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# BRIEF NOTES

## Numerical treatment of the Boltzmann-equation

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DIFFERENT types of Gauss-Hermite quadrature procedures are used as a tool of solution of the nonlinear BGK-equation. The comparison of these methods is presented in the paper.

### 1. Introduction

THE NUMERICAL treatment of the Boltzmann-equation with the non-linear BHATNAGAR-GROSS-KROOK-collision operator [1] on the base of the discrete ordinate method due to HUANG [2] uses approximation formulas for the moments of the velocity distribution function. The calculated results for the flow of a monoatomic gas in a slit of finite length show a strong dependence on the type of applied quadrature formula. Figure 1 shows three curves according to the Gauss-Hermitean quadrature formula (I) and other formulas proposed by HUANG and HARTLEY [3] (II, III) which lead to qualitatively and

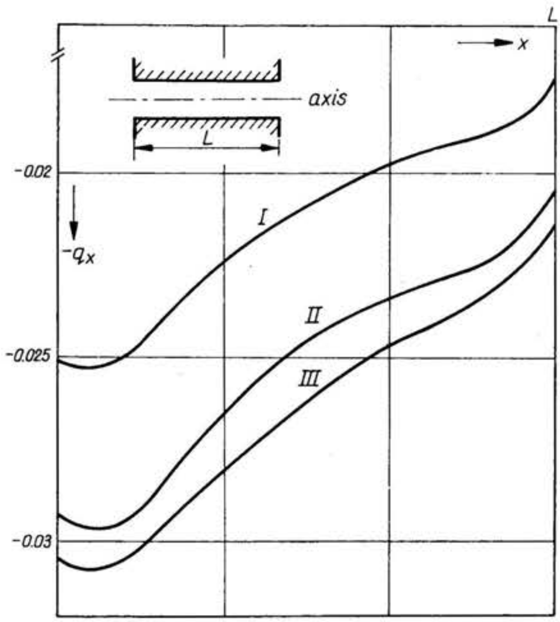


FIG. 1. Dimensionless velocity distribution of a monoatomic gas along the channel-axis (pressure ratio 1.5).

quantitatively different results. Therefore, it is necessary to know the error induced by the quadrature formulas especially when determine the particle number density. As we cannot compare the numerical results with an exact solution of the Boltzmann-equation we will introduce a test equation which resembles the Boltzmann-equation formally.

## 2. Test equation

In this paper we shall compare the numerical results of the non-linear partial differential equation

$$\mathbf{c}\cdot\nabla g = -\frac{2\pi}{n(\mathbf{r})}\mathbf{c}^2(\mathbf{r}\cdot\mathbf{c})g \tag{2.1}$$

gained by the discrete ordinate method with respect to $\mathbf{c} = c_x, c_y$. Formally we will call the vector $\mathbf{c}$ a velocity vector, the components of which may vary in a two-dimensional real space $V^2$. The non-linearity of Eq. (2.1) is due to the denominator which is a functional of the unknown solution $g$

$$n(\mathbf{r}) := \iint\limits_{-\infty}^{\infty} g(\mathbf{r},\mathbf{c})\,dc_x\,dc_y.$$

The domain in which the solution is sought is a rectangle $G$

$$G:\quad -L \leqslant x \leqslant L, \qquad -0.5 \leqslant y \leqslant 0.5.$$

The exact solution of Eq. (2.1) which is defined for all $\mathbf{r}\in R^2$ and all $\mathbf{c}\in V^2$ is given by

$$\gamma(\mathbf{r},\mathbf{c}) = \exp[-\mathbf{c}^2\exp(\mathbf{r}^2)]. \tag{2.2}$$

For $\gamma$ the following relations hold:

(a) symmetry: $\gamma(\mathbf{r},\mathbf{c}) = \gamma(-\mathbf{r},-\mathbf{c})$,

(b) positiveness: $\gamma(\mathbf{r},\mathbf{c}) > 0$,

(c) existence of the double and fourfold integral:

$$\iint\limits_{-\infty}^{\infty} \gamma(\mathbf{r},\mathbf{c})\,dc_x\,dc_y = \pi\exp[-\mathbf{r}^2],$$

$$\iint\limits_{-\infty}^{\infty}\Big[\iint\limits_{-\infty}^{\infty} \gamma(\mathbf{r},\mathbf{c})\,dc_x\,dc_y\Big]\,dx\,dy = \pi^2.$$

Physically speaking the function $\nu(\mathbf{r}) := \pi\exp(-\mathbf{r}^2)$ shows the same behaviour as a particle number density which decreases very rapidly to 0 when $|\mathbf{r}|\to\infty$. Using $\nu(\mathbf{r})$ we may rewrite the exact solution in the form

$$\gamma(\mathbf{r},\mathbf{c}) = \exp[-\pi\mathbf{c}^2/\nu(\mathbf{r})].$$

## 3. Quadrature formulas

For the application of the Gauss-Hermitean quadrature formula we introduce a new function $\Phi$ by the separation ansatz

$$g(\mathbf{r},\mathbf{c}) = \exp[\mathbf{c}^2\cdot\Phi]\exp[-\mathbf{c}^2)].$$

According to this assumption the partial differential equation for $\Phi$ is of the following form:

(2.1′)
$$\mathbf{c}\cdot\nabla\Phi = -\frac{2\pi}{n(\mathbf{r})}(\mathbf{r}\cdot\mathbf{c}),$$
$$n(\mathbf{r}) = \iint\limits_{-\infty}^{\infty} \exp[\mathbf{c}^2\Phi]\exp[-\mathbf{c}^2]\,dc_x\,dc_y.$$

The exact solution of (2.1′) is given by

$$\varphi(\mathbf{r},\mathbf{c}) = 1-\exp[\mathbf{r}^2].$$

As initial conditions for $\Phi$ we pose

$$\Phi(\pm L, y, \mathbf{c}) = 1-\exp[L^2+y^2].$$

$n(\mathbf{r})$ will be determined by one of the following approximating formulas:

I Gauss-Hermite: $n(\mathbf{r}) \approx \sum\limits_{i,k} A_i A_k \Phi(r, \alpha_i, \alpha_k)$,

II Huang-Hartley: $n(\mathbf{r}) \approx \sum\limits_{i,k} B_i B_k \Phi(r, \beta_i, \beta_k)$,

III Huang-Hartley: $n(\mathbf{r}) \approx \sum\limits_{i,k} C_i C_k \Phi(r, \gamma_i, \gamma_k)$.

The weighting factors $A_j$, $B_j$, $C_j$ together with the discrete ordinates $\alpha_j, \beta_j, \gamma_j$, $j = 1, \ldots, 4$, are listed in Appendix A.

## 4. Difference scheme

Defining $a := c_y/c_x$ and $F(\mathbf{r}, a; n) := -2\pi(x+ay)/n(\mathbf{r})$ the differential equation (2.1′) can be written in the form

(2.1″)
$$\frac{\partial\Phi}{\partial x} + a\frac{\partial\Phi}{\partial y} = F(\mathbf{r}, a; n).$$

As equation (2.1″) is hyperbolic we will pose the Cauchy initial value problem. For the numerical calculation we introduce a difference scheme in the physical space (Fig. 2) by the formula

(4.1)
$$\frac{\Phi_P^{R+1}-\Phi_P^R}{h} + a\,\frac{\Phi_{P+1}^R-\Phi_P^R}{k} = F_P^R.$$

The initial value distribution is prescribed by the values of the exact solution along the left and right part of the boundary:

$$\Phi_P^1 = \varphi_P;$$

$$\Phi_P^R := \Phi\big(-L+(R-1)h,\ -0.5+(P-1)k\big), \quad h := \frac{2L}{N}, \quad k := \frac{0.5}{M},$$

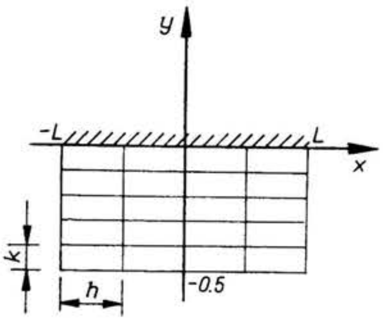


FIG. 2. Domain of the numerical solution.

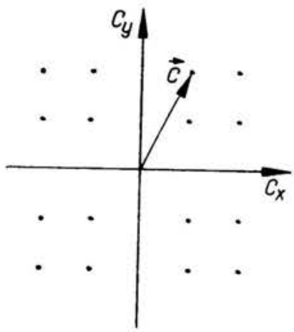


FIG. 3. Velocity space (64 points were used for the calculation).

$R = 1, \ldots, N+1$; $P = 1, \ldots, M+1$. $N$ is the number of intervals in the $x$-direction, $M$ the number of intervals in the $y$-direction. Typical values for calculation have been $N = 9$, $M = 10$.

A stability analysis of the explicit difference scheme (4.1) leads to the necessary stability criterion:

$$\alpha := \left|\frac{c_y}{c_x}\right| \frac{h}{k} < 1. \tag{4.2}$$

Applying the discrete ordinate method we have to introduce a set of points in the velocity space (Fig. 3) at which we solve the equation (2.1″) by an iterative process. Summing up the contribution of each velocity point according to the chosen quadrature formula we obtain the desired moment $n(\mathbf{r})$. It is obvious that the larger the number of points in the velocity space, the better will $n(\mathbf{r})$ be approximated. Nevertheless, we have to fulfil the stability criterion (4.2) as a consequence of which the grid spacing in the $x$-direction shrinks drastically when we admit velocity points close to the $c_y$-axis. Thus, the stability parameter $\alpha$ depends strongly on the quadrature formula.

## 5. Results

In Appendix $B$ for two values of $L$ the moment $n(\mathbf{r})$ is compared for the three formulas I, II, III. It follows that formula I leads to the smallest absolute error taken over all grid points at which $\Phi$ was calculated. The maximal absolute difference between two successive approximations of $n(\mathbf{r})$ drops to 0 very rapidly but the corresponding maximal absolute error is about one order of magnitude larger. Fig. 4 shows a perspective view of the exact solution as a surface above the domain $G$ for $y < 0$. The Figs. 5a, b, c give, in a relative measure, the error behaviour in the whole field of computation.

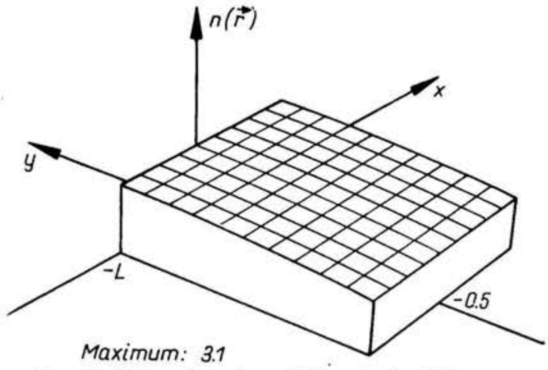


FIG. 4. Perspective view of the exact solution.

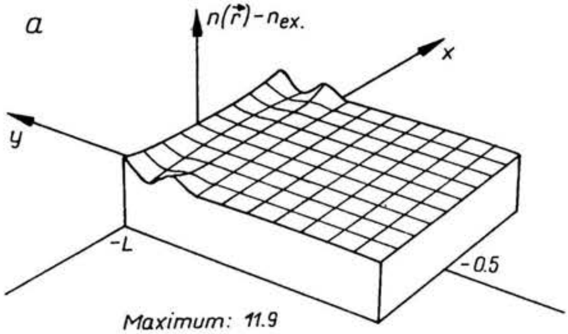


FIG. 5a. (I) GAUSS-HERMITE.

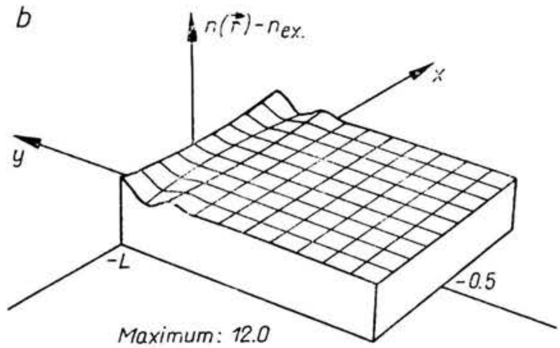


FIG. 5b. (II) HUANG-HARTLEY (even equally spaced).

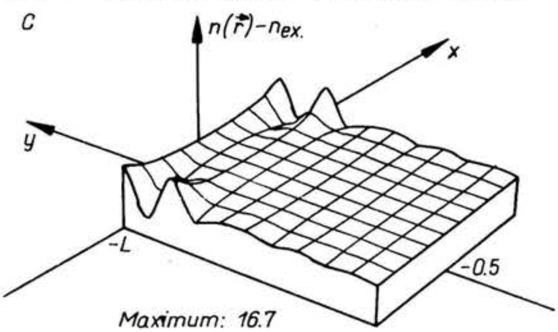


FIG. 5c. (III) HUANG-HARTLEY (odd equally spaced).

## Appendix A

| | | Weighting factors | Discrete ordinates |
|---|---|---|---|
| I | Gauss-Hermite | $A_1 = 0.66114701$<br>$A_2 = 0.20780233$<br>$A_3 = 0.17077988E{-}1$<br>$A_4 = 0.19960407E{-}3$ | $\alpha_1 = 0.38118699$<br>$\alpha_2 = 1.1571937$<br>$\alpha_3 = 1.9816568$<br>$\alpha_4 = 2.9306374$ |
| II | Huang-Hartley | $B_1 = 0.72186$<br>$B_2 = 0.15334$<br>$B_3 = 0.12349$<br>$B_4 = 0.19421$ | $\beta_1 = 0.32$<br>$\beta_2 = 0.64$<br>$\beta_3 = 0.96$<br>$\beta_4 = 1.28$ |
| III | Huang-Hartley | $C_1 = 0.18219$<br>$C_2 = 0.80680$<br>$C_3 = 0.62089$<br>$C_4 = 0.51812$ | $\gamma_1 = 0.16$<br>$\gamma_2 = 0.54$<br>$\gamma_3 = 0.80$<br>$\gamma_4 = 1.12$ |

## Appendix B

| | $L$ | Number of iterations $i$ | Stability parameter $\alpha$ | max $\lvert n^i - n^{i-1}\rvert$ | $\max\lvert n^i - n\,\text{exact}\rvert$ |
|---|---|---|---|---|---|
| I | | 2 | 0.3417 | 0.00316 | 0.0015 |
| II | 0.01 | 2 | 0.1778 | 0.00397 | 0.0019 |
| III | | 2 | 0.3111 | 0.00697 | 0.0031 |
| I | | 3 | 0.6834 | 0.000426 | 0.00957 |
| II | 0.02 | 3 | 0.3556 | 0.000241 | 0.0102 |
| III | | 3 | 0.6222 | 0.00840 | 0.0334 |

### References

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