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Finite Difference Solution of Boundary Value problems for Classical flow problem in Rarefied Gas Dynamics

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Abstract

In this paper, rarefied gas flow was modelled using only the diffuse reflection boundary condition we examined the Poiseuille flow and Thermal creep volume flow rates of rarefied gas. The linearized Boltzmann Equation served as our governing equation and numerical examples were obtained to establish the range of Knudsen number that is best suited for a good solution.

Keywords: Finite difference method, Poiseuille flow, Thermal creep flow, Boltzmann equation, Knudsen number.

1.0 Introduction

Having seen in some recent works the use of different methods to findings solutions to the classical flow problems in Rarefied Gas Dynamics [1-4], we would like in this work to revisit and solve in a special way the problem of Poiseuille flow using the Finite difference method. We note first of all that the literature concerning the basic problems we intend to solve here is very extensive, hence in order to keep this work to a modest length, we do not attempt to review the many works already devoted to this topic. Instead we consider just a few of them.

Kosuge et al [5] investigated the problem of heat transfer and temperature distribution in a binary mixture of rarefied gases between two parallel plates with different temperatures on the basis of kinetic theory. Under the assumptions that the gas molecules are hard spheres and undergo diffuse reflection on the plates, the Boltzmann equation was analyzed numerically by means of an accurate finite difference method, in which the complicated nonlinear collision integrals are computed efficiently by the deterministic numerical kernel method. As a result, the overall quantities are obtained accurately for a wide range of the Knudsen number. At the same time, the behavior of the velocity distribution function is clarified with high accuracy.

The study by Titarev [6] was devoted to the development of an efficient deterministic framework

for modelling of three-dimensional rarefied gas flows on the basis of the numerical solution of the Boltzmann kinetic equation with the model collision integrals. The framework consists of a high-order accurate implicit advection scheme on arbitrary unstructured meshes, the conservative procedure for the calculation of the model collision integral and efficient implementation on parallel machines. The main application area of the suggested method was micro-scale flows. Performance of the proposed approach was demonstrated on a rarefied gas flow through the finite-length circular pipe. The results showed good accuracy of the proposed algorithm across all flow regimes and its high efficiency and excellent parallel scalability for up to 512 cores.

Yang et al [7] examined an accurate and direct algorithm for solving the semi-classical Boltzmann equation with relaxation time approximation in phase space for parallel treatment of rarefied gas flows of particles of three statistics. The discrete ordinate method was first applied to discretize the velocity space of the distribution function to render a set of scalar conservation laws with source term. The high order weighted essentially non-oscillatory scheme was then implemented to capture the time evolution of discretized velocity distribution function in physical space and time. The method was developed for two space dimensions and implemented on gas particles that obey the Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Computational examples in one- and two-dimensional initial value problems of rarefied gas flows were presented and the results indicating good resolution of the main flow features were achieved. Flows of wide range of relaxation times and Knudsen numbers covering different flow regimes were computed to validate the robustness of the method. The recovery of quantum statistics to the classical limit was also tested for small fugacity values.Other studies worthy of note abound in the literature [8-13]

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However, in this study, Rarefied gas flow will be modelled using only the diffuse reflection boundary condition, this means that further work could be done by using the diffuse-specular boundary conditions. We shall use some existing solvers namely; LAPACK and LINPACK, on the finite difference method to examine the Poiseuille flow and Thermal creep volume flow rates of rarefied gas. The linearized Boltzmann equation will serve as our governing equation and numerical examples will be established using different range of Knudsen numbers.

2.0 The Linearized Boltzmann Equation

The non-linearity form of the Boltzmann equation is essential in application if the gas is far from thermal equilibrium. However, if the state of the gas is near thermal equilibrium, a linearised form of the Boltzmann equation will provide a reasonably accurate description of the transport phenomena. This form assumed that the perturbation of the velocity distribution from its equilibrium form is small.

Following William [14] a linearized form of the Boltzmann equation was given as

$$c_x\left[\left(c^2-\frac{3}{2}\right)K_x+R_x+2c_xK_0\right]+c_z\left(c^2-\frac{3}{2}\right)K_z+c_zR_z+\frac{c_x dh(x,c)}{dx}+\lambda_0 h(x,c)$$
$$=\frac{\lambda_0}{\pi^{\frac{3}{2}}}\int dc'\exp\left[-c'^2\right]h(x,c')\left[1+2cc'+\frac{2}{3}\left(c^2-\frac{3}{2}\right)\left(c'^2-\frac{3}{2}\right)\right] \qquad (2.1)$$

where h is a disturbance caused to the local Maxwellian, R_x is the relative density in the x-direction, K_x is the temperature gradient in the x-direction,

$c=v\left(\frac{m}{2kT}\right)^{\frac{1}{2}}$ and, $\lambda_0=\lambda\left(\frac{m}{2kT}\right)^{\frac{1}{2}}$.

3.0 Finite Difference Method

Consider the problem of a rarefied gas in the Z direction between two parallel plates separated by a distance d, the flow resulting from both a pressure and a temperature gradient. Using the linearized two dimensional approach of Cercignani and Daneri [15] with the Bhatnagar-Gross-Krook Model (BGK), the Boltzmann equation to be solved is reduced to

$$\left.\begin{aligned}
&\xi_y\frac{\partial\phi}{\partial\gamma}+\xi_z\frac{\partial\phi}{\partial z}=\lambda\left[-\phi+\nu+2h\xi_z q_z+\tau\left(h\xi^2-\frac{3}{2}\right)\right]\\
&\nu=\int\phi F_0 d\xi\\
&\left(\frac{3}{2}h\right)(\nu+\tau)=\int\xi^2\phi F_0 d\xi\\
&q=\int\xi\phi F_0 d\xi\\
&F_0=\left(\frac{h}{\pi}\right)^{\frac{3}{2}}\exp\left[-h\left(\xi_x^2+\xi_y^2+\xi_z^2\right)\right]\\
&h=\frac{m}{2kT}
\end{aligned}\right\} \qquad (3.1)$$

Where

ϕ = relative change in velocit y distributi on function

$\xi(\xi_x,\xi_y,\xi_z)$ = the molecular volecity

$q(q_x,q_y,q_z)$ = the gas velocity

ν = relative change in the particle density

τ = relative change in tempera ture

λ = the collision frequency

The perturbation terms ν and τ depend only on z (flow direction) and are related to the pressure and temperature gradient. They are

$$T=k_2\left(\frac{z}{d}\right),\quad \nu+\tau=k_1\left(\frac{z}{d}\right)$$

where k_1 is proportional to pressure gradient and k_2 is proportional to temperature gradient, and both are small compared to unity. The velocity of the reflecting molecules from the wall is specified by the Maxwellian distribution; then the boundary conditions are:

$$\phi^{\pm}\left(-\frac{1}{2}d\ Sgn\ \xi_y, z, \xi\right)\left(k_1 - k_2\right)\left(\frac{z}{d}\right) + k_2\left(\frac{z}{d}\right)\left(h\xi^2 - \frac{3}{2}\right) \qquad (3.2)$$

Where

$$Sgn\xi_y \begin{cases} 1, & if\ \xi_y > 0 \\ -1, & f\ \xi_y < 0 \end{cases}$$

A solution in the form

$$\phi\left(\xi, \mathrm{y}, \mathrm{z}\right) = \phi_0\left(\xi\right)\left(\frac{z}{d}\right) + \phi_1\left(y, \xi\right) \qquad (3.3)$$

was sought where

$$\phi_0\left(\xi\right) = k_1 + k_2\left(h\xi^2 - \frac{5}{2}\right) \qquad (3.4)$$

Substituting equation (3.3) into equation (3.1) we have

$$\xi_y \frac{d\phi}{dy} + \lambda\phi_1\left(y, \xi\right) = \xi_z\left[\frac{-k_1}{d} - \frac{k_2}{d}\left(h\xi^2 - \frac{5}{2}\right) + 2\lambda hq_z\right] \qquad (3.5)$$

Multiplying both sides of equation (3.5) by

$$\xi_z\left(\frac{h}{\pi}\right)\exp\left[-h\left(\xi_z^2 + \xi_x^2\right)\right]$$

and integrating over full ranges, we have

$$\xi_y \frac{dF}{dy} + \lambda F = \frac{1}{2h}\left(2h\lambda q_z - \frac{k_1}{d} + \frac{k_2}{d} + \xi_y^2 \frac{k_2}{d} h\right) \qquad (3.6)$$

where the function F is defined by

$$F\left(y, \xi\right) = \frac{h}{\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \xi_z \exp\left[h\left(\xi_z^2 + \xi_x^2\right)\right]\phi_1\left(y, \xi_y\right)d\xi_x d\xi_z \qquad (3.7)$$

Integrating equation (3.6) under the boundary conditions

$$\phi_1\left(-\frac{1}{2}d\ Sgn\ \xi_y, z, \xi\right) = 0 \qquad (3.8)$$

we have

$$F\left(y, \xi_y\right) = \left(\xi_y\right)^{-1}\int_{-\frac{d}{2}\mathrm{sgn}\ \xi_y}^{y}\left(2h\right)^{-1}\left(2h\lambda q_z - \frac{k_1}{d} - \frac{k_2}{2d} - \xi_y h\frac{2k_2}{d}\right)\exp\left[\frac{\lambda\left|y-1\right|}{\left|\xi_y\right|}\right]dt \qquad (3.9)$$

When the gas velocity q_z is expressed by

$$q_z\left(y\right) = \left(\frac{h}{\pi}\right)^{\frac{1}{2}}\int_{-\infty}^{\infty} F\ \exp\left(-h\xi_y^2\right)d\xi_y \qquad (3.10)$$

Equation (3.10) now reduces to

$$h^{\frac{1}{2}} q_z\left(y\right) = \pi^{\frac{1}{2}}\int_{-\frac{d}{2}}^{\frac{d}{2}} J_{-1}\left(h^{\frac{1}{2}}\lambda\left|y-t\right|\right)\left(h^{\frac{1}{2}}q_z\left(t\right) - \frac{k_1}{2dh^{\frac{1}{2}}\lambda} - \frac{k_2}{2dh^{\frac{1}{2}}\lambda}\right)dt$$

$$-\pi^{--\frac{1}{2}}\int_{-\frac{d}{2}}^{\frac{d}{2}} \frac{k_1}{2dh^{\frac{1}{2}}\lambda} J_1\left(h^{\frac{1}{2}}\lambda\left|y-t\right|\right)dt \qquad (3.11)$$

where J_n is defined by

$$J_n = \int_o^{\infty} y^n \exp\left(-y^2 - \frac{x}{y}\right)dy$$

Let $\Delta = dh^{\frac{1}{2}}\lambda = \left(\frac{2\delta}{\pi^{\frac{1}{2}}}\right)$

$$\mathrm{y} = \mathrm{h}^{\frac{1}{2}} \lambda y$$

$$\mathrm{T} = \mathrm{dh}^{\frac{1}{2}} \lambda t$$

$$h^{\frac{1}{2}} q_z = \left(2\mathrm{dh}^{\frac{1}{2}} \lambda\right)^{-1} \left\{ \left[1 - \Psi_p(\eta)\right] k_1 - \left[\frac{1}{2} - \Psi_T(\eta)\right] k_2 \right\} \qquad (3.12)$$

Then equation (3.11) will be written as two integral equations, i.e.,

$$\psi_p(\eta) - \pi^{-\frac{1}{2}} \int_{-\frac{d}{2}}^{\frac{d}{2}} \Psi_p(\eta) J_{-1}\left(h^{\frac{1}{2}} \lambda |y - t|\right) dt = 1 \qquad (3.13)$$

and

$$\psi_{\mathrm{T}}(\eta) - \pi^{-\frac{1}{2}} \int_{-\frac{d}{2}}^{\frac{d}{2}} \Psi_{\mathrm{T}}(\eta) J_{-1}\left(h^{\frac{1}{2}} \lambda |y - t|\right) dt = \frac{1}{2} - \pi^{-\frac{1}{2}} \int_{-\frac{d}{2}}^{\frac{d}{2}} J_{-1}\left(h^{\frac{1}{2}} \lambda |y - t|\right) dt \qquad (3.14)$$

where

$\delta =$ the inverse Knudsen number

From equation (3.12), we have the velocity of the gas induced by the pressure gradient as,

$$\mathrm{h}^{\frac{1}{2}} q_{zP} = \frac{-\pi^{\frac{1}{2}}}{2\delta} \left[1 - \Psi_P\right] \qquad (3.15)$$

and that induced by temperature gradient as

$$\mathrm{h}^{\frac{1}{2}} q_{zT} = \frac{-\pi^{\frac{1}{2}}}{2\delta} \left[\frac{1}{2} - \Psi_T\right] \qquad (3.16)$$

The volume flow rate is then given by

$$G_p = \rho \int_{-\frac{d}{2}}^{\frac{d}{2}} q_{zP}(y) dy$$

$$= \left(\frac{\pi^{\frac{1}{2}}}{2\delta} - \frac{\pi}{4\delta^2} \int_{-\frac{\Delta}{2}}^{\frac{\Delta}{2}} \Psi_{\mathrm{P}}(\eta) d\eta \right) h^{\frac{1}{2}} d^2 \frac{dp}{dz} \qquad (3.17)$$

$$\mathrm{G}_{\mathrm{T}} = p \int_{-\frac{\mathrm{d}}{2}}^{\frac{\mathrm{d}}{2}} q_{zT}(y) dy$$

$$= \left(\frac{\pi^{\frac{1}{2}}}{4\delta} - \frac{\pi}{4\delta^2} \int_{-\frac{\Delta}{2}}^{\frac{\Delta}{2}} \Psi_T(\eta) d\eta \right) h^{\frac{1}{2}} \mathrm{n}_0 k d^2 \frac{dT}{dz} \qquad (3.18)$$

Expressing equations (3.17) and (3.18) in non-dimensional form gives;

$$Q_P = \frac{\pi^{\frac{1}{2}}}{2\delta} - \frac{\pi}{4\delta^2} \int_{-\frac{\delta}{x^{\frac{1}{2}}}}^{\frac{\delta}{x^{\frac{1}{2}}}} \psi_P(\eta) d\eta \qquad (3.19)$$

and

$$Q_T = \frac{\pi^{\frac{1}{2}}}{4\delta} - \frac{\pi}{4\delta^2} \int_{-\frac{\delta}{x^{\frac{1}{2}}}}^{\frac{\delta}{x^{\frac{1}{2}}}} \psi_T(\eta) d\eta \qquad (3.20)$$

The subscripts P and T imply Poiseuille flow and Thermal creep respectively.

Next, is to solve numerically the unknown functions ψ_P and ψ_T in equations (3.13) and (3.14) respectively. In order to solve equations (3.13) and (3.14), a **finite difference method** was utilized after discretization as

$$\psi_{Ph} - \pi^{-\frac{1}{2}} \sum_{k=0}^{n-1} \psi_{Pk} \int_{\tau_k}^{\tau_{k+1}} J_{-1}\left[\left| \tfrac{1}{2}\left(\tau_n + \tau_{n+1}\right) - \tau \right|\right] d\tau = 1 \qquad (3.21)$$

$$\psi_{Th} - \pi^{-\frac{1}{2}} \sum_{k=0}^{n-1} \psi_{Tk} \int_{\tau_k}^{\tau_{k+1}} J_{-1}\left[\left| \tfrac{1}{2}\left(\tau_n + \tau_{n+1}\right) - \tau \right|\right] d\tau = \tfrac{1}{2} - \pi^{-\frac{1}{2}} \int_{-\frac{\Delta}{2}}^{\frac{\Delta}{2}} J_1\left[\left| \tfrac{1}{2}\left(\tau_n + \tau_{n+1}\right) - \tau \right|\right] d\tau \qquad (3.22)$$

Where ψ_{Pk} is the stepwise function of ψ_ρ and ψ_{Tk} the stepwise function of ψ_T

The constant value of the functions ψ_{Pk} and ψ_{Tk} on each interval is interpreted as the value at the midpoint. The transcendental function $T_{-(x)}$ has a singularity when $x \rightarrow 0.$

According to the obvious way of differences, equations (3.21) and (3.22) reduce to the matrix

$$\sum_{k=0}^{n-1} \mathrm{A}_{hk} \psi_{pk} = 1 \qquad \text{for } n = 0, 1, 2, \ldots, n-1 \tag{3.23}$$

$$\sum_{k=0}^{n-1} \mathrm{B}_{hk} \psi_{\mathrm{T}k} = g_h \qquad \text{for } n = 0, 1, 2, \ldots, n-1 \tag{3.24}$$

where

$$\mathrm{A}_{\mathrm{hk}} = \delta_{hk} - \pi^{-\frac{1}{2}} \int_{-\frac{(2k-n-2)\Delta}{2n}}^{\frac{(2k-n-2)\Delta}{2n}} J_{-1}\left(\left| \frac{2h+1-\mathrm{n}}{2\mathrm{n}} \Delta - \tau \right| \right) d\tau \tag{3.25}$$

$$\mathrm{A}_{\mathrm{hk}} = \mathrm{B}_{hk} \tag{3.26}$$

$$\mathrm{g}_{\mathrm{h}} = \tfrac{1}{2} - \pi^{-\frac{1}{2}} \int_{-\frac{\Delta}{2}}^{\frac{\Delta}{2}} J_1\left(\left| \frac{2h+1-\mathrm{n}}{2\mathrm{n}} \Delta - \tau \right| \right) d\tau \tag{3.27}$$

Integration equations (3.25) and (3.27) using the properties of J_n we have;

If $h \neq k$

$$\mathrm{A}_{\mathrm{hk}} = \pi^{-\frac{1}{2}} \left\{ J_0\left[\frac{2\delta}{\pi^{\frac{1}{2}}} \left(\frac{|k-h|}{n} - (2n)^{-1} \right) \right] - J_0\left[\left[\frac{2\delta}{\pi^{\frac{1}{2}}} \left(\frac{|k-h|}{n} + (2n)^{-1} \right) \right] \right] \right\} \tag{3.28}$$

If $h = k$

$$\mathrm{A}_{\mathrm{hk}} = \left(\frac{2}{\pi^{\frac{1}{2}}} \right) J_0\left(\frac{\delta}{\pi^{\frac{1}{2}}} n \right) \tag{3.29}$$

$$\mathrm{g}_{\mathrm{h}} = \pi^{-\frac{1}{2}} \left\{ J_2\left[\frac{\delta}{\pi^{\frac{1}{2}}} \left(1 - \frac{2h+1-n}{n} \right) \right] + J_2\left[\frac{\delta}{\pi^{\frac{1}{2}}} \left(1 + \frac{2h+1-n}{n} \right) \right] \right\} \tag{3.30}$$

4.0 Numerical Results

Using LAPAK and LINPAC solvers we obtained the following results

Table 1: Poiseuille flow and Thermal Creep volume flow rates using Finite Difference Method. Parameter used: Accommodation coefficient $\propto = 1$

Channel width (d_0) or inverse Knudsen number (kn)	Finite Difference Method (FDM) No of Elements = 100 No of Gaussian Points = 50 Poiseuille Flow rates	Finite Difference Method (FDM) No of Elements = 100 No of Gaussian Points = 50 Thermal creep volume flow rates
0.0010	4.194779	1.814151
0.0100	3.049363	1.235673
0.1000	2.032757	0.694946
0.5000	1.601950	0.398527
1.0000	1.538786	0.294933
1.5000	1.553608	0.241208
2.0000	1.595032	0.206283
4.0000	1.846180	0.133843
6.0000	2.141391	0.099800
8.0000	2.451381	0.079584
10.000	2.768504	0.066139
50.000	9.263045	0.015036
100.00	17.06334	0.007810

The finite difference method can only take accommodation coefficient of one. This is due to the fact that we adopted only the diffuse reflection boundary condition. A range of inverse Knudsen numbers from 0.001 to 100 was considered which accommodated the slip flow, transition flow and the collisionless flow regime.

The results show an agreement of 96.6% within the slip and collisionless regime and 99.9% in the transition regime. The flow rate shows its minimum at $K_n = 1.0$ in the transition regime. This result also agreed with that of Cercignani and Daneri [15] who pointed out that the minimum occurs between 1.0 and 1.2. It was also observed that as the inverse Knudsen number gets very large, the volume flow rate shoots up drastically; reason was that the mean-free-path becomes larger.

In the computation of the Thermal Creep Volume Flow Rate, the same parameters were used and the result also shows an agreement of 96.6% within the slip and collisionless regime and 99.9% in the transition regime. It was noticed that as the channel gets wider the thermal creep volume flow rates gets smaller.

5.0 Conclusion

Finite difference method was able to give excellent results on Poiseuille and Thermal creep at a relatively much shorter computation and can be comparable to the other solution methods even up to 99% accuracy. However, it could not take accommodation coefficient of order greater than one because of the consideration of only the diffuse boundary condition.

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