

A new Well-Balanced scheme for a hyperbolic model of chemotaxis

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Hyperbolic model of chemotaxis

$$\partial_t \rho + \partial_x (\rho u) = 0, \quad (1)$$

$$\partial_t (\rho u) + \partial_x (\rho u^2 + p) = \chi \rho \partial_x \phi - \alpha \rho u, \quad (2)$$

$$\partial_t \phi - D \partial_{xx} \phi = a \rho - b \phi, \quad (3)$$

where

- $\rho(x, t) \geq 0$: particles density,
- $u(x, t) \in \mathbb{R}$: mean velocity,
- $\phi(x, t) \geq 0$: concentration of chemoattractant,
- $p(\rho) = \varepsilon \rho^\gamma$: pressure law, with $\gamma > 1$ adiabatic exponent and $\varepsilon > 0$ a constant,
- $\chi \geq 0, \alpha \geq 0, D > 0, a > 0$ and $b > 0$ some parameters.

Objectives

- Preserve equilibrium states (at rest, with $u = 0$), that are given by

$$\begin{cases} \frac{\varepsilon}{\chi} \frac{\gamma}{\gamma-1} \rho^{\gamma-1} - \phi = K, \\ -D \partial_{xx} \phi = a\rho - b\phi, \end{cases} \quad (4)$$

with a constant K .

- W-B scheme on the hyperbolic part (1)-(2)^{1,2}, and also on the equation (3) for ϕ .

¹Natalini, Ribot, Twarogowska, CMS 2014.

²Twarogowska, PhD Thesis 2011.

Outline

- Hyperbolic model
- Full model
- Numerical results

Hyperbolic model

We first look at the two first equation (1)-(2), that we rewrite as

$$\partial_t w + \partial_x F(w) = S(w) \quad (5)$$

with

$$w = \begin{pmatrix} \rho \\ \rho u \end{pmatrix}, F(w) = \begin{pmatrix} \rho u \\ \rho u^2 + p \end{pmatrix} \text{ and } S(w) = \begin{pmatrix} 0 \\ \chi \rho \partial_x \phi - \alpha \rho u \end{pmatrix},$$

considering ϕ as a known source term.

- First study: without friction ($\alpha = 0$).
- Second study: with friction ($\alpha > 0$).

Approximate Riemann solver

Approximate Riemann solver $\tilde{w}(\frac{x}{t}, w_L, w_R)$ defined by:

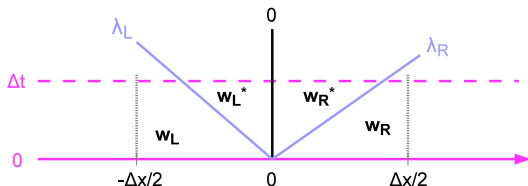
- velocities $\lambda_L < 0 < \lambda_R$:

$$\lambda_L = \min(0^-, \lambda_L^-, \lambda_R^-) \quad \text{and} \quad \lambda_R = \max(0^+, \lambda_L^+, \lambda_R^+),$$

where λ_L^\pm and λ_R^\pm denote the eigenvalues of the flux Jacobian matrix:

$$\lambda^\pm = u \pm c \quad \text{where} \quad c = c(\rho) = \sqrt{P'(\rho)} = \sqrt{\varepsilon \gamma \rho^{\gamma-1}},$$

- intermediate states w_L^* and w_R^* (will be defined later),
- the CFL condition: $\frac{\Delta t}{\Delta x} \max(|\lambda_L|, |\lambda_R|) \leq \frac{1}{2}$.



HLL consistency condition

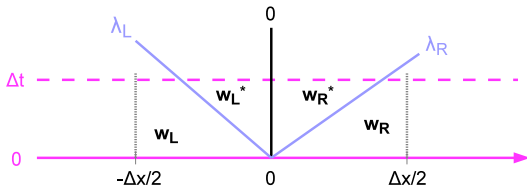
Consistency condition from Harten, Lax and van Leer:

$$\underbrace{\frac{1}{\Delta x} \int_{-\frac{\Delta x}{2}}^{\frac{\Delta x}{2}} \tilde{w}\left(\frac{x}{\Delta t}, w_L, w_R\right) dx}_{\tilde{A}} = \underbrace{\frac{1}{\Delta x} \int_{-\frac{\Delta x}{2}}^{\frac{\Delta x}{2}} w_R\left(\frac{x}{\Delta t}, w_L, w_R\right) dx}_{A_R},$$

with $w_R\left(\frac{x}{\Delta t}, w_L, w_R\right)$ the exact solution of the Riemann problem.

- Left side:

$$\tilde{A} = \frac{1}{2} (w_L + w_R) + \frac{\Delta t}{\Delta x} (\lambda_L (w_L - w_L^*) + \lambda_R (w_R^* - w_R)).$$



$$\partial_t w + \partial_x F(w) = S(w) \quad (5)$$

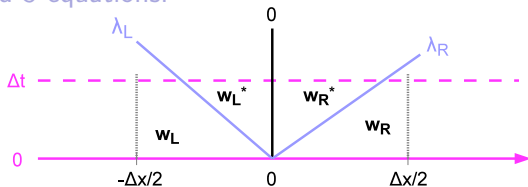
- Right side (by integrating on $[0, \Delta t] \times [-\frac{\Delta x}{2}, \frac{\Delta x}{2}]$ the exact equation (5)) in the case $\alpha = 0$:

$$A_{\mathcal{R}} = \frac{1}{2} (w_L + w_R) - \frac{\Delta t}{\Delta x} (F(w_R) - F(w_L)) + \Delta t \begin{pmatrix} 0 \\ S_{\mathcal{R}} \end{pmatrix}.$$

- Exact source term $S_{\mathcal{R}} = \frac{1}{\Delta t \Delta x} \int_0^{\Delta t} \int_{-\frac{\Delta x}{2}}^{\frac{\Delta x}{2}} \chi \rho \partial_x \phi dx dt$ approximated by S^* .

- Four other unknowns: $w_L^* = \begin{pmatrix} \rho_L^* \\ \rho_L^* u_L^* \end{pmatrix}$ and $w_R^* = \begin{pmatrix} \rho_R^* \\ \rho_R^* u_R^* \end{pmatrix}$.

→ We need 5 equations.



- Two first equation: $\tilde{A} = A_{\mathcal{R}} \Leftrightarrow$

$$\lambda_L (\rho_L - \rho_L^*) + \lambda_R (\rho_R^* - \rho_R) = \rho_L u_L - \rho_R u_R,$$

$$\lambda_L (\rho_L u_L - \rho_L^* u_L^*) + \lambda_R (\rho_R^* u_R^* - \rho_R u_R) = \rho_L u_L^2 + p_L - \rho_R u_R^2 - p_R + \Delta x S^*.$$

- Third equation: $\rho_L^* u_L^* = \rho_R^* u_R^* =: q^*$.
- Two last equations: study the steady states at rest.

Steady states at rest

- Steady states at rest associated to (5) given by:
$$\begin{cases} u = 0, \\ e - \chi\phi = K, \end{cases}$$

where $e(\rho)$ is defined by $\partial_x e = \frac{1}{\rho} \partial_x P$ which is, since $P(\rho) = \varepsilon \rho^\gamma$:

$$e(\rho) = \varepsilon \frac{\gamma}{\gamma - 1} \rho^{\gamma-1} + e_0$$

with e_0 an arbitrary constant.

- In the Riemann problem:
$$\begin{cases} u_L = u_R = 0, \\ e_L - \chi\phi_L = e_R - \chi\phi_R = K. \end{cases}$$
- Approximated Riemann solver preserves steady states at rest:

$$\begin{cases} u_L^* = u_R^* = 0 \quad (\Rightarrow q^* = 0), \\ e_L^* - \chi\phi_L = e_R^* - \chi\phi_R = K. \end{cases}$$

Source-term approximation³

- We are at steady state $\Rightarrow \tilde{A} = A_{\mathcal{R}}$ becomes

$$\begin{cases} \lambda_L(\rho_L - \rho_L^*) + \lambda_R(\rho_R^* - \rho_R) = 0, \\ (\lambda_R - \lambda_L)q^* + p_R - p_L = \Delta x S^*. \end{cases}$$

- We want to preserve steady states \Rightarrow we have to ensure $q^* = 0$
 \Rightarrow we suggest to put the following consistent expression of S^* :

$$S^* = \frac{\chi}{\Delta x} \frac{p_R - p_L}{e_R - e_L} (\phi_R - \phi_L).$$

- \rightarrow Fourth equation.
- \rightarrow Necessary condition for Well-Balanced property.

³Berthon, Chalons, submitted.

- For the last equation, we choose to impose

$$e_L \frac{\rho_L^*}{\rho_L} - \chi \phi_L = e_R \frac{\rho_R^*}{\rho_R} - \chi \phi_R,$$

which is consistent with $e_R - e_L = \phi_R - \phi_L$ and gives a linearization of the equation $\partial_x e = \chi \partial_x \phi$.

→ Sufficient condition for Well-Balanced property.

- Solving the system of five equations \Rightarrow expressions for ρ_L^* , ρ_R^* , q^* and S^* .

Case with friction: $\alpha > 0$

- What changes? The second equation:

$$\partial_t (\rho u) + \partial_x (\rho u^2 + p) = \chi \rho \partial_x \phi - \alpha \rho u.$$

- Integrating on $[0, \Delta t] \times [-\frac{\Delta x}{2}, \frac{\Delta x}{2}]$ gives

$$\mathcal{F}(\Delta t) = \frac{1}{2} (\rho_L u_L + \rho_R u_R) - \frac{\Delta t}{\Delta x} (\rho_R u_R^2 + p_R - \rho_L u_L^2 - p_L) + \Delta t S_{\mathcal{R}} - \alpha \int_0^{\Delta t} \mathcal{F}(t) dt,$$

where

$$\mathcal{F}(t) = \frac{1}{\Delta x} \int_{-\Delta x/2}^{\Delta x/2} (\rho u)_{\mathcal{R}}(x, t) dx.$$

→ Equation in $\mathcal{F}(\Delta t)$:

$$\mathcal{F}'(\Delta t) = \frac{1}{2} (\dots) - \frac{\Delta t}{\Delta x} (\dots) + \Delta t S_{\mathcal{R}} - \alpha \mathcal{F}(\Delta t).$$

- Solution:

$$\mathcal{F}(\Delta t) = Ke^{-\alpha\Delta t} + \frac{1}{\alpha} \left[-\frac{1}{\Delta x} (\rho_R u_R^2 + p_R - \rho_L u_L^2 - p_L) + S_{\mathcal{R}} \right],$$

with

$$K = \frac{1}{2} (\rho_L u_L + \rho_R u_R) - \frac{1}{\alpha} \left[-\frac{1}{\Delta x} (\rho_R u_R^2 + p_R - \rho_L u_L^2 - p_L) + S_{\mathcal{R}} \right].$$

- HLL consistency condition: $\tilde{A}_2 = \mathcal{F}(\Delta t)$.
- Approximation of $S_{\mathcal{R}}$ in order to preserve equilibrium ($u = 0$): S^* defined previously suits.
- ρ_L^* and ρ_R^* not changed.
- q^* is the only quantity that has to be modified when taking $\alpha > 0$.

Correction for the positivity

Min-Max procedure in order to ensure $\rho_L^* \geq 0$ and $\rho_R^* \geq 0$, where

$$\rho_L^* = \rho_L + \frac{\lambda_R \mathcal{R}}{\delta_R \lambda_L - \delta_L \lambda_R} - \delta_R \frac{\rho_L u_L - \rho_R u_R}{\delta_R \lambda_L - \delta_L \lambda_R},$$

$$\rho_R^* = \rho_R + \frac{\lambda_L \mathcal{R}}{\delta_R \lambda_L - \delta_L \lambda_R} - \delta_L \frac{\rho_L u_L - \rho_R u_R}{\delta_R \lambda_L - \delta_L \lambda_R},$$

with $\delta_R := \frac{e_R}{\rho_R}$, $\delta_L := \frac{e_L}{\rho_L}$ and $\mathcal{R} := \chi(\phi_R - \phi_L) - e_R$.

- For simplicity reasons: $\lambda_R = -\lambda_L$.
- Consistency gives now:

$$\tilde{A}_1 = A_{\mathcal{R},1} \Leftrightarrow \rho_L^* + \rho_R^* = \rho_L + \rho_R - \frac{\rho_R u_R - \rho_L u_L}{\lambda_R} =: 2\rho_{HLL}.$$

- We take:

$$\rho_R^* = \min(\max(0, \rho_R^*), 2\rho_{HLL}),$$

$$\rho_L^* = \min(\max(0, \rho_L^*), 2\rho_{HLL}).$$

Full model

We now look at the equation (3) on ϕ , that we rewrite as:

$$\partial_t \phi - D \partial_x \psi = a \rho - b \phi,$$

where ρ is assumed to be known (since computed previously) and $\psi := \partial_x \phi$.

HLL consistency condition

Consistency condition from Harten, Lax and van Leer:

$$\underbrace{\frac{1}{\Delta x} \int_{-\Delta x/2}^{\Delta x/2} \tilde{\phi} \left(\frac{x}{\Delta t}, \phi_L, \phi_R \right) dx}_{\tilde{A}} = \underbrace{\frac{1}{\Delta x} \int_{-\Delta x/2}^{\Delta x/2} \phi_{\mathcal{R}} \left(\frac{x}{\Delta t}, \phi_L, \phi_R \right) dx}_{A_{\mathcal{R}}},$$

with $\phi_{\mathcal{R}}$ the exact Riemann solver and $\tilde{\phi}$ the approximated one.

- Left side:

$$\tilde{A} = \frac{1}{2} (\phi_L + \phi_R) + \frac{\Delta t}{\Delta x} (\lambda_L (\phi_L - \phi_L^*) + \lambda_R (\phi_R^* - \phi_R)).$$

$$\partial_t \phi - D \partial_x \psi = a \rho - b \phi \quad (3)$$

- Right side (by integrating on $[0, \Delta t] \times [-\frac{\Delta x}{2}, \frac{\Delta x}{2}]$ the exact equation (3)):

$$A_{\mathcal{R}} = \frac{1}{2} (\phi_L + \phi_R) + \frac{D \Delta t}{\Delta x} (\psi_R - \psi_L) + \frac{1}{\Delta x} \int_0^{\Delta t} \int_{-\Delta x/2}^{\Delta x/2} a \rho_{\mathcal{R}} - b \phi_{\mathcal{R}} dx dt.$$

- First part of the model:

$$\frac{1}{\Delta x} \int_{-\Delta x/2}^{\Delta x/2} \rho_{\mathcal{R}}(x, t) dx = \frac{1}{2} (\rho_L + \rho_R) - \frac{t}{\Delta x} (\rho_R u_R - \rho_L u_L).$$

- We get:

$$\begin{aligned} \mathcal{F}(\Delta t) := A_{\mathcal{R}} &= \frac{1}{2} (\phi_L + \phi_R) + \frac{D \Delta t}{\Delta x} (\psi_R - \psi_L) \\ &+ a \left(\frac{\Delta t}{2} (\rho_L + \rho_R) - \frac{\Delta t^2}{2 \Delta x} (\rho_R u_R - \rho_L u_L) \right) - b \int_0^{\Delta t} \mathcal{F}(t) dt. \end{aligned}$$

→ Equation on $\mathcal{F}(\Delta t)$:

$$\mathcal{F}'(\Delta t) + b\mathcal{F}(\Delta t) = \frac{D}{\Delta x} (\psi_R - \psi_L) + a \left(\frac{1}{2} (\rho_L + \rho_R) - \frac{\Delta t}{\Delta x} (\rho_R u_R - \rho_L u_L) \right).$$

- Solution:

$$\mathcal{F}(\Delta t) = \frac{1}{2} (\phi_L + \phi_R) e^{-b\Delta t} + \alpha \Delta t + \beta (1 - e^{-b\Delta t})$$

with $\alpha = -\frac{a}{b\Delta x} (\rho_R u_R - \rho_L u_L)$ and

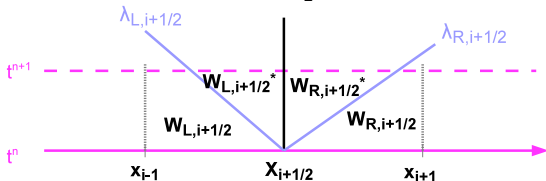
$$\beta = \frac{D}{b\Delta x} (\psi_R - \psi_L) + \frac{a}{2b} (\rho_L + \rho_R) + \frac{a}{b^2\Delta x} (\rho_R u_R - \rho_L u_L).$$

- Consistency condition: $\tilde{A} = A_{\mathcal{R}} = \mathcal{F}(\Delta t)$.
- + Choice: $\phi_L - \phi_L^* = \phi_R - \phi_R^*$.
- Expressions for ϕ_L^* and ϕ_R^* .
- And what about ψ_L and ψ_R ? Answer later...

Finite Volumes scheme

- 1D domain $[0, L]$ discretized by $N + 1$ points: $x_i = i\Delta x$, $i = 0, \dots, N$, $\Delta x = \frac{L}{N}$.
- Evolution in time of $w_i^n \approx \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} w(x, t^n) dx$ and $\phi_i^n \approx \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} \phi(x, t^n) dx$, where $t^n = n\Delta t$ for a time step Δt .
- Scheme coming from the previously defined Riemann solvers:

$$\begin{cases} w_i^{n+1} = w_i^n - \frac{\Delta t}{\Delta x} \left(\lambda_{i-\frac{1}{2},R} \left(w_i^n - w_{i-\frac{1}{2},R}^* \right) - \lambda_{i+\frac{1}{2},L} \left(w_i^n - w_{i+\frac{1}{2},L}^* \right) \right), \\ \phi_i^{n+1} = \phi_i^n - \frac{\Delta t}{\Delta x} \left(\lambda_{i-\frac{1}{2},R} \left(\phi_i^n - \phi_{i-\frac{1}{2},R}^* \right) - \lambda_{i+\frac{1}{2},L} \left(\phi_i^n - \phi_{i+\frac{1}{2},L}^* \right) \right). \end{cases}$$



Definition of ψ_i^n

- ψ_i^n such that good approximation of $(\partial_x \phi)_i^n$, for example of the form

$$\psi_i^n = \frac{1}{2\Delta x} (\phi_{i+1}^n - \phi_{i-1}^n) \times 1(\Delta x)$$

where $1(\Delta x)$ has to be consistent with 1 when Δx tends to 0.

- $1(\Delta x)$: correction term such that $\phi_i^{n+1} = \phi_i^n$ at equilibrium in the particular case $\gamma = 2$.

Equilibrium for $\gamma = 2$

- Equilibrium given by:

$$\begin{cases} u = 0, \\ \phi = \frac{2\varepsilon}{\chi}\rho + K, \\ D\partial_{xx}\phi - b\phi = -a\rho, \end{cases} \Rightarrow \begin{cases} u = 0, \\ \partial_{xx}\rho - \frac{\chi}{2\varepsilon D} \left(\frac{2\varepsilon b}{\chi} - a \right) \rho = Kb \frac{\chi}{2\varepsilon D}. \end{cases}$$

- Solutions^{1,2}:

if $\rho = 0$: $\phi(x) = A \cosh(x\sqrt{b}) + B \sinh(x\sqrt{b})$,

if $\rho > 0$, $C < 0$: $\phi(x) = A \cos(x\sqrt{|C|}) + B \sin(x\sqrt{|C|}) - \phi_p$, $\rho(x) = \frac{\chi}{2\varepsilon}(\phi(x) - K)$,

if $\rho > 0$, $C > 0$: $\phi(x) = A \cosh(x\sqrt{C}) + B \sinh(x\sqrt{C}) - \phi_p$, $\rho(x) = \frac{\chi}{2\varepsilon}(\phi(x) - K)$,

where A and B are some constants, $C = \frac{1}{D} \left(b - \frac{a\chi}{2\varepsilon} \right)$ and $\phi_p = \frac{Ka\chi}{2\varepsilon b - a\chi}$.

¹Natalini, Ribot, Twarogowska, CMS 2014.

²Twarogowska, PhD Thesis 2011.

- Injecting these solutions in the Finite Volumes scheme and imposing $\phi_i^{n+1} = \phi_i^n$ gives the appropriate expression of $I(\Delta x)$:

$$\text{if } \rho = 0 : \quad I(\Delta x) = \frac{\Delta x^2}{2} \frac{b}{\cos(\sqrt{b}\Delta x) - 1},$$

$$\text{if } \rho > 0, C < 0 : \quad I(\Delta x) = \frac{\Delta x^2}{2} \frac{C}{\cos(\sqrt{|C|}\Delta x) - 1},$$

$$\text{if } \rho > 0, C > 0 : \quad I(\Delta x) = \frac{\Delta x^2}{2} \frac{C}{\cosh(\sqrt{C}\Delta x) - 1}.$$

- Expression of ψ_i^n

$$\psi_i^n = \frac{1}{2\Delta x} (\phi_{i+1}^n - \phi_{i-1}^n) \times I(\Delta x)$$

with this $I(\Delta x) \Rightarrow$ steady states exactly preserved for $\gamma = 2$ and approximated for $\gamma > 2$.

- Min-Max procedure in order to ensure $\phi \geq 0$.

Testcase 1: perturbation of an equilibrium solution

- Exact equilibrium solution^{1,2}:

$$\phi(x) = \begin{cases} \frac{2\varepsilon bK}{\tau\chi D} \frac{\cos(\sqrt{\tau}x)}{\cos(\sqrt{\tau}\bar{x})} - \frac{aK}{\tau D}, & \text{for } x \in [0, \bar{x}], \\ -\frac{2\varepsilon K}{\chi} \frac{\cosh\left(\sqrt{\frac{b}{D}}(x-L)\right)}{\cosh\left(\sqrt{\frac{b}{D}}(\bar{x}-L)\right)}, & \text{for } x \in]\bar{x}, L], \end{cases}$$

$$\rho(x) = \begin{cases} \frac{\chi}{2\varepsilon} \phi(x) + \frac{D}{b} \frac{M\tau^{3/2}}{\tan(\sqrt{\tau}\bar{x}) - \sqrt{\tau}\bar{x}}, & \text{for } x \in [0, \bar{x}], \\ 0, & \text{for } x \in]\bar{x}, L], \end{cases}$$

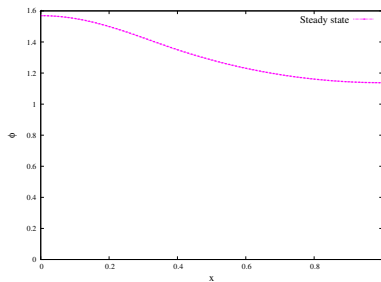
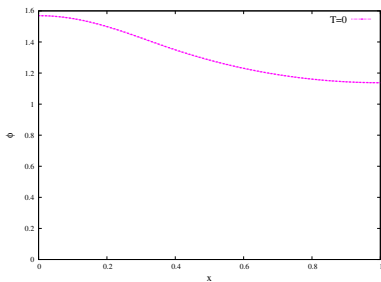
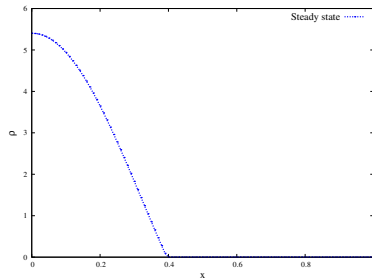
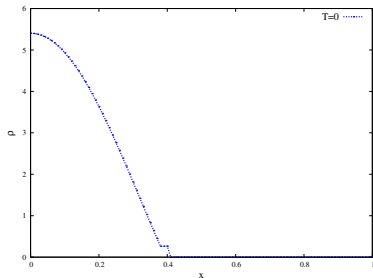
$$u(x) = 0,$$

where $\tau = \frac{1}{D} \left(\frac{a\chi}{2\varepsilon} - b \right)$ and \bar{x} s.t. $\sqrt{\frac{b}{\tau D}} \tan(\sqrt{\tau}\bar{x}) = \tanh\left(\sqrt{\frac{b}{D}}(\bar{x}-L)\right)$.

¹Natalini, Ribot, Twarogowska, CMS 2014.

²Twarogowska, PhD Thesis 2011.

ρ and ϕ with $a = b = D = \varepsilon = 1$, $\gamma = 2$, $\chi = 50$, $L = 1$, $\Delta x = 0.01$.



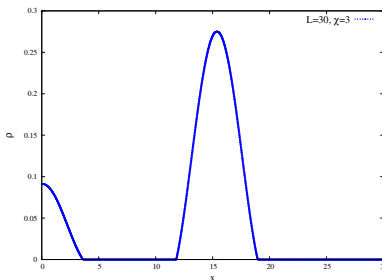
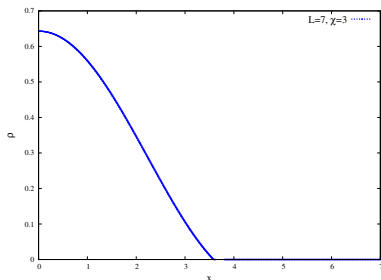
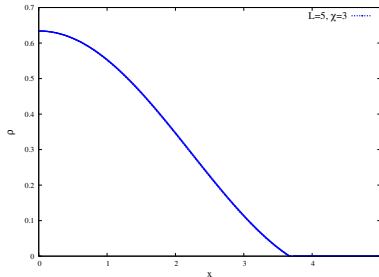
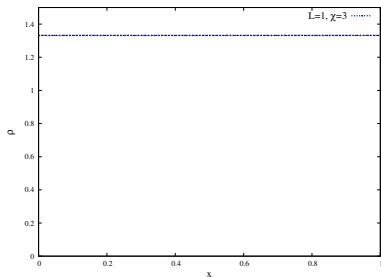
Testcase 2: influence of parameters on the steady state

- Initial conditions: $\rho(x, 0) = 1 + \sin\left(4\pi\left|x - \frac{L}{4}\right|\right)$,
 $u(x, 0) = 0$,
 $\phi(x, 0) = 0$.
- Study
 - Density ρ as a function of x at steady state.
 - Influence of L and χ with $a = b = D = \varepsilon = 1$.
 - Influence of γ with $a = 20$, $b = 10$, $D = 0.1$, $\varepsilon = 1$.
- Validation? No analytical solution. But results similar to those of Twarogowska^{1,2}.

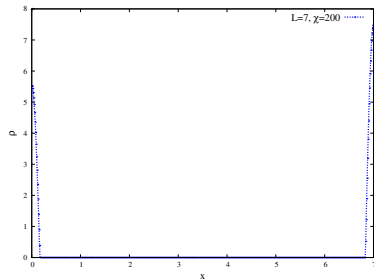
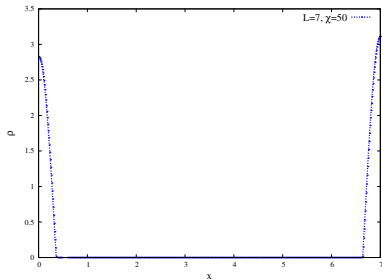
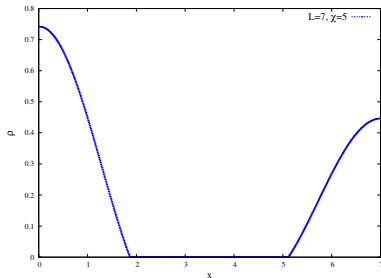
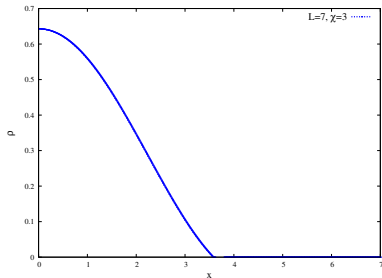
¹Natalini, Ribot, Twarogowska, CMS 2014.

²Twarogowska, PhD Thesis 2011.

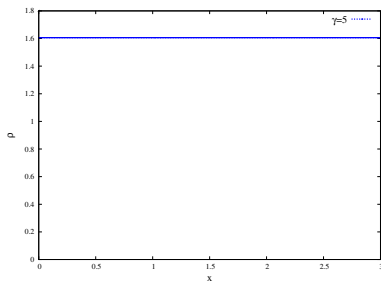
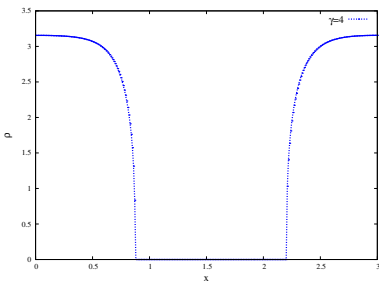
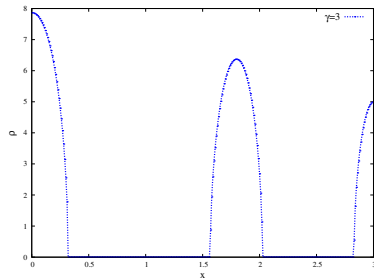
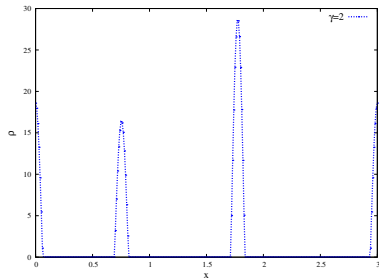
Influence of L at $\gamma = 2$, $\chi = 3$, $\Delta x = 0.01$.



Influence of χ at $\gamma = 2$, $L = 7$, $\Delta x = 0.01$.



Influence of γ at $\chi = 10$, $L = 3$, $\Delta x = 0.01$.



Conclusions...

- HLL consistent Riemann solver.
- Positivity of ρ and ϕ .
- Equilibrium states exactly preserved when $\gamma = 2$ and well approached when $\gamma > 2$.
- No problem with vacuum $\rho = 0$.
- We can prove that the scheme is AP in the case $\alpha > 0$.

... and perspectives

- Understand the behaviour of the asymptotic-parabolic model.
- Extension of the model to the 2D.

References

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Thank you for your attention!