On a discrete Boltzmann equation

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(joint work with A.J.Soares, U. Minho)

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Boltzmann 1870

Description of the dynamics of a rarefied ideal gas. $f(\vec{x},\vec{v},t)$: distribution function of particles in the phase space (position,momentum) at time t.

$$\frac{Df}{Dt} = \frac{\partial f}{\partial t}(\vec{x},\vec{v},t) + \vec{v}.\vec{\nabla}_{\vec{x}} f(\vec{x},\vec{v},t) = < f, f > .$$

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Collision operator:

$$< f, f >= \int \int_{\Omega, \vec{v}_2} (f^* f_2^* - f f_2) |\vec{v} - \vec{v}_2| \sigma(\Omega) d\Omega d\vec{v}_2,$$

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where

$$f=f(\vec{x},\vec{v},t)\ ,\ f_2=f(\vec{x},\vec{v}_2,t),\ f^*=f(\vec{x},\vec{v}^*,t)\ ,\ f_2^*=f(\vec{x},\vec{v}_2^*,t),$$

$\vec{v}^*$, $\vec{v}_2^*$ functions of $\vec{v}$, $\vec{v}_2$, Ω.

Statistical Entropy (Boltzmann, Gibbs 1872).
Milestone: Boltzmann $\mathcal{H}$ function,

$$\mathcal{H}(\vec{x}, t) = \int_V f(\vec{x}, \vec{v}, t) \log(f(\vec{x}, \vec{v}, t)) dv$$

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$\mathcal{H}$-Theorem

$$\frac{\partial}{\partial t}\mathcal{H}(\vec{x}, t) \leq 0.$$

Discrete Boltzmann Models: the Broadwell Model (1964)

We will allow particles to travel at a finite number of preselected velocities only.
6-velocity Broadwell Model:

$v_1 = (c, 0, 0), \ v_2 = (0, c, 0), \ v_3 = (0, 0, c)$
and $v_{j+3} = -v_j$ for $j = 1, 2, 3$.

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$N_i(\vec{x}, t)$: Number density of particles travelling with speed v_i.

Evolution system for $N = (N_1, \ldots, N_6)$

Admissible (inelastic) collisions:
Conservation of kinetic energy and momentum.

Particles with velocity v_i collide with particles with velocity $-v_i = v_{i+3}$ with 3 possible outcomes
(each with probability $p = 1/3$.)

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We will focus on the one-dimensional evolution. The Broadwell system becomes:

$$\begin{cases} \dfrac{\partial N_1}{\partial t} + c\dfrac{\partial N_1}{\partial x} & = & \frac{4cS}{3}(N_2^2 - N_1 N_3) \\ \dfrac{\partial N_2}{\partial t} & = & \frac{2cS}{3}(N_1 N_3 - N_2^2) \\ \dfrac{\partial N_3}{\partial t} - c\dfrac{\partial N_3}{\partial x} & = & \frac{4cS}{3}(N_2^2 - N_1 N_3) \end{cases}$$

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Kawashima (Nonlinear analysis-TMA, 1990):
Existence of strong global solutions for this system.

A model for a chemically active gas

1997: R. Monaco, M. Pandolfi Bianchi and A.J. Soares.

Three species: A, A_2, A^* undergoing an autocatalytic reaction

$$A_2 + M \rightleftharpoons A + A^* + M \ , \quad M = A, A^*, A_2$$

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Kinetic equations: $(v_1, v_2, v_3) = (c, 0, -c)$

$$\begin{cases} \dfrac{\partial}{\partial t} N_i^A(x,t) + v_i \dfrac{\partial}{\partial x} N_i^A(x,t) = F_i^A(N(x,t)) & (i \in \{1;2;3\}), \\[2ex] \dfrac{\partial}{\partial t} N_i^{A_2}(x,t) + \dfrac{v_i}{2} \dfrac{\partial}{\partial x} N_i^{A_2}(x,t) = F_i^{A_2}(N(x,t)) & (i \in \{1;2;3\}), \\[2ex] \dfrac{\partial}{\partial t} N_i^{A^*}(x,t) + v_i \dfrac{\partial}{\partial x} N_i^{A^*}(x,t) = F_i^{A^*}(N(x,t)) & (i \in \{1;3\}), \end{cases}$$

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$$N = \left(N_1^A, N_2^A, N_3^A, N_1^{A^*}, N_3^{A^*}, N_1^{A_2}, N_2^{A_2}, N_3^{A_3} \right) .$$

Structure of the collision terms:

$$F_i^M(N) = \left(P_{i,M}^{(1)}(N) + P_{i,M}^{(2)}(N)\right) - N_i^M \left(Q_{i,M}^{(1)}(N) + Q_{i,M}^{(2)}(N)\right)$$

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- $P_{i,M}^{(1)}(N)$ and $P_{i,M}^{(2)}(N)$: polynomials of degree 2 and 3, representing the creation of particles M with velocity v_i due to inert or reactive collisions.

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- $Q_{i,M}^{(1)}(N)$ and $Q_{i,M}^{(2)}(N)$: polynomials of degree 1 and 2, representing the disappearance of particles M with velocity v_i due to inert or reactive collisions.

We will study the mixed problem in the half-space: $(x, t) \in [0; +\infty[\times[0; +\infty[$.

- Initial conditions

$$N_i^M(x,0) = N_{i_0}^M(x)\ ,\ x \geq 0$$

- Boundary conditions

$$\begin{pmatrix} N_1^A(0,t) \\ N_1^{A^*}(0,t) \\ N_1^{A_2}(0,t) \end{pmatrix} = \begin{pmatrix} \beta_A^A & \beta_{A^*}^A & \beta_{A_2}^A \\ \beta_A^{A^*} & \beta_{A^*}^{A^*} & \beta_{A_2}^{A^*} \\ \beta_A^{A_2} & \beta_{A^*}^{A_2} & \beta_{A_2}^{A_2} \end{pmatrix} \begin{pmatrix} N_3^A(0,t) \\ N_3^{A^*}(0,t) \\ N_3^{A_2}(0,t) \end{pmatrix}$$

$$\sum_{M'} \beta_{M'}^M \leq 1\,,\ \ \beta_M^A + \beta_M^{A^*} + \frac{1}{2}\beta_M^{A_2} \leq \delta_M,$$

where $\delta_M = 1$ if $M = A, A^*$ and $\delta_{A_2} = \frac{1}{2}$.

We set

$$\mathcal{B}^1(X) = C^1(X) \cap W^{1,\infty}(X) = \left\{ f \in C^1(X) \ / \ f, \frac{\partial f}{\partial x}, \frac{\partial f}{\partial t} \in L^\infty(X) \right\}.$$

Local solutions

Let $N_o \in \mathcal{B}^1_+([0;+\infty[)$. Then there exists a unique solution

$$N \in \mathcal{B}^1_+([0;+\infty[\times[0;T_o])$$

for the mixed-problem, where the life-span $T_o > 0$ depends exclusively on

$$E_o = \max_{i,M} \sup_{x\in\mathbb{R}^+} N^M_{i_o}(x).$$

sketch of the proof

We will use a Banach fixed-point technique.

$$\frac{\partial}{\partial t} N_i^M + v_i^M \, \frac{\partial}{\partial x} N_i^M = F_i^M(N).$$

We sum λN_i^M:

$$\frac{\partial}{\partial t} N_i^M + v_i^M \, \frac{\partial}{\partial x} N_i^M + \lambda N_i^M = F_i^M(N) + \lambda N_i^M := F_i^{M,\lambda}(N) \quad (1)$$

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We fix (x, t) and integrate (1) along the v_i^M-characteristic through (x, t).

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1. If $x - v_i^M(t) \geq 0$:

$$N_i^M(x,t) = e^{-\lambda t} N_{i_o}(x - v_i^M t) + \\ + \int_0^t e^{-\lambda(t-\tau)} F_i^{M,\lambda}(N)(x - v_i^M(t-\tau),\tau) d\tau := expr_1(N).$$

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2. If $x - v_i^M(t) < 0$:

$$N_i^M(x,t) = e^{-\lambda(t-t_i^M)} N_i^M(0,t_i^M) + \\ + \int_{t_i^M}^t e^{-\lambda(t-\tau)} F_i^{M,\lambda}(N)(x - v_i^M(t-\tau),\tau)d\tau.$$

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We use the boundary condition:

$$N_i^M(x,t) = e^{-\lambda(t-t_i^M)} \sum_{M'} \beta_{M'}^M N_3^{M'}(0, t_i^M) + \\ + \int_{t_i^M}^{t} e^{-\lambda(t-\tau)} F_i^{M,\lambda}(N)(x - v_i^M(t-\tau), \tau) d\tau.$$

We integrate once again along the characteristics:

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$$N_i^M(x,t) = e^{-\lambda t} \sum_{M'} \beta_{M'}^M e^{-\lambda t_i^M} N_{3_0}^{M'}(-v_3^{M'} t_i^M) + \\ + e^{-\lambda t} \sum_{M'} \beta_{M'}^M \int_0^{t_i^M} e^{-\lambda(t_i^M - \tau)} F_3^{M',\lambda}(N)(x - v_3^{M'}(t-\tau),\tau)d\tau \\ + \int_{t_i^M}^t e^{-\lambda(t-\tau)} F_i^{M,\lambda}(N)(x - v_i^M(t-\tau),\tau)d\tau := expr_2(N).$$

We set:

- $\Omega_T = [0; +\infty[\times [0; T]$
  $\Omega^+_{M,i,T} = \{(x,t) \in \Omega_T \; ; \; x \geq v_i^M t\}$
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- $X^1(T) = \left\{ N = (N_i^M)_{i,M} \ ; \ \ N, \dfrac{\partial N_i^M}{\partial x} \in C^o \cap L^\infty(\Omega_T) \right\}$
- $S(T, E, G) \subset X^1(T)$ the close and convex set of functions N such that
  $\forall i, M$
  - $N_i^M(x, 0) = N_{i_o}^M(x) \ , \ x \in [0; +\infty[$
  - $0 \leq N_i^M(x,t) \leq E \ , \ |\dfrac{\partial N_i^M}{\partial x}(x,t)| \leq G \ , \ (x,t) \in \Omega_T$.

We now set

- $$\psi : S(T,E,G) \rightarrow S(T,E,G)$$
  $$N_i^M(x,t) \rightarrow \ expr_1(N) \ \text{ if } (x,t) \in \Omega^+_{M,i,T}$$
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We can prove that for adequate values of S, T, G, λ, ψ is a contraction of $S(T, E, G)$.

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The time regularity is easy ro get.

Global solutions (2005)

Let $N_o \in \mathcal{B}^1_+([0;\infty[) \cap L^1([0;+\infty[)$.
Then there exists $\epsilon, \epsilon' > 0$ such that if

$$m_o = \int_0^{+\infty} \left(\sum_{i=1}^{3} (N_{i_o}^{A} + 2N_{i_o}^{A_2}) + \sum_{i=1,3} N_{i_o}^{A^*} \right)(x)dx < \epsilon$$

and

$$E_o = \max_{i,M} \sup_{x \in \mathbb{R}^+} N_{i_o}^{M}(x) < \epsilon',$$

the mixed problem has a unique solution

$$N \in \mathcal{B}^1_+([0;\infty[\times[0;\infty[.$$

Proof: We set $E(T_o) = \max_{i,M} \sup_{x\in\mathbb{R}^+,\, t\in[0;T_o]} {N_i}^M(x,t)$.

We show an a priori estimate of the type $\forall t \in [0;T[,\ E(t) \leq M$.

Conservation laws:

- $$\frac{\partial}{\partial t}\left(\sum_{i=1}^{3}(N_i^A + N_i^{A_2})\right) + \frac{\partial}{\partial x}\left(\sum_{i=1}^{3} v_i(N_i^A + \frac{1}{2}N_i^{A_2})\right) = 0$$

- $$\frac{\partial}{\partial t}\left(\sum_{i=1}^{3} N_i^{A_2} + \sum_{i=1,3} N_i^{A^*}\right) + \frac{\partial}{\partial x}\left(\sum_{i=1}^{3} \frac{1}{2} v_i N_i^{A_2} + \sum_{i=1,3} v_i N_i^{A^*}\right) = 0$$

- $$\frac{\partial}{\partial t}\left(\sum_{i=1}^{3} v_i(N_i^A + N_i^{A_2}) + \sum_{i=1,3} v_i N_i^{A^*}\right)$$
$$+\frac{\partial}{\partial x}\left(\sum_{i=1}^{3} v_i^2(N_i^A + \frac{1}{2}N_i^{A_2}) + \sum_{i=1,3} v_i^2 N_i^{A^*}\right) = 0\,.$$

From the conservation laws, we build two exact forms:

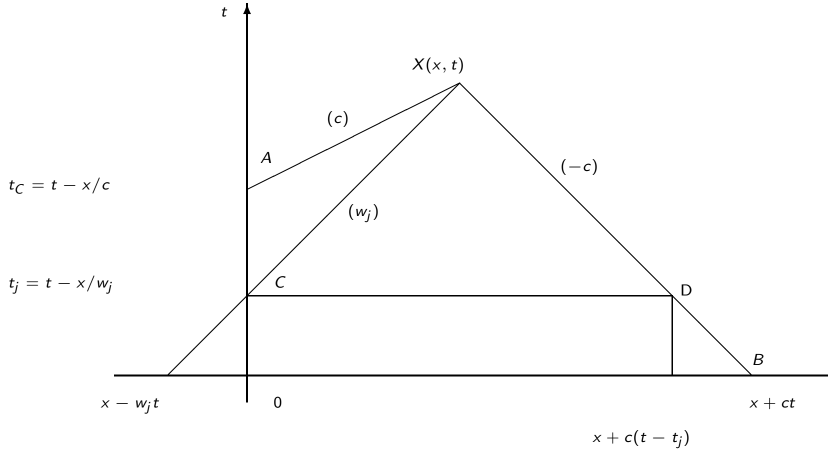
$$w = -\left(\sum_{i=1}^{3}(N_i^A + 2N_i^{A_2}) + \sum_{i=1,3} N_i^{A^*}\right) dx +$$

$$\left(\sum_{i=1}^{3} v_i(N_i^A + N_i^{A_2}) + \sum_{i=1,3} v_i N_i^{A^*}\right) dt.$$

$$w' = -\left(\sum_{i=1}^{3}((w_j - v_i)N_i^A + (2w_j - v_i)N_i^{A_2}) + \sum_{i=1,3}(w_j - v_i)N_i^{A^*}\right) dx$$

$$+\left(\sum_{i=1}^{3} v_i((w_j - v_i)N_i^A + (w_j - \frac{1}{2}v_i)N_i^{A_2}) + \sum_{i=1,3} v_i(w_j - v_i)N_i^{A^*}\right) dt.$$

We integrate the 1-forms w and w'in cycles:



, Eventually, we will get the inequality

$$E(t) \leq CE_o + C' m_o (E(t) + E(t)^2).$$