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NUMERICAL STUDY OF GAS EXPANSION IN A BOX USING THE GENERAL FOUR VELOCITY BROADWELL MODEL

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ABSTRACT. In this paper we investigate the expansion of a gas in a box in the scope of discrete kinetic theory. The box is initially at rest and half-full filled of a gas. The general four velocity discrete model of Broadwell is retained for the modelling and the resulting mild problem is solved numerically using a fractional step method. The starting motion into the empty part of the box and the behaviour at large times of the gas is studied. An equilibrium state is attained after a transitional phase where the behaviour of the macroscopic variables of the flow depend on the set of the velocities of the model. The influence of the set of the velocities of the model vanishes in the steady state.

1. INTRODUCTION

After the pioneering works of Broadwell who solved the Couette and the Rayleigh flows and the shock wave problem analytically using discrete velocity models [?,1], many problems of rarefied gas dynamics have been investigated in the scope of discrete kinetic theory. Owing to the fact that global existence question is well understood in one space dimension for discrete velocity models [4], several

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analytical and numerical results in good accordance whith those obtained using other methods of resolution of the Boltzmann Equation have been established [4, 6–8]. Recent progress in the proof of the existence of solution for boundary value and mild problems for discrete velocity models in more than one dimension [5, 11–13] allow to investigate gas dynamics problems in higher spatial dimensions.

The aim of this paper is to solve numerically the problem of the expansion of a gas in a box initially at rest and half-full filled of a gas.

The paper is organized as follows. In section 2 we briefly present the model used to perfom the computations and state the mathematical problem in consideration in the paper. The numerical method of resolution is described in section 3. In section 4 we present and analyse the numerical results obtained.

2. Statement of the problem

2.1. The discrete velocity model. The general plane four velocity discrete models of Broadwell denoted by B_{θ} are among the simplest discrete velocity models and have been used to study initial and boundary value problems in one dimension [4], [6] and to build exact solutions [10]. In the basis $(\vec{e_1}, \vec{e_2})$ of orthonormal reference $(O, \vec{e_1}, \vec{e_2})$ of the plane \mathbb{R}^2 its velocities are $\vec{u_1} = c(\cos\theta, \sin\theta)$, $\vec{u_2} = c(-\sin\theta, \cos\theta)$, $\vec{u_3} = -\vec{u_2}$, $\vec{u_4} = -\vec{u_1}$, where $\theta = angle(\vec{e_1}, \vec{u_1})$ accounts of the orientation of the discrete velocity model with respect to the reference.



FIGURE 1. The model

Let $N'_i(t', x', y')$ be the number density of the gas molecules with velocity $\vec{u_i}$, i = 1, 2, 3, 4 at the time t' and at the position M(x', y') the kinetic equations of the model are:

$$(2.1) \begin{cases} \frac{\partial N_1'}{\partial t'} + ccos\theta \frac{\partial N_1'}{\partial x'} + csin\theta \frac{\partial N_1'}{\partial y'} &= Q' \\ \frac{\partial N_2'}{\partial t'} - csin\theta \frac{\partial N_2'}{\partial x'} + ccos\theta \frac{\partial N_2'}{\partial y'} &= -Q' \\ \frac{\partial N_3'}{\partial t'} + csin\theta \frac{\partial N_3'}{\partial x'} - ccos\theta \frac{\partial N_3'}{\partial y'} &= -Q' \\ \frac{\partial N_4'}{\partial t'} - ccos\theta \frac{\partial N_4'}{\partial x'} - csin\theta \frac{\partial N_4'}{\partial y'} &= Q' \end{cases}$$

(2.2)
$$Q' = 2cs (N'_2 N'_3 - N'_1 N'_4).$$

The total density ρ' and the macroscopic velocity $\overrightarrow{U}'(U', V')$ of a gas described by the model are defined by:

(2.3)

$$\rho' = N'_1 + N'_2 + N'_3 + N'_4,$$

$$\rho'U' = \cos(\theta)[N'_1 - N'_4] - \sin(\theta)[N'_2 - N'_3],$$

$$\rho'V' = \sin(\theta)[N'_1 - N'_4] + \cos(\theta)[N'_2 - N'_3].$$

The Maxwellian densities of the model associated with the macroscopic variables ρ' , U' and V' are given by the relations:

$$N_{1M}' = \frac{N'}{4} \Big[1 + \cos(2\theta) \Big(u^2 - v^2 \Big) + 2uv \sin(2\theta) + 2u \cos(\theta) + 2v \sin(\theta) \Big],$$

$$N_{2M}' = \frac{N'}{4} \Big[1 - \cos(2\theta) \Big(u^2 - v^2 \Big) - 2uv \sin(2\theta) + 2v \cos(\theta) - 2u \sin(\theta) \Big],$$

$$N_{3M}' = \frac{N'}{4} \Big[1 - \cos(2\theta) \Big(u^2 - v^2 \Big) - 2uv \sin(2\theta) - 2v \cos(\theta) + 2u \sin(\theta) \Big],$$

$$N_{4M}' = \frac{N'}{4} \Big[1 + \cos(2\theta) \Big(u^2 - v^2 \Big) + 2uv \sin(2\theta) - 2u \cos(\theta) - 2v \sin(\theta) \Big],$$
with $u = U'/c$ et $v = V'/c$

with u = U'/c et v = V'/c.

2.2. The mathematical problem. We consider a gas flow described by the general four velocity discrete model in a rectangular box of lenght *L* and width *h* $(0 < h \le L)$. The walls of the box are impermeable. Initially the box is divided in two compartments of the same capacity. The first compartment is filled by a

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gas at rest and the second compartment is empty. The origin *O* of the orthonormal reference introduced above is chosen so that the edges of the box are located on the lines $x' = -\frac{L}{2}$, $x' = \frac{L}{2}$, $y' = -\frac{h}{2}$ and $y' = \frac{h}{2}$ and the angle θ belongs to the interval $\left[0, \frac{\pi}{2}\right]$.



FIGURE 2. The box

The initial densities are denoted by $N'_i(0, x', y') = N'_{i,0}$, i = 1, 2, 3, 4. We use the diffuse reflection boundary conditions on the walls. The microscopic densities of the discrete gas in Maxwellian equilibrium with a wall, respectively denoted by N^{\pm}_{iw} and $N_{iw_{\pm}}$ at $y = \pm \frac{h}{2}$ and $x = \pm \frac{L}{2}$, are the Maxwellian densities associated with 1 and the longitudinal and transversal velocities of the wall respectively denoted by U^{\pm}_w and V^{\pm}_w . Let λ^{\pm} be the respective accommodation coefficients. The boundary conditions of diffuse reflection are written in the form [2,8]:

(2.5)

$$N_{1}'(t', -L/2, y') = \lambda_{-}(t', -L/2, y')N_{1w_{-}},$$

$$N_{3}'(t', -L/2, y') = \lambda_{-}(t', -L/2, y')N_{3w_{-}},$$

$$N_{2}'(t', L/2, y') = \lambda_{+}(t', L/2, y')N_{2w_{+}},$$

$$N_{4}'(t', L/2, y') = \lambda_{+}(t', L/2, y')N_{4w_{+}},$$

$$N_{1}'(t', x', -h/2) = \lambda^{-}(t', x', -h/2)N_{1w}^{-},$$

$$N_{2}'(t', x', -h/2) = \lambda^{-}(t', x', -h/2)N_{2w}^{-},$$

$$N_{3}'(t', x', h/2) = \lambda^{+}(t', x', h/2)N_{3w}^{+},$$

$$N_{4}'(t', x', h/2) = \lambda^{+}(t', x', h/2)N_{4w}^{+}.$$

In the sequel, we assume naturally that the walls are at rest. The impermeability of the box's walls means that the normal velocity at each wall vanishes. Therefore:

$$\vec{U}\cdot\vec{n}=0$$

where \vec{n} denote the inward-pointing (i.e. into the gas) unit vectors normal to the wall.

The problem is put in dimensionless form. The reference quantities are ρ'_0 , the initial total density, for the density, *c* for the velocity, t_0 for the time and *L* and *h* for the length respectively for the *x'* axis and the *y'* axis. t_0 is the characteristic time of the unsteady flow. The dimensionless variables are:

(2.7)
$$\begin{aligned} x &= x'/L, \ y &= y'/h, \ t' &= t/t_0, \ \varepsilon &= h/L, \ \mathrm{Kn} &= (sn_0L)^{-1}, \ \mathrm{St} &= L/ct_0, \\ N_i &= N_i'/n_0, \ \rho &= \rho'/\rho_0', \ \rho_0 &= \rho_0'/\rho_0' &= 1, \\ u_0 &= U_0/c, \ v_0 &= V_0/c, \ u &= U/c, \ v &= V/c. \end{aligned}$$

The parameter ε is the aspect ratio of the box, Kn is the Knudsen number and St is the Strouhal number. The dimensionless problem to solve is:

$$\begin{aligned} \operatorname{St} \frac{\partial N_{1}}{\partial t} + \cos(\theta) \frac{\partial N_{1}}{\partial x} + \frac{1}{\varepsilon} \sin(\theta) \frac{\partial N_{1}}{\partial y} &= \frac{2}{Kn} (N_{2}N_{3} - N_{1}N_{4}), \\ \operatorname{St} \frac{\partial N_{1}}{\partial t} - \sin(\theta) \frac{\partial N_{1}}{\partial x} + \frac{1}{\varepsilon} \cos(\theta) \frac{\partial N_{1}}{\partial y} &= \frac{2}{Kn} (N_{1}N_{4} - N_{2}N_{3}), \\ \operatorname{St} \frac{\partial N_{1}}{\partial t} + \sin(\theta) \frac{\partial N_{1}}{\partial x} - \frac{1}{\varepsilon} \cos(\theta) \frac{\partial N_{1}}{\partial y} &= \frac{2}{Kn} (N_{1}N_{4} - N_{2}N_{3}), \\ \operatorname{St} \frac{\partial N_{1}}{\partial t} - \cos(\theta) \frac{\partial N_{1}}{\partial x} - \frac{1}{\varepsilon} \sin(\theta) \frac{\partial N_{1}}{\partial y} &= \frac{2}{Kn} (N_{2}N_{3} - N_{1}N_{4}), \\ N_{i}(0, x, y) &= N_{i,0}, \quad i = 1, 2, 3, 4, \end{aligned}$$

$$(2.8) \qquad N_{3w_{-}}N_{1}(t, -1/2, y) - N_{1w_{-}}N_{3}(t, -1/2, y) &= 0, \\ N_{4w_{+}}N_{2}(t, 1/2, y) - N_{2w_{+}}N_{4}(t, 1/2, y) &= 0, \\ N_{2w}N_{1}(t, x, -1/2) - N_{1w}^{-}N_{2}(t, x, -1/2) &= 0, \\ N_{4w}^{+}N_{3}(t, x, 1/2) - N_{3w}^{+}N_{4}(t, x, 1/2) &= 0, \\ \cos(\theta)[N_{1}(t, -1/2, y) - N_{4}(t, -1/2, y)] \\ &-\sin(\theta)[N_{2}(t, -1/2, y) - N_{3}(t, -1/2, y)] &= 0, \end{aligned}$$

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$$\begin{split} &-\sin(\theta) \left[N_2(t,1/2,y) - N_3(t,1/2,y) \right] = 0, \\ &\sin(\theta) \left[N_1(t,x,-1/2) - N_4(t,x,-1/2) \right] \\ &+\cos(\theta) \left[N_2(t,x,-1/2) - N_3(t,x,-1/2) \right] = 0, \\ &\sin(\theta) \left[N_1(t,x,1/2) - N_4(t,x,1/2) \right] \\ &+\cos(\theta) \left[N_2(t,x,1/2) - N_3(t,x,1/2) \right] = 0, \end{split}$$

where $(t, x, y) \in [0, T] \times [-1/2, 1/2] \times [-1/2, 1/2]$ with *T* a positive arbitrary number.

The problem (2.8) is solved using the classic fractional step method [3, 10]. The numerical resolution is done in two steps. Firstly the problem is solved for a spatial homogeneous flow (equations (2.9)), and secondly it is solved in the free molecular regime (equations (2.10)).

$$(2.9) \qquad \begin{cases} \operatorname{St} \frac{N_{1}^{m+\frac{1}{2}} - N_{1}^{m}}{\Delta t} = \frac{2}{Kn} \left(N_{2}^{m+1/2} N_{3}^{m+1/2} - N_{1}^{m+1/2} N_{4}^{m+1/2} \right) & ((2.9).1) \\ \operatorname{St} \frac{N_{2}^{m+\frac{1}{2}} - N_{2}^{m}}{\Delta t} = \frac{2}{Kn} \left(N_{1}^{m+1/2} N_{4}^{m+1/2} - N_{2}^{m+1/2} N_{3}^{m+1/2} \right) & ((2.9).2) \\ \operatorname{St} \frac{N_{3}^{m+\frac{1}{2}} - N_{3}^{m}}{\Delta t} = \frac{2}{Kn} \left(N_{1}^{m+1/2} N_{4}^{m+1/2} - N_{2}^{m+1/2} N_{3}^{m+1/2} \right) & ((2.9).3) \\ \operatorname{St} \frac{N_{4}^{m+\frac{1}{2}} - N_{4}^{m}}{\Delta t} = \frac{2}{Kn} \left(N_{2}^{m+1/2} N_{3}^{m+1/2} - N_{1}^{m+1/2} N_{4}^{m+1/2} \right) & ((2.9).4) \end{cases} \\ \left(\operatorname{St} \frac{N_{1}^{m+1} - N_{1}^{m+\frac{1}{2}}}{\Delta t} + \cos(\theta) \frac{\partial}{\partial x} \left(N_{1}^{m+1} \right) + \frac{1}{\varepsilon} \sin(\theta) \frac{\partial}{\partial y} \left(N_{1}^{m+1} \right) = 0 & ((2.10).1) \end{cases} \right)$$

$$(2.10) \begin{cases} \operatorname{St} \frac{N_2^{m+1} - N_2^{m+\frac{1}{2}}}{\Delta t} - \sin(\theta) \frac{\partial}{\partial x} \left(N_2^{m+1} \right) + \frac{1}{\varepsilon} \cos(\theta) \frac{\partial}{\partial y} \left(N_2^{m+1} \right) = 0 \quad ((2.10).2) \\ \operatorname{St} \frac{N_3^{m+1} - N_3^{m+\frac{3}{2}}}{\Delta t} + \sin(\theta) \frac{\partial}{\partial x} \left(N_3^{m+1} \right) - \frac{1}{\varepsilon} \cos(\theta) \frac{\partial}{\partial y} \left(N_3^{m+1} \right) = 0 \quad ((2.10).3) \\ \operatorname{St} \frac{N_4^{m+1} - N_4^{m+\frac{1}{2}}}{\Delta t} - \cos(\theta) \frac{\partial}{\partial x} \left(N_4^{m+1} \right) - \frac{1}{\varepsilon} \sin(\theta) \frac{\partial}{\partial y} \left(N_4^{m+1} \right) = 0 \quad ((2.10).4) \end{cases}$$

In the above equations the discretisation of time interval is made with step Δt and N_i^m and $N_i^{m+1/2}$ represent the values of the function N_i at $t = m\Delta t$ and $t = (m + 1/2)\Delta t$ respectively. The resolution of equations (2.9) gives:

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$$N_{1}^{m+\frac{1}{2}} = \frac{N_{1}^{m} + \sigma\left(N_{1}^{m} + N_{2}^{m}\right)\left(N_{1}^{m} + N_{3}^{m}\right)}{1 + \sigma\left(N_{1}^{m} + N_{2}^{m} + N_{3}^{m} + N_{4}^{m}\right)}, N_{2}^{m+\frac{1}{2}} = \frac{N_{2}^{m} + \sigma\left(N_{1}^{m} + N_{2}^{m}\right)\left(N_{2}^{m} + N_{4}^{m}\right)}{1 + \sigma\left(N_{1}^{m} + N_{3}^{m}\right)\left(N_{3}^{m} + N_{4}^{m}\right)}, N_{4}^{m+\frac{1}{2}} = \frac{N_{2}^{m} + \sigma\left(N_{1}^{m} + N_{2}^{m}\right)\left(N_{2}^{m} + N_{4}^{m}\right)}{1 + \sigma\left(N_{1}^{m} + N_{3}^{m}\right)\left(N_{3}^{m} + N_{4}^{m}\right)}, N_{4}^{m+\frac{1}{2}} = \frac{N_{2}^{m} + \sigma\left(N_{1}^{m} + N_{2}^{m}\right)\left(N_{2}^{m} + N_{4}^{m}\right)}{1 + \sigma\left(N_{1}^{m} + N_{2}^{m} + N_{3}^{m}\right)}, N_{4}^{m+\frac{1}{2}} = \frac{N_{4}^{m} + \sigma\left(N_{1}^{m} + N_{2}^{m}\right)\left(N_{3}^{m} + N_{4}^{m}\right)}{1 + \sigma\left(N_{1}^{m} + N_{2}^{m} + N_{3}^{m}\right)}, N_{4}^{m+\frac{1}{2}} = \frac{N_{4}^{m} + \sigma\left(N_{2}^{m} + N_{4}^{m}\right)\left(N_{3}^{m} + N_{4}^{m}\right)}{1 + \sigma\left(N_{1}^{m} + N_{2}^{m} + N_{3}^{m}\right)}, N_{4}^{m+\frac{1}{2}} = \frac{N_{4}^{m} + \sigma\left(N_{2}^{m} + N_{4}^{m}\right)\left(N_{3}^{m} + N_{4}^{m}\right)}{1 + \sigma\left(N_{1}^{m} + N_{2}^{m} + N_{3}^{m}\right)}, N_{4}^{m+\frac{1}{2}} = \frac{N_{4}^{m} + \sigma\left(N_{2}^{m} + N_{4}^{m}\right)\left(N_{3}^{m} + N_{4}^{m}\right)}{1 + \sigma\left(N_{1}^{m} + N_{2}^{m} + N_{3}^{m}\right)}, N_{4}^{m+\frac{1}{2}} = \frac{N_{4}^{m} + \sigma\left(N_{4}^{m} + N_{4}^{m}\right)\left(N_{3}^{m} + N_{4}^{m}\right)}{1 + \sigma\left(N_{1}^{m} + N_{2}^{m} + N_{3}^{m}\right)}, N_{4}^{m+\frac{1}{2}} = \frac{N_{4}^{m} + \sigma\left(N_{4}^{m} + N_{4}^{m}\right)\left(N_{3}^{m} + N_{4}^{m}\right)}{1 + \sigma\left(N_{4}^{m} + N_{4}^{m} + N_{4}^{m}\right)},$$

where $\sigma = \frac{2\text{St}\Delta t}{Kn}$. The quantities N_i^m and $N_i^{m+1/2}$ depend on x and y. We perform a discretisation of the domain $[-1/2, 1/2] \times [-1/2, 1/2]$ in a regular grid with the steps $\Delta x = 1/(J-1)$ and $\Delta y = 1/(K-1)$ where $J, K \in \mathbb{N} \setminus \{0, 1\}$. Let $N_{i;j,k}^{m+1}$ be the value of N_i^{m+1} at the point $M_{jk}(x_j, y_k) \in [0, 1] \times [-1/2, 1/2]$. The $N_{i;j,k}^{m+1}$ are the solutions of the following equations which are finite difference approximations of the equations (2.10):

$$(2.12) \begin{cases} \operatorname{St} \frac{N_{1;j,k}^{m+1} - N_{1;j,k}^{m+\frac{1}{2}}}{\Delta t} + \cos(\theta) \frac{N_{1;j,k}^{m+1} - N_{1;j-1,k}^{m+1}}{\Delta x} + \frac{1}{\varepsilon} \sin(\theta) \frac{N_{1;j,k}^{m+1} - N_{1;j,k-1}^{m+1}}{\Delta y} = 0 \quad ((2.12).1), \\ \operatorname{St} \frac{N_{2;j,k}^{m+1} - N_{2;j,k}^{m+\frac{1}{2}}}{\Delta t} - \sin(\theta) \frac{N_{2;j+1,k}^{m+1} - N_{2;j,k}^{m+1}}{\Delta x} + \frac{1}{\varepsilon} \cos(\theta) \frac{N_{2;j,k}^{m+1} - N_{2;j,k-1}^{m+1}}{\Delta y} = 0 \quad ((2.12).2), \\ \operatorname{St} \frac{N_{3;j,k}^{m+1} - N_{3;j,k}^{m+\frac{1}{2}}}{\Delta t} + \sin(\theta) \frac{N_{3;j,k}^{m+1} - N_{3;j-1,k}^{m+1}}{\Delta x} - \frac{1}{\varepsilon} \cos(\theta) \frac{N_{3;j,k+1}^{m+1} - N_{3;j,k}^{m+1}}{\Delta y} = 0 \quad ((2.12).3), \\ \operatorname{St} \frac{N_{4;j,k}^{m+1} - N_{4;j,k}^{m+\frac{1}{2}}}{\Delta t} - \cos(\theta) \frac{N_{4;j+1,k}^{m+1} - N_{4;j,k}^{m+1}}{\Delta x} - \frac{1}{\varepsilon} \sin(\theta) \frac{N_{4;j,k+1}^{m+1} - N_{4;j,k}^{m+1}}{\Delta y} = 0 \quad ((2.12).4) \end{cases}$$

3. Consistence and stability

The analysis developped in this section is based on the stability and the convergence study of the numerical scheme done in [9,10].

3.1. **Consistence.** Consider the equations ((2.9).1) and ((2.12).1). By addition one can write

(3.1)
$$\frac{\frac{n_{1;j,k}^{m+1} - n_{1;j,k}^{m}}{\Delta t} + \cos(\theta) \frac{n_{1;j+1,k}^{m+1} - n_{1;j,k}^{m+1}}{\Delta x} + \frac{1}{\varepsilon} \sin(\theta) \frac{n_{1;j,k}^{m+1} - n_{1;j,k-1}^{m+1}}{\Delta y}}{\frac{\sqrt{2} + \sqrt{3}}{Kn} \left(n_{2}^{m+1/2} n_{3}^{m+1/2} - n_{1}^{m+1/2} n_{4}^{m+1/2} \right)}$$

Making a Taylor expansion we have:

$$\begin{aligned} \frac{n_{1;j,k}^{m+1} - n_{1;j,k}^m}{\Delta t} &= \frac{\partial n_1}{\partial t} (t_{m+1}, x_j, y_k) + O(\Delta t), \\ \frac{n_{1;j+1,k}^{m+1} - n_{1;j,k}^{m+1}}{\Delta x} &= \frac{\partial n_1}{\partial x} (t_{m+1}, x_j, y_k) + O(\Delta x), \\ \frac{n_{1;j,k}^{m+1} - n_{1;j,k-1}^{m+1}}{\Delta y} &= \frac{\partial n_1}{\partial y} (t_{m+1}, x_j, y_k) + O(\Delta y). \end{aligned}$$

Then

$$\begin{pmatrix} \frac{n_{1;j,k}^{m+1} - n_{1;j,k}^m}{\Delta t} + \cos(\theta) \frac{n_{1;j+1,k}^{m+1} - n_{1;j,k}^{m+1}}{\Delta x} + \frac{1}{\varepsilon} \sin(\theta) \frac{n_{1;j,k}^{m+1} - n_{1;j,k-1}^{m+1}}{\Delta y} \end{pmatrix}$$

$$- \left(\frac{\partial n_1}{\partial t} (t_{m+1}, x_j, y_k) + \cos(\theta) \frac{\partial n_1}{\partial x} (t_{m+1}, x_j, y_k) + \frac{1}{\varepsilon} \sin(\theta) \frac{\partial n_1}{\partial y} (t_{m+1}, x_j, y_k) \right)$$

$$= O(\Delta t + \Delta x + \Delta y).$$

The same argumentation hold for i = 2, 3, 4. We can thus conclude that the scheme is accurate of order 1 in time and space.

3.2. Stability. We made the stability analysis by the Fourier analysis. We put:

(3.2)
$$n_{i,j,k}^m = \widetilde{n}_i^m(\xi,\eta) \exp\left(q(\xi j \Delta x + \eta k \Delta y)\right),$$

(3.3)
$$\rho_{j,k}^{m} = 2 \sum_{i=1}^{4} n_{i,j,k}^{m} = \widetilde{\rho}^{m}(\xi,\eta) \exp\left(q(\xi j \Delta x + \eta k \Delta y)\right),$$

with $\tilde{\rho}^m(\xi,\eta) = 2\left(\tilde{n}_1^m(\xi,\eta) + \tilde{n}_2^m(\xi,\eta) + \tilde{n}_3^m(\xi,\eta) + \tilde{n}_4^m(\xi,\eta)\right)$, where (ξ,η) is an arbitrary wave vector and q is the complex number such that $q^2 = -1$.

The boundedness of $\tilde{n}_i^m(\xi, \eta)$, i = 1, 2, 3, 4 is equivalent to that of $\tilde{\rho}^m(\xi, \eta)$. Using the conservation of mass in equations (2.9), we have $\tilde{\rho}^{m+\frac{1}{2}}(\xi, \eta) = \tilde{\rho}^m(\xi, \eta)$.

We have:

(3.4)
$$n_{i,j-1,k}^{m} = n_{i,j,k}^{m} \exp\left(-q\xi\Delta x\right),$$
$$n_{i,j+1,k}^{m} = n_{i,j,k}^{m} \exp\left(q\xi\Delta x\right),$$
$$n_{i,j,k-1}^{m} = n_{i,j,k}^{m} \exp\left(-q\eta\Delta y\right),$$
$$n_{i,j,k+1}^{m} = n_{i,j,k}^{m} \exp\left(q\eta\Delta y\right).$$

We replace these relations in the equations (2.12) to obtain:

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(3.5)
$$F_i(\xi,\eta)n_{i,j,k}^{m+1} = n_{i,j,k}^{m+1/2}, \qquad i = 1, 2, 3, 4.$$

with

$$\begin{cases} F_1(\xi,\eta) = 1 + \alpha \cos(\theta) + \gamma \sin(\theta) - \alpha \cos(\theta) \exp(-q\xi\Delta x) - \gamma \sin(\theta) \exp(-q\eta\Delta y) \\ F_2(\xi,\eta) = 1 + \alpha \sin(\theta) + \gamma \cos(\theta) - \alpha \sin(\theta) \exp(q\xi\Delta x) - \gamma \cos(\theta) \exp(-q\eta\Delta y) \\ F_3(\xi,\eta) = 1 + \alpha \sin(\theta) + \gamma \cos(\theta) - \alpha \sin(\theta) \exp(-q\xi\Delta x) - \gamma \cos(\theta) \exp(q\eta\Delta y), \\ F_4(\xi,\eta) = 1 + \alpha \cos(\theta) + \gamma \sin(\theta) - \alpha \cos(\theta) \exp(q\xi\Delta x) - \gamma \sin(\theta) \exp(q\eta\Delta y) \\ \text{and } \alpha = \frac{\Delta t}{St\Delta x} \text{ et } \gamma = \frac{\Delta t}{\varepsilon St\Delta y}. \text{ By taking the module, we can write:} \\ [F_1(\xi,\eta)]^2 = [1 + \alpha \cos(\theta)(1 - \cos(\xi\Delta x)) + \gamma \sin(\theta)(1 - \cos(\eta\Delta y))]^2 + [\alpha \cos(\theta)\sin(\xi\Delta x) + \gamma \sin(\theta)\sin(\eta\Delta y)]^2 \\ [F_2(\xi,\eta)]^2 = [1 + \alpha \cos(\theta)(1 - \cos(\xi\Delta x)) + \gamma \sin(\theta)(1 - \cos(\eta\Delta y))]^2 + [-\alpha \cos(\theta)\sin(\xi\Delta x) + \gamma \sin(\theta)\sin(\eta\Delta y)]^2 \\ [F_3(\xi,\eta)]^2 = [1 + \alpha \cos(\theta)(1 - \cos(\xi\Delta x)) + \gamma \sin(\theta)(1 - \cos(\eta\Delta y))]^2 + [-\alpha \cos(\theta)\sin(\xi\Delta x) - \gamma \sin(\theta)\sin(\eta\Delta y)]^2 \\ [F_4(\xi,\eta)]^2 = [1 + \alpha \cos(\theta)(1 - \cos(\xi\Delta x)) + \gamma \sin(\theta)(1 - \cos(\eta\Delta y))]^2 + [-\alpha \cos(\theta)\sin(\xi\Delta x) - \gamma \sin(\theta)\sin(\eta\Delta y)]^2 \\ [F_4(\xi,\eta)]^2 = [1 + \alpha \cos(\theta)(1 - \cos(\xi\Delta x)) + \gamma \sin(\theta)(1 - \cos(\eta\Delta y))]^2 + [-\alpha \cos(\theta)\sin(\xi\Delta x) - \gamma \sin(\theta)\sin(\eta\Delta y)]^2 \\ [F_4(\xi,\eta)]^2 = [1 + \alpha \cos(\theta)(1 - \cos(\xi\Delta x)) + \gamma \sin(\theta)(1 - \cos(\eta\Delta y))]^2 + [-\alpha \cos(\theta)\sin(\xi\Delta x) - \gamma \sin(\theta)\sin(\eta\Delta y)]^2 \\ [F_4(\xi,\eta)]^2 = [1 + \alpha \cos(\theta)(1 - \cos(\xi\Delta x)) + \gamma \sin(\theta)(1 - \cos(\eta\Delta y))]^2 + [-\alpha \cos(\theta)\sin(\xi\Delta x) - \gamma \sin(\theta)\sin(\eta\Delta y)]^2 \\ [F_4(\xi,\eta)]^2 = [1 + \alpha \cos(\theta)(1 - \cos(\xi\Delta x)) + \gamma \sin(\theta)(1 - \cos(\eta\Delta y))]^2 + [-\alpha \cos(\theta)\sin(\xi\Delta x) - \gamma \sin(\theta)\sin(\eta\Delta y)]^2 \\ [F_4(\xi,\eta)]^2 = [1 + \alpha \cos(\theta)(1 - \cos(\xi\Delta x)) + \gamma \sin(\theta)(1 - \cos(\eta\Delta y))]^2 + [-\alpha \cos(\theta)\sin(\xi\Delta x) - \gamma \sin(\theta)\sin(\eta\Delta y)]^2 \\ [F_4(\xi,\eta)]^2 = [1 + \alpha \cos(\theta)(1 - \cos(\xi\Delta x)) + \gamma \sin(\theta)(1 - \cos(\eta\Delta y))]^2 + [-\alpha \cos(\theta)\sin(\xi\Delta x) - \gamma \sin(\theta)\sin(\eta\Delta y)]^2 \\ [F_4(\xi,\eta)]^2 = [1 + \alpha \cos(\theta)(1 - \cos(\xi\Delta x)) + \gamma \sin(\theta)(1 - \cos(\eta\Delta y))]^2 + [-\alpha \cos(\theta)\sin(\xi\Delta x) - \gamma \sin(\theta)\sin(\eta\Delta y)]^2 \\ As \theta \in [0, \pi/2[, \text{ one has } \cos(\theta) > 0 \text{ and } \sin(\theta) > 0. \text{ Furthermore, for any } X \in \mathbb{R}, \\ 1 - \cos(X) \ge 0. \text{ Then we have } |F_i(\xi,\eta)| > 1, i = 1, 2, 3, 4. \text{ Thus all the amplification factors } \frac{1}{F_i(\xi,\eta)} \sin(\xi,\eta) \le \widetilde{n_i}^{m+1/2}(\xi,\eta), i = 1, 2, 3, 4. \end{cases}$$

Making the sum, we have:

(3.9)
$$\widetilde{\rho}^{m+1}(\xi,\eta) \leq \widetilde{\rho}^{m+1/2}(\xi,\eta) \\ \leq \widetilde{\rho}^{m}(\xi,\eta), \quad \forall m.$$

Finally

(3.10)
$$\widetilde{\rho}^m(\xi,\eta) \leq \widetilde{\rho}^0(\xi,\eta), \quad \forall m.$$

We can then conclude to the stability of the scheme and therefore it converge.

4. Discussion of the results

A point of interest in the study of gas flows in the scope of discrete kinetic theory is the study of the influence of the geometry of the models on the behaviour •

of the macroscopic variables. The four velocity plane models of Broadwell B_{θ} are one speed models whose sets of velocities depend on the angle θ . One speed models have linearly independant summational invariants associated to the mean density and the macroscopic velocity. This work therefore focuses on the analysis of the dependence of the mean density and the macroscopic velocity of the flow upon θ . The numerical results shown here are those of computation made for fixed values of the nondimensional parameters namely $\varepsilon = 0.5$, St = 0.1 and Kn = 0.05 and for angle $\theta \in \left\{0, \frac{\pi}{8}, \frac{\pi}{4}, \frac{3\pi}{8}\right\}$. We point out the fact that the models B_{θ} are isotropic for $\theta = 0, \pi/4$.

For all the chosen values of θ , after an unsteady phase where the macroscopic variables depend clearly upon θ the flow reaches a steady state independent of the latter. The macroscopic velocity decreases in the flow when time grows and at the steady state the gas is at rest. Similarly the macroscopic density decreases and reaches at the steady state the half of its initial value uniformly in the box. The motion of the gas only results of the difference of density initially maintained between the two parts of the box which is at rest. Moreover the process is athermal so these results seem normal. Although it depends on θ , the unsteady phase exhibit some general features.

4.1. **General behaviour of the macroscopic velocity.** When the fictitous diaphragm separating the two compartments of the box is removed, the particles of the discrete gas enter the initially empty part of the box. The flow direction depend completely on θ and for $\theta = 0$ and $\theta = \pi/4$ it is symmetrical with respect to the horizontal line of cordinate (see Table 1). At the onset, the particles move from the full part to the empty part of the box are driven back in the flow but their number is not high enough to influence the flow direction. The mean velocity of the flow is very low in the initially full part and high in the initially empty part of the box: the jump of the macroscopic density generates a flow whose velocity increases with the distance to the separation zone. The mean speed of the flow is maximum when the first particles hit the wall of the empty part of the box parallel to the diaphragm. As soon as the time increases the particles returning into the flow after the impact with the walls generate near the latters flows in their opposite normal directions. These flowbacks first slow down the mean flow

and little by little reverse its direction first in the initially empty part, then in the whole box. The same phenomena occur in the initially full compartment of the box and an inversion of the direction of the mean flow take place there and after in the whole box. The time evolution of the fow is thus a succession of inversions of the flow direction until the mean velocity vanishes. The maximum of the mean speed of the flow decreases with time and is no longer attained near the walls where it tends towards zero. The mean velocity is non monotonic and its extrema are attained anywhere in the box during the unsteady phase. It vanishes in the box at the steady phase (figures 3,4,6,8,9,11,12).

4.2. General behaviour of the mean density. Initially the mean density has constant values in the two compartments of the box: the nondimensional values are one in the full part and zero in the empty part. This profil becomes strictly decreasing at the beginning of the process due to the mass flow. As soon as time increases the strictly decreasing profil of the mean density evolves towards a constant profil after several inversions: partial inversions leading to non monotonic profils and total inversions leading alternatively to increasing and decreasing profils of the density in the box. The maximum of the macroscopic density which can be attained anywhere in the box in the unsteady phase decreases from the nondimensional value one at the beginning of the process to the constant value 0.5 in the whole box at the steady state. These results are shown on figure 10 but the value of the Knudsen number induces a jump of the macroscopic density at the wall which reduces the values of the maxima at the beginning of the process and at the steady state (figure 10).

4.3. **Special effects due to the geometry of the model.** We report here some additionnal features of the flow resulting from the influence of the angle θ . The study of the profils of the macroscopic velocity of the flow in the unsteady phase shows a clear difference between the trajectories and the streamlines for zero and nonzero θ . The trajectories and streamlines are always lines for $\theta = 0$ while they are curves with nonzero curvature for nonzero θ even in the symmetrical case $\theta = \pi/4$ (table 1, figures 3,4,6,8). This result suggests the presence of zones of strong melting where dissipation and rotational effects occur in the flows described by the model for nonzero θ . A convenient analysis of these effects can not be done using the general four velocity Broadwell model which is athermal.







Figure 3. Macroscopic velocity fields for $\theta = 0$



Figure 4. Macroscopic velocity fields for $\theta = \pi/8$







Figure 6. Macroscopic velocity fields for $\theta = \pi/4$



Figure 6. Macroscopic velocity fields for $\theta = \pi/4$



Figure 7. Velocity field for $\theta = \pi/4$



Figure 8. Macroscopic velocity fields for $\theta = 3\pi/8$



FIGURE 8. Macroscopic velocity fields for $\theta = 3\pi/8$



FIGURE 9. Macroscopic velocity fields for $\theta = 3\pi/8$



FIGURE 10. Density at the center



Figure 11. Velocity u at the center



Figure 12. Velocity v at the center



FIGURE 12. Velocity v at the center

5. Conclusion

We solve numerically, using the fractional step method, the problem of the expansion of a gas in a box initially at rest and half-full filled. We analyze the influence of the model orientation on the macroscopic velocity and density. We show that the model orientation influences the flow in the unsteady state but not in the steady state. The steady state is quantitatively and qualitatively the same for all the chosen values of θ used for the study. Interesting features of the flow are brought to the fore in the unsteady phase. Their dependence upon θ is obvious. However their analysis deserves the use of multispeed models in order to take into account energetic properties of the flow.

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