A well-balanced numerical scheme for solution with vacuum to a 1d quasilinear hyperbolic model of chemotaxis

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Outline

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Chemotaxis

Directed movement of mobile species towards lower/higher concentration of chemical substance present in the surrounding environment

Example: Vasculogenesis

- a process of de novo formation of blood vessels
- chemotactic factor: VEGF-A released by cells
- percolative and ”Swiss cheese” transitions depending on the initial mass

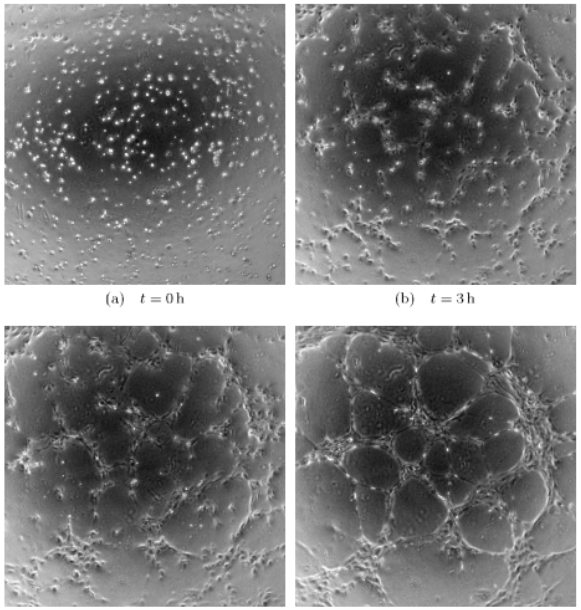

Figure: In vitro experiments of Vasculogenesis (Serini et. al)

Hyperbolic model of vasculogenesis [Gamba A., Preziosi L. et al. (2003)]

$$\begin{cases} \rho_t + div(\rho\vec{u}) = 0 \\ (\rho\vec{u})_t + div(\rho\vec{u} \otimes \vec{u}) = \chi\rho\nabla\phi - \alpha\rho\vec{u} - \nabla P(\rho) \\ \phi_t = D\Delta\phi + a\rho - b\phi \end{cases}$$

- ρ - density of endothelial cells
- ϕ - concentration of chemical factor VEGF

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Forces acting on cells:

- internal force $\mathcal{F}_{vol} = -\nabla P(\rho),$ where $P(\rho) = \varepsilon\rho^{\gamma}, \quad \varepsilon > 0, \gamma > 1$
- body force - chemotaxis $\mathcal{F}_{chem} = \chi\rho\nabla\phi, \quad \chi > 0$
- contact force $\mathcal{F}_{diss} = -\alpha\rho u, \quad \alpha > 0$

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$\Rightarrow$ **solutions containing vacuum**

Di Russo, C. and Sepe, A. - "Existence and Asymptotic Behavior of Solutions to a Quasilinear Hyperbolic-Parabolic Model of Vasculogenesis" (2011), preprint.

Outline

Hyperbolic model of chemotaxis: stationary solutions

Problem:

We look for non constant stationary solutions of system

$$\begin{cases} \rho_t + (\rho u)_x = 0 \\ (\rho u)_t + (\rho u^2 + P(\rho))_x = -\alpha \rho u + \chi \rho \phi_x \\ \phi_t = D\phi_{xx} + a\rho - b\phi \end{cases} \tag{1}$$

defined on a bounded domain $\Omega = [0, L]$ with homogeneous Neumann boundary conditions

$$\rho_x|_{\partial\Omega} = 0, \quad \phi_x|_{\partial\Omega} = 0, \quad u|_{\partial\Omega} = 0$$

and the total mass, conserved in time, given by $M = \int_0^L \rho(x,t)dx$.

Motivation: description and study of vascular-like networks observed in the in vitro experiments with human, endothelial cells [Serini et.al.]

General case: $P(\rho) = \varepsilon\rho^\gamma, \quad \gamma > 1$

$$
\begin{aligned}
(\rho u)_x &= 0, \\
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Solutions:

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$$\phi: \quad \begin{aligned} -D\phi_{xx} &= a\rho - b\phi \quad \text{if} \quad \rho > 0 \\ D\phi_{xx} &= b\phi \quad \text{if} \quad \rho = 0 \end{aligned}$$

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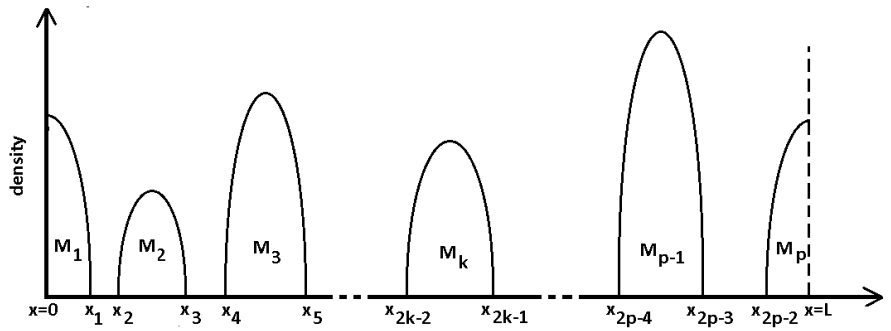

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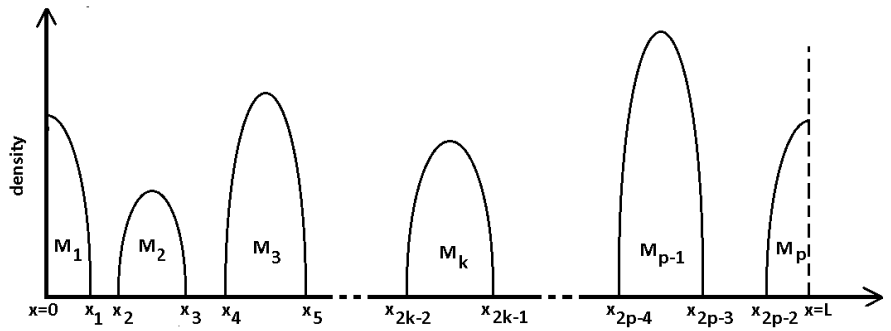


Problems in finding an explicit solution I:

- number of bumps $p \in \mathbf{N}$ is not known a priori
- for $p > 1$: more unknown constants than available equations
- for $\gamma > 2$ finding ϕ_k is not trivial

Lateral bump

If $\alpha = \frac{a\chi}{2\varepsilon D} - \frac{b}{D} > 0$ and $L > \frac{\pi}{\sqrt{\alpha}}$ then there exists a unique, positive solution of the form

$$\text{on} \quad [0, \bar{x}], \quad \phi(x) = \frac{2\varepsilon\beta K}{\alpha\chi}\frac{\cos(\sqrt{\alpha}x)}{\cos(\sqrt{\alpha}\bar{x})} - \frac{aK}{\alpha D}, \quad \rho(x) = \frac{\chi}{2\varepsilon}\phi(x) + K$$

$$\text{on} \quad [\bar{x}, L], \quad \phi(x) = \frac{2\varepsilon bK}{\chi}\tan(\sqrt{\beta}L)\frac{\sinh(\sqrt{\beta}(x-L))}{\cosh(\sqrt{\beta}(\bar{x}-L))}, \quad \rho(x) = 0$$

given by the smallest $\bar{x} \in \frac{1}{\sqrt{\alpha}}]\frac{\pi}{2}, \pi[$ satisfying

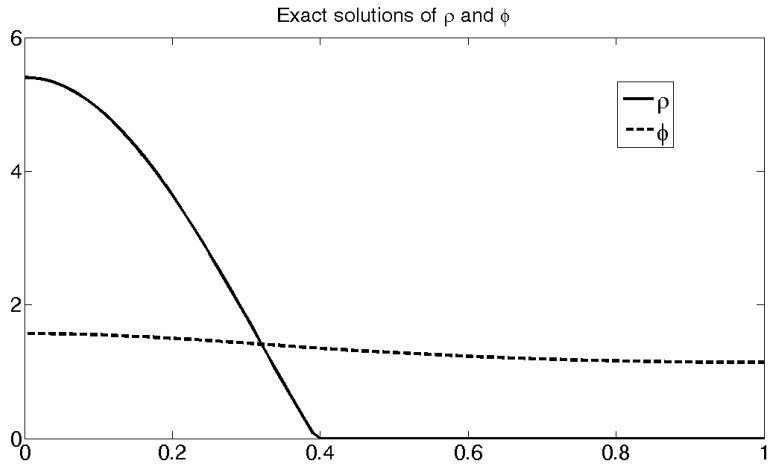
$$\sqrt{\frac{\beta}{\alpha}}\tan(\sqrt{\alpha}\bar{x}) = \tanh(\sqrt{\beta}(\bar{x}-L)) \tag{2}$$

and K equal to $K = \frac{\alpha M}{\frac{\beta}{\sqrt{\alpha}}\tan(\sqrt{\alpha}\bar{x}) - \beta\bar{x}}$.

Assumption: $p = 1$, $P(\rho) = \varepsilon\rho^2$

Lateral bump

$$\rho(x) = \begin{cases} \frac{\chi}{2\varepsilon}\phi(x) + K & x \in [0, \bar{x}] \\ 0 & x \in (\bar{x}, L] \end{cases}$$



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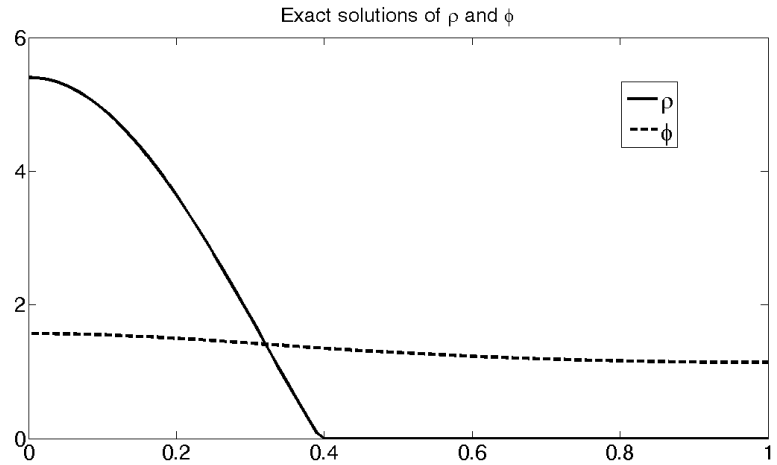
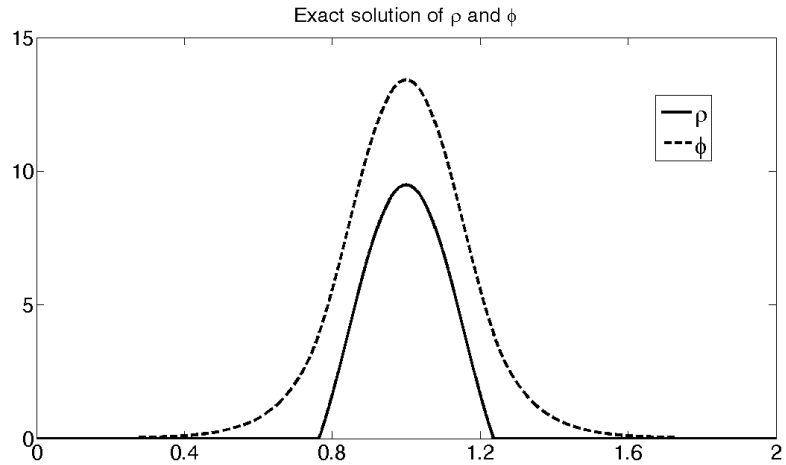


Centered bump

$$\rho(x) = \begin{cases} 0 & x \in [0, \bar{x}) \\ \frac{\chi}{2\varepsilon}\phi(x) + K & x \in [\bar{x}, L - \bar{x}] \\ 0 & x \in (L - \bar{x}, L] \end{cases}$$



Solution is SYMMETRIC

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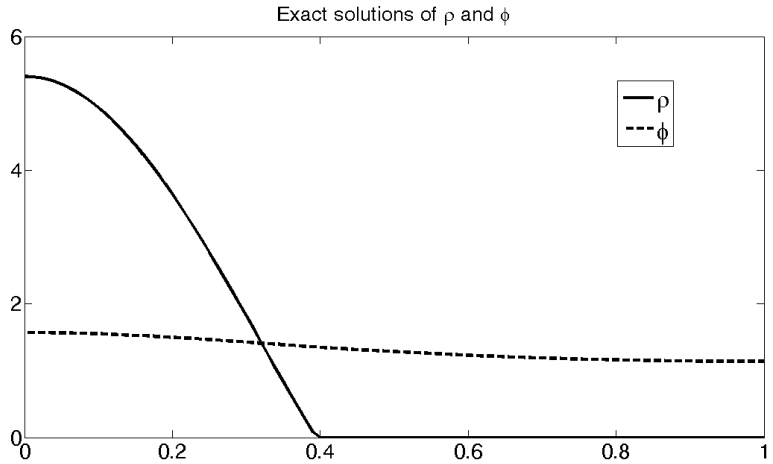

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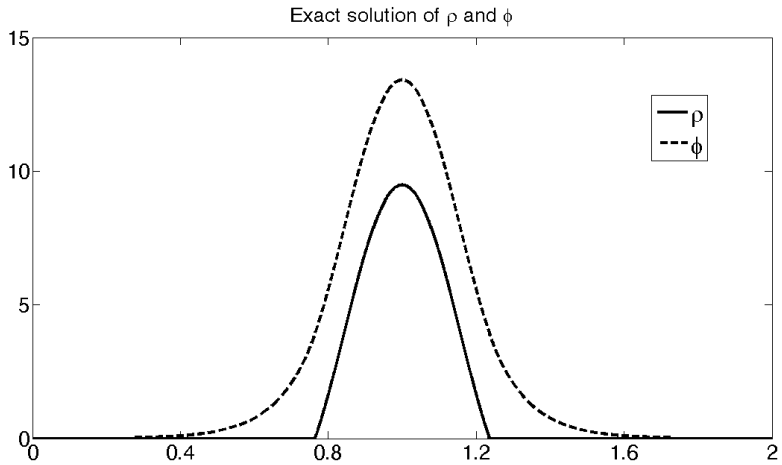

Solution is SYMMETRIC

Problems in finding an explicit solution II: existence of interface points $\bar{x}_k$ in the case $p > 1$ is an open problem

Outline

Numerical scheme for a 1d quasilinear model of vasculogenesis

$$\begin{cases} \rho_t + (\rho u)_x = 0 \\ (\rho u)_t + (\rho u^2 + P(\rho))_x = -\alpha \rho u + \chi \rho \phi_x \\ \phi_t = D\phi_{xx} + a\rho - b\phi \end{cases}$$

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Requirements for a numerical scheme:

- consistency with the original system
- preservation of the non negativity of densities and concentrations
- preservation of the total mass
- treatment of vacuum states
- good approximation of non constant steady states
- low numerical viscosity

Approach I: standard finite difference scheme

$$U_t + F(U)_x = S(U),$$

$$U = \begin{pmatrix} \rho \\ \rho u \end{pmatrix}, \quad F(U) = \begin{pmatrix} \rho u \\ \rho u^2 + P(\rho) \end{pmatrix}, \quad S(U) = \begin{pmatrix} 0 \\ -\alpha \rho u + \chi \rho \phi_x^n \end{pmatrix}.$$

Standard finite difference scheme on uniform grid with centered approximation of the source term

$$U_i^{n+1} = U_i^n + \Delta t H_i(U^n) + \Delta t \begin{pmatrix} 0 \\ \chi \rho_i^n \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} - \alpha \rho_i^{n+1} u_i^{n+1} \end{pmatrix}$$

$H_i(U^n)$ - space discretization of the homogeneous part

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Problems at non constant steady states:

- Mass conservation
- Approximation of velocity field

Approach II: Well-balanced, finite volume scheme

General semi-discrete finite volume scheme

$$\Delta x \frac{d}{dt} U_i + F_{i+1/2} - F_{i-1/2} = S_i$$

where

- $U_i = (\rho_i(t),\, \rho_i(t) u_i(t))$ is a cell-average vector of discrete unknowns
- $F_{i+1/2} = \mathcal{F}(U^-_{i+1/2}, U^+_{i+1/2})$, with $\mathcal{F}$ - consistent C^1 numerical flux function

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Well-balancing:

- $S_i = \mathcal{S}^-_{i+1/2} + \mathcal{S}^+_{i-1/2} = F(U^-_{i+1/2}) - F(U_i) + F(U_i) - F(U^+_{i-1/2})$

  $\Longrightarrow$ ansatz motivated by the balance relation $F(U)_x = S(U)$

- Reconstruction of $U^{\pm}_{i+1/2}$ using the equilibrium system

Approach II: Well-balanced, finite volume scheme

First order Euler forward time discretization

$$U_i^{n+1} = U_i^n + \frac{\Delta t}{\Delta x}\left(\mathcal{F}\left(U_{i+1/2}^-, U_{i+1/2}^+\right) - \mathcal{F}\left(U_{i-1/2}^-, U_{i-1/2}^+\right)\right) + \frac{\Delta t}{\Delta x}\left(F\left(U_{i+1/2}^-\right) - F\left(U_{i-1/2}^+\right)\right)$$

- $\mathcal{F}$ is a C^1 numerical flux function
- F is an analytical flux

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Reconstruction of $\mathbf{U^{\pm}_{i+1/2}}$: Approximate integration of the equilibrium system in suitable intervals

$$\begin{cases} (\rho u)_x = 0 \\ (\rho u^2 + P(\rho))_x = -\alpha\rho u + \chi\rho\phi_x \end{cases} \quad \text{in} \quad \begin{array}{lll} \left[x_i, x_{i+1/2}\right] & \rightarrow & U^-_{i+1/2} \\ \left[x_{i+1/2}, x_{i+1}\right] & \rightarrow & U^+_{i+1/2} \end{array}$$

under the assumption: $\boxed{u_x = 0}$.

Numerical method: well-balanced schemes

- Equilibrium schemes for scalar conservation laws [R.Botchorishvili, B. Perthame, A.Vasseur]
- U.S.I. for Euler equations with high friction [F.Bouchut, H.Ounaissa, B.Perthame]

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- Asymptotically high order scheme (AHO) for Cattaneo model of chemotaxis (that works only for the semilinear model) [R.Natalini, M.Ribot]
- Well-balanced scheme in the framework of non-conservative products for Cattaneo model of chemotaxis [L.Gosse]

Reconstruction of the interface variables $U^{\pm}_{i+1/2}$

- We introduce the internal energy $e(\rho)$ such that

$$e'(\rho) = \frac{P(\rho)}{\rho^2} \quad \text{and} \quad \Psi(\rho) = e(\rho) + \frac{P(\rho)}{\rho} \text{ is finite for } \rho \to 0$$

and rewrite the equilibrium system in the form

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- Integrating for example in $\left[x_i, x_{i+1/2}\right]$ yields:

$$\begin{cases} u^-_{i+1/2} = u_i, \\ \Psi(\rho^-_{i+1/2}) = \Psi(\rho_i) - \alpha \displaystyle\int_{x_i}^{x_{i+1/2}} u dx + \chi(\phi_{i+1/2} - \phi_i) \end{cases}$$

$\Rightarrow$ **How to assure consistency and non negativity of density?**

Proposition

Let $F = (F^\rho, F^{\rho u})^T$ be the analytical flux of the quasilinear model of chemotaxis and let $\mathcal{F}$ be a consistent, $\mathcal{C}^1$ numerical flux preserving the non negativity of ρ for the homogeneous problem.
The finite volume scheme

$$\Delta x \frac{d}{dt} U_i + \mathcal{F}\left(U^-_{i+1/2}, U^+_{i+1/2}\right) - \mathcal{F}\left(U^-_{i-1/2}, U^+_{i-1/2}\right) = S_i$$

with

$$S_i = \mathcal{S}^-_{i+1/2} + \mathcal{S}^+_{i-1/2} = \begin{pmatrix} 0 \\ F^{\rho u}\left(\rho^-_{i+1/2}\right) - F^{\rho u}(\rho_i) \end{pmatrix} + \begin{pmatrix} 0 \\ F^{\rho u}(\rho_i) - F^{\rho u}\left(\rho^+_{i+1/2}\right) \end{pmatrix}$$

and the reconstruction

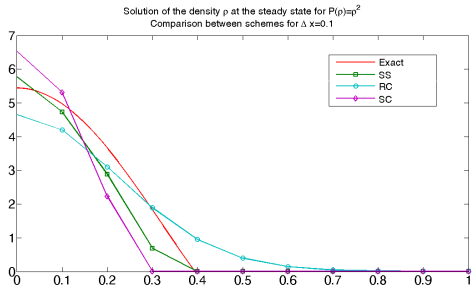
$$\begin{aligned} \left(\rho^-_{i+1/2}, u^-_{i+1/2}\right) &= \left(\Psi^{-1}[\Psi(\rho_i) - \alpha(u_i)_+ \Delta x + \chi(\min(\phi_i, \phi_{i+1}) - \phi_i)]_+, u_i\right), \\ \left(\rho^+_{i+1/2}, u^+_{i+1/2}\right) &= \left(\Psi^{-1}[\Psi(\rho_{i+1}) + \alpha(u_{i+1})_- \Delta x + \chi(\min(\phi_i, \phi_{i+1}) - \phi_{i+1})]_+, u_{i+1}\right), \end{aligned}$$

i) is **consistent** away from the vacuum

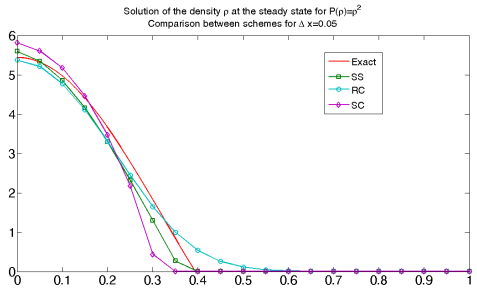
ii) **preserves the non negativity** of $\rho_i(t)$

iii) **preserves the non constant steady states**.

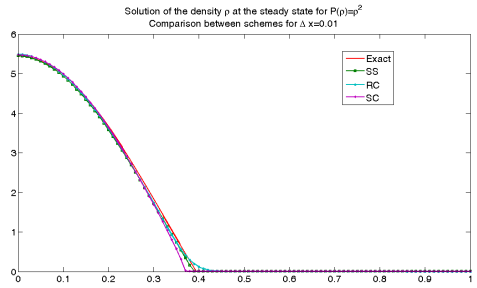
Numerical test: approximation of the free boundary



$\Delta x = 0.1$



$\Delta x = 0.05$

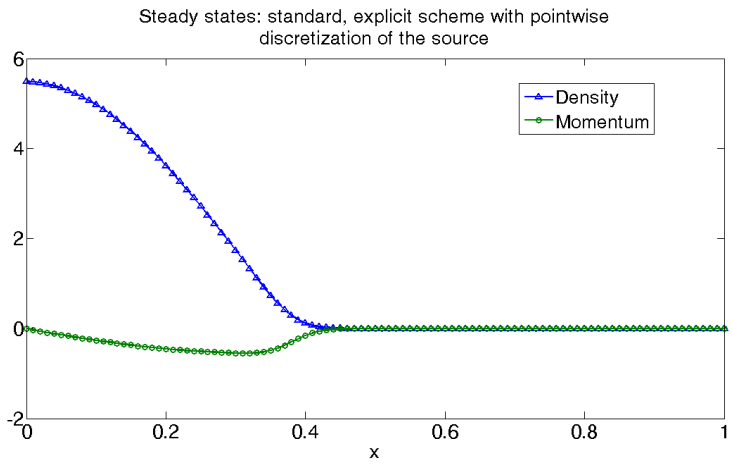


$\Delta x = 0.01$

Figure: Comparison between different approximations of the source term:

SS	(green)	-	Well-balanced finite volume method
SC	(pink)	-	Finite volume method with centered in space approx. of the source
RC	(blue)	-	Finite difference method with centered in space approx. of the source

Numerical test: approximation of the velocity field



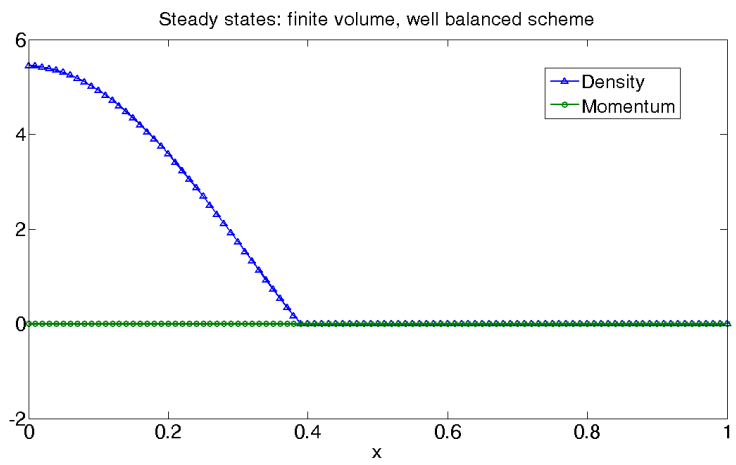


Figure: Density and momentum profiles:

On the left: - Finite difference method with centered in space approx. of the source

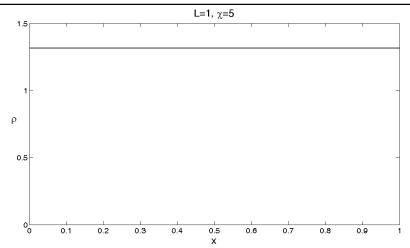
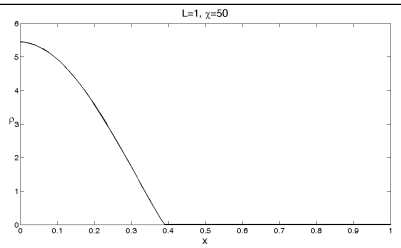
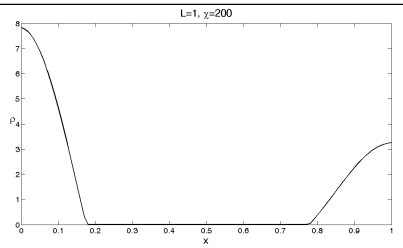
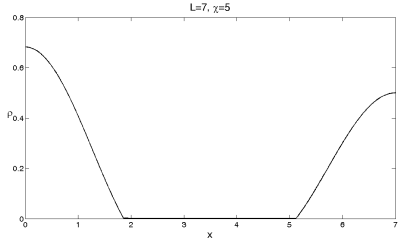
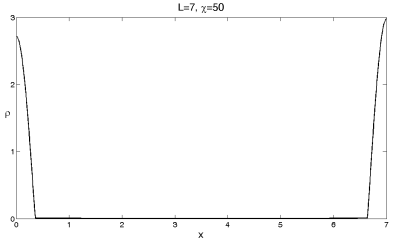
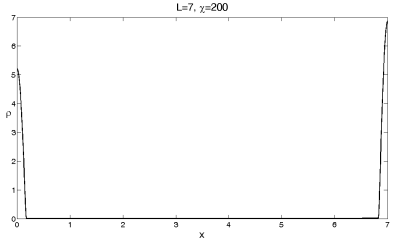
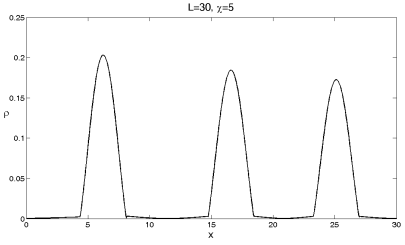
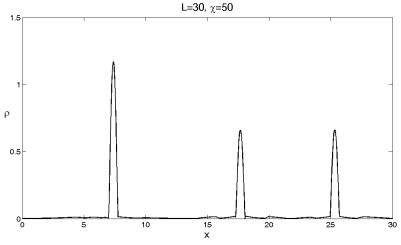
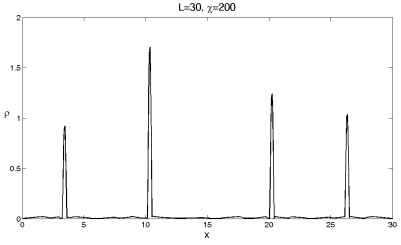
On the right - Well-balanced finite volume method

Summary

	FDM - centered source	FVM - WB source
free boundary	high numerical viscosity	approximate Riemann solvers
mass conservation	Additional conditions	Ok
non constant s.s.	No for velocity field	Ok
$\mathbf{M >> 1}$	Ok	No
$\gamma > \mathbf{5}$	Ok	No

Outline

Numerical results: dependence on L and χ

$L\backslash\chi$	5	50	200
1			
7			
30			

- $\alpha = \frac{a\chi}{2\varepsilon D} - \frac{b}{D} < 0$ or ($\alpha > 0$ and $L < \frac{\pi}{\sqrt{\alpha}}$) $\rightarrow$ only constant steady states
- non constant states: enough space + chemotaxis ”dominant”
- condition determining the number of bumps at any domain ???

Numerical results: dependence on γ and total mass M

Dependence on the adiabatic exponent γ

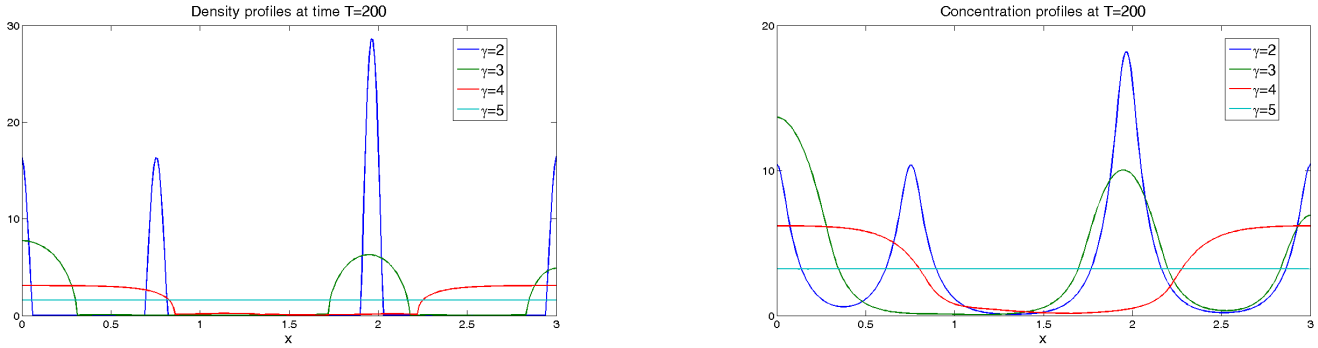
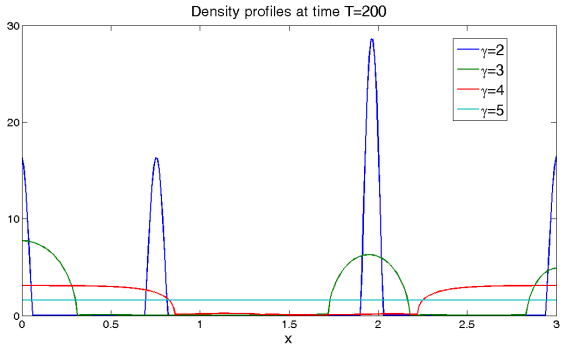


Figure: Profiles of the density (on the left) and the concentration (on the right) at steady states. Comparison for $\gamma = \{2, 3, 4, 5\}$.

Numerical results: dependence on γ and total mass M

Dependence on the adiabatic exponent γ



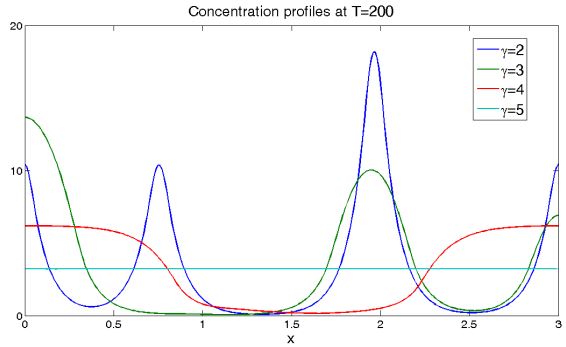
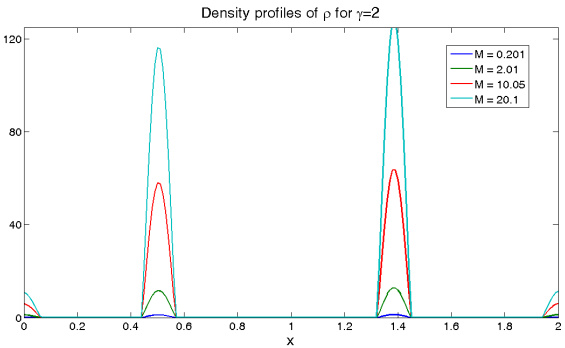


Figure: Profiles of the density (on the left) and the concentration (on the right) at steady states. Comparison for $\gamma = \{2, 3, 4, 5\}$.

Dependence on the total mass $M = \int_0^L \rho(x,t)dx$ for $\gamma = 2$ and $\gamma = 3$



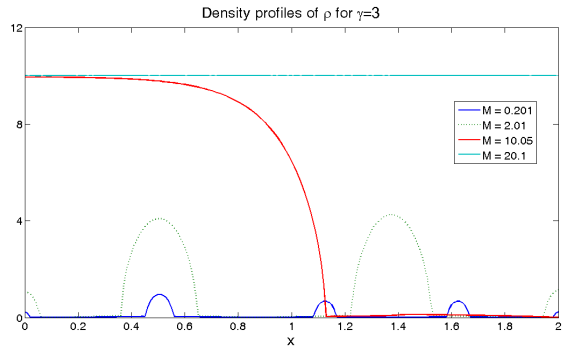


Figure: Density profiles for $\gamma = 2$ (on the left) and for $\gamma = 3$ (on the right). Comparison for $M = \{0.201, 2.01, 10.05, 20.1\}$

Relation between numerical results and experimental observations

Experiment	Numerical results
formation of vascular network	non - constant steady states containing regions where $\rho > 0$ and where $\rho = 0$
characteristic length of chords	minimal size of the domain to form non constant steady states
communication between cells via VEGF-A	chemotaxis ”dominant” to form non constant equilibria
incompressibility of cells	estimates of the adiabatic coefficient γ
percolative and ”swiss cheese” transitions	$\gamma = 2$ doesn’t reproduce the influence of the initial mass, while $\gamma = 3$ does

Thank you for your attention.