The Appropriate Grid Size of *N* Layer Loosely Coupled Hexagonal Model for Equilibria of Boltzmann Equation

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Abstract

The discrete equilibrium solutions (equilibria) f of the Boltzmann equation can be expressed in terms of four parameters characterizing mass, (x, y)-momenta and kinetic energy. We present an error estimation by comparing the discrete equilibria with the corresponding Maxwellian which leads to determine the appropriate grid size N of the N-layer loosely coupled hexagonal grid for given temperature and bulk-velocity. We calculate numerical results showing how temperature depends on the parameter μ, characterizing kinetic energy and bulk-velocity depends on the parameter κ's, characterizing (x, y) momenta and μ as well.

Keywords— The Boltzmann equation, loosely coupled hexagonal grid, discrete equilibrium solution.

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1 INTRODUCTION

To derive an efficient scheme for the numerical simulation of the Boltzmann collision operator, one immediately faces two major difficulties: (i) The computational cost for the numerical simulation of the Boltzmann equation is very high. This is due to the complexity of the five dimensional integral Boltzmann collision operator, which has to be numerically evaluate at each point (x, y) in the (discretize) six-dimensional space and (ii) The discretization of the Boltzmann collision operator has to be modeled carefully so that it satisfies the features of kinetic theory like conservation laws, H-theorem, properties of linearized collisions operator etc. Several numerical techniques have been proposed in recent years to deal with the complexity of the Boltzmann collision operator. Simplified Collision model have been introduced in rectangular grid in [1][2][3], but there appears many artificial invariants which have to be eliminated by further techniques.

Therefore, in [4] has developed a kinetic theory for the discrete Boltzmann equation based on hexagonal grid in $\mathbf{R}^2$. The Boltzmann collision sphere can be much more suited in the hexagonal grid than rectangular grid model. The system of binary collisions contains artificial invariants and to avoid the artificial invariants a ternary interaction law is introduced. It is shown that the conservation laws, the H-theorem, the correct number of invariants and the properties of linearized operator are satisfied for the discrete Boltzmann equation in the hexagonal grid. In [5], has developed an automatic generation of the Boltzmann collision operator based on a hexagonal grid and made some numerical simulations based on the grid in. In [6], introduced a discrete model Boltzmann equation based on a loosely coupled hexagonal discretization of $\mathbf{R}^2$. The model satisfies the basic features of kinetic theory like conservation laws, H theorem, correct dimension of the null-space of the linearized collision operator etc. In [7] showed that the model Boltzmann equation, based on only binary collision law, discretized on the loosely coupled hexagonal grid in $\mathbf{R}^2$ provides two artificial invariants. In [8], developed a generalized layer-wise construction of a loosely coupled N-layer hexagonal mesh for a discrete model Boltzmann equation. This work also described some properties of the N-layer loosely coupled hexagonal grid and identify the regular hexagons belonging to the mash in order to generate collision model for the Boltzmann equation.

The discrete equilibrium solutions (equilibria) of the Boltzmann equation based on a generalize N -layer loosely coupled hexagonal grid is determine in [9][10]. The equilibria f of the discrete Boltzmann equation can be expressed in terms of four parameters characterizing mass, (x, y) -momenta and kinetic energy. A necessary algorithm for the computation of the equlibria is also constructed by them.

In this article, several numerical simulations for a 6-layer loosely coupled hexagonal grid in $\mathbf{R}^2$ are performed. Also we present an error estimation by comparing the discrete equilibria with the corresponding Maxwellian which leads to determine the appropriate grid size N of the N -layer loosely coupled hexagonal grid for given temperature and bulk-velocity. We also observe temperature depends on the kinetic energy and bulk-velocity depends on the (x, y) momenta and kinetic energy.

2 BOLTAZMANN EQUATION

The Boltzmann equation is a prominent representative of kinetic equations, describes the evolution of rarefied gases. With the conservation of momentum and energy, the dynamics of the Boltzmann equation is given by a free flow step and a particle interactions step. The free flow step is modeled by the Liouville-equation and the particle interaction step is modeled by the Boltzmann collision operator. As a simple mathematical consequence of the Boltzmann equation is $\left(\partial_t + v.\nabla_x\right) f\left(t,x,v\right) = \mathrm{J}[\mathrm{f},\mathrm{f}]$, where, $\mathrm{J}\left[\mathrm{f},\mathrm{f}\right] = \int_{R^d} \int_{S^{d-1}} k(\mathrm{v}-\mathrm{w},\eta)[\mathrm{f}(\mathrm{v}')\,\mathrm{f}(\mathrm{w}') - \mathrm{f}(\mathrm{v})\,\mathrm{f}(\mathrm{w})] d^{d-1}\eta \, d^d \mathrm{w}$ is the Boltzmann collision operator and $f = f(t,x,v)$, a density function which depends on time, space and velocity. Here $k(.,.)$ is the collision kernel in the operator satisfying some symmetry properties, the post collision velocities $(\mathrm{v}', \mathrm{w}')$ result from the pre-collision velocities (v, w) satisfying the collision relations, conservation of momentum, $\mathrm{v} + \mathrm{w} = \mathrm{v}' + \mathrm{w}'$ and conservation of kinetic energy, $(|\mathrm{v}|^2 + |\mathrm{w}|^2) = (|\mathrm{v}'|^2 + |\mathrm{w}'|^2)$.

3 N-LAYER LOOSELY COUPLED HEXAGONAL MESH

Any two neighboring hexagons have only one common vertex on a loosely coupled hexagonal discretization in $\mathbf{R}^2$. A generalized layer-wise construction of a loosely coupled N-layer hexagonal mesh for a discrete velocity model Boltzmann equation is presented in this section. A 72-velocity model which is constructed by adding two-layer of hexagons centering to a center one and called two layers loosely coupled hexagonal mesh is shown in Fig.3.1. Similarly, by adding one more layer of regular basic hexagons, one can obtain a 3-layer hexagonal mesh and so on. In general, we may call this a N -layer loosely coupled hexagonal mesh and the collision model based on the mesh can be called a N -layer hexagonal model which is a regular collision model so that it satisfies the basic kinetic features and can be divided into six symmetric partitions (Fig.3.1).

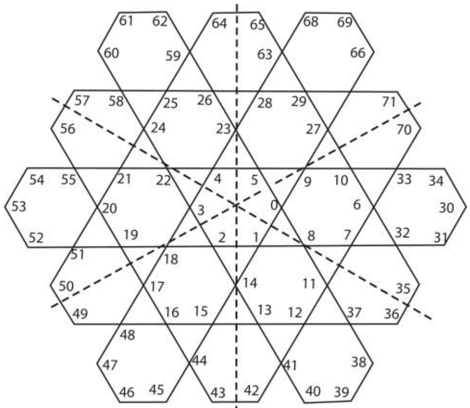


Figure 3.1: 72-velocity Model as a Two-Layer Model.

4 EQUILIBRIA FOR A N-LAYER MODEL

Strictly positive density vectors $\mathrm{f} = \left(f_i\right)_{i=0}^{(3N+2)^2 + (3N+1)}$ is said to be the equilibrium solutions (equilibria) if $\mathrm{J}[\mathrm{f},\mathrm{f}] \equiv 0$ for a N -layer hexagonal model. The i^{th} equilibrium of the n^{th} layer is $f(n,i) = z\mu^{m(n,i)} \kappa_{0+}^{\bar{\kappa}_0(n,i)} \kappa_{1+}^{\bar{\kappa}_1(n,i)} \kappa_{2+}^{\bar{\kappa}_2(n,i)}$; where $z, \kappa_{0+}, \kappa_{1+}, \kappa_{2+} > 0$ are satisfying arbitrary quantities $\kappa_{0+}\kappa_{1-}\kappa_{2+} = 1$. The equilibria at the six nodes of 0-st layer (i.e. at the nodes of the central basic hexagon) are givenby $(f_0, f_1, f_2, f_3, f_4, f_5) = z.(\kappa_{0+}, \kappa_{1+}, \kappa_{2+}, \kappa_{0-}, \kappa_{1-}, \kappa_{2-})^{\mathrm{T}}$.

For a 3-layer model, presents the equilibria for the nodes of the partition as

$$z(\mu\kappa_{0+}\kappa_{1+},\ \mu^3\kappa_{0+}\kappa_{1+}^2,\ \mu^4\kappa_{1+}^3,\ \mu^3\kappa_{1+}^2\kappa_{2+}) \in \text{1st layer}$$

$$z(\mu^9\kappa_{0+}^2\kappa_{1+}^3,\ \mu^6\kappa_{0+}\kappa_{1+}^3,\ \mu^{10}\kappa_{0+}\kappa_{1+}^4,\ \mu^{12}\kappa_{1+}^5,\ \mu^{10}\kappa_{1+}^4\kappa_{2+},\ \mu^6\kappa_{1+}^3\kappa_{2+},\ \mu^9\kappa_{1+}^3\kappa_{2+}^2) \in \text{2nd layer}$$

$$z(\mu^{13}\kappa_{0+}^3\kappa_{1+}^3,\ \mu^{18}\kappa_{0+}^3\kappa_{1+}^4,\ \mu^{19}\kappa_{0+}^2\kappa_{1+}^5,\ \mu^{15}\kappa_{0+}\kappa_{1+}^5,\ \mu^{21}\kappa_{0+}\kappa_{1+}^6,\ \mu^{24}\kappa_{1+}^7,\ \mu^{21}\kappa_{1+}^6\kappa_{2+},\ \mu^{15}\kappa_{1+}^5\kappa_{2+},\ \mu^{19}\kappa_{1+}^5\kappa_{2+}^2,\ \mu^{18}\kappa_{1+}^4\kappa_{2+}^3) \in \text{3rd layer}$$

Where z parameterizes mass, $(\kappa_{0+}, \kappa_{2+})$ characterize non-vanishing bulk-velocity, μ responsible kinetic energy.

Fig. 4.1 shows each n^{th} layer of a partition has $(3n+1)$ nodes and the node numbering is from the top to bottom of at each layer.

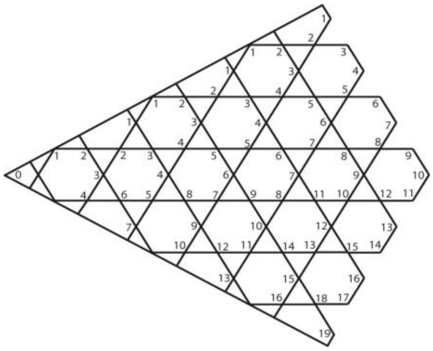


Figure 4.1: A partition of a Six-Layer Model.

We generalize nodes values of a partition for equilibra of *N*-layer model as a proposition in [9], [10]. Also establish a theorem in [9][10] for equilibria of *N*-layer loosely coupled hexagonal model and prove the theorem in [9].

5 Computation of Equilibrium

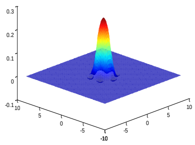
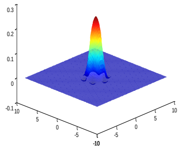
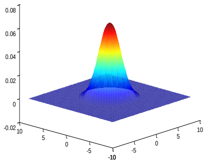
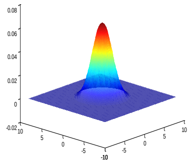
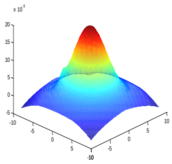
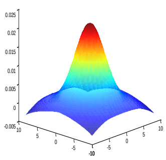
Here the discrete equilibria are computed, which are described by the parameters $z, \mu, \kappa_{0+}, \kappa_{2+}$ characterizing respectively mass, temperature, and bulk-velocity. It is evident that $\bar{v}_x = 0,\ <0,\ >0$ according as $\kappa_{0+}\kappa_{2+} = \kappa_{1+} = 1,\ <1,\ >1$; $\bar{v}_y = 0,\ <0,\ >0$ according as $\kappa_{0+} - \kappa_{2+} = 0,\ <0,\ >0$ and $\kappa_{0+} - \kappa_{2+} = \kappa_{0+} - \dfrac{\kappa_{1+}}{\kappa_{0+}}$.

Now the discrete equlibria $\tilde{\mathrm{f}}^h \in \varepsilon$ given by the theorem in [9], [10] for the case of zero bulk-velocity on a 4-layer grid (of 210 grid points) with discretization parameter $h = 1$ for three different values of $\mu = 0.25,\ 0.55,\ 0.95$ is computed and the corresponding Maxwellian given by $\tilde{f} = \dfrac{\rho}{(2\pi T)^{d/2}} \exp\left(\dfrac{-(\mathrm{v}-\bar{\mathrm{v}})^2}{2T}\right),\ d = 2$, where $\rho = \sum_i \tilde{f}_i^h$ is the mass density, $\bar{\mathrm{v}} = \left(\frac{1}{\rho}\right)\sum_i \mathrm{v}_i \tilde{f}_i^h$ is defined as the bulk velocity, $T = \left(\frac{1}{2\rho}\right)\sum_i (\mathrm{v}_i - \bar{\mathrm{v}})^2 \tilde{f}_i^h$ is the temperature. The normalized discrete equilibrium state f^h is compared with the normalized Maxwellian f and calculated the error $err = \left\|\mathrm{f} - \mathrm{f}^h\right\|_1$ and the moments, temperature as shown in the table 1.1.

Here three interesting cases of three different temperatures with zero bulk-velocities are presented.

1. In the first case, for $\mu = 0.25$ the calculated temperature is $T = 0.8293$. The main part of the configuration is centered at the origin with a small radius and a small part of the mass occurred on the grid. That is the resolution of the grid is too low to present such low temperature and this causes a noticeable 5% error.
2. This is a good situation because the main part of the mass of the function f lies inside of the domain. In this case it occurs very little error for $\mu = 0.55$ in which the calculated temperature $T = 1.6759$.
3. Here the grid is not large enough to present such high temperature $T = 11.0488$ for a given $\mu = 0.95$ and a significant fraction of the mass of the function f is cut down the boundary which causes 20% error. Thus to avoid this error it requires to further extension of the 4-layer grid model.

Table 1.1
In varying temperatures Discrete equilibria and Maxwellian are on a 4-layer grid

f^h = **Discrete equilibria**	f **= Maxwellian**	**Err =** $\left\| f - f^h \right\|_{L_1}$
		$\rho = 1.000$ $\bar{v}_x = 0$ $\bar{v}_y = 0$ $\mu = 0.25$ $T = 0.8293$ $err = 0.0501$
		$\rho = 1.000$ $\bar{v}_x = 0$ $\bar{v}_y = 0$ $\mu = 0.55$ $T = 1.6759$ $err = 0.0013$
		$\rho = 1.000$ $\bar{v}_x = 0$ $\bar{v}_y = 0$ $\mu = 0.95$ $T = 11.0488$ $err = 0.1920$

It is thus seen that a larger model is needed to restrict the error to a reasonable range for high temperature otherwise a noticeable error due to boundary effect.

6 Appropriate Grid Size

In order to determine the appropriate size grid for given values of μ, κ_{0+}, κ_{2+}, we compute the error $err = \left\| f - f^h \right\|_1$ for different sizes N of the N-layer model and chose the smallest N as an appropriate size for which the error restricted to a given tolerance. Fig.6.1 shows the error with respect to the size N for zero bulk velocity with four increasing values of temperature for $\mu = 0.3,\ 0.5,\ 0.7,\ 0.75$. In the first case for $\mu = 0.3$, it shows that the error goes below 1.2% for $N = 2$ and thus for given tolerance 0.012. $N = 2$ is the appropriate size for $\mu = 0.3$. Similarly, the rest three cases show that $N = 3, 4, 5$ are the appropriate size for given values of $\mu = 0.5,\ 0.7,\ 0.75$ respectively. For given temperature and bulk-velocity we can determine the appropriate size (az) of the model by the few steps as shown in algorithm 6.1.

```
Initialize N = 1
Calculate err = ||f - f^h||_L1
If err < tol
   az = N
   BREAK
   ELSE
   N = N + 1
   END
CONTINUE
```

Algorithm 6.1

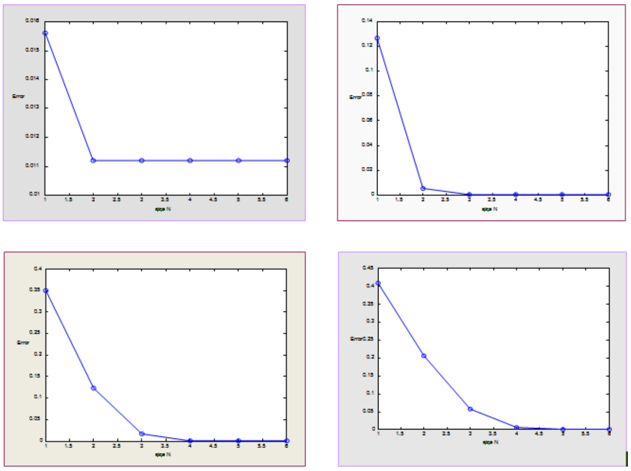


Figure 6.1: Error w.r.to size N for increasing temperature T in zero bulk-velocity v.

Now Figure 6.2, shows temperature depends on the parameter μ, characterizing kinetic energy.

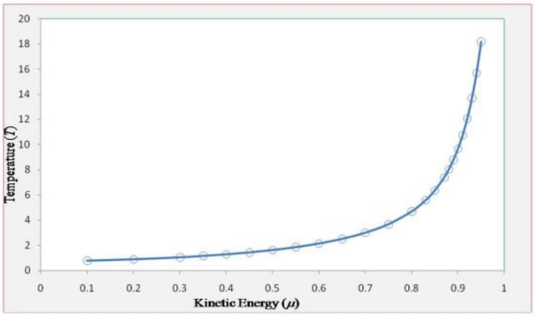


Figure 6.2: temperature depends on the parameter μ

It is clearly seen in the Figure 6.2 that temperature depends upon the values of the kinetic energy μ which is expected.

Figure 6.3, shows the calculated bulk-velocity for given $\mu \in [0.1,\ 0.9]$ at the three different choices of $(\kappa_{0+}, \kappa_{2+})$.

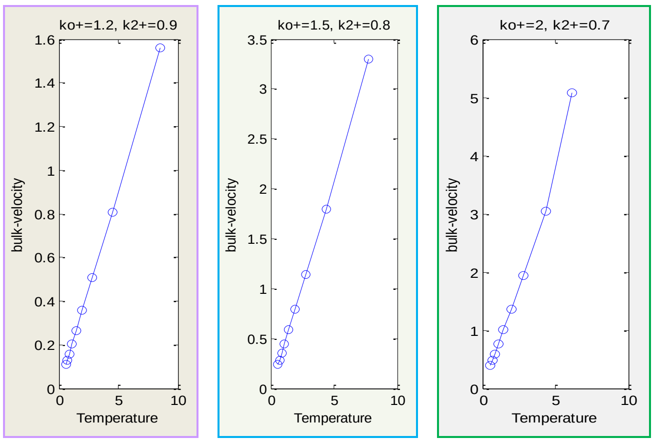


Figure 6.3: Bulk-velocity depends on $T(\mu)$ and κ's.

As expected, it is clearly seen in the Figure 6.3 that the modulus of the bulk-velocity $|v|$ depends upon the choice of temperature as well as the values of the parameters κ_{0+}, κ_{2+}.

Figure 6.4 shows appropriate size $N(T,|\mathrm{v}|)$ for two different choices of the pairs $(\kappa_{0+},\kappa_{2+})$ and some varying values of μ . For both the cases of $(\kappa_{0+},\kappa_{2+}) = (2,1),\ (3,1)$ (in the figure the upper and lower respectively), we observe that the temperature profiles are the same but the velocity profiles are changing as expected.

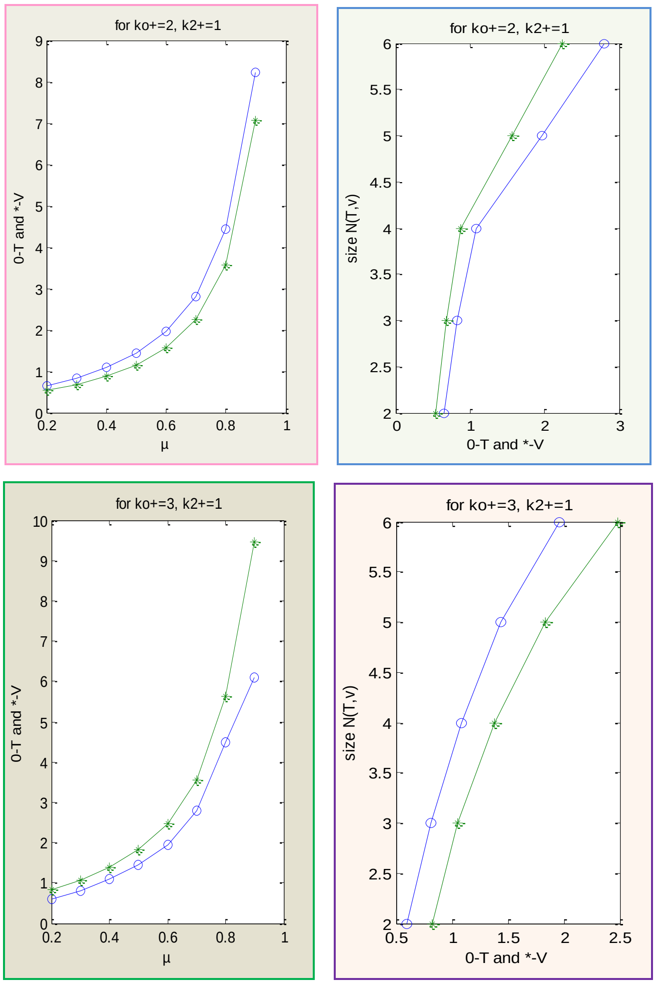


Figure 6.4: Size $N(T,|\mathrm{v}|)$ depends on temperature T and bulk-velocity v .

7 Conclusion

Using four parameters, characterizing mass, (x,y)-momenta and kinetic energy, the equilibria f of the Boltzmann equation can be expressed. The computation of discrete equilibria of the Boltzmann equation is effected by varying temperature and bulk-velocity. The temperature depends on the parameter μ , characterizing kinetic energy. The bulk-velocity depends on the parameters κ's , characterizing (x,y) momenta and μ as well. Error estimation of the discrete equilibria of the discrete model leads to determine the appropriate grid size for a given mass, bulk-velocity and temperature. Restricting the error in a given tolerance one can investigates efficient numerical scheme to solve the space inhomogeneous Boltzmann equation which we may investigate in our future work.

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