

# Well-balanced schemes for linear models of Boltzmann equation: a legacy of Chandrasekhar, Case, Cercignani and Siewert

Laurent Gosse

IAC-CNR (Bari and then Rome)



# Plan of the talk

## 1 Introduction

- What need for well-balanced ?
- Localization process with  $BV$  theory

## 2 Cercignani's decomposition of linear Boltzmann equation

- Decoupling shear effects/heat transfer
- Shear flows :  $\Psi_3, \Psi_4$  and  $\Psi_5$
- Heat transfer :  $\Psi := (\Psi_1 \ \Psi_2)^T$
- Well-balanced Godunov schemes

## 3 Numerical results

- Radiative transfer with discontinuous opacity (R. Sentis)
- Couette flow with  $\neq$  accommodation coefficients
- Heat transfer with different Knudsen's (C.W. Siewert)
- Linear 1-D chemotaxis (Othmer-Hillen, Natalini)
- 1-D  $n^+nn^+$  MOSFET simulation (I.Gamba, A.Jungel)
- Gravitational Vlasov-Poisson (Dolbeault, Bouchut)



## Well-Balanced schemes : a quick story

A.-Y. LeRoux, may 1995, during the Ph.D. of Alain Zelmanse :

*If you simulate a glass of water with a small stone inside, it makes any numerical scheme unstable.*

The best discretization of  $\partial_t u = Au + Bu$  with  $A, B$  of different nature (e.g.  $Au = -\partial_x f(u)$ ,  $B(u) = g(x, u)$  or differential and Fredholm operators) is probably not a linear combination of already existing ones for  $\partial_t u = Au$  and  $\partial_t u = Bu$  alone.

Main ingredients :

- introduce the auxiliary equation for  $\Delta x > 0$ ,

$$\partial_t u + \partial_x f(u) = \Delta x \sum_j g(x, u) \delta(x - (j - \frac{1}{2})\Delta x)$$

- define correctly the non-conservative products
- set up the Godunov scheme for NC homogeneous eqn
- homogeneous Godunov has no viscosity at steady-state



## Several remaining open problems

- justify the "localization step" for general 1-D hyperbolic systems of balance laws (the limit  $\Delta x \rightarrow 0$  has been studied with wavefront-tracking techniques in [Amadori, L.G., Guerra, ARMA 2002]) and prove the definition of NC products.
- understand the "nonlinear resonance" phenomenon when  $\det(f_u)$  vanishes : intricate Riemann problems (cf. Liu, Isaacson-Temple, Vasseur, Goatin, Le Floch, [A.G.G. JDE'04]). Is it really useful numerically ?
- extend to multi-D, to high order ...
- extend to more general equations (the topic of today).



## The "localization step" : results with $BV$ theory

- 1-D scalar balance law :  $\partial_t u + \partial_x f(u) = k(x)g(u)$ ,  $f' > 0$ ,
- 2-velocity kinetic model :  $\partial_t f^\pm \pm \partial_x f^\pm = \mp(f^+ - f^-)$ .

Write  $k(x) = \partial_x a^1(x)$ , define a sequence  $a^\varepsilon(x) \rightarrow a(x) \in BV(\mathbb{R})$  which induces a sequence  $u^\varepsilon$  of usual Kruzkov solutions. Following early computations, [L.G., MCOM 2002], the  $2 \times 2$  system

$$\partial_t u + \partial_x f(u) - g(u)\partial_x a = 0, \quad \partial_t a = 0,$$

is Temple class. Its Riemann invariants are  $a$ ,  $w(u, a) = \phi^{-1}(\phi(u) - a)$ ,  $\phi' = f'/g$ .  $BV$  norm decays with time and 1-to-1 if  $f' > 0$ . Thus  $u^\varepsilon$  is uniformly  $BV$ -bounded and compact in  $L^1_{loc}$ . Hence  $g(u^\varepsilon)\partial_x a^\varepsilon$  becomes a well-defined non-conservative product in the sense of LeFloch-Tzavaras. NC product uses steady-state eqns  $\partial_x f(u) = k(x)g(u)$ .



## Linear models of Boltzmann equation

For simplicity, let's start with BGK model ( $\rightarrow$  Gross-Jackson) :

$$\partial_t f + \xi \partial_x f = \nu (\mathcal{M}(f) - f) := \mathcal{J}f, \quad \xi := \mathbf{v}_1,$$

If  $f(t, x, \mathbf{v}) = M(\mathbf{v})[1 + h(t, x, \mathbf{v})]$ , the eqn can be linearized :  
 $\partial_t h + \xi \partial_x h = -\nu (Id - \mathcal{P})h$ , with  $\mathcal{P}$  the orthogonal projection onto the vector space spanned by 5 collisional invariants.  $\mathcal{P}h(t, x, \mathbf{v}) =$

$$\int_{\mathbb{R}^3} M(\mathbf{v}') \left[ 1 + 2\mathbf{v} \cdot \mathbf{v}' + \frac{2}{3} \left( |\mathbf{v}|^2 - \frac{3}{2} \right) \left( |\mathbf{v}'|^2 - \frac{3}{2} \right) \right] h(t, x, \mathbf{v}') d\mathbf{v}'.$$

For  $\Delta x > 0$  the space-step of the computational grid,

$$\partial_t h + \xi \partial_x h = \nu \Delta x \sum_{j \in \mathbb{Z}} (\mathcal{P} - Id)h \delta \left( x - (j - \frac{1}{2})\Delta x \right).$$



Define the 5-components vector :

$$\Phi(\mathbf{v}) = \frac{1}{\pi^{\frac{3}{4}}} \left( 1 \quad \sqrt{\frac{2}{3}}(|\mathbf{v}|^2 - \frac{3}{2}) \quad \sqrt{2}\mathbf{v}_2 \quad \sqrt{2}\mathbf{v}_3 \quad \sqrt{2}\mathbf{v}_1 \right)^T.$$

A direct computation shows that : ( $T$  denotes transposition)

$$\mathcal{P}h(t, x, \mathbf{v}) = \int_{\mathbb{R}^3} M(\mathbf{v}') \left[ \Phi(\mathbf{v})^T \Phi(\mathbf{v}') \right] h(t, x, \mathbf{v}') d\mathbf{v}'.$$

Cercignani introduces the (normalized) functions :

$$\mathbf{G}(\mathbf{v}_2, \mathbf{v}_3) = \begin{pmatrix} g_1(\mathbf{v}_2, \mathbf{v}_3) \\ g_2(\mathbf{v}_2, \mathbf{v}_3) \\ g_3(\mathbf{v}_2, \mathbf{v}_3) \\ g_4(\mathbf{v}_2, \mathbf{v}_3) \end{pmatrix} = \frac{1}{\sqrt{\pi}} \begin{pmatrix} 1 \\ (\mathbf{v}_2^2 + \mathbf{v}_3^2 - 1) \\ \sqrt{2}\mathbf{v}_2 \\ \sqrt{2}\mathbf{v}_3 \end{pmatrix},$$

which are orthogonal in the following sense,

$$\int_{\mathbb{R}^2} g_i(\mathbf{v}_2, \mathbf{v}_3) g_j(\mathbf{v}_2, \mathbf{v}_3) \exp(-\mathbf{v}_2^2 - \mathbf{v}_3^2) d\mathbf{v}_2 d\mathbf{v}_3 = \delta_{i,j}.$$



With the notation  $\mathbf{v}_1 = \xi$ ,  $h(t, x, \mathbf{v})$  can be expanded :

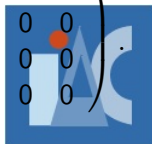
$$h(t, x, \mathbf{v}) = \sum_{i=1}^4 \Psi_i(t, x, \xi) g_i(\mathbf{v}_2, \mathbf{v}_3) + \Psi_5(t, x, \mathbf{v}),$$

where the components  $\Psi_i$  are “unusual moments” which read,

$$\Psi_i(t, x, \xi) = \int_{\mathbb{R}^2} h(t, x, \mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3) g_i(\mathbf{v}_2, \mathbf{v}_3) \exp(-\mathbf{v}_2^2 - \mathbf{v}_3^2) d\mathbf{v}_2 d\mathbf{v}_3.$$

$$\partial_t \Psi + \xi \partial_x \Psi + \Psi = \int_{\mathbb{R}} [\mathbf{P}(\xi) \mathbf{P}(\xi')^T + \mathbf{Q}(\xi) \mathbf{Q}(\xi')^T] \Psi(\xi') \frac{\exp(-|\xi'|^2)}{\sqrt{\pi}} d\xi',$$

$$\mathbf{P}(\xi) = \begin{pmatrix} \sqrt{\frac{2}{3}}(\xi^2 - \frac{1}{2}) & 1 & 0 & 0 \\ \sqrt{\frac{2}{3}} & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \mathbf{Q}(\xi) = \sqrt{2}\xi \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$





Microscopic (easy) eqn :  $\partial_t \Psi_5 + \xi \partial_x \Psi_5 + \Psi_5 = 0$ . Shear flows realize slns of “reduced viscosity equation” for  $\psi := \Psi_3, \Psi_4$  :

$$\partial_t \psi + \xi \partial_x \psi = \int_{\mathbb{R}} \psi(t, x, \xi') \frac{\exp(-|\xi'|^2)}{\sqrt{\pi}} d\xi' - \psi,$$

Well-balanced stems on solving the “forward-backward problem” :

$$\xi \partial_x \psi = \int_{\mathbb{R}} \psi(x, \xi') \frac{\exp(-|\xi'|^2)}{\sqrt{\pi}} d\xi' - \psi, \quad x \in (0, \Delta x),$$

with inflow boundary conditions. According to Chandrasekhar,  $\psi(x, \xi) = \exp(-x/\nu) \varphi_\nu(\xi)$  [translation invariance, Sturm-Liouville] which leads to a third kind linear integral eqn (cf. [Bart, Warnock, SIMA'73]) which admits “elementary slns” (Case, Zweifel, Cercignani, Siewert ...) and a superposition principle :

$$\psi(x, \xi) = \alpha + \beta(x - \xi) + \int_{\mathbb{R}} A(\nu) \exp(-x/\nu) \varphi_\nu(\xi) d\nu.$$



Forward-backward boundary-value problem for  $\Psi(x, \xi) \in \mathbb{R}^2$  :

$$\xi \partial_x \Psi + \Psi = \int_{\mathbb{R}} [\mathbf{P}(\xi) \mathbf{P}(\xi')^T + 2\xi\xi' \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}] \Psi(\xi') \frac{\exp(-|\xi'|^2)}{\sqrt{\pi}} d\xi',$$

Flux  $J = \int_{\mathbb{R}} \xi' \begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot \Psi(x, \xi') \frac{\exp(-|\xi'|^2)}{\sqrt{\pi}} d\xi'$  doesn't depend on  $x$ .

Same technique of "elementary slns" yields the explicit sln :

$$\Psi(x, \xi) = \sum_{i=1}^2 \mathbf{P}(\xi) [\alpha_i + \beta_i(x - \xi)] \vec{e}_i + \int_{\mathbb{R}} A_i(\nu) \Phi_i(\nu, \xi) \exp(-x/\nu) d\nu.$$

We have stationary slns and so we can build WB schemes !

Gaussian quadrature for strictly hyperbolic *DO* eqns :

$$\xi = (\xi_1, \xi_2, \dots, \xi_N) \in (0, 1)^N, \quad \omega = (\omega_1, \dots, \omega_N) \in \mathbb{R}^+.$$



# NC Riemann solver and WB Godunov scheme

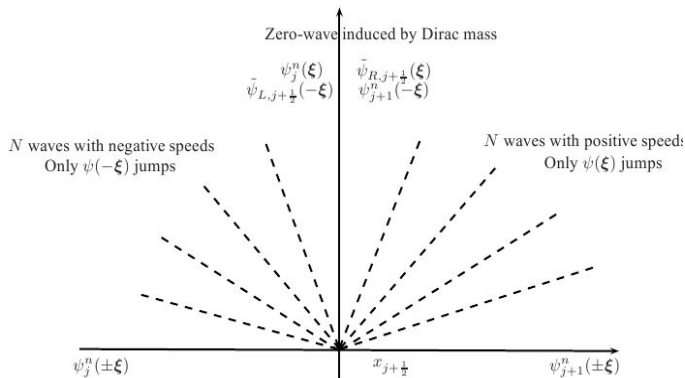


FIGURE 3. Self-similar solution of non-conservative Riemann problem.



Consistent Godunov scheme for shear or heat flows :

$$\begin{cases} \psi_j^{n+1}(\xi_k) = \psi_j^n(\xi_k) - \xi_k \frac{\Delta t}{\Delta x} \left( \psi_j^n(\xi_k) - \tilde{\psi}_{R,j-\frac{1}{2}}(\xi_k) \right), \\ \psi_j^{n+1}(-\xi_k) = \psi_j^n(-\xi_k) + \xi_k \frac{\Delta t}{\Delta x} \left( \tilde{\psi}_{L,j+\frac{1}{2}}(-\xi_k) - \psi_j^n(-\xi_k) \right), \end{cases}$$

with for all  $j$  in the computational domain and  $N \in \mathbb{N}$  :

$$\begin{pmatrix} \tilde{\psi}_{R,j+\frac{1}{2}}(\xi) \\ \tilde{\psi}_{L,j+\frac{1}{2}}(-\xi) \end{pmatrix} = \tilde{M} M^{-1} \begin{pmatrix} \psi_j^n(\xi) \\ \psi_{j+1}^n(-\xi) \end{pmatrix}.$$

$M$  and  $\tilde{M}$  are matrices of passage between the base of elementary slns and the usual space  $(x, \xi)$ . (pre-processing step)

We are exact in  $x$ , only  $\xi$  has been discretized.



At each interface  $j + \frac{1}{2}$ , solve a linear problem :

$$M \begin{pmatrix} \mathbf{A} \\ \alpha \\ \mathbf{B} \\ \beta \end{pmatrix} = \begin{pmatrix} \psi_j^n(\xi) \\ \psi_{j+1}^n(-\xi) \end{pmatrix} \in \mathbb{R}_+^{2N},$$

where the  $2N \times 2N$  matrices  $M, \tilde{M}$  read for  $\nu := \{\nu_1, \nu_2, \dots, \nu_{N-1}\}$ ,

$$M = \begin{pmatrix} (1 - \xi \otimes \nu^{-1})^{-1} & \mathbf{1}_{\mathbb{R}^N} & (1 + \xi \otimes \nu^{-1})^{-1} \exp(-\frac{\Delta x}{\nu}) & -\xi \\ (1 + \xi \otimes \nu^{-1})^{-1} \exp(-\frac{\Delta x}{\nu}) & \mathbf{1}_{\mathbb{R}^N} & (1 - \xi \otimes \nu^{-1})^{-1} & \Delta x + \xi \end{pmatrix}.$$

$$\tilde{M} = \begin{pmatrix} (1 - \xi \otimes \nu^{-1})^{-1} \exp(-\frac{\Delta x}{\nu}) & \mathbf{1}_{\mathbb{R}^N} & (1 + \xi \otimes \nu^{-1})^{-1} & \Delta x - \xi \\ (1 + \xi \otimes \nu^{-1})^{-1} & \mathbf{1}_{\mathbb{R}^N} & (1 - \xi \otimes \nu^{-1})^{-1} \exp(-\frac{\Delta x}{\nu}) & \xi \end{pmatrix},$$

the interface values are given by :

$$\begin{pmatrix} \tilde{\psi}_{R,j+\frac{1}{2}}(\xi) \\ \tilde{\psi}_{L,j+\frac{1}{2}}(-\xi) \end{pmatrix} = \tilde{M} M^{-1} \begin{pmatrix} \psi_j^n(\xi) \\ \psi_{j+1}^n(-\xi) \end{pmatrix}.$$



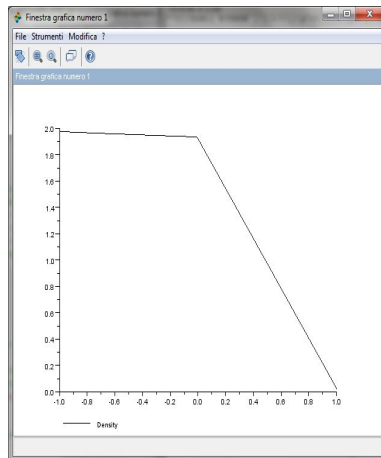
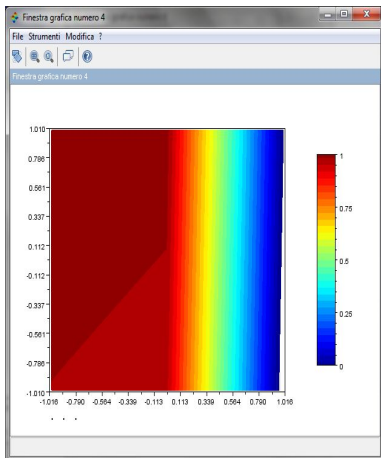
## Numerical results with several models

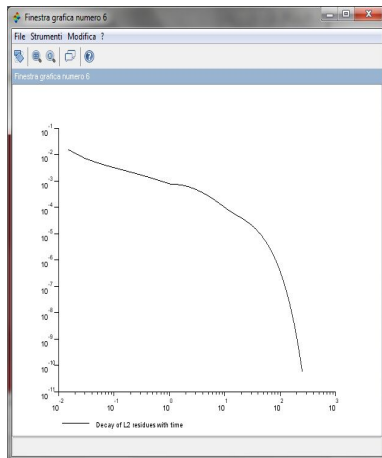
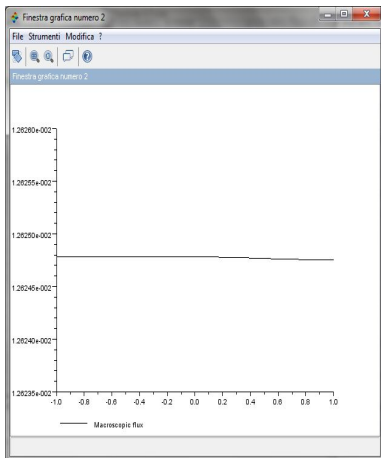
IBVP for linear kinetic equation :

$$\partial_t f + v \partial_x f = \kappa(x) \left( \frac{1}{2} \int_{-1}^1 f(t, x, v') dv' - f \right),$$

with variable (discontinuous) opacity  $\kappa$  and inflow boundary conditions.  $\kappa(x) = 1 + 49\chi(x > 0)$  with  $x \in ]-1, 1[$ . We want the flow  $\int_{-1}^1 v' f(t, x, v') dv'$  to be constant at numerical steady-state! Positive inflow in the transparent region ( $x < 0, \kappa = 1$ ) and zero re-entry in the opaque zone ( $x > 0, \kappa = 50$ ). [JQSRT'11]  
The WB Godunov scheme can be converted into an AP scheme for the diffusion approximation in the parabolic scaling (exactly like in [G-Toscani, 2002 & 2004]).









IBVP for linear kinetic equation :

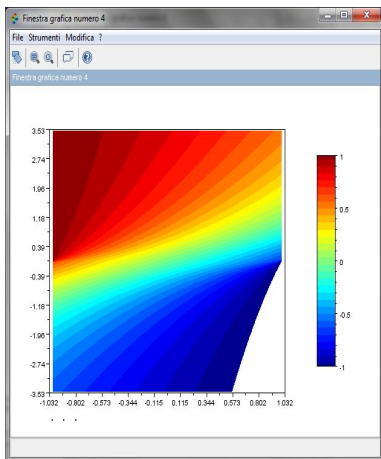
$$\partial_t \psi + v \partial_x \psi = \int_R \psi(t, x, v') \frac{\exp(-|v'|^2)}{\sqrt{\pi}} dv' - \psi,$$

with inflow boundary conditions corresponding to infinite plates moving at  $\pm u_{wall}$  and  $\alpha \in [0, 1]$  is the accommodation coefficient :

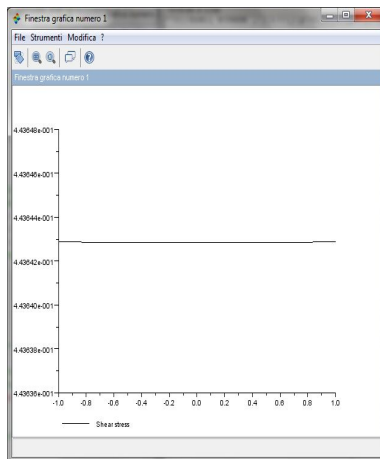
$$\psi(t, x = \pm 1, \mp |v|) = \mp \alpha u_{wall} + (1 - \alpha) \psi(t, x = \pm 1, \pm |v|).$$

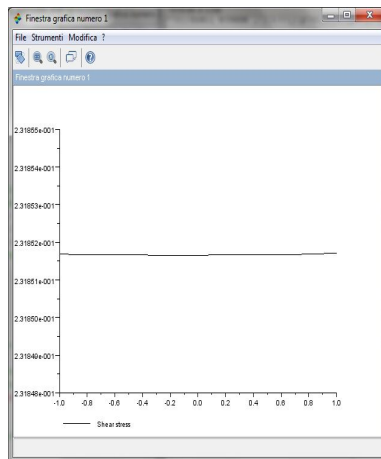
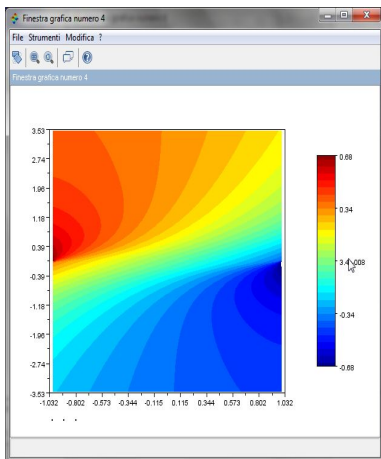
We want the shear stress  $\int_{-1}^1 v' \psi(t, x, v') dv'$  to be constant at numerical steady-state! (cf. papers by L. Barichello & C.W. Siewert + collaborators)





$\alpha = 1$  : no specular reflection.





$\alpha = \frac{1}{2}$  : half specular reflection.



$2 \times 2$  kinetic system for density and temperature fluctuations :

$$\partial_t \Psi + \xi \partial_x \Psi + \Psi = \int_{\mathbb{R}} [\mathbf{P}(\xi) \mathbf{P}(\xi')^T + \mathbf{Q}(\xi) \mathbf{Q}(\xi')^T] \Psi(\xi') \frac{\exp(-|\xi'|^2)}{\sqrt{\pi}} d\xi,$$

$$\mathbf{P}(\xi) = \begin{pmatrix} \sqrt{\frac{2}{3}}(\xi^2 - \frac{1}{2}) & 1 \\ \sqrt{\frac{2}{3}} & 0 \end{pmatrix}, \quad \mathbf{Q}(\xi) = \sqrt{2}\xi \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.$$

We want the macroscopic mass flow and the normalized heat flow to be constant at numerical steady-state with  $\neq$  acc. coeffs  $\alpha_i$ .

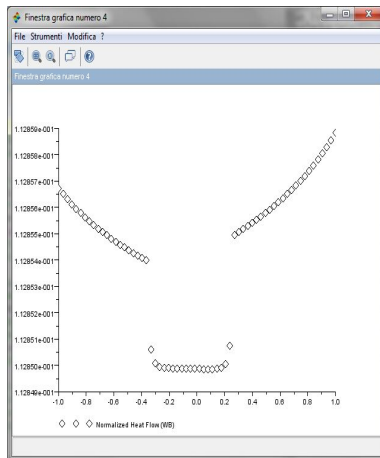
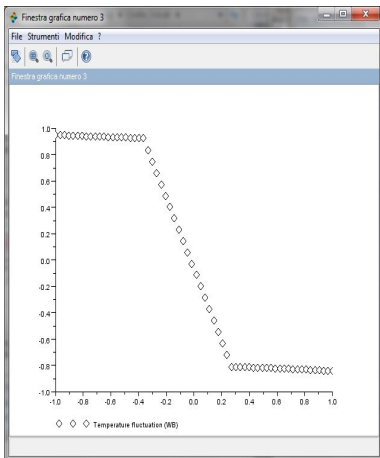
$$\Psi(t, \pm 1, \mp |\xi|) = (1 - \alpha_i) \Psi(t, \pm 1, \pm |\xi|) \mp \alpha_i \delta_i \sqrt{\pi} \begin{pmatrix} \xi^2 + \beta_i \\ 1 \end{pmatrix}.$$

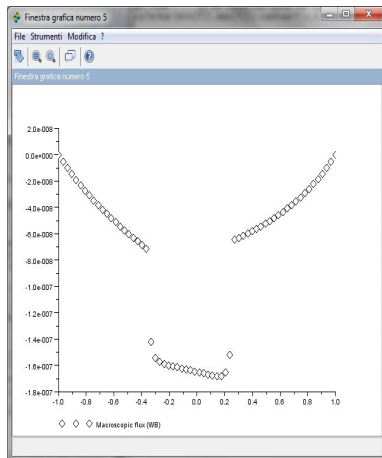
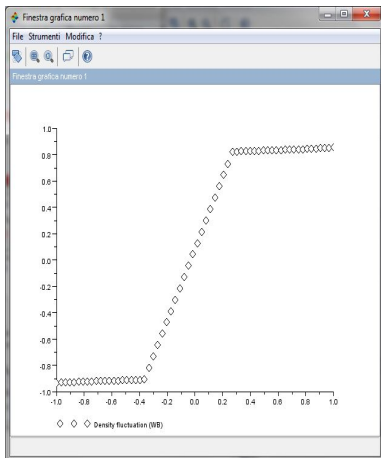
Zero macroscopic flux through the infinite walls [L.G.'11].

Variable Knudsen number in the domain :

$$\varepsilon = 1 \text{ for } x \in \left(-1, -\frac{1}{3}\right) \cup \left(\frac{1}{3}, 1\right), \quad \varepsilon = 10^{-2} \text{ elsewhere.}$$







Weakly nonlinear system with "biased" velocity redistribution :

$$\partial_t f + v \partial_x f + f = \frac{1}{2} \int_{-1}^1 [1 + 2v \cdot (a(\partial_x S) v')] f(t, x, v') dv' - f,$$

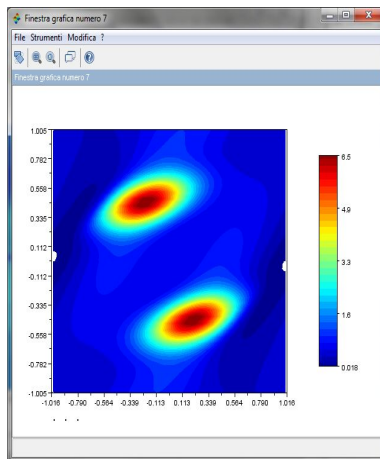
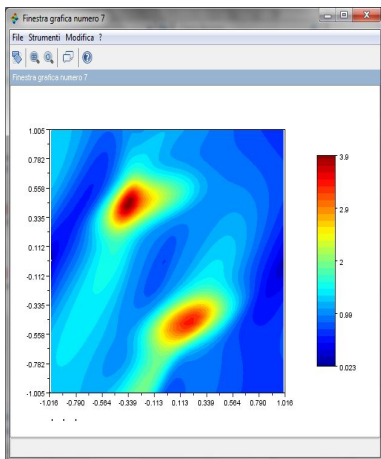
specular BC, and  $S(t, x)$  chemo-attractant concentration sln of

$$\partial_t S - D \partial_{xx} S = \alpha \rho - \beta S \quad + \text{Neumann BC.}$$

Steady-states are constant in  $x$  [OH] : we want to see the differences due to  $\partial_x S$  compared to radiative transfer eqn.  $2 \times 2$  model studied in detail by extending [G.Toscani '04]. Especially,  $v \in \{-1, 1\}$  implies that : any numerical stationary-state with non-zero flux is not Maxwellian :

$$f^+ = f^- \Rightarrow J = f^+ - f^- = 0, \quad [\text{Natalini, Ribot, G.}]$$

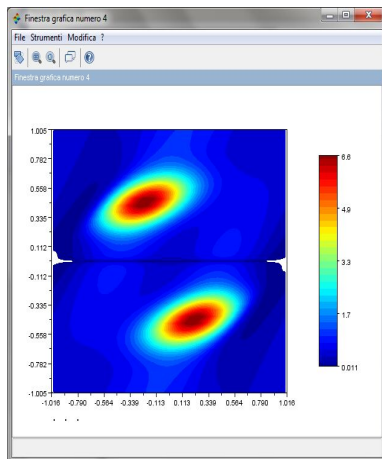
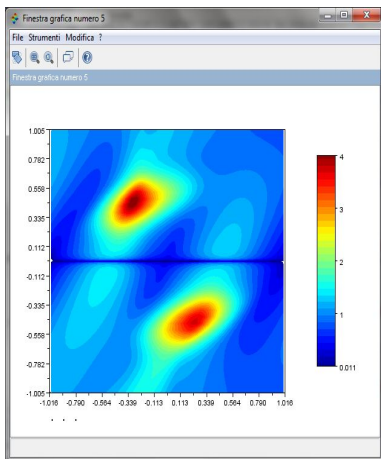




Numerical solution with time-splitting. (viscous!)







Numerical solution with kinetic well-balanced.



Weakly nonlinear system (Vlasov-Poisson + linear collisions) :

$$\partial_t f + v \partial_x f + E(t, x) \partial_v f = \frac{1}{\varepsilon} \left( \frac{\exp(-|v|^2)}{\sqrt{\pi}} \int_{\mathbb{R}} f(t, x, v') dv' - f \right),$$

with the electric field  $E = -\partial_x \Phi$  and

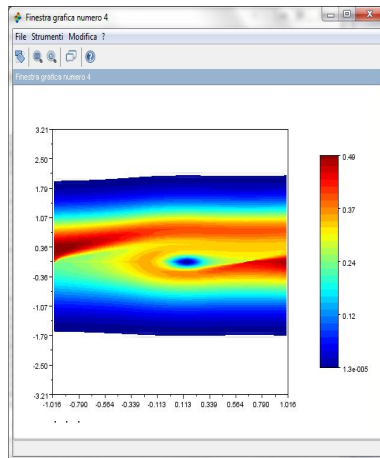
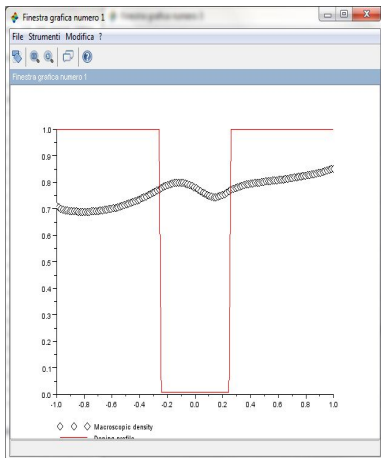
$$-\lambda^2 \partial_{xx} \Phi(t, x) = \int_{\mathbb{R}} f(t, x, v) dv - D(x),$$

$D$  the discontinuous doping profile and the relaxation time passes from  $\varepsilon \simeq 0.01/0.0001$  in doped areas to  $\varepsilon \simeq 1/\infty$  in the channel (few collisions or ballistic).  $\lambda =$  scaled Debye length.

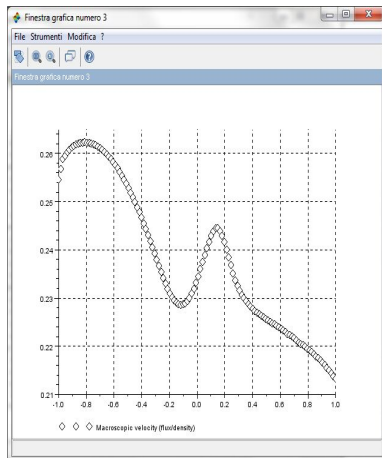
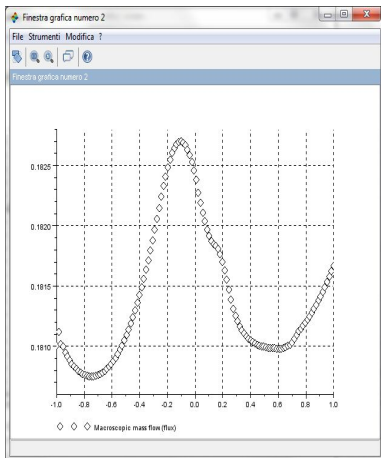
We want  $\int_{\mathbb{R}} v f(t, x, v) dv$  at least continuous in  $x$ , or even constant at numerical steady-state in order to compute the current-voltage relation without (too much ?) averaging.

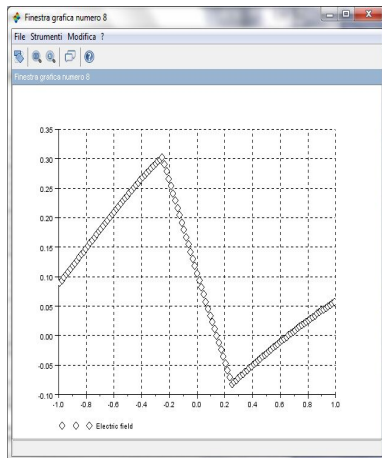
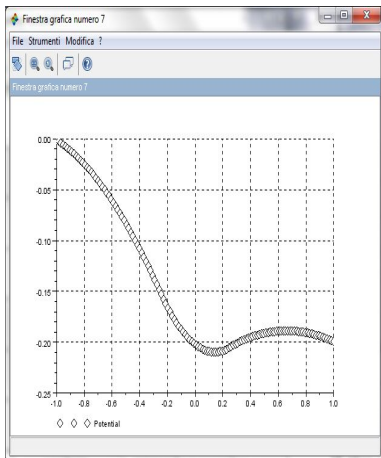


# Big value of $\varepsilon$ : Vlasov-type behavior

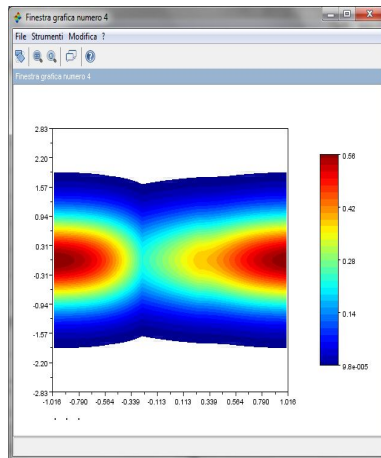
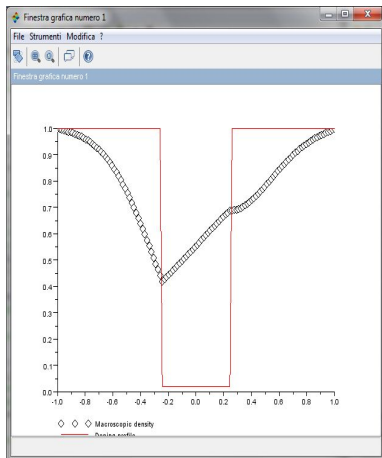


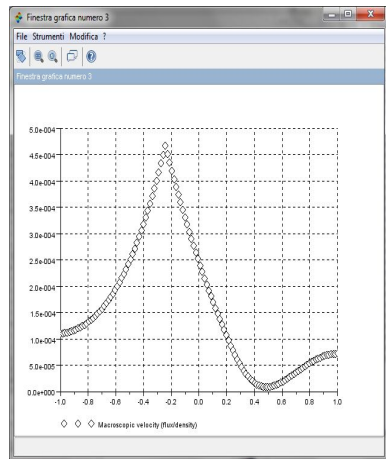
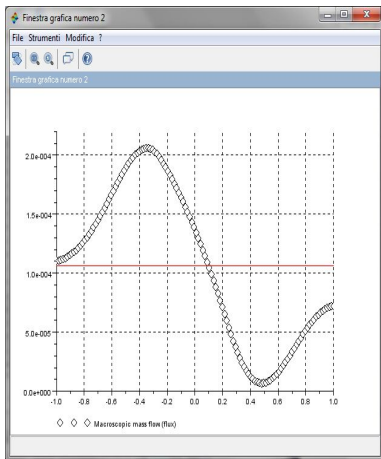
Maxwellian boundary conditions ( $\alpha = 1$ , no spec reflexion).





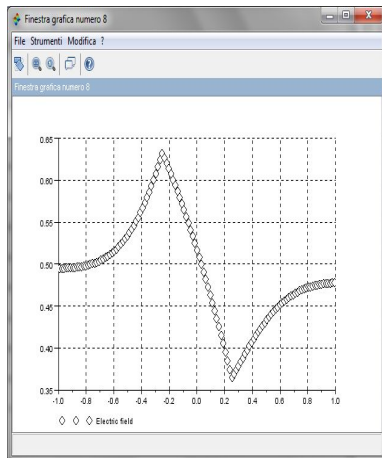
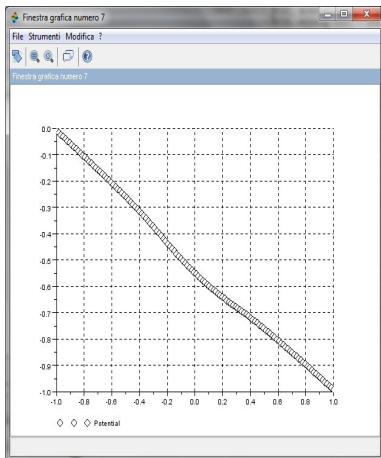
## Numerical results

1-D  $n^+ nn^+$  MOSFET simulation (I.Gamba, A.Jungel) $\varepsilon = 0.0002$  & 1 (channel) : strong collisions"Neighbor" boundary conditions ( $\alpha = 1$ , no spec reflexion).



Macroscopic flow (current) continuous but not constant.







## Approximate elementary solutions for Vlasov-collisions model :

$$v\partial_x f + E\partial_v f = M(v) \int f(v') dv' - f + B.C.$$

Observe that  $\tilde{M}(x, v) = \exp(-v^2 + 2Ex)$  is an exact solution (both sides vanish). One seeks  $f$  in the form :  $f(x, v) = \tilde{M}(x, v)g(x, v)$ ,

$$v\partial_x(g\tilde{M}) + E\partial_v(g\tilde{M}) = \tilde{M} \left[ v\partial_x g + \underbrace{E\partial_v g}_{=0!} \right] = M(v) \int \tilde{M}' g' dv' - \tilde{M} g.$$

Simplify by  $\tilde{M}$  and observe that :  $\frac{M(v)}{\tilde{M}(x, v)} \tilde{M}(x, v') = M(v')$ . Thus

$v\partial_x g + g = \int M(v') g(x, v') dv'$  and this admits usual elementary solutions by writing  $g(x, v) = \exp(-x/\nu) \varphi_\nu(v)$  and then ...

Note :  $g(x, v) \exp(2Ex)$  "nearly" satisfies Vlasov eqn.



Weakly nonlinear system (Vlasov-Poisson) :

$$\partial_t f + v \partial_x f + E(t, x) \partial_v f = 0,$$

with the attractive gravity field  $E = -\partial_x \Phi$  and

$$\partial_{xx} \Phi(t, x) = \int_{\mathbb{R}} f(t, x, v) dv.$$

We want to see circular motion even if macroscopic quantities display strong discontinuities by using a variant of the Perthame-Simeoni scheme [PS Calcolo'01] which consists in rewriting it with interface values computed with matrix products (matrix depends on interpolation in  $v$ ).



