Nonlinear Boltzmann Equation for the Homogeneous Isotropic case (HIBE)

Some improvements to deterministic methods and perspectives

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7th International Conference for
Mesoscopic Methods in Engineering and Science
University of Alberta, Edmonton, Alberta, Canada, July 12–16th, 2010

Outline of this talk

1. Motivation of this work
2. Preliminary considerations
   - Adopted notation for the Boltzmann Equation (BE)
   - Isotropic filtering and vanishing Mach model
3. Homogeneous Isotropic case (HIBE)
4. Discretization of the velocity formulation
5. Discretization of the energy formulation
   - Aristov's deterministic method
   - Proposed DVM-like correction (Discrete-Velocity-Model)
6. Numerical example

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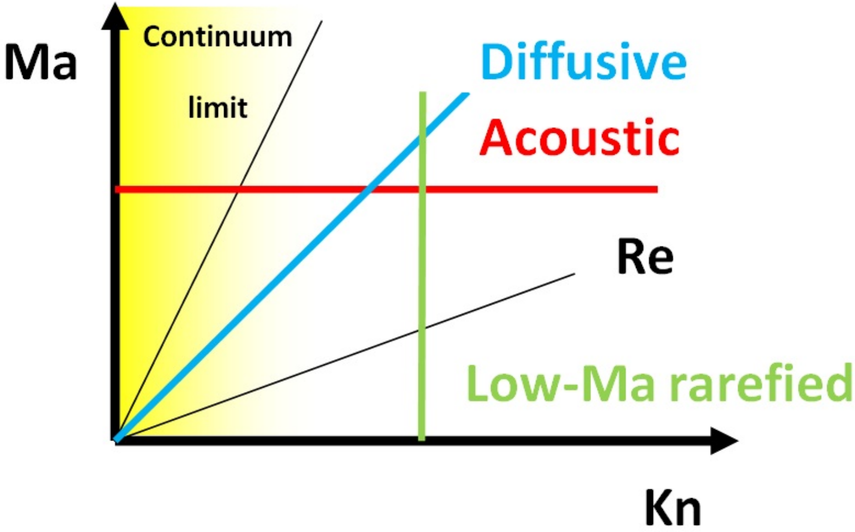
Micro-electro-mechanical systems (MEMs)

- The von Kármán's relation, namely $\mathrm{Ma} \sim \mathrm{Re}\,\mathrm{Kn}$, is the key tool for discriminating different regimes.
- If one wants to catch some rarefied effect, then a finite value of the Knudsen number Kn must be considered and a full kinetic description must be considered in general.
- Nowadays, a lot of attention is attracted by micro – electro – mechanical systems (MEMs). These devices are increasingly applied to a great variety of industrial and medical problems. In these problems, given the small dimensions of the devices, it may be necessary to use the kinetic theory, instead of the usual fluid–dynamics.
- However the motion of dilute gases in the small gaps of these devices is usually extremely small.[1]

[1] C. Cercignani, *Slow rarefied flows: theory and application to micro – electro – mechanical systems*, Birkhauser, 2006.

Beyond usual fluid–dynamic description ?



The regime under investigation

- Hence the fluid–dynamic regime we want to investigate is given by vanishing Mach number (Ma) and finite Knudsen number (Kn).
- Let us consider

$$\mathsf{Ma} \sim \epsilon \ll 1, \qquad \mathsf{Kn} \sim 1, \qquad (\mathsf{Re} \sim \epsilon).$$

- This means that one could try to derive consistently model equations from the full Boltzmann equation in the limit of vanishing Mach numbers.
- It comes out (anticipation, see next) that, in this regime, the distribution function is weakly anisotropic and this allows one to simplify (eventually) the description of the small anisotropic dynamics (while retaining the leading isotropic dynamics).

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Post-collision Velocities (or Pre-collision Velocities ?)

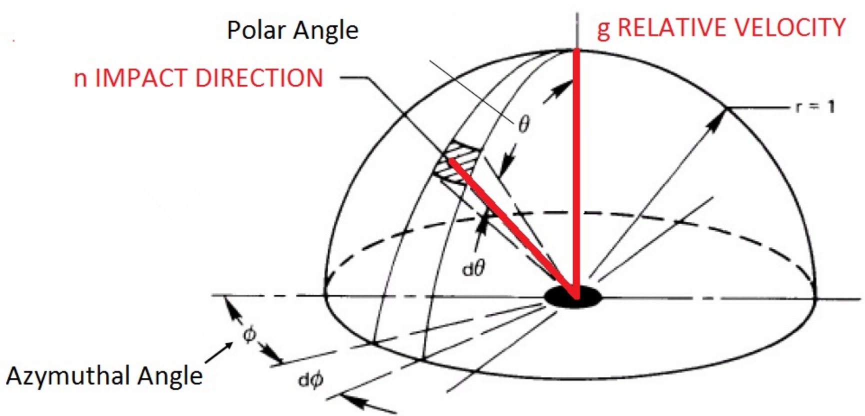
- Let us focus our attention on a test particle $\boldsymbol{\xi} \in \mathbb{R}^3_{\boldsymbol{\xi}}$ and let us consider all possible interactions with any other field particle $\boldsymbol{\xi}_* \in \mathbb{R}^3_{\boldsymbol{\xi}}$ (integration dummy variable).
- $\boldsymbol{g} = \boldsymbol{\xi}_* - \boldsymbol{\xi}$ is the relative velocity (of the field particle with regards to the test particle).
- $\boldsymbol{\xi}'$, $\boldsymbol{\xi}'_* \in \mathbb{R}^3_{\boldsymbol{\xi}}$ are the post–collision (conventional since the collision is reversible) test and field particle velocities respectively

$$\boldsymbol{\xi}' = \boldsymbol{\xi} + (\boldsymbol{g} \cdot \boldsymbol{n})\, \boldsymbol{n}, \tag{1}$$

$$\boldsymbol{\xi}'_* = \boldsymbol{\xi}_* - (\boldsymbol{g} \cdot \boldsymbol{n})\, \boldsymbol{n}, \tag{2}$$

  where $\boldsymbol{n} \in \mathbb{R}^3$ is the unit vector along the direction connecting the centers of the two particles during the instantaneous collision and versus pointing from particle $\boldsymbol{\xi}$ to $\boldsymbol{\xi}_*$.
- There are many possible outcomes $(\boldsymbol{\xi}', \boldsymbol{\xi}'_*)$ from a given pair of incoming particle velocities $(\boldsymbol{\xi}, \boldsymbol{\xi}_*)$, depending on two additional degrees of freedom ($\boldsymbol{n}$ is a versor).

Geometrical Schematic



Boltzmann Equation (1 of 2)

- According to the kinetic theory of gases, the probability density function of a dilute gas

$$f(t, \boldsymbol{x}, \boldsymbol{\xi})$$

with elastic binary interactions satisfies the Boltzmann transport equation

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \nabla_{\boldsymbol{x}} f = Q(f, f), \tag{3}$$

where the collisional integral is given by

$$Q(f, f) \doteq \int_{\mathbb{R}^3_{\boldsymbol{\xi}}} \int_{\boldsymbol{g} \cdot \boldsymbol{n} < 0} B(\boldsymbol{g}, \boldsymbol{n}) \left[f(\boldsymbol{\xi}') f(\boldsymbol{\xi}'_*) - f(\boldsymbol{\xi}) f(\boldsymbol{\xi}_*) \right] d\boldsymbol{n} \, d\boldsymbol{\xi}_*,$$

where $d\boldsymbol{n}$ is the infinitesimal solid angle (two–fold integration) and $d\boldsymbol{\xi}_*$ is the infinitesimal volume around the field particle in the velocity space (three–fold integration).

Boltzmann Equation (2 of 2)

- $B(\boldsymbol{g}, \boldsymbol{n})$ is a volumetric particle flux or collision kernel. Let us assume the following expression

$$B(|\boldsymbol{g} \cdot \boldsymbol{n}|) = a^2 \, c_s \, \left(\frac{|\, \boldsymbol{g} \cdot \boldsymbol{n} \,|}{c_s} \right)^{\beta}, \qquad (4)$$

  where a is the particle radius, c_s is a characteristic mean particle velocity (i.e. statistical mean of the particle velocity deviations) and β is a tunable parameter (natural number).
- In particular, some meaningful cases follow:
  - if $\beta = 0$, then the constant kernel model (CKM) is recovered (degenerate case of Maxwell molecules corresponding to the Kac's Ring Model);
  - if $\beta = 1$, then the hard sphere model (HSM) is recovered (finite–size elastically rigid particles).

Equilibrium distribution function

- It is possible to verify that the collisional operator is null, namely $Q(f_E, f_E) = 0$, for a special distribution function describing the local equilibrium, namely

$$f_E = \frac{n}{(2\pi E_B)^{3/2}} \exp\left(-\frac{(\boldsymbol{\xi} - \boldsymbol{u})^2}{2\, E_B}\right), \tag{5}$$

  where n is the number density, $\boldsymbol{u}$ is the macroscopic velocity, $E_B = 2e/3$ and e is the internal energy, which are macroscopic quantities (moments), depending on f (hence $f_E = f_E(f)$).

- Even though the equilibrium function represents a local attractor for the distribution function, one can not assume the smallness of the distance (according to some proper metrics in phase space $||\cdot||$) of f with regards to f_E.

Isotropic filtering

- Let us apply an isotropic filter to f, namely

$$f_I(\xi) = \frac{1}{4\pi} \int_0^{2\pi} \int_0^{\pi} f \, d\boldsymbol{n} = \frac{1}{4\pi} \int_0^{2\pi} \int_0^{\pi} f \sin(\alpha_x) \, d\alpha_x \, d\beta_x, \qquad (6)$$

where $\xi = |\boldsymbol{\xi}|$, $\boldsymbol{\xi}$ (test) is assumed as polar axis for $d\boldsymbol{n}$, α_x is the angle between $\boldsymbol{\xi}$ (test) and $\boldsymbol{n}$, and finally β_x is the corresponding azimuthal angle.

- In the considered regime

$$||f - f_I|| \sim \text{Ma} \sim \epsilon \ll 1,$$

and consequently

$$f = f_I \,(1 + \varphi_A) = f_I \,(1 + \epsilon \, \hat{\varphi}_A),$$

where $\varphi_A = \epsilon \, \hat{\varphi}_A$ is the anisotropic correction (the definition follows from direct comparison between the previous equations).

Isotropic filtering of the equilibrium distribution function

- Let us apply the previous filter to the equilibrium distribution function

$$f_E = \frac{n}{(2\pi E_B)^{3/2}} \exp\left(-\frac{(\boldsymbol{\xi}-\boldsymbol{u})^2}{2\,E_B}\right) = f_{IE}\ (1+\varphi_{AE}) + O(\epsilon^2), \quad (7)$$

where

$$f_{IE} = \frac{n}{(2\pi E_B)^{3/2}} \exp\left(-\frac{\xi^2}{2\,E_B}\right), \qquad \varphi_{AE} = \frac{\boldsymbol{\xi}\cdot\boldsymbol{u}}{2\,E_B}. \quad (8)$$

- Neglecting the quadratic terms yields[2]

$$f_{AE} = f_{IE}\ (1+\varphi_{AE}) = f_{IE}\ (1+\epsilon\,\hat{\varphi}_{AE})\,. \quad (9)$$

[2]This derivation is for illustration purposes only, but it allows one to consider the revisited Stokes problem: see V. Yakhot, C. Colosqui, J. Fluid Mech., vol. 586 (2007).

Simplified model for vanishing Mach (1 of 2)

- Introducing the previous expansion in Eq. (3) and neglecting the second order terms (with regards to Mach) yields

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \nabla_{\boldsymbol{x}} f = Q(f_I, f_I) + 2\, Q(f_I, f_A), \tag{10}$$

where

$$Q(f_I, f_A) = \int_{\mathbb{R}^3_{\boldsymbol{\xi}}} \int_{\boldsymbol{g}\cdot\boldsymbol{n}<0} B(\boldsymbol{g}, \boldsymbol{n}) \left[f_I' f_{I*}' (\varphi_A' + \varphi_{A*}') - f_I f_{I*} (\varphi_A + \varphi_{A*}) \right] d\boldsymbol{n}\, d\boldsymbol{\xi}_*.$$

- In the following, let us assume small deviations from local equilibrium (note: for the anisotropic part only).

Simplified model for vanishing Mach (2 of 2)

- Consequently the pre–factors become

$$f_I' f_{I*}' = f_{IE}' f_{IE*}' = f_{IE} f_{IE*} = f_I f_{I*},$$

and the deviations φ_A', φ_{A*}' and φ_{A*} are assumed in local equilibrium, namely

$$\varphi_A' + \varphi_{A*}' = \varphi_{AE}' + \varphi_{AE*}' = \varphi_{AE} + \varphi_{AE*}.$$

- Introducing the previous assumptions in Eq. (10) yields

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \nabla_{\boldsymbol{x}} f = \overbrace{Q(f_I, f_I)}^{\text{Isotropic BE}} + \overbrace{\nu_A\, f_{IE}\, (\varphi_{AE} - \varphi_A)}^{\text{Anisotropic BGK}}, \qquad (11)$$

where

$$\nu_A = 2 \int_{\mathbb{R}^3_{\boldsymbol{\xi}}} \int_{\boldsymbol{g}\cdot\boldsymbol{n}<0} B(\boldsymbol{g}, \boldsymbol{n}) f_{IE}(\xi_*) d\boldsymbol{n}\, d\boldsymbol{\xi}_*.$$

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Homogeneous case (in physical space)

- Let us consider first the homogeneous case (in space). Consequently the probability density function becomes $f(t, \boldsymbol{\xi})$ and the homogeneous Boltzmann equation becomes

$$\frac{\partial f}{\partial t} = Q(f, f), \tag{12}$$

where the collisional integral is rewritten equivalently as

$$Q(f, f) = \int_{-\infty}^{+\infty} \int_{0}^{4\pi} S(q)\, B(q) \left[f(\boldsymbol{\xi}') f(\boldsymbol{\xi}'_*) - f(\boldsymbol{\xi}) f(\boldsymbol{\xi}_*) \right] d\boldsymbol{n}\, d\boldsymbol{\xi}_*, \tag{13}$$

where $q = \boldsymbol{g} \cdot \boldsymbol{n}$, $B(q) = B(|q|)$ for simplicity and $S(q)$ is an auxiliary function introduced for simplifying the integration domain (at the price of making more complex the integrand), namely

$$S(q) = \begin{cases} 1, & q < 0, \\ 0, & q \geq 0. \end{cases} \tag{14}$$

Isotropic case (in velocity space) (1 of 3)

- The probability density function is further simplified $f(t, \xi)$, for the time $t \in \mathbb{R}^+$ and for the magnitude of the molecular velocity $\xi = \|\boldsymbol{\xi}\| \in \mathbb{R}_\xi^+$.
- In this way, the distribution function allows one to compute the infinitesimal probability to find some molecules in the time interval between t and $t + dt$ with a velocity magnitude between ξ and $\xi + d\xi$, namely $f(t, \xi) dt d\xi$.
- Let us introduce the unit vector $\boldsymbol{n}_*$ along the direction $\boldsymbol{\xi}_*$ (field) and the unit vector $\boldsymbol{n}_\odot$ along the direction $\boldsymbol{\xi}$ (test), namely

$$\boldsymbol{n}_* = \frac{\boldsymbol{\xi}_*}{\|\boldsymbol{\xi}_*\|}, \qquad \boldsymbol{n}_\odot = \frac{\boldsymbol{\xi}}{\|\boldsymbol{\xi}\|}, \tag{15}$$

consequently

$$Q(f, f) = \int_0^{+\infty} \int_0^{4\pi} \int_0^{4\pi} \left(f' f'_* - f f_* \right) S(q)\, B(q)\, \xi_*^2 \, d\boldsymbol{n} \, d\boldsymbol{n}_* \, d\xi_* . \tag{16}$$

Isotropic case (in velocity space) (2 of 3)

- q is the only parameter dependent on directions $\boldsymbol{n}$ and $\boldsymbol{n}_*$, namely

$$q = \boldsymbol{\xi}_* \cdot \boldsymbol{n} - \boldsymbol{\xi} \cdot \boldsymbol{n} = \xi_* \cos(\alpha_y) - \xi \cos(\alpha_x) = \xi_* \, y - \xi \, x, \qquad (17)$$

  where α_x is the angle between $\boldsymbol{\xi}$ (test) and $\boldsymbol{n}$, α_y is the angle between $\boldsymbol{\xi}_*$ (field) and $\boldsymbol{n}$, $x = \cos(\alpha_x)$ and $y = \cos(\alpha_y)$.
- Let us express the surface elements in Eq. (16) by using
  - $\boldsymbol{\xi}$ (test) as polar axis for $d\boldsymbol{n}$, namely $d\boldsymbol{n} = \sin(\alpha_x)\, d\alpha_x\, d\beta_x$,
  - and $\boldsymbol{n}$ as polar axis for $d\boldsymbol{n}_*$ (field), namely $d\boldsymbol{n}_* = \sin(\alpha_y)\, d\alpha_y\, d\beta_y$,

  where β_x and β_y are the corresponding azimuthal angles.
- Taking the square of Eqs. (1, 2) and recalling that $q = \boldsymbol{g} \cdot \boldsymbol{n}$ yields

$$(\xi')^2 = \xi^2 + q^2 + 2\, q\, \xi\, x = \xi^2 (1 - x^2) + \xi_*^2\, y^2, \qquad (18)$$

$$(\xi_*')^2 = {\xi_*}^2 + q^2 - 2\, q\, \xi_*\, y = \xi_*^2 (1 - y^2) + \xi^2\, x^2. \qquad (19)$$

Isotropic case (in velocity space) (3 of 3)

- In case of homogeneous and isotropic conditions

$$Q(f,f) = N(f,f) - \nu(f)\, f, \tag{20}$$

where

$$\frac{N(f,f)}{2\,\pi^2\, a^2 c_s^{1-\beta}} = \int_0^{+\infty} \xi_*^2 \int_{-1}^{+1} \int_{-1}^{+1} f(\xi') f(\xi_*') \left|\xi_*\, y - \xi\, x\right|^\beta dx\, dy\, d\xi_*, \tag{21}$$

$$\frac{\nu(f)}{2\,\pi^2\, a^2 c_s^{1-\beta}} = \int_0^{+\infty} f(\xi_*)\, \xi_*^2 \int_{-1}^{+1} \int_{-1}^{+1} \left|\xi_*\, y - \xi\, x\right|^\beta dx\, dy\, d\xi_*. \tag{22}$$

- The previous expressions are three–fold integrals. Dimensionality has been reduced but not dramatically ($5 \to 3$).
- The basic idea is to discretize the velocity magnitude and to analytically integrate over the collision parameters (x, y).

Bhatnagar–Gross–Krook limit (1 of 2)

- Let us consider Eq. (22) for HSM (i.e. $\beta = 1$), in the limit $f(\xi) \approx f_e(\xi)$, which yields $\nu \approx \nu_e$, where

$$\nu_e = \nu(f_e) = 2\,\pi^2\,a^2 \int_0^{+\infty} f_e(\xi_*)\,\xi_*^2 \int_{-1}^{+1} \int_{-1}^{+1} S(q)\,|q|\,dx\,dy\,d\xi_* . \tag{23}$$

- Recalling Eq. (5) with $\boldsymbol{u} = 0$ (since isotropicity is assumed) yields

$$\nu_e(\xi) = \frac{n\pi\,a^2\sqrt{k_B T}}{\sqrt{2}}\,\zeta\,\left(\frac{1}{\zeta\sqrt{\pi}}\,\mathrm{exp}(-\zeta^2) + \frac{1}{2\,\zeta^2}\,\mathrm{erf}\,(\zeta) + \mathrm{erf}\,(\zeta)\right), \tag{24}$$

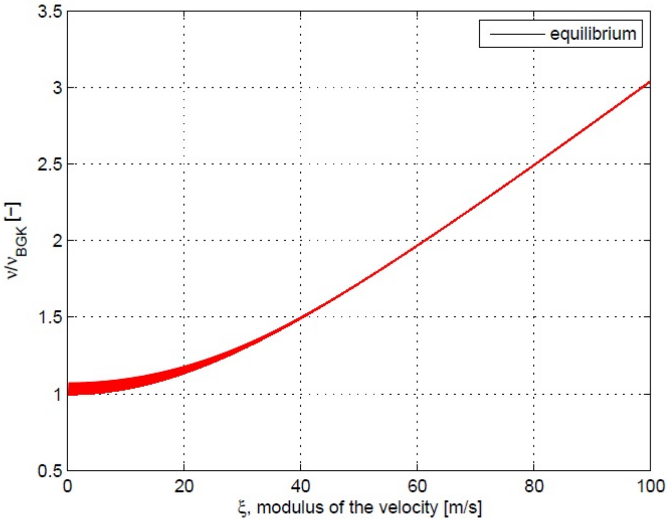
where $\zeta = \xi/\sqrt{2\,k_B T}$.

- In the following, let us consider two limits of the previous function

$$\nu_{BGK} = \lim_{\xi \ll \sqrt{k_B T}} \nu_e(\xi) \approx \sqrt{2\pi}\,a^2\,n\,\sqrt{k_B T}, \tag{25}$$

$$\nu_\infty = \lim_{\xi \gg \sqrt{k_B T}} \nu_e(\xi) \approx \frac{n\,\pi\,a^2}{2}\,\xi. \tag{26}$$

Bhatnagar–Gross–Krook limit (2 of 2)



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Constraints on the velocity discretization

- Let us recall the definitions of the post–collision velocities

$$
\begin{aligned}
(\xi')^2 &= \xi^2 + q^2 + 2\,q\,\xi\,x = \xi^2\,(1 - x^2) + \xi_*^2\,y^2, \qquad (27)\\
({\xi_*}')^2 &= {\xi_*}^2 + q^2 - 2\,q\,\xi_*\,y = \xi_*^2\,(1 - y^2) + \xi^2\,x^2. \qquad (28)
\end{aligned}
$$

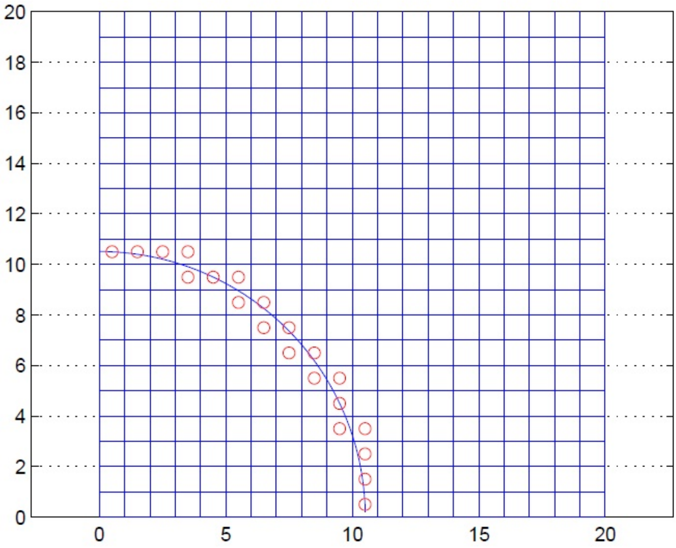
- Summing the previous definitions yields

$$
(\xi')^2 + ({\xi_*}')^2 = \xi^2 + \xi_*^2,
$$

  which must be ensured exactly (even in the numerical implementation), in order to satisfy the energy conservation.

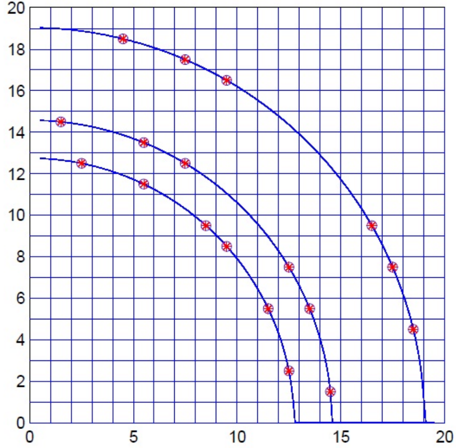
- From one hand, one needs to use regular grid in the discretization of the microscopic velocities, but, on the other hand, regular grids poorly match with quadratic constraints.

Regular grids poorly match quadratic constraints



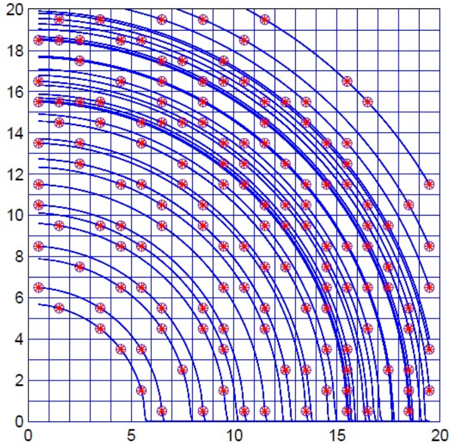
Circles with maximum number of regular points

Velocity grid made of $M \times M = 20 \times 20$ points. The maximum number of regular points matching a circle is $R(M) = 6$ and only $C(M, R(M)) = 3$ circles exist satisfying this condition.



Circles with smaller number of regular points

The maximum number of regular points matching a circle is $R(M) = 6$ but, considering also circles with a smaller number ($4 < 6$) of regular points, it is possible to find up to $C(M, 4 < R(M) = 6) = 35$ circles.



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Energy formulation

- Let us introduce a change of variables in the previous expressions. Let us introduce $E = \xi^2/2$, $E_* = \xi_*^2/2$, $E' = (\xi')^2/2$ and $E'_* = (\xi'_*)^2/2$, namely

$$\frac{N(f,f)}{F c_s^{-\beta}} = \int_0^{+\infty} E_*^{1/2} \int_{-1}^{+1} \int_{-1}^{+1} f(E') f(E'_*) \, |q|^\beta \, dx \, dy \, dE_*, \quad (29)$$

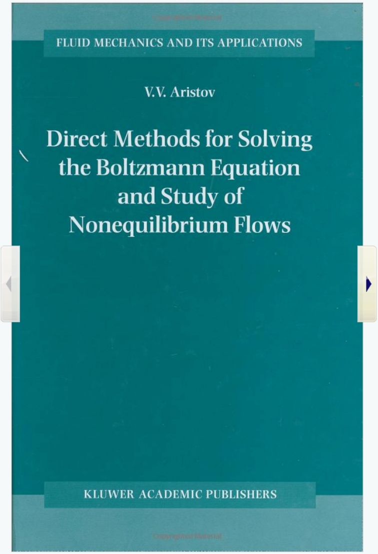
$$\frac{\nu(f)}{F c_s^{-\beta}} = \int_0^{+\infty} f(E_*) \, E_*^{1/2} \int_{-1}^{+1} \int_{-1}^{+1} |q|^\beta \, dx \, dy \, dE_*, \quad (30)$$

where $q = y\, E_*^{1/2} - x\, E^{1/2}$ and $F = 2^{(\beta+3)/2} \pi^2 a^2 c_s$ has the dimensions of a volumetric flow rate. Consequently the collision relations become (linear w.r.t. E and E_*)

$$E' = E\,(1 - x^2) + E_*\, y^2, \quad (31)$$

$$E'_* = E\, x^2 + E_*\,(1 - y^2). \quad (32)$$

Reference for the Aristov's method



Numerical integration of the LOSS term

- Let us assume a maximum value for the test particle kinetic energy E, namely E_M. Let us divide the interval $[0,\, E_M]$ in M equal parts, with length $\Delta E = E_M/M$. Each cell is identified by index $1 \leq i \leq M$, such that $E_i = (i-1/2)\,\Delta E$, and the probability distribution function is discretized accordingly, namely $f_i = f(E_i)$.
- For example, concerning the LOSS term

$$\nu_i = \nu(f_i) \approx \tilde{\nu}_i = \tilde{F}\,\Delta E \sum_{j=1}^{M} f_j\, E_j^{1/2}\, A_{ij}, \tag{33}$$

where

$$\begin{aligned} A_{ij} &= \Delta E^{-\beta/2} \int_{-1}^{+1} \int_{-1}^{+1} \left| y\, E_j^{1/2} - x\, E_i^{1/2} \right|^{\beta} dx\, dy = \\ &= 2\,\Delta E^{-\beta/2} \frac{\left| E_i^{1/2} + E_j^{1/2} \right|^{2+\beta} - \left| E_i^{1/2} - E_j^{1/2} \right|^{2+\beta}}{E_i^{1/2} E_j^{1/2} (2+3\beta+\beta^2)}. \end{aligned} \tag{34}$$

Numerical integration of the GAIN term

- Concerning the GAIN term

$$N_i = N(f_i, f_i) \approx \tilde{N}_i = \tilde{F}\,\Delta E \sum_{j=1}^{M} E_j^{1/2} \sum_{k=1}^{M}\sum_{l=1}^{M} f_k f_l\, B_{ij}^{kl}, \tag{35}$$

where

$$B_{ij}^{kl} = C(E_{k+}) - C(E_{k-}), \tag{36}$$

$$C(E_{k\pm}) = \Delta E^{-\theta/2} \int_{\Omega_\pm(E_{k\pm})} \left| y\, E_j^{1/2} - x\, E_i^{1/2} \right|^{\theta} dx\, dy. \tag{37}$$

- In particular, the shape of the domains $\Omega_\pm$ on the plane (x, y) depend on the relative magnitude of the energies E_i, E_j, E_{k-} and E_{k+}. Six cases are possible, but the domain is always made of two strips between two hyperbolas and/or boundaries of the square domain $(x, y) \in [-1, 1] \times [-1, 1]$.

Proposed DVM-like correction (1 of 2)

- The previous outlined method may produce some inaccuracies close to the equilibrium, because density and energy are not perfectly conserved.
- The computation of the dynamics can be improved by a sort-of Discrete-Velocity-Model (DVM) correction, which allows one to satisfy exactly the macroscopic conservation laws [Asinari, 2010].
- The first problem is that there is a net loss of particles, because

$$\sum_{k=1}^{M}\sum_{l=1}^{M} B_{ij}^{kl} = A_{ij}, \qquad \text{for} \qquad E_i + E_j \leq E_M, \tag{38}$$

$$\sum_{k=1}^{M}\sum_{l=1}^{M} B_{ij}^{kl} < A_{ij}, \qquad \text{for} \qquad E_i + E_j > E_M. \tag{39}$$

- Hence in the following, let us use instead $\hat{A}_{ij} = \sum_{k=1}^{M} \sum_{l=1}^{M} B_{ij}^{kl}$.

Proposed DVM-like correction (2 of 2)

- Consequently the following master equation holds

$$\frac{\partial f_i}{\partial t} = \frac{F \Delta E^2}{E_i^{1/2}} \sum_{j,k,l=1}^{M} \Gamma_{ij}^{kl} \left(f_k f_l - f_i f_j \right), \qquad \Gamma_{ij}^{kl} = \frac{\sqrt{E_i \, E_j}}{\Delta E} B_{ij}^{kl}. \tag{40}$$

- Let us define by $\{\Gamma_{ij}^{kl}\}$ the set of transition frequencies obtained by permutations of the indexes (i, j, k, l) conserving kinetic energy. The DVM correction is defined as

$$\forall \, (i, j, k, l) : \Gamma_{ij}^{kl} \in \{\Gamma_{ij}^{kl}\}, \qquad \tilde{\Gamma}_{ij}^{kl} = \overline{\{\Gamma_{ij}^{kl}\}}, \tag{41}$$

where the overline means the arithmetic mean (symmetrization).

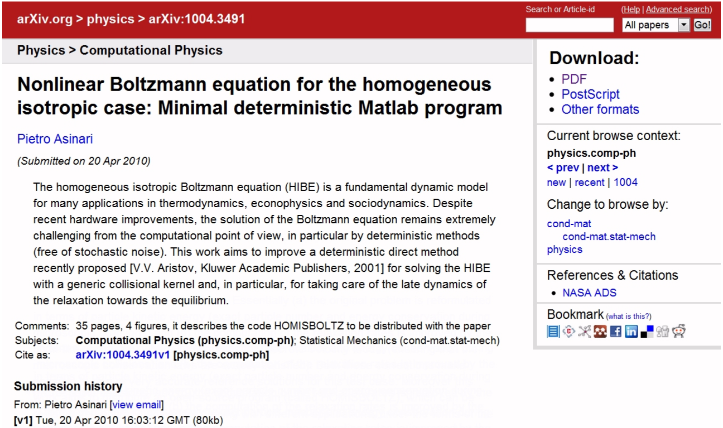
- Consequently for the dimensionless frequencies

$$\tilde{B}_{ij}^{kl} = \frac{\Delta E}{\sqrt{E_i \, E_j}} \tilde{\Gamma}_{ij}^{kl}, \qquad \tilde{A}_{ij} = \sum_{k=1}^{M} \sum_{l=1}^{M} \tilde{B}_{ij}^{kl}, \tag{42}$$

which ensure perfectly the conservation laws.

Reference for the numerical code HOMISBOLTZ

P. Asinari, *Nonlinear Boltzmann equation for the homogeneous isotropic case: Minimal deterministic Matlab program*, accepted in "Computer Physics Communications", arXiv: 1004.3491, 2010. (FEEL FREE TO ASK ME FOR A COPY OF THE CODE !!!)



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Nonlinear Boltzmann equation for the homogeneous isotropic case: Minimal deterministic Matlab program

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(Submitted on 20 Apr 2010)

The homogeneous isotropic Boltzmann equation (HIBE) is a fundamental dynamic model for many applications in thermodynamics, econophysics and sociodynamics. Despite recent hardware improvements, the solution of the Boltzmann equation remains extremely challenging from the computational point of view, in particular by deterministic methods (free of stochastic noise). This work aims to improve a deterministic direct method recently proposed [V.V. Aristov, Kluwer Academic Publishers, 2001] for solving the HIBE with a generic collisional kernel and, in particular, for taking care of the late dynamics of the relaxation towards the equilibrium.

Comments: 35 pages, 4 figures, it describes the code HOMISBOLTZ to be distributed with the paper

Subjects: **Computational Physics (physics.comp-ph)**; Statistical Mechanics (cond-mat.stat-mech)

Cite as: **arXiv:1004.3491v1 [physics.comp-ph]**

Submission history

From: Pietro Asinari [view email]

[v1] Tue, 20 Apr 2010 16:03:12 GMT (80kb)

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Outline Compass

1. Motivation of this work
2. Preliminary considerations
   - Adopted notation for the Boltzmann Equation (BE)
   - Isotropic filtering and vanishing Mach model
3. Homogeneous Isotropic case (HIBE)
4. Discretization of the velocity formulation
5. Discretization of the energy formulation
   - Aristov's deterministic method
   - Proposed DVM-like correction (Discrete-Velocity-Model)
6. Numerical example

Numerical example setup

- The interactions among the molecules can be described by means of the collision kernel given by Eq. (4) with[3]

$$a = 1, \qquad c_s = 50, \qquad \beta = 1 \qquad \text{Hard Sphere Model (HSM)}.$$

- Let us consider the following initial condition $f(t=0,E) = f_I(E)$, where

$$f_I(f_0, G_0, G_{00}) = f_0 \exp\left[-\frac{\left(\sqrt{E}-\sqrt{G_0}\right)^2}{G_{00}}\right]. \tag{43}$$

In the considered test case, the values of these parameters are

$$E_M = 5000, \qquad f_0 = 5\times 10^{-4}, \qquad G_0 = 600, \qquad G_{00} = 35. \tag{44}$$

[3] International System of Units (SI) applies.

Measured macroscopic quantities

- Let us consider the following macroscopic moments

$$\Phi_p(t) = 4\pi\sqrt{2}\int_0^{+\infty} f\, E^{p+1/2}\, dE. \tag{45}$$

- Moreover let us introduce the relaxation rate R_p for the macroscopic moment Φ_p, namely

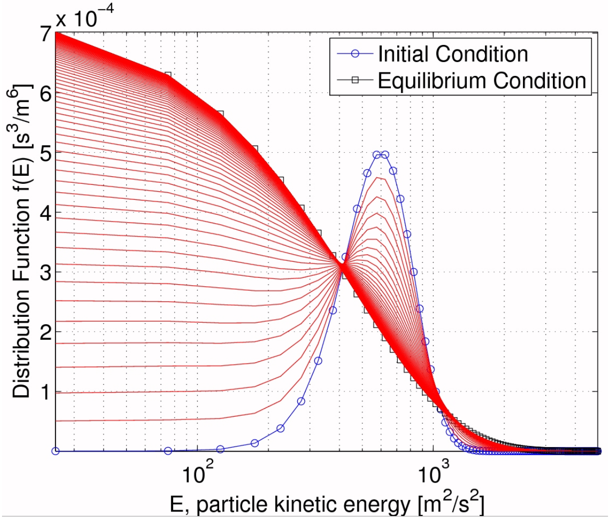
$$R_p(t) = \frac{\Phi_p - \Phi_p^E}{\Phi_p^E}, \tag{46}$$

and the (time-dependent) effective relaxation frequency ν_p for the moment p, namely

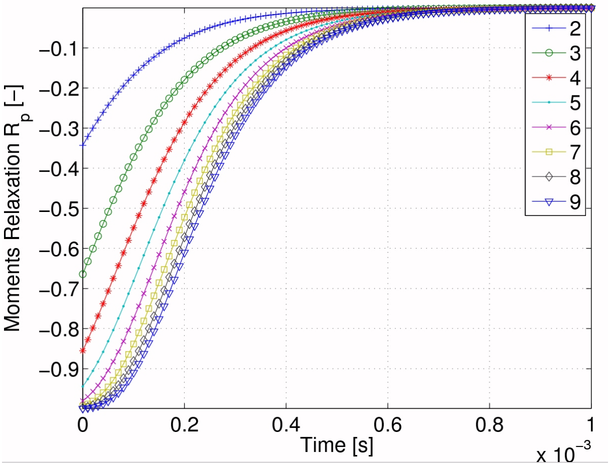
$$\nu_p(t) = \frac{\Phi_p^Q}{\Phi_p^E - \Phi_p}, \tag{47}$$

where $\Phi_p^Q = \Phi_p(Q)$ and Q is the collisional operator.

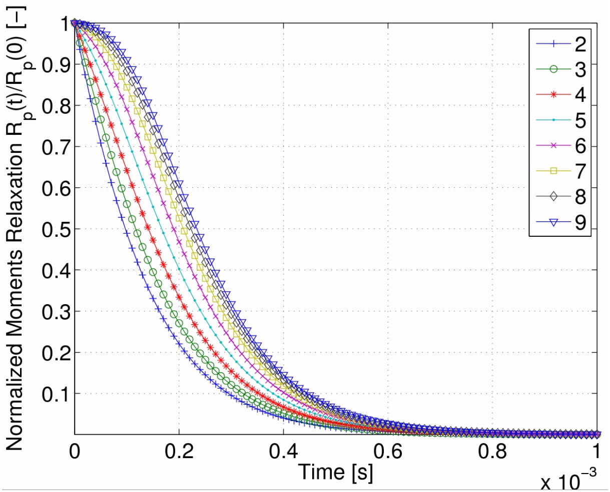
Example dynamics: distribution function



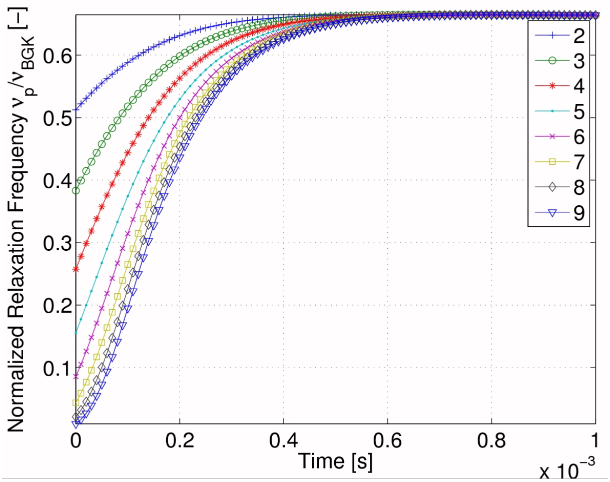
Macroscopic moment relaxation rates



Normalized macroscopic moment relaxation rates



Effective (time-dependent) relaxation frequencies



Conclusions

- In this work, some improvements to the deterministic numerical method proposed by Aristov for the homogeneous isotropic Boltzmann equation (HIBE) are discussed.
- In particular, the DVM-like correction allows one to satisfy exactly the macroscopic conservation laws and it is particularly suitable for dealing with the late dynamics of the relaxation towards the equilibrium.
- An open-source program (called `HOMISBOLTZ`) was developed, which can be easily understood and modified for dealing with different applications (thermodynamics, econophysics and sociodynamics).
- This work represents the first preliminary step towards the development of physical models for micro – electro – mechanical systems (MEMs) in the vanishing Mach number limit (but finite Knudsen number) by isotropic / anisotropic decomposition.

- Thank you for your attention !
- Any question ?