timestep is chosen such that the fastest molecular group anywhere in the domain streams no more than a set fraction of a grid spacing, typically ≤ 0.5 .

The mass, momentum and energy carried by these fluxes are then determined and stored for each destination cell.

Fluxes are calculated assuming some distribution of molecular number density in the source cell: piecewise-constant (first order spatial accuracy) and piecewise linear (second order) have been used, as have higher order reconstruction schemes.

At the end of the streaming phase the fluxes of mass, momentum and energy into each cell are collected and summed with the quantities remaining in the cell from molecules which did not leave.

In the collision phase, a molecular distribution function is determined from the quantities of mass, momentum and energy in each cell. In most of the computations performed to date by the authors, an infinite collision rate was assumed and a Maxwellian distribution forced. A distribution calculation from the first order Chapman-Enskog distribution has also been applied. This of course requires information on the shear stresses and heat fluxes, computed from local property gradients.

Boundary conditions are applied with ghost cells lying outside the flow domain, with properties set so as to achieve the desired boundary fluxes.

Further details of the implementation are given in [5].

Comparison with LBM

The QDS scheme has several similarities with LBM. A regular mesh, discretised molecular velocity distribution, explicit Euler time integration, streaming and collision are handled separately, transport is based on the advection of groups of molecules with no requirement to determine pressure (no Poisson problem to be solved as in incompressible Navier-Stokes methods). Further, computations are based on local information (compact stencil): only nearest neighbour information required for second order spatial accuracy. Also, each streaming and collision computation requires few floating point operations, with no exponential or error functions to be evaluated. These features lead, as in LBM, to straightforward meshing, good stability, and good parallel speedup.

The QDS scheme has some important differences with LBM:

- The Maxwell distribution, where used, is discretised with the computationally efficient Gauss-Hermite quadrature, which is very computationally efficient
- The scheme is conceptually simpler and easier to program
- Discrete molecular velocities are determined locally according to bulk velocity and temperature
- With a fixed grid spacing, a timestep determined by a global kinetic CFL criterion and locally varying molecular speeds, it is not possible to stream directly to adjacent grid nodes. Most molecular groups travel some fraction of the distance to the neighbouring cell centre.

These differences lead to some advantages and disadvantages compared to LBM:

- Locally varying molecular speeds mean it is possible to model flows with strong variations in bulk velocity and temperature. The basic scheme is valid in compressible flows and flows with strong temperature gradients.
- The molecules travel less than one grid spacing, and terminate their flight away from the centre of the cell. However cell properties are stored at the cell centre. Without proper interpolation this leads to further high numerical dissipation, except where corrected by a reconstruction scheme of sufficiently high order.
- No parameter of the modelled gas relates to viscosity. The effective viscosity of the modelled gas, as will be shown below, is a function of temperature and grid spacing.

Issues with the basic QDS scheme

The QDS scheme lacks the errors, inherent in LBM, which grow with Mach number. It contains errors related to the thermal transport, which diminish with Mach number, making it well suited for high speed, virtually inviscid flows. However in its current formulation it is not valid for low speed viscous flows, for two principal reasons:

In real gas, collisions modify the speeds of the molecules at every collision. Collisionless streaming, lacking collisions during streaming, ignores the reduction in speed which the faster molecules experience and leads to transport of momentum and energy in excess of that encountered in a physical gas.

The distribution forced during the collision phase should take into account evolution of the molecular speeds during streaming, and the finite time required for relaxation. This is

These two problems are analysed separately in the following sections.

VALIDITY OF THE ASSUMPTION OF INFINITE COLLISION RATE

In the basic QDS scheme, the Maxwell molecular velocity distribution is forced at the end of each streaming phase. This distribution is valid for a gas in local thermal equilibrium, and is derived assuming an infinite time has elapsed for relaxation, and that no spatial gradients in density, bulk velocity or temperature exist to disturb the equilibrium. In practice the distribution relaxes quickly towards the Maxwellian quickly. Titov and Levin [6] found, in collision-limited DSMC, that two collisions per time step per particle are sufficient for the computed non-equilibrium distribution to relax to one differing negligibly from the corresponding Maxwell-Boltzmann equilibrium distribution.

The validity of the assumption of a Maxwellian distribution may be tested by considering the number of collisions per timestep, and the strength of local gradients in property, for each cell.

The number of collisions per timestep is given by: $\frac{\overline{t_{col}}}{\Delta t} = \frac{\lambda}{c\Delta t}$ (3)

Where $\overline{t_{col}}$ is the average time between collisions, $\lambda = \frac{1}{\sqrt{2\pi}nd^2}$ the mean free path and \overline{c} the average thermal velocity. The density gradient length Knudsen number may be calculated with [7]

$$Kn_{GLL} = \frac{\lambda}{\rho \frac{\Delta \rho}{\Delta x}} \quad (4)$$

The value of these parameters and hence the validity of the equilibrium assumption depends on the flow being modelled, the CFL criterion and grid spacing used. This issue is discussed for one particular flow in a companion paper in this conference, by the same authors.

ANALYSIS OF NUMERICAL DISSIPATION IN THE BASIC SCHEME

The numerical dissipation in the basic scheme may be quantified for a two dimensional shear flow in which the bulk u-velocity is aligned with the grid. A scheme with three molecular speeds is assumed. The central speed in the y-direction will be zero and this group of molecules will not transport any momentum in the y-direction. The two outlying molecular speeds will be nonzero and will transport y-momentum in the x direction. By considering the quantity of momentum transported and the relation between shear stress and viscosity for a real fluid, the effective viscosity of the modelled gas may be quantified. Figure X shows two adjacent cells. The gas in the top cell (in blue) is moving at an average speed of $\bar{u} = u + \Delta u$ and the gas in the lower cell (in red) at $\bar{u} = u$, in the x-direction. The highest of the molecular speeds in the y-direction carries a flux of u-momentum into the adjacent cell.

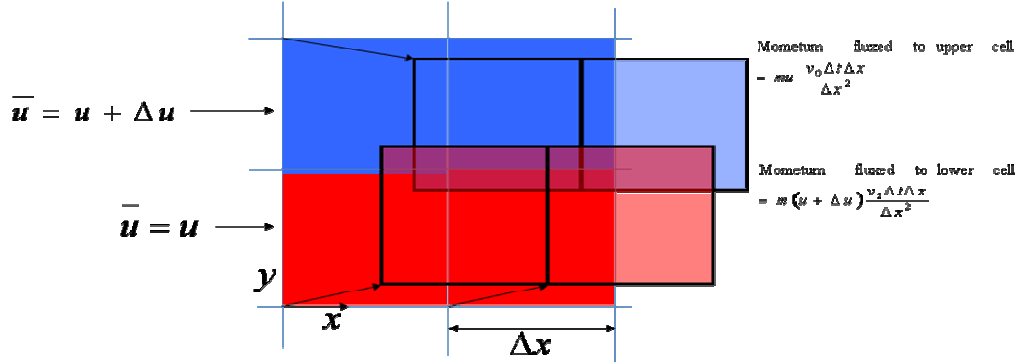


FIGURE 1. Schematic of a simple shear flow on a regular Cartesian grid showing the computed fluxes.

Net momentum fluxed to lower cell

$$\begin{aligned} \Delta p &= \sum_{i=0}^2 \left\{ m \frac{w_i}{\sqrt{\pi}} \frac{w_2}{\sqrt{\pi}} (u + \Delta u + \sqrt{2RT} q_i) \frac{|v_2 \Delta t|}{\Delta x} - m \frac{w_i}{\sqrt{\pi}} \frac{w_0}{\sqrt{\pi}} (u + \sqrt{2RT} q_i) w_i \frac{|v_0 \Delta t|}{\Delta x} \right\} \\ &= \sum_{i=0}^2 m \frac{w_i}{\sqrt{\pi}} \frac{w_2}{\sqrt{\pi}} \Delta u \frac{|v_2 \Delta t|}{\Delta x} \text{ as } |v_0| = |v_2| \text{ and } w_0 = w_2 \\ &= \rho \frac{w_2}{\sqrt{\pi}} \Delta u |v_2 \Delta t| \Delta x \end{aligned}$$

The effective shear stress is calculated from this quantity of momentum transferred:

$$\tau_{\text{scheme}} = \frac{1}{A} \frac{\partial p}{\partial t} = \frac{\rho w_2 \Delta u |v_2 \Delta t| \Delta x}{\sqrt{\pi} \Delta x \Delta t} = \frac{\rho w_2 \Delta u |v_2| \Delta x}{\sqrt{\pi} \Delta x}$$

which may be compared to the shear stress $\tau = \mu \frac{\partial u}{\partial y}$ where μ is the absolute viscosity.

$$\mu_{\text{scheme}} = \frac{\rho w_2 |v_2| \Delta x}{\sqrt{\pi}} \quad (5)$$

$$v_{\text{scheme}} = \frac{w_2 |v_2| \Delta x}{\sqrt{\pi}}$$

where :

$$\frac{w_2}{\sqrt{\pi}} = \frac{1}{6}; v_2 = \sqrt{\frac{2kT}{m}} q_2 = 1.22474 \sqrt{\frac{2kT}{m}}$$

This may be compared to the result that the kinematic viscosity of a gas is equal to [6]:

$$v_{\text{physical}} = \frac{1}{3} \bar{c} \lambda = \frac{1}{3} \sqrt{\frac{3kT}{m}} \lambda \quad (6)$$

So the ratio of the effective numerical to true physical viscosity is:

$$\frac{v_{scheme}}{v_{physical}} = \frac{\frac{1.22474\sqrt{2}}{6} \sqrt{\frac{kT}{m}} \Delta x}{\frac{1}{\sqrt{3}} \sqrt{\frac{kT}{m}} \lambda} \approx 0.5 \frac{\Delta x}{\lambda} \quad (7)$$

The basic scheme will only reproduce the correct viscous behaviour if the grid spacing is of the order of the mean free path. In air at standard temperature and pressure this is of order 10^{-8} m, such grids are not feasible with currently available computing speeds and memory.

The results of this analysis are checked by modelling a 2D channel flow with the basic QDS scheme with three discrete speeds in each spatial dimension. A uniform Cartesian grid of $M \times M$ cells is used where $M=10, 20$ and 50 representing a flow domain of 1m long by 1m wide. The upper and lower walls bounding the flow are modelled with ghost cells implementing the bounce-back boundary condition, equivalent to a no-slip condition. The left and right boundaries are periodic. In each timestep, the velocity of each molecular group is incremented by an amount equivalent to the acceleration that would be achieved by a pressure gradient of -0.01 Pa/m. Second order spatial reconstruction is used, with an MC slope limiter and a maximum kinetic CFL number of 0.1. The gas modelled has $R=1$, $T=1$, $\gamma=5/3$ and the molar mass of argon 39.948g/mol. An initial mean velocity of zero is applied everywhere. The gas is evolved until a steady state is reached. The velocity profile on the axis is extracted and plotted in Figure 2.

The analytical velocity distribution is also plotted, fitted to the modelled velocity distribution by setting the kinematic viscosity to that calculated with the formula above.

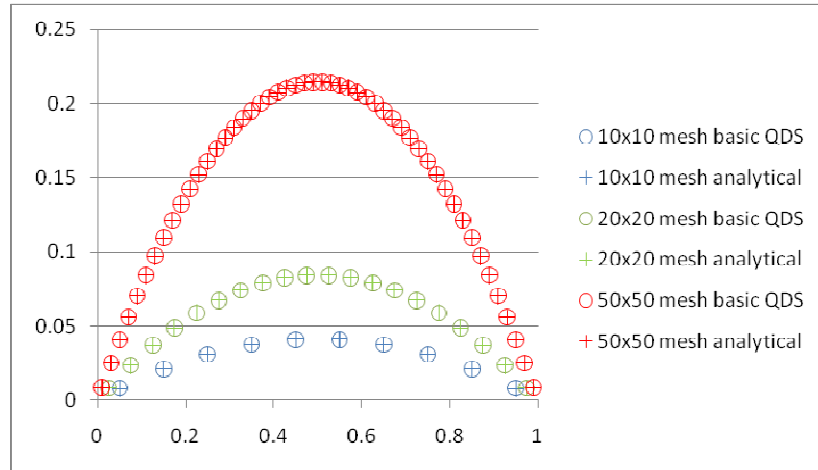


FIGURE 2. 2D channel flow computed with the basic QDS scheme.

The values of fitted kinematic viscosity and that predicted by the analysis above are compared in Figure Y. Good agreement is reached.

COLLISION DURING STREAMING

If low Mach number flows are to be modelled with QDS at acceptable computational and memory cost it is necessary to find ways of reducing the inherent numerical viscosity. One possibility is to compute the effects of collision during streaming. Below, a simple model is used to calculate the retardation of the particles due to collisions with the surrounding gas. Several assumptions are made which may be questioned. Nevertheless, this simple model serves to demonstrate the principle.

The flight of molecules of group j with speed u_j are considered. Collisions between these molecules and the other molecules in the distribution $i \neq j$ are considered. Each spatial direction is treated independently. The number of collisions experienced on average while the molecule traverses the source cell is computed with a simple hard sphere model with a fixed molecular diameter. The collisions experienced in the destination cell are neglected as these are considered in the collision step, when the Maxwellian distribution is applied.

The average number of collisions is calculated as follows:

For each set of molecules moving at speed u_i

each such molecule experiences ϕ_{ij} collisions with molecules travelling at speed u_j in time Δt

$$\phi_{ij} = |u_i - u_j| \Delta t n_j \sigma_{ij}$$

where n is the local number density of molecules travelling at speed u_j and σ_{ij} is the collision cross section

It is assumed the velocities and number densities do not change during Δt .

Summing over all $j \neq i$:

$$\phi_i = \sum_{j=1}^J |u_i - u_j| \Delta t n_j \sigma_{ij} (1 - \delta_{ij})$$

where δ_{ij} is the Kronecker delta.

Assuming hard sphere collisions, the collision cross section is not a function of the velocities of the collision partners and $\sigma_{ij} = \sigma = \frac{\pi d^2}{4}$

where d is the effective molecular diameter, noting that $|u_i - u_i| = 0 = (1 - \delta_{ii})$ so the Kronecker delta can be eliminated,

and that $n_j = n w_j$ where n is the total number density, including molecules at all speeds

$$\phi_i = \sum_{j=1}^J |u_i - u_j| \Delta t n \frac{w_j}{\sqrt{\pi}} \frac{\pi d^2}{4}$$

which can be rearranged as :

$$\phi_i = \Delta t n \frac{\pi d^2}{4} \left| u_i \sum_{j=1}^J \frac{w_j}{\sqrt{\pi}} - \sum_{j=1}^J u_j \frac{w_j}{\sqrt{\pi}} \right| = \Delta t n \frac{\pi d^2}{4} |u_i - \bar{u}|$$

It is assumed that the speed of the other molecules is not diminished during the timestep.

The collisions are assumed to be wholly elastic and one dimensional. The effect of each collision is to reduce the difference in velocity between the collision partners by one half.

For one collision:

$$u_{post,1} = \frac{u_{pre} + \bar{u}}{2}$$

where

$u_{post,1}$ = post - collision velocity of fluxing gas molecules after one collision

u_{pre} = pre - collision velocity of fluxing gas molecules

For two collisions:

$$u_{post,2} = \frac{u_{post,1} + \bar{u}}{2} = \frac{\frac{u_{pre} + \bar{u}}{2} + \bar{u}}{2} = \frac{u_{pre}}{4} + \frac{3\bar{u}}{4}$$

where

$u_{post,2}$ = post - collision velocity of fluxing gas molecules after two collisions

After n collisions:

$$u_{post,\phi} = \frac{u_{pre}}{2^\phi} + \bar{u} \left(1 - \frac{1}{2^\phi} \right) \quad (10)$$

where

$u_{post,\phi}$ = post - collision velocity of fluxing gas molecules after ϕ collisions

This model is implemented in a code solving 2D channel flow. The boundary conditions (including pressure gradient) and details of the solver are identical with those in the previous section, except for the addition of the collision model. Results are presented in Figure 3 for the basic scheme, collision en route (CER) with the model described above with molecular diameter set equal to 2.5×10^{-12} m, and for two fixed collision numbers $\phi=0.5$ and 2.0 applied to all speeds in all cells.

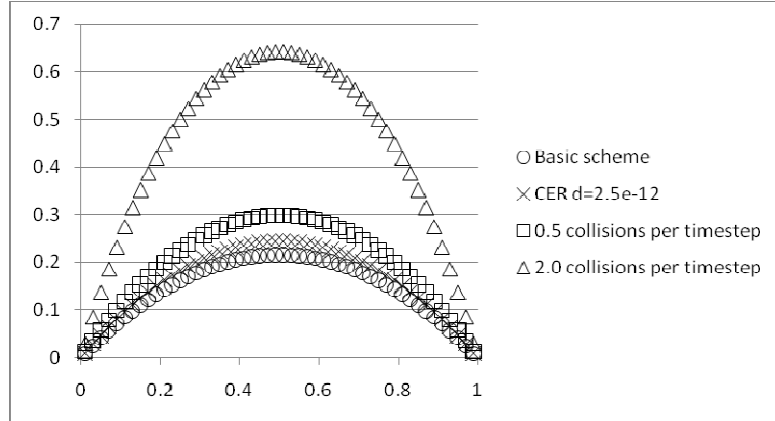


FIGURE 3. 2D channel flow computed with the basic and viscosity reducing schemes.

The effective viscosity is clearly reduced, with the smallest values achieved with the highest collision numbers, as expected. The molecular diameter used is small for a noble gas of this mass. $D=2.25 \times 10^{-12}$ m gives a collision number $\phi \approx 0.2$. The hard sphere diameter may be calculated for argon using [8]

$$\mu = \frac{5}{16} \frac{\sqrt{\pi m k T}}{\sigma} \quad (11)$$

With $\mu \approx 1.8 \times 10^{-5}$ Pa.s at $T=300$ K this gives a molecular diameter of $d \approx 8 \times 10^{-10}$ m which would give a collision number $\phi \approx 20,000$ resulting in yet smaller viscosities. However in the present case, instabilities appeared at smaller molecular diameters, yet did not appear with large fixed collision numbers ϕ . Future work will address the origin of these instabilities which are thought to be caused by an error in the periodic boundary conditions leading to reversal of velocities in some cells immediately after initialisation.

CONCLUSIONS

The QDS scheme is similar in many respects to LBM, but differs in some important points, most particularly the scalable molecular velocities which suit it to compressible flows and flows with strong thermal gradients. The Maxwellian distribution is forced at each timestep. The validity of this assumption depends on the flow, grid spacing and timestep. The major flaw in the scheme is the effective viscosity of the gas is a function of grid spacing, and is large compared to the physical viscosity of most gases of interest, if a computationally feasible grid is used. The effective viscosity of the modelled gas is quantified, for simple shear flows. A means of reducing this viscosity by modelling collisions during the streaming phase is considered. A model, based on crude assumptions, was shown to reduce the effective viscosity of the modelled gas, and suggests further work on more accurate models.

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