

Discrete Kinetic Theory of Gases

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Discrete Kinetic Theory of Gases: Outline

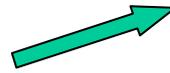
- 1. Introduction**
- 2. Discrete kinetic theory**
- 3. Hydrodynamical description for regular discrete models**
- 4. Boundary conditions**
- 5. Applications**
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1. Introduction

Introduction

Boltzmann equation

$$\mathcal{D}f = \mathcal{J}(f, f)$$



Balance laws



Entropy inequality



Constitutive laws

Dimensionless



$$\varepsilon \ll 1$$

**Euler, Navier-Stokes,
Burnett, ... equations**

Boltzmann equation



$$\varepsilon \gg 1$$

Free molecular flows

$$\mathcal{D}f = (1/\varepsilon) \mathcal{J}(f, f)$$



$$\varepsilon \cong 1$$

**Transition flows: Wave
shock structure, Knudsen
layer, ...**

$$\varepsilon = \lambda / L$$



Need models

Introduction: The first works

	Authors	Velocity number	Subject
1957	Carleman	2	H-Theorem
1960	Gross		The velocity discretization is emphasized
1964	Broadwell	6	Shock wave structure
« «	Broadwell	8	Couette and Rayleigh problems
1965	R. G.	6	Shock wave structure
1966	Harris	6	Ternary collisions and H-Theorem
1967	Harris	4	Study of the H-function
1970	R.G.	p	Discrete kinetic theory
1971	Godunov & Sultangazin	6	Kinetic and hydrodynamical descriptions
1972	Hardy & Pomeau	4	Lattice gases

R. G.

1965 - 1972	6 CRAS	Shock structure, H-Theorem, General kinetic equations, Chapman-Enskog expansion, ...
1970	Zeitschrift für Flugwissenschaften	« Théorie cinétique des gaz à répartition discrète de vitesses »
1975	Lecture Notes in Physics (Vol. 39)	
1975	Physics Fluids	Discrete kinetic theory
1977	Physics of Fluids	Boundary conditions
1965 - ...	4 theses, about 20 papers and 20 proceedings	

H. Cabannes

1975	J. de Mécanique	Shock structure (14 velocities)
1977 - ...	On the solutions of the discrete kinetic equations (existence theorems, exact solutions)	
1980	Lecture notes, Berkeley University, « The discrete Boltzmann Equation »	

2. Discrete Kinetic Theory of Gases

Discrete Kinetic Theory of Gases

- In discrete kinetic theory, the main idea is that the velocities of the molecules belong to a given set of vectors
- The Boltzmann equation is replaced by a system of partial differential equations
- This system has an interesting mathematical structure (H. Cabannes, Bellomo, Cercignani, Kawashima, ...)
- The discrete models, by their simplicity, help to understand the fundamental problems of rarefied gas dynamics
- The hydrodynamic description of discrete gases is obtained via the Chapman-Enskog expansion

Discrete kinetic theory: Binary collisions

The particles are identical

The particle velocities belong to a given set of vectors:

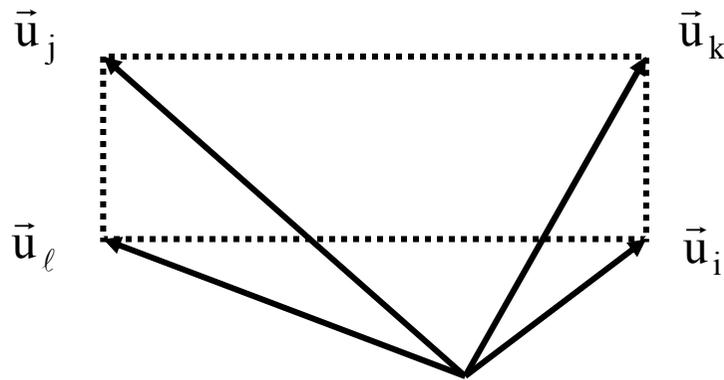
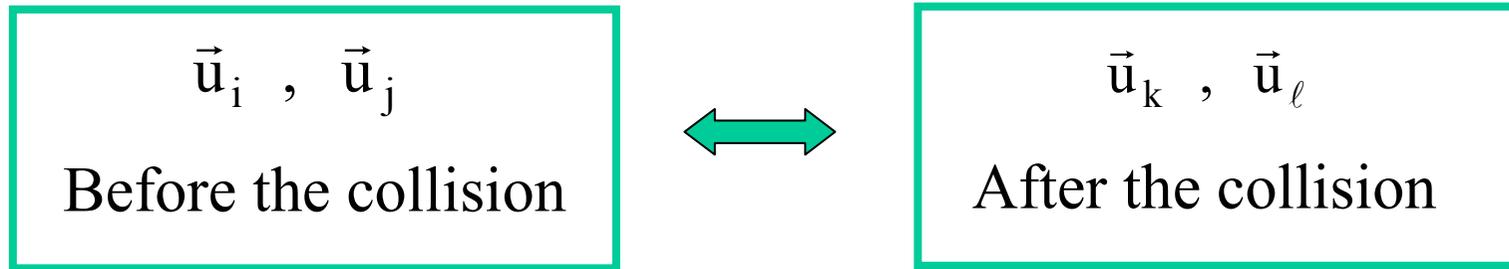
$$\vec{u}_k, k = 1, 2, \dots, p$$

$N_k(\vec{x}, t)$ denotes the number of particles with velocity \vec{u}_k
(i.e. particle « k ») per unit of volume

Macroscopic quantities

$$\left\{ \begin{array}{l} n = \sum_k N_k \\ n \vec{u} = \sum_k N_k \vec{u}_k \\ n e = \frac{m}{2} \sum_k N_k (\vec{u}_k - \vec{u})^2 \end{array} \right. \quad \left\{ \begin{array}{l} \vec{P} = m \sum_k N_k (\vec{u}_k - \vec{u})(\vec{u}_k - \vec{u}) \\ \vec{q} = \frac{m}{2} \sum_k N_k (\vec{u}_k - \vec{u})^2 (\vec{u}_k - \vec{u}) \end{array} \right.$$

Binary collision



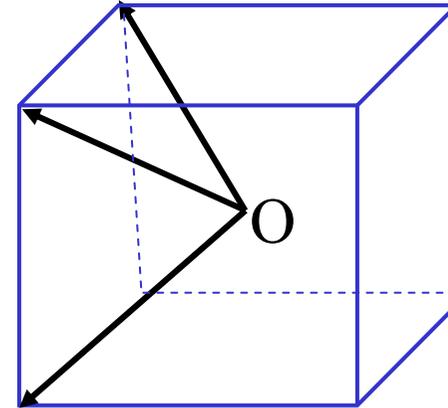
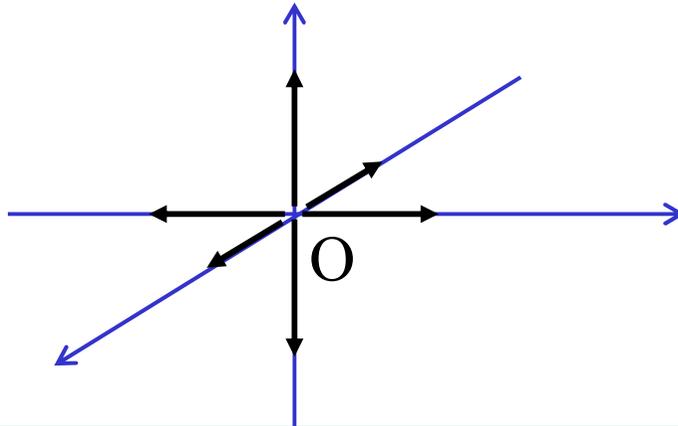
In the collision, the mass, momentum and energy are conserved

Transition probability A_{ij}^{kl}

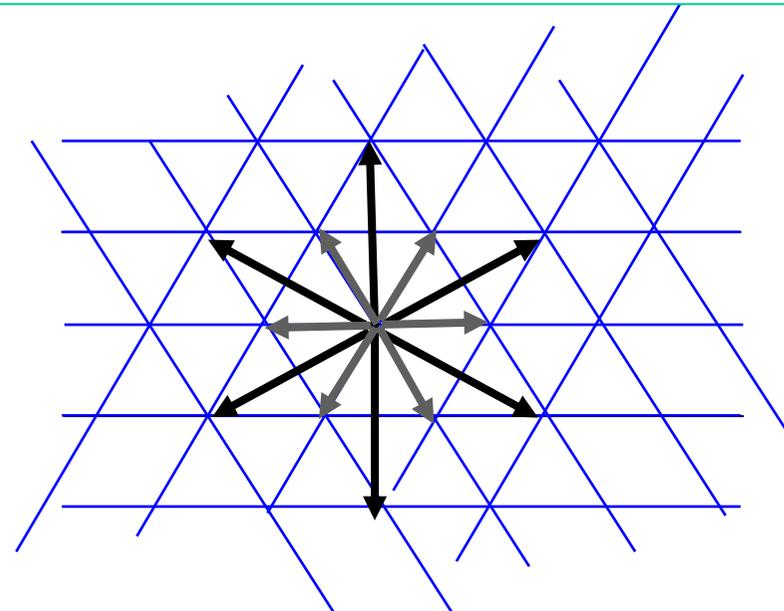
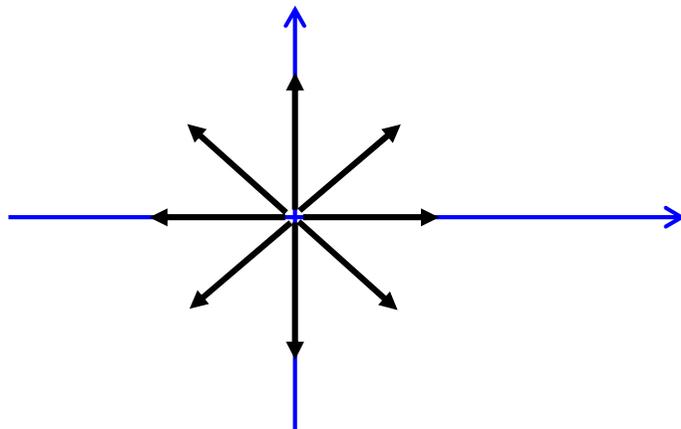
Microreversibility property $A_{ij}^{kl} = A_{kl}^{ij}$

Discrete kinetic theory: Examples

Spatial models with 6 velocities or with 8 velocities
(Broadwell, 1964)



Coplanar models



Kinetic equations (binary collisions)

$$\left\{ \begin{array}{l} \frac{\partial}{\partial t} N_k + \vec{u}_k \cdot \vec{\nabla} N_k = G_k - L_k, \quad k = 1, 2, \dots, p \\ \frac{\partial}{\partial t} N_k + \vec{u}_k \cdot \vec{\nabla} N_k = \frac{1}{2} \sum_{ij\ell} \left(A_{ij}^{k\ell} N_i N_j - A_{k\ell}^{ij} N_k N_\ell \right), \quad k = 1, 2, \dots, p \end{array} \right.$$

Notations

$$\mathbf{N} = (N_1, N_2, \dots, N_p)$$

$$\langle \mathbf{U}, \mathbf{V} \rangle = \sum_k U_k V_k$$

$\mathcal{F}(\mathbf{U}, \mathbf{V})$ Linear mapping of $\mathbb{R}^p \times \mathbb{R}^p$ into \mathbb{R}^p

Kinetic equations

$$\frac{\partial}{\partial t} \mathbf{N} + \mathcal{A} \mathbf{N} = \mathcal{F}(\mathbf{N}, \mathbf{N})$$

Symmetry property

$$\langle \phi, \mathcal{F}(\mathbf{U}, \mathbf{V}) \rangle = -\frac{1}{8} \sum_{ijkl} A_{kl}^{ij} (\varphi_k + \varphi_l - \varphi_i - \varphi_j) (U_i V_j + U_j V_i)$$

$$\phi = (\varphi_1, \varphi_2, \dots, \varphi_p) \in \mathbb{R}^p$$

Summational invariants: $\phi \in \mathbb{R}^p$ such as

$$A_{ij}^{kl} (\varphi_k + \varphi_l - \varphi_i - \varphi_j) = 0 \quad \forall i, j, k, l$$

→ Linear subspace \mathbf{F} ($\mathbf{F} \subset \mathbb{R}^p$ dimension of $\mathbf{F} = q$)

Base in \mathbf{F} : $\mathbf{v}^1, \mathbf{v}^2, \dots, \mathbf{v}^q$

Base in \mathbb{R}^p : $\mathbf{v}^1, \mathbf{v}^2, \dots, \mathbf{v}^q, \mathbf{w}^{q+1}, \dots, \mathbf{w}^p$

Kinetic densities

$$\mathbf{N} = \sum_{\alpha=1}^{\alpha=q} \mathbf{a}_{\alpha} \mathbf{v}^{\alpha} + \sum_{\beta=q+1}^{\beta=p} \mathbf{b}_{\beta} \mathbf{w}^{\beta}$$

Macroscopic variable

Microscopic variable

$$\frac{\partial}{\partial t} \mathbf{N} + \mathcal{A} \mathbf{N} = \mathcal{F}(\mathbf{N}, \mathbf{N})$$

Equations for the \mathbf{a}_α and the \mathbf{b}_β variables

$$\left\{ \begin{array}{l} \frac{\partial \mathbf{a}_\alpha}{\partial t} + \langle \mathcal{A} \mathbf{N}, \mathbf{V}^\alpha \rangle = 0, \quad \alpha = 1, 2, \dots, q \quad \text{conservation laws} \\ \frac{\partial \mathbf{b}_\beta}{\partial t} + \langle \mathcal{A} \mathbf{N}, \mathbf{W}^\beta \rangle = \langle \mathcal{F}(\mathbf{N}, \mathbf{N}), \mathbf{W}^\beta \rangle, \quad \beta = q+1, q+2, \dots, p \end{array} \right.$$

H – Theorem: H is decreasing with $H = \langle \mathbf{N}, \ln \mathcal{F}(\mathbf{N}, \mathbf{N}) \rangle$

Maxwellian state: $\ln \mathbf{N} \in \mathbf{F} \Leftrightarrow \mathcal{F}(\mathbf{N}, \mathbf{N}) = 0 \Leftrightarrow \ln \mathbf{N} = \sum_{\alpha=1}^{\alpha=q} \mathbf{c}_\alpha \mathbf{V}^\alpha$

Euler equations associated with the model: Equations for the variables \mathbf{a}_α or equivalently for the \mathbf{c}_α variables

$$\sum_{\delta=1}^{\delta=q} \frac{\partial^2 \mathcal{L}(\mathbf{c}_1, \mathbf{c}_2, \dots, \mathbf{c}_q)}{\partial \mathbf{c}_\alpha \partial \mathbf{c}_\delta} \frac{\partial \mathbf{c}_\delta}{\partial t} + \sum_{\delta=1}^{\delta=q} \frac{\partial^2 \mathcal{M}(\mathbf{c}_1, \mathbf{c}_2, \dots, \mathbf{c}_q)}{\partial \mathbf{c}_\alpha \partial \mathbf{c}_\delta} \frac{\partial \mathbf{c}_\delta}{\partial \mathbf{x}} = 0, \quad \alpha = 1, 2, \dots, q$$

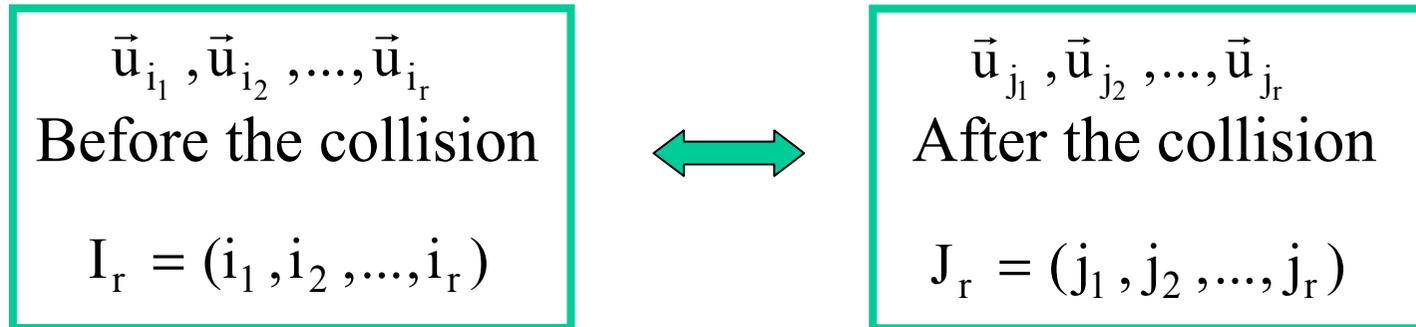
Two problems are present in discrete kinetic theory:

- 1. The existence of macroscopic variables other than mass, momentum and energy**
- 2. The anisotropic character generally related to the discrete models**

In order to reduce and possibly to eliminate them, multiple collisions are introduced and some symmetry properties on the models are adopted

The multiple collisions

A r – collision is a collision between r particles:



Transition probability: $A_{I_r}^{J_r}$

$\delta(k, I_r, J_r)$ is the algebraic number of particles « k » created in the r – collision $I_r \rightarrow J_r$

$\sum_{I_r, J_r} \delta(k, I_r, J_r) A_{I_r}^{J_r} N_{i_1} N_{i_2} \dots N_{i_r}$ is the algebraic number of particles « k » created in all the r – collisions (per unit time)

Kinetic equations with r – collisions ($r = 2, 3, \dots, R$)

$$\frac{\partial}{\partial t} N_k + \vec{u}_k \cdot \vec{\nabla} N_k = \frac{1}{2} \sum_{r=2,3,\dots,R} \sum_{I_r J_r} \delta(k, I_r, J_r) A_{I_r}^{J_r} N_{i_1} N_{i_2} \dots N_{i_r}$$

$$k = 1, 2, \dots, p$$

$$\frac{\partial}{\partial t} \mathbf{N} + \mathcal{A} \mathbf{N} = \mathcal{C}(\mathbf{N})$$

Summational invariants $\phi = (\phi_1, \phi_2, \dots, \phi_p) \in \mathbb{R}^p$

$$A_{I_r}^{J_r} \sum_k \delta(k, I_r, J_r) \phi_k = 0 \quad \forall I_r, J_r, r$$

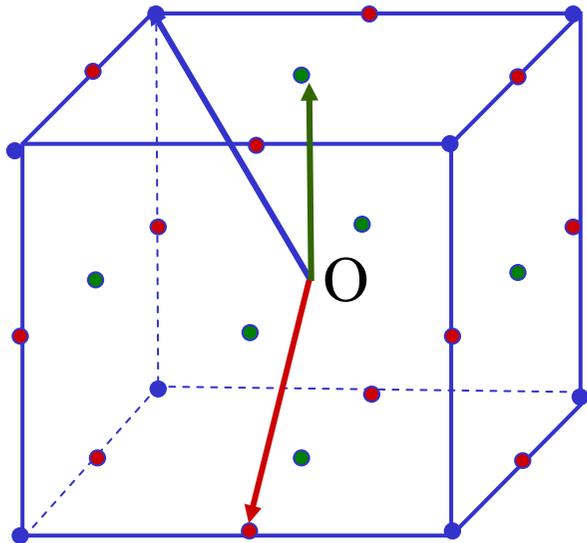
→ Linear subspace \mathbf{F} ($\mathbf{F} \subset \mathbb{R}^p$)

Two remarks

- By taking into account multiple collisions, the dimension of \mathbf{F} is decreasing
- By taking into account all the r – collisions, it is possible to find the dimension of \mathbf{F} , without explicitly determining all the collisions between the particles (Ph. Chauvat)

Examples: Dimension of \mathbf{F} is 4 or 5

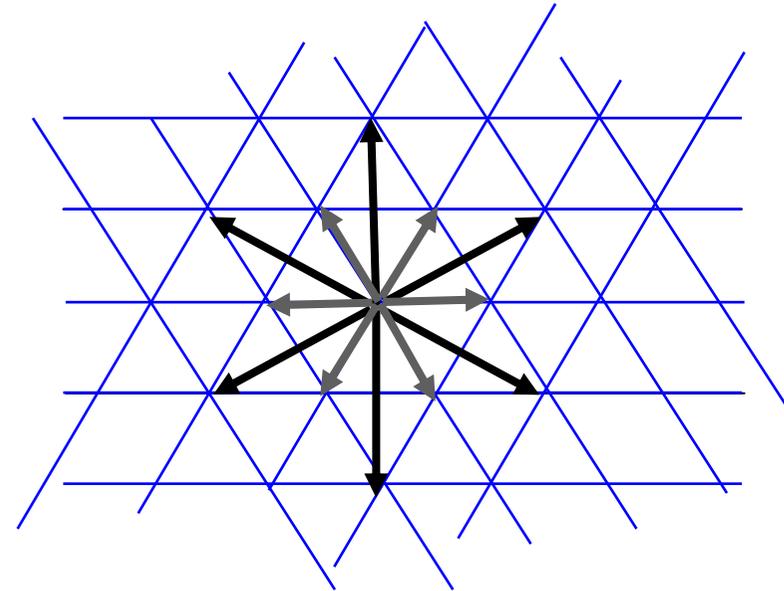
Spatial models related to the cube



Velocity number

- 6 •
- 8 •
- 14 • •
- 26 • • •

Coplanar models related to the hexagonal lattice



Generalizations

$$\vec{u}_k = a_k \vec{I} + b_k \vec{J} + c_k \vec{K},$$

$$(a_k, b_k, c_k) \in \mathbb{Z}^3$$

$$\dim \mathbf{F} = 5$$

Chapman – Enskog expansion

$$\frac{\partial}{\partial t} \mathbf{N} + \mathcal{A} \mathbf{N} = \frac{1}{\varepsilon} C(\mathbf{N}, \mathbf{N}) \quad \varepsilon \ll 1 \quad (\varepsilon \text{ Knudsen number})$$

But: To obtain balance laws for the variables \mathbf{a}_α

$$\left\{ \begin{array}{l} \frac{\partial \mathbf{a}_\alpha}{\partial t} + \langle \mathcal{A} \mathbf{N}, \mathbf{V}^\alpha \rangle = 0, \quad \alpha = 1, 2, \dots, q \\ \text{with } \mathbf{N} = \mathbf{N}(\mathbf{a}_\alpha, \mathbf{b}_\beta), \text{ the variables } \mathbf{b}_\beta \text{ depending on the } \mathbf{a}_\alpha \end{array} \right.$$

Chapman – Enskog expansion

$$\mathbf{N} = \mathbf{N}^{(0)} + \varepsilon \mathbf{N}^{(1)} + \varepsilon^2 \mathbf{N}^{(2)} + \dots$$

$$\mathcal{J}(\mathbf{N}^{(1)}) = \frac{\partial}{\partial t} \mathbf{N}^{(0)} + \mathcal{A} \mathbf{N}^{(0)}$$

$$\left\{ \begin{array}{l} C(\mathbf{N}^{(0)}, \mathbf{N}^{(0)}) = 0 \end{array} \right.$$

$\mathbf{N}^{(0)}$ Maxwellian densities

Euler equations for \mathbf{a}_α

$\mathcal{J}(\mathbf{N}^{(1)})$ Linearized collision operator

$\mathbf{N}^{(0)} + \varepsilon \mathbf{N}^{(1)}$ Navier – Stokes

equations for \mathbf{a}_α

3. Hydrodynamical description for regular discrete models

Regular discrete models

The successful simulations undertaken with the lattice gas method introduced by Frisch, Hasslacher and Pomeau, ... have provided a new light on the discrete models of gas

" Quasi – isotropic " models (Chauvat, Coulouvrat, R.G.)

$$\mathcal{V}_\ell = \left\{ \vec{u}_k^\ell, \left| \vec{u}_k^\ell \right| = c_\ell, k = 1, 2, \dots, p_\ell \right\}$$

$$\mathcal{V} = \left\{ \vec{u}_k, k = 1, 2, \dots, p \right\} = \bigcup_{\ell=1}^L \mathcal{V}_\ell$$

Mean properties

- + \mathcal{G} : Isometry group in \mathbb{R}^D
- + $g(\mathcal{V}) = \mathcal{V} \quad \forall g \in \mathcal{G}$
- + $\dim F = D + 2$ (The multiple collisions are introduced)

Examples: Coplanar models related to the hexagonal lattice,
Spatial models related to the cubic lattice

Hydrodynamical description of the gas

Maxwellian state $N_k^{(0)} = \exp\left(\alpha + \vec{\beta} \cdot \vec{u}_k + \gamma (\vec{u}_k^2 - a^2)\right)$

$$n = \sum_k N_k^{(0)}, \quad n \vec{u} = \sum_k N_k^{(0)} \vec{u}_k, \quad n e = \frac{1}{2} \sum_k N_k^{(0)} \vec{u}_k^2$$

$$\alpha, \vec{\beta}, \gamma \Leftrightarrow n, \vec{u}, e \quad \text{Bijection}$$

Homogeneous Maxwellian state $N_k^{(0)} = \frac{n}{p} \quad (\vec{u} = 0, e = \frac{1}{2} a^2)$

Quasi-homogeneous Maxwellian state $\Delta e / a^2 \ll 1, \quad |\vec{u}| / a \ll 1$

$$N_k^{(0)} = \frac{n}{p} \left\{ 1 + \frac{D}{a^2} \vec{u} \cdot \vec{u}_k + \frac{2(\vec{u}_k^2 - a^2)}{a^4 - a^4} \left(e - \frac{a^2}{2} \right) + \frac{D^2}{2a^4} \left(\vec{u}_k \vec{u}_k - \frac{\vec{u}_k^2}{D} \vec{I} \right) : \vec{u} \vec{u} \right. \\ \left. + \frac{2D^2}{a^2} \left(\frac{\vec{u}_k^2 - a^2}{a^4 - a^4} - \frac{1}{a^2} \right) \left(e - \frac{a^2}{2} \right) (\vec{u} \cdot \vec{u}_k) \right\}$$

Notations: $a_r = \left(\frac{1}{p} \sum_k |\vec{u}_k|^{2r} \right)^{1/2r} \quad a_1 = \left(\frac{1}{p} \sum_k |\vec{u}_k|^2 \right)^{1/2} \equiv a$

Euler equations associated with the model

$$\left\{ \begin{array}{l} \frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\rho \vec{u}) = 0 \\ \frac{\partial (\rho \vec{u})}{\partial t} + \eta \vec{\nabla} \cdot (\rho \vec{u} \vec{u}) + \vec{\nabla} \varpi = (\eta - 1) \vec{\nabla} \left(\rho \frac{\vec{u}^2}{D} \right) + \vec{\nabla} \cdot \left(\rho \vec{M}_{an} \right) \\ \frac{\partial}{\partial t} \left(\rho e + \rho \frac{\vec{u}^2}{2} \right) + \eta \vec{\nabla} \cdot \left(\left(\rho e + \rho \frac{\vec{u}^2}{2} + \varpi \right) \vec{u} \right) = \varphi \vec{\nabla} \cdot \left(\rho \left(e - \rho \frac{a^2}{2} \right) \vec{u} \right) \end{array} \right.$$

$$\eta = \frac{a_2^4}{a^4} \frac{D}{D+2}$$

$$\varphi = \frac{2a_2^8 - a^4 a_2^4 - a^2 a_3^6}{a^4 (a_2^4 - a^4)}$$

η and φ depend on the discrete models

Continuous fluids: $\eta = 1$ $\varphi = 0$

Remarks: We can provide equivalent forms of the Euler equations; for example with a pressure tensor not necessarily spherical or a vector heat flux not necessarily zero

Numerical results for the transport coefficients

Model	$\bar{\mu}$	$\bar{\kappa}$	Pr
I	0.15	0.24	0.62
II	0.24	0.33	0.73
III	0.22	0.24	0.92
IV	0.25	0.41	0.61
Chauvat (1989)*	<u>0.14</u>	<u>0.50</u>	<u>0.28</u>
Chahine (1967)**	<u>0.14</u>	<u>0.56</u>	<u>0.25</u>

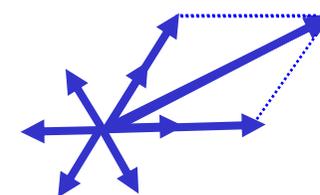
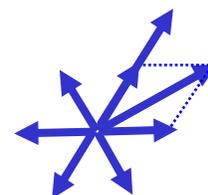
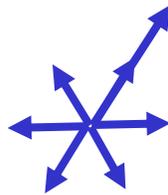
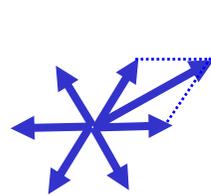
$$\mu = \frac{ma}{S\sqrt{2}} \bar{\mu}$$

$$\kappa = \frac{ma}{S\sqrt{2}} \bar{\kappa}$$

$$Pr = \frac{\mu}{\kappa}$$

* model I ($\eta = 0.67, \phi = 0$)

** coplanar continuous model



Models: I (12)

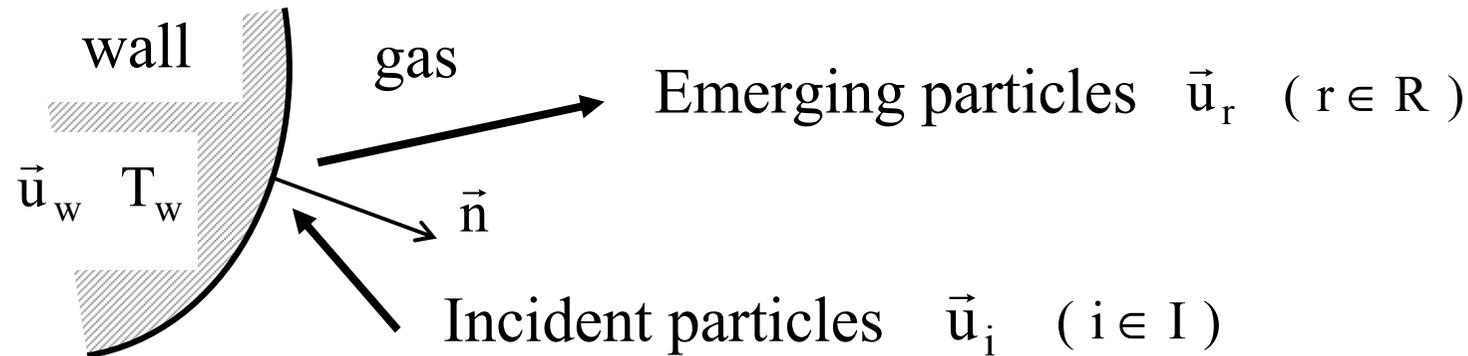
II (12)

III (18)

IV (18)

4. Boundary Conditions

Boundary conditions on an impermeable wall (R.G., 1975)



$$|(\vec{u}_r - \vec{u}_w) \cdot \vec{n}| N_r = \sum_{i \in I} B_{ir} |(\vec{u}_i - \vec{u}_w) \cdot \vec{n}| N_i \quad \forall r \in R$$

B_{ir} : probability for a particle of velocity \vec{u}_i impinging the wall, to be reflected with the velocity \vec{u}_r

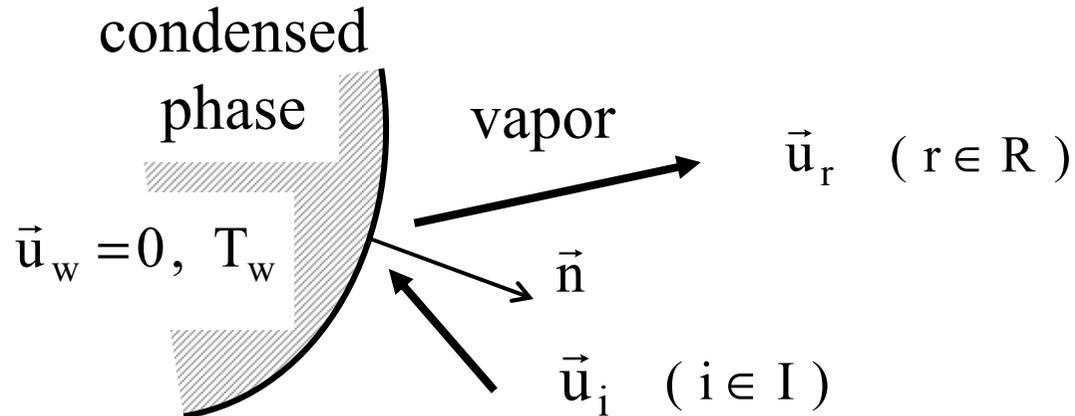
H – Theorem in a vessel

Particular case of the diffuse reflexion: $N_r = \lambda N_{rw}$

The densities N_{rw} are Maxwellian densities associated with the macroscopic variables of the wall $n_w = 1, \vec{u}_w, T_w, \dots$

λ (as n) is unknown; $\hat{\lambda}$ is known when the problem is solved

Boundary conditions on an interface



Gas in Maxwellian equilibrium with the condensed phase

$$N_{kw} = \exp\left(\alpha + \vec{\beta} \cdot \vec{u}_k + \gamma |\vec{u}_k|^2\right)$$

$$\sum_k N_{kw} = 1, \quad \sum_k N_{kw} \vec{u}_k = 0, \quad \frac{1}{2} \sum_k N_k (\vec{u}_k - \vec{u})^2 = \frac{3}{2} \frac{k T_w}{m}$$

Boundary conditions for the vapor $N_r = n_{\text{sat}} N_{rw}, \quad \forall r \in R$

n_{sat} : saturation density of the vapor at the temperature T_w

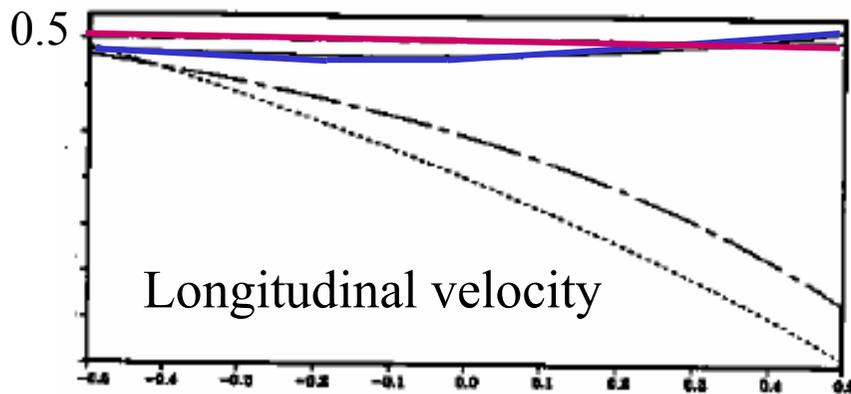
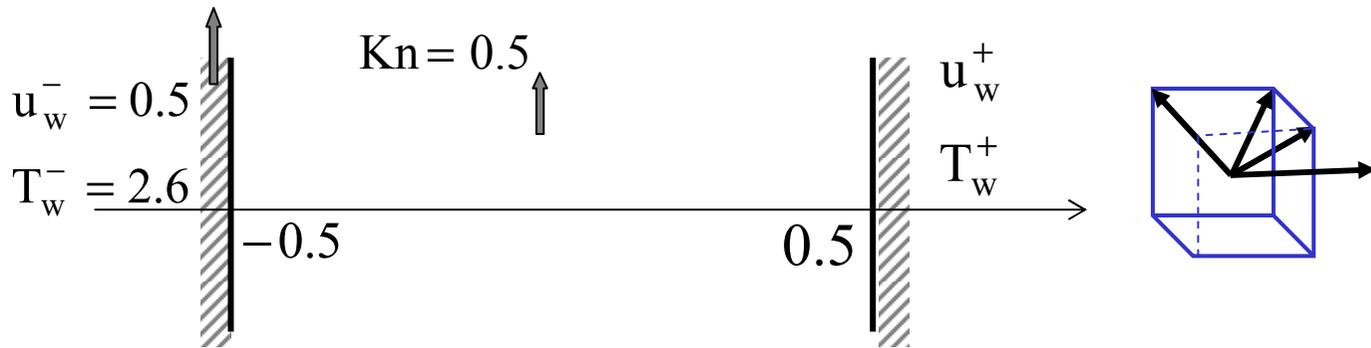
Remark: This boundary condition is valid only when the models are symmetrical about the normal \vec{n} . This condition is similar to that of the continuous kinetic theory

5. Applications

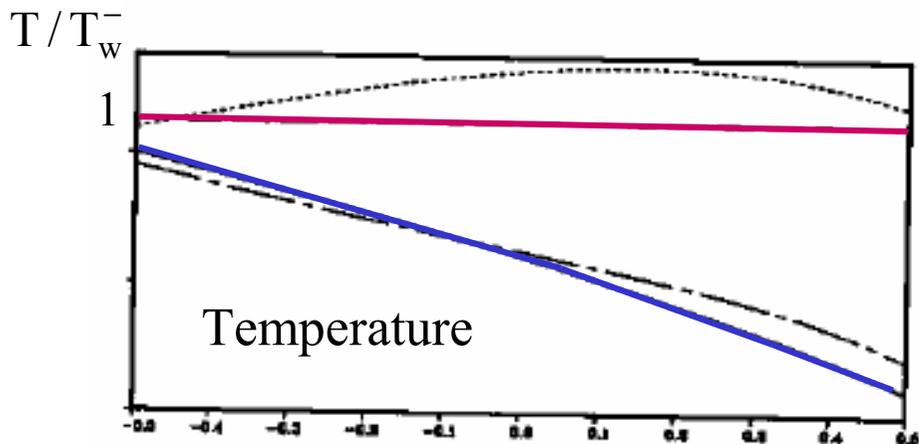
Applications

- **Shock wave structure**
- **Unsteady and steady Couette flows (Knudsen layer, initial layer, ...)**
- **Flow and heat transfer between two parallel plates**
- **Evaporation / condensation between two interfaces (temperature inversion)**
- **Evaporation or condensation on a liquid interface**
- **Flow in a microchannel**
- **...**

Flow and heat transfer between two parallel plates (d'Almeida)

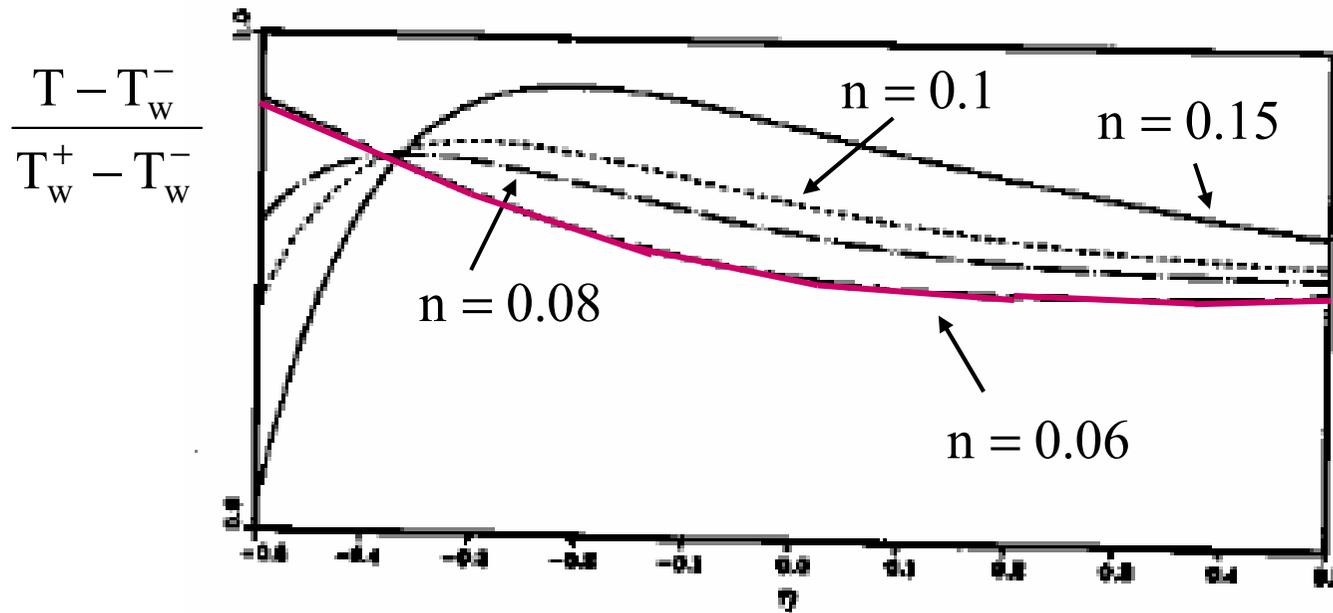
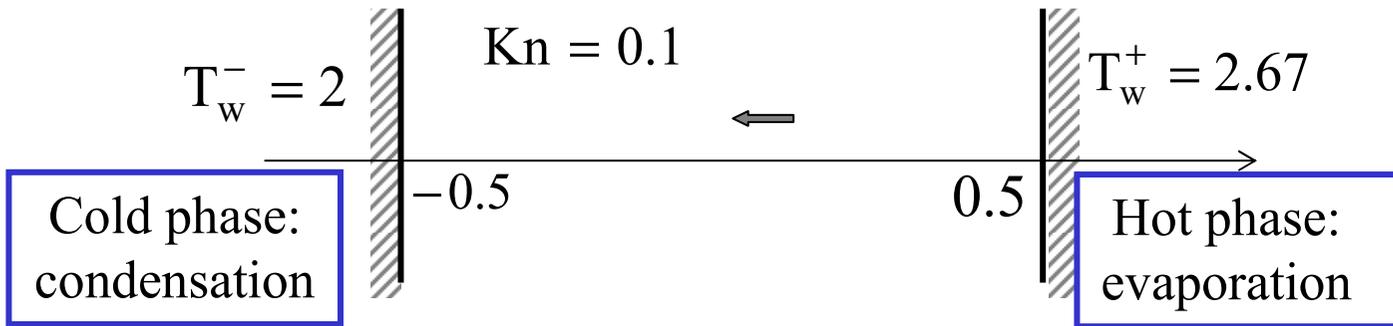


Red line: test case
 $T_w^+ = 2.6$, $u_w^+ = 0.5$

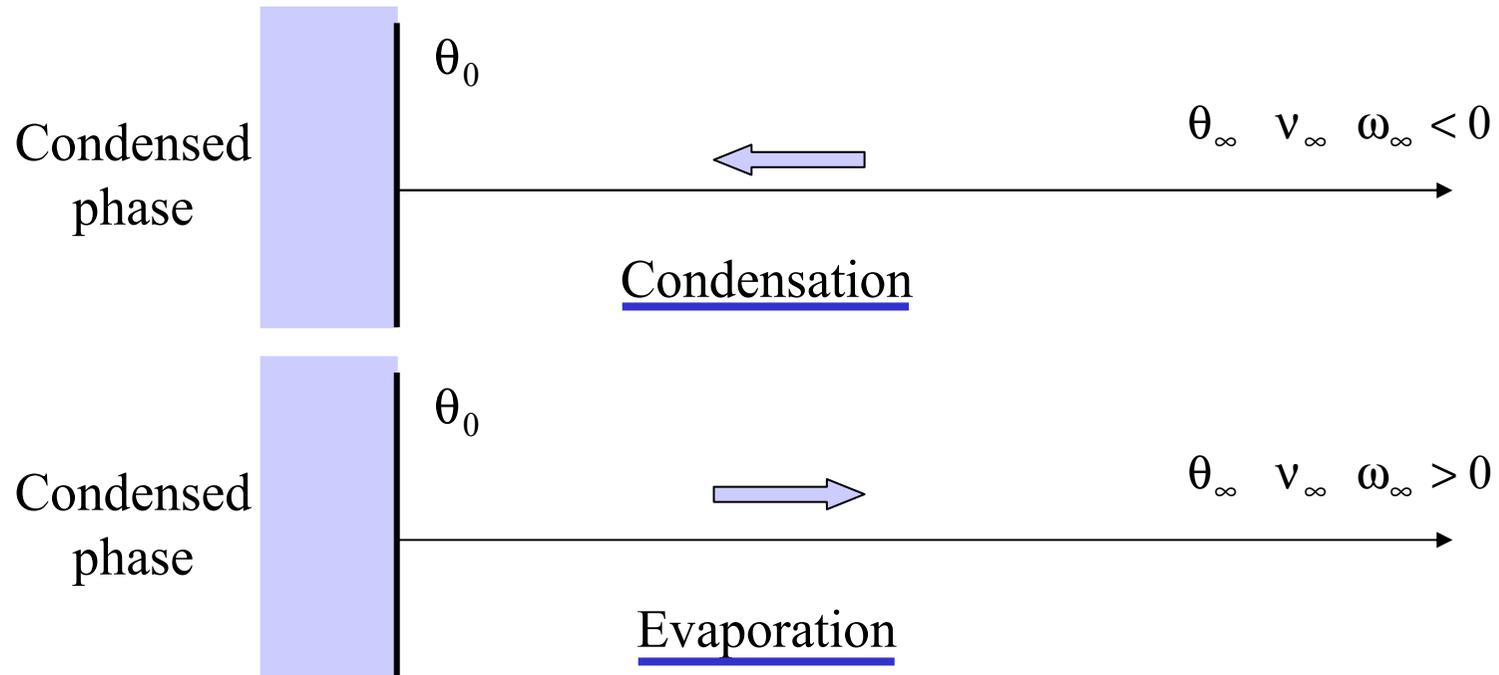


Blue line: Thermophoresis phenomenon
 $T_w^+ = 2$, $u_w^+ = 0.2$

Evaporation / condensation between two interfaces (d'Almeida)



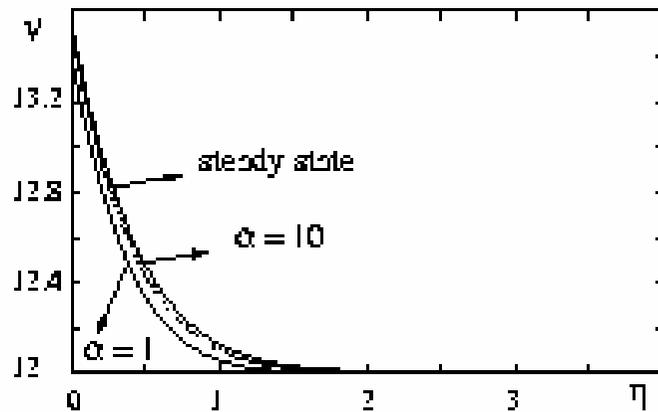
Evaporation or condensation on a liquid interface (Nicodin)



These problems depend on 3 parameters : $\frac{\theta_\infty}{\theta_0}$, v_∞ , $M_\infty = \frac{|\omega_\infty|}{\sqrt{\theta_\infty}} > 0$

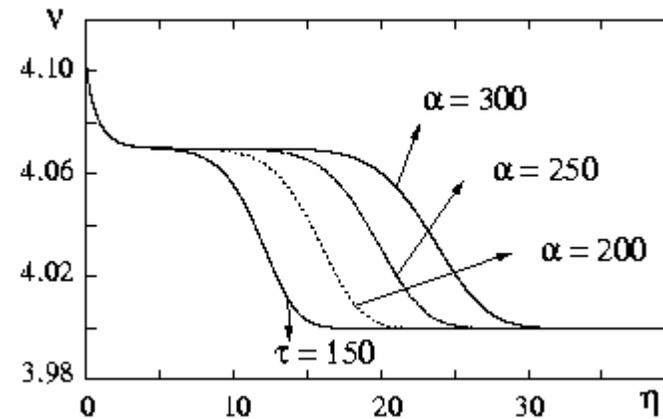
The results obtained with a very simple model (16 velocities only) are in very good agreement with those of Sone, Aoki and their collaborators with continuous theory

Condensation problem (Nicodin)



$$\frac{\theta_{\infty}}{\theta_0} = 1, \quad v_{\infty} = 12, \quad M_{\infty} = 1.414$$

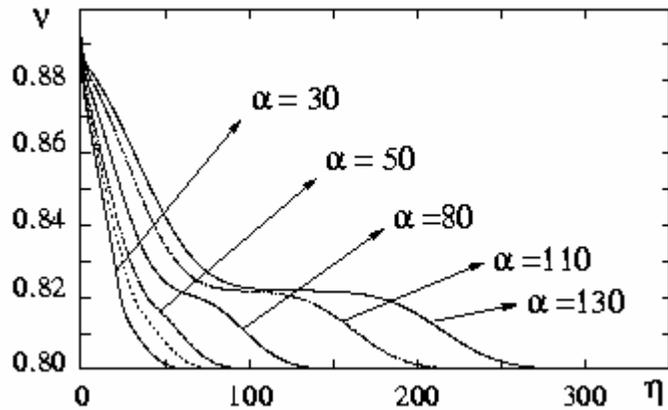
The vapor is compressed on the condensed phase ($\eta = 0$). The steady state is obtained for about 30 mean free times



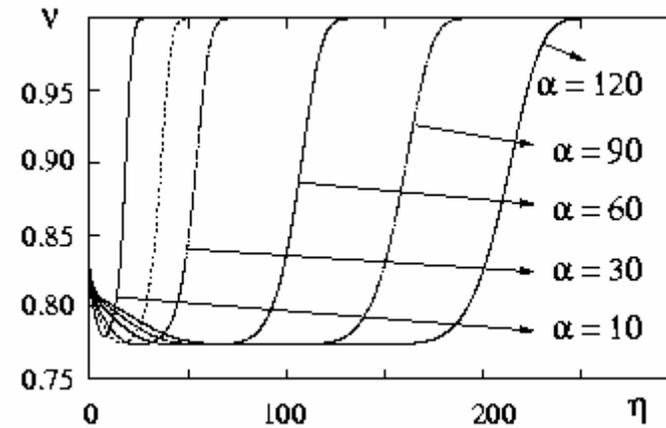
$$\frac{\theta_{\infty}}{\theta_0} = 1, \quad v_{\infty} = 4, \quad M_{\infty} = 0.707$$

There is a Knudsen layer near the condensed phase ($\eta = 0$). A compression wave (shock wave) propagates to infinity

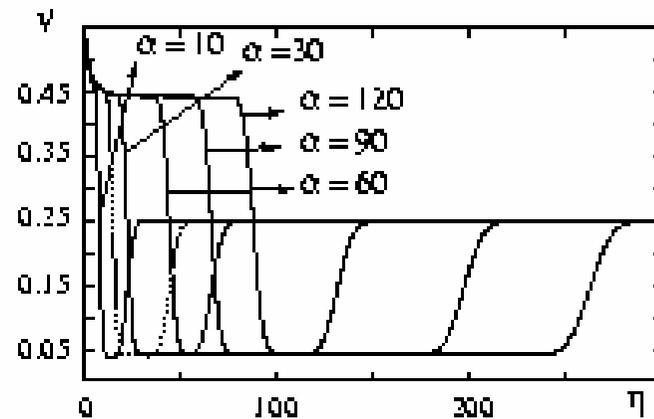
Evaporation problem (Nicodin)



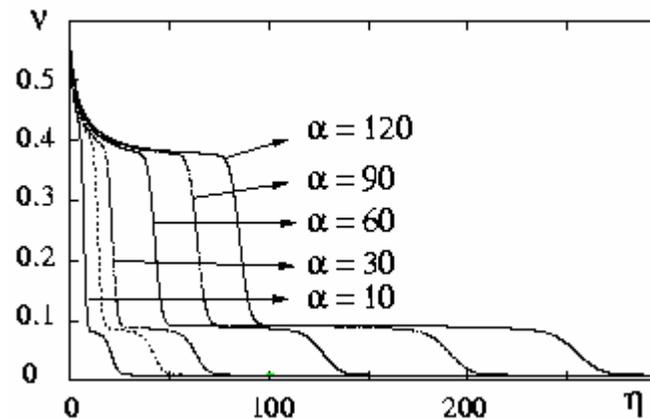
$$\frac{\theta_\infty}{\theta_0} = 1, \quad v_\infty = 0.8, \quad M_\infty = 0.058$$



$$\frac{\theta_\infty}{\theta_0} = 1, \quad v_\infty = 1, \quad M_\infty = 0.316$$



$$\frac{\theta_\infty}{\theta_0} = 1, \quad v_\infty = 0.01, \quad M_\infty = 1$$



$$\frac{\theta_\infty}{\theta_0} = 1, \quad v_\infty = 0.25, \quad M_\infty = 1.73$$

6. Conclusion

Conclusion

Many generalizations

Gas mixtures (Cercignani, Cornille, ...)

Chemical reactions (Pandolfi, ...)

Numerical approaches (Leguillon, Teman, Golstein, ...)

Semi discrete Boltzmann equation (Cabannes, Toscani, ...)

...

Many mathematical papers

Existence theorems, exact solutions, asymptotic analysis, ...

Cabannes, Bardos, Beale, Bellomo, Bobylev, Bony,
Cercignani, Cornille, Godunov, Golse, Hamdache, Illner,
Kawashimha, Levermore, Nishida, Platkowski, Sultangazin,
Tartar, Vedenyapin, ...

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Alain Fanget (Thesis, 1980)

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Mohammed Kane (DEA, 1977)

Ayaovi Bodjrenou (DEA, 2000)

Yassine Benbouali (DEA, 2003)

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Thank you for your attention