Asymptotic preserving schemes for nonlinear kinetic equations leading to volume-exclusion chemotaxis in the diffusive limit

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Online seminar (CSIAM: TM20)

Outline

Motivation

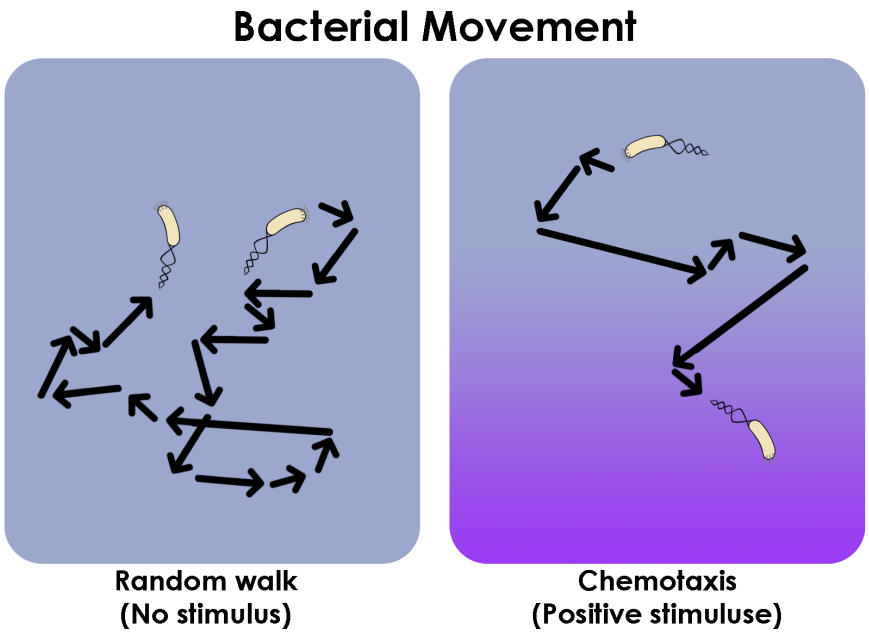

Figure: Cell movement without/with chemotaxis [1]

- run and tumble: cells move along a straight line in the running phase and reorient in the tumbling phase
- chemotaxis: cells adapt movement in response to a chemical stimulus

[1] http://2016.igem.org/Team:Technion_Israel/Chemotaxis

Patlak-Keller-Segel (PKS) model

A popular macroscopic model:

$$\partial_t \rho - D_\rho \Delta \rho + \chi_0 \nabla \cdot \{\rho \nabla c\} = h(\rho, c),$$
$$D_c \Delta c + g(\rho, c) = 0.$$

- ρ – cell density, c – chemical concentration
- D_ρ, D_c – diffusion constant
- $h(\rho, c) = r_0 \rho(1 - \rho/\rho_{\max})$ – proliferation or death of cells
- $g(\rho, c) = \rho - c$ – production or consumption of chemoattractant
- Simple yet able to demonstrate pattern forming for suitable kinetics
- Solutions have a tendency to exhibit finite-time blow-up
  - Density-dependent chemotactic sensitivity and motility

Outline

1D discrete random walk [2]

Notations:

- $u_i(t)$ – prob. at $i \in \mathbb{Z}$ at time t
- $c_i(t)$ – chemical concentration
- T_i^+ – prob. per unit time of one-step jump to $i+1$
- T_i^- – prob. per unit time of one-step jump to $i-1$

$$\frac{\partial u_i}{\partial t} = T_{i-1}^+ u_{i-1} + T_{i+1}^- u_{i+1} - (T_i^+ + T_i^-)u_i$$

[2] Kevin Painter and Thomas Hillen (2002)

Relation with classical PKS

Assume

$$T_i^{\pm} = \alpha + \frac{\beta}{2}(c_{i\pm1} - c_i)$$

then

$$\frac{\partial u_i}{\partial t} = \alpha(u_{i+1} - 2u_i + u_{i-1}) - \frac{\beta}{2}((u_{i+1} + u_i)(c_{i+1} - c_i) - (u_i + u_{i-1})(c_i - c_{i-1}))$$

Relation with classical PKS

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With some scaling and taking the limit

$$\frac{\partial u}{\partial t} = D_u \frac{\partial^2 u}{\partial x^2} - \frac{\partial}{\partial x}(\beta u \frac{\partial c}{\partial x})$$

volume-filling model

Taking into account the volume limitations

$$T_i^{\pm} = q(u_{i\pm1})(\alpha + \frac{\beta}{2}(c_{i\pm1} - c_i)),$$

where

- $q(u)$ – prob. finding space at its neighbouring location
- $q(U_{\max})$ – finite capacity
- $q(u) \geq 0$ for $0 \leq u \leq U_{\max}$

volume-filling model

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- $q(U_{\max})$ – finite capacity
- $q(u) \geq 0$ for $0 \leq u \leq U_{\max}$

An example:

$$q(u) = 1 - \frac{u}{U_{\max}}$$

Volume-exclusion PKS

$$\begin{aligned}\frac{\partial u_i}{\partial t} =& \alpha(q_i u_{i+1} - (q_{i+1} + q_{i-1})u_i + q_i u_{i-1}) \\ & - \frac{\beta}{2}((q_i u_{i+1} + q_{i+1} u_i)(c_{i+1} - c_i) - (q_{i-1} u_i + q_i u_{i-1})(c_i - c_{i-1}))\end{aligned}$$

In the limit, we arrive at

$$\frac{\partial u}{\partial t} = D_u \left(q(u) \frac{\partial^2 u}{\partial x^2} - u \frac{\partial^2 q(u)}{\partial x^2} \right) - \frac{\partial}{\partial x}(\beta q(u) u \frac{\partial c}{\partial x})$$

or equivalent divergence form

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left(D_u (q(u) - q'(u)u) \frac{\partial u}{\partial x} - \beta q(u) u \frac{\partial c}{\partial x} \right)$$

Volume-exclusion PKS

$$\begin{aligned}\frac{\partial u_i}{\partial t} =& \alpha(q_i u_{i+1} - (q_{i+1} + q_{i-1})u_i + q_i u_{i-1}) \\ & - \frac{\beta}{2}((q_i u_{i+1} + q_{i+1} u_i)(c_{i+1} - c_i) - (q_{i-1} u_i + q_i u_{i-1})(c_i - c_{i-1}))\end{aligned}$$

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or equivalent divergence form

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left(D_u (q(u) - q'(u)u) \frac{\partial u}{\partial x} - \beta q(u) u \frac{\partial c}{\partial x} \right)$$

Well defined: $q(u) - q'(u)u > 0$ if $q'(u) \leq 0$

Framework of kinetic model

General form of the kinetic model:

$$\partial_t f + \mathbf{v} \cdot \nabla (F[\rho](t, \mathbf{x}, \mathbf{v}) f) = \lambda q(\rho)(-f + \rho T(\mathbf{v}, \rho, \nabla c)) \ .$$

- $f(t, \mathbf{x}, \mathbf{v})$ – density, $\rho(t, \mathbf{x}) = \int_V f(t, \mathbf{x}, \mathbf{v}) \mathrm{d}\mathbf{v}$ with V unit sphere
- $c(t, \mathbf{x})$ – chemical concentration
- $q(\rho)$ – probability to find space at its neighbouring locations
- λ – constant turning rate
- $F[\rho](t, \mathbf{x}, \mathbf{v})$ – anisotropic transport due to density limitation
- $T(\mathbf{v}, \rho, \nabla c)$ – prob. of a velocity jump to velocity $\mathbf{v}$ satisfying

$$\int_V T(\mathbf{v}, \rho, \nabla c) \, \mathrm{d}\mathbf{v} = 1$$

Choice of $F[\rho]$ and T

- Assume cells only move to non-overcrowded regions

$$F[\rho](t, \mathbf{x}, \mathbf{v}) = q\big(\rho(t, \mathbf{x} + \mathbf{v})\big) \ .$$

- Assume cells only make a turn in directions where space is available

$$T(\mathbf{v}, \rho, \nabla c) = \tilde{c}(t, \mathbf{x})\psi(\mathbf{v}, \nabla c)q(\rho(t, \mathbf{x} + \mathbf{v})) \ ,$$

  where $\tilde{c}(t, \mathbf{x})$ is a normalisation factor.

Remark

The assumptions imply cells will only make a turn

- *if they are not already trapped in a high density region*
- *only in directions where the density is not too large*

Diffusion scaling

- Introduce characteristic speed s and characteristic length scale L
- Assuming the space scaling such that

$$\tau_{run} \ll \tau_{drift} \ll \tau_{diff}$$

where

- $\tau_{run} = \frac{1}{\lambda}$
- $\tau_{drift} = \frac{L}{s}$
- $\tau_{diff} \approx \frac{L^2\lambda}{s^2}$ since the diffusion coefficient $D \approx \mathcal{O}(\frac{s^2}{\lambda})$

- Introduce $\varepsilon \ll 1$ such that

$$\tau_{run} = \mathcal{O}(1), \quad \tau_{drift} = \mathcal{O}(\frac{1}{\varepsilon}), \quad \tau_{diff} = \mathcal{O}(\frac{1}{\varepsilon^2})$$

Scaled kinetic model

With the diffusion scaling, we get the dimensionless equation

$$\varepsilon^2 \partial_t f^\varepsilon + \varepsilon \mathbf{v} \cdot \nabla (F_\varepsilon[\rho](t, \mathbf{x}, \mathbf{v}) f^\varepsilon) = q(\rho)(-f^\varepsilon + \rho T_\varepsilon(\mathbf{v}, \rho, \nabla c))$$

where

$$F_\varepsilon[\rho](t, \mathbf{x}, \mathbf{v}) = q(\rho(t, \mathbf{x} + \varepsilon \mathbf{v}))$$

$$T_\varepsilon(\mathbf{v}, \rho, \nabla c) = \frac{\psi_\varepsilon(\mathbf{v}, \nabla c) q(\rho(t, \mathbf{x} + \varepsilon \mathbf{v}))}{\int_V \psi_\varepsilon(\mathbf{v}, \nabla c) q(\rho(t, \mathbf{x} + \varepsilon \mathbf{v})) \, \mathrm{d}\mathbf{v}}$$

$$\psi_\varepsilon(\mathbf{v}, \nabla c) = \psi_0(\mathbf{v}) + \varepsilon \psi_1(\mathbf{v}, \nabla c)$$

To recover the volume-exclusion PKS, we make the assumptions:

- $\int_V \psi_0(\mathbf{v}) \, \mathrm{d}\mathbf{v} = 1 \ , \quad \int_V \psi_1(\mathbf{v}, \nabla c) \, \mathrm{d}\mathbf{v} = 0$
- $\int_V \mathbf{v} \psi_0(\mathbf{v}) \, \mathrm{d}\mathbf{v} = 0 \ , \quad \psi_1(\mathbf{v}, \nabla c) = \phi(\mathbf{v}) \cdot \nabla c$

Macroscopic limit

Theorem (formal)

The limit $\varepsilon \to 0$ *of* f^ε *is* $f^0 = \rho(t,\mathbf{x})\psi_0(\mathbf{v})$*, where* ρ *solves*

$$\partial_t \rho - \nabla \cdot \big(D_0\big(q(\rho) - \rho q'(\rho)\big)\nabla\rho - \beta\rho q(\rho)\nabla c\big) = 0 \ ,$$

with the diffusion coefficient D_0 *and the chemotactic sensitivity parameter* β *given by*

$$D_0 = \langle(\mathbf{v}\otimes\mathbf{v})\psi_0(\mathbf{v})\rangle \qquad \text{and} \qquad \beta = \langle \mathbf{v}\otimes\phi(\mathbf{v})\rangle \ .$$

where $\langle f(\mathbf{v})\rangle = \int_V f(\mathbf{v})\,\mathrm{d}\mathbf{v}$.

General idea of proof: Consider a regular expansion of f^ε

$$f^\varepsilon(t,\mathbf{x},\mathbf{v}) = f^0(t,\mathbf{x},\mathbf{v}) + \varepsilon f^1(t,\mathbf{x},\mathbf{v}) + \mathcal{O}(\varepsilon^2) \ .$$

Do expansions to the kinetic model and compare terms with the same order in ε.

Asymptotic expansion

- Expansion of $F_\varepsilon[\rho] = q(\rho(t, \mathbf{x} + \varepsilon \mathbf{v}))$:

$$F_\varepsilon[\rho] = q(\rho) + \varepsilon q'(\rho)\mathbf{v} \cdot \nabla \rho + \mathcal{O}(\varepsilon^2)$$

- Expansion of $T_\varepsilon = \tilde{c}_\varepsilon(t, \mathbf{x})\psi(\mathbf{v}, \nabla c)q(\rho(t, \mathbf{x} + \varepsilon \mathbf{v}))$:

$$T_\varepsilon(\mathbf{v}, \rho, \nabla c) = \psi_0(\mathbf{v}) + \varepsilon\left(\psi_1(\mathbf{v}, \nabla c) + \frac{q'(\rho)}{q(\rho)}(\mathbf{v} \cdot \nabla \rho)\psi_0(\mathbf{v})\right) + \mathcal{O}(\varepsilon^2)$$

Identifying equations in powers of ε, we obtain

$$\varepsilon^0 : f^0(t, \mathbf{x}, \mathbf{v}) = \rho(t, \mathbf{x})\psi_0(\mathbf{v})$$

$$\varepsilon^1 : \mathbf{v} \cdot \nabla(q(\rho)f^0) = q(\rho)\left(-f^1 + \rho\left(\psi_1(\mathbf{v}, \nabla c) + \frac{q'(\rho)}{q(\rho)}(\mathbf{v} \cdot \nabla \rho)\psi_0(\mathbf{v})\right)\right)$$

$$\varepsilon^2 : \partial_t f^0 + \mathbf{v} \cdot \nabla\left(q(\rho)f^1 + q'(\rho)(\mathbf{v} \cdot \nabla \rho)f^0\right) = \mathcal{O}(1)$$

Formal proof of the limit $\varepsilon \to 0$

Replacing f^0 by $\rho(t,\mathbf{x})\psi_0(\mathbf{v})$, integrating ε^2-equation over $\mathbf{v} \in V$

$$\partial_t f^0 + \mathbf{v}\cdot\nabla\Big(q(\rho)f^1 + q'(\rho)(\mathbf{v}\cdot\nabla\rho)f^0\Big) = \mathcal{O}(1)$$

and noticing the right hand terms integrate to zero, we get

$$\partial_t\rho + \nabla\cdot\big(q(\rho)\langle\mathbf{v}f^1\rangle + D_0\rho q'(\rho)\nabla\rho\big) = 0, \tag{1}$$

where $D_0 = \langle(\mathbf{v}\otimes\mathbf{v})\psi_0(\mathbf{v})\rangle$.
Replacing f^0 by $\rho(t,\mathbf{x})\psi_0(\mathbf{v})$, multiplying ε-equation

$$\mathbf{v}\cdot\nabla(q(\rho)f^0) = q(\rho)\left(-f^1 + \rho\left(\psi_1(\mathbf{v},\nabla c) + \frac{q'(\rho)}{q(\rho)}(\mathbf{v}\cdot\nabla\rho)\psi_0(\mathbf{v})\right)\right)$$

by $\mathbf{v}$ and integrating over $\mathbf{v}\in V$, we get

$$q(\rho)\langle\mathbf{v}f^1\rangle = -\nabla\cdot\big(D_0\rho q(\rho)\big) + \rho q(\rho)\langle\mathbf{v}\psi_1\rangle + D_0\rho q'(\rho)\nabla\rho \tag{2}$$

Combining (1) and (2), we recovered the volume-exclusion PKS model.

Outline

Approximate kinetic model

As we are interested in the limit $\varepsilon \to 0$, we truncate F_ε and T_ε and solve

$$\varepsilon^2 \partial_t f + \varepsilon \mathbf{v} \cdot \nabla (\tilde{F}_\varepsilon(\rho) f) = q(\rho) \left(-f + \rho \tilde{T}_\varepsilon(\mathbf{v}, \rho, \nabla c) \right) + \varepsilon^2 r_0 f \left(1 - \rho/\rho_{\mathsf{max}}\right)_+ ,$$

where

$$\begin{aligned} \tilde{F}_\varepsilon &= q(\rho(t,\mathbf{x})) + \varepsilon q'(\rho(t,\mathbf{x})) \mathbf{v} \cdot \nabla \rho(t,\mathbf{x}) , \\ \tilde{T}_\varepsilon &= \psi_0(\mathbf{v}) + \varepsilon \left(\psi_1(\mathbf{v}, \nabla c) + \frac{q'(\rho)}{q(\rho)} (\mathbf{v} \cdot \nabla \rho) \psi_0(\mathbf{v}) \right) . \end{aligned}$$

Remark

The approximate kinetic model converges to the same macroscopic limit (with proliferation term) as $\varepsilon \to 0$.

Micro-macro decomposition [3]

To design an asymptotic preserving scheme, we decompose

$$f(t,\mathbf{x},\mathbf{v}) = \rho(t,\mathbf{x})\psi_0(\mathbf{v}) + \varepsilon g(t,\mathbf{x},\mathbf{v}),$$

where g is the perturbation satisfying $\langle g \rangle = 0$.

Equation for ρ

Integrating the approximate kinetic model

$$\partial_t f + \frac{1}{\varepsilon}\mathbf{v}\cdot\nabla(\tilde{F}_\varepsilon(\rho)f) = \frac{1}{\varepsilon^2}q(\rho)\left(-f + \rho\tilde{T}_\varepsilon(\mathbf{v},\rho,\nabla c)\right) + r_0 f\left(1-\rho/\rho_{\max}\right)_+$$

over $\mathbf{v}$*, we have*

$$\partial_t \rho + \langle \mathbf{v}\cdot\nabla(q(\rho)g)\rangle + \nabla\cdot(q'(\rho)\rho D_0\nabla\rho) = r_0\rho\left(1-\rho/\rho_{\max}\right)_+ \ .$$

[3] M. Lemou and L. Mieussens (2008)

Equation for g

To get equation for g, we introduce the projection

$$\Pi f(t,\mathbf{v},\mathbf{x}) = \langle f(t,\mathbf{v},\mathbf{x})\rangle \psi_0(\mathbf{v})$$

Equation for g

Taking $I-\Pi$ into the kinetic equation, we get

$$\begin{aligned}&\partial_t g + \frac{1}{\varepsilon}(I-\Pi)\left[\mathbf{v}\cdot\nabla(q(\rho)g) + \nabla\cdot(\rho q'(\rho)(\mathbf{v}\otimes\mathbf{v})\nabla\rho\psi_0)\right]\\ =&\frac{1}{\varepsilon^2}\left[-q(\rho)(\mathbf{v}\cdot\nabla\rho)\psi_0 + \rho q(\rho)\psi_1 - q(\rho)g\right] + r_0 g\left(1-\rho/\rho_{\max}\right)_+ \ .\end{aligned}$$

Micro-macro formulation

Micro-macro formulation

$$\begin{cases} \partial_t \rho + \langle \mathbf{v} \cdot \nabla (q(\rho) g) \rangle + D_0 \nabla \cdot (\rho q'(\rho) \nabla \rho) = r_0 \rho \left(1 - \rho/\rho_{\max}\right)_+ \ , \\ \partial_t g + \frac{1}{\varepsilon}(I - \Pi) K_\varepsilon = \frac{1}{\varepsilon^2} S_\varepsilon + r_0 g \left(1 - \rho/\rho_{\max}\right)_+ \ , \\ \Delta c + \rho - c = 0 \ , \end{cases}$$

where $D_0 = \langle (\mathbf{v} \otimes \mathbf{v}) \psi_0 \rangle$, *and*

$$K_\varepsilon = \mathbf{v} \cdot \nabla (q(\rho) g) + \nabla \cdot (\rho \psi_0 (\mathbf{v} \otimes \mathbf{v}) \nabla q(\rho)) \ ,$$
$$S_\varepsilon = -q(\rho)(\mathbf{v} \cdot \nabla \rho) \psi_0 + \rho q(\rho) \psi_1 - q(\rho) g \ .$$

Remark

In the limit $\varepsilon \to 0$, *we can recover the volume-exclusion PKS model by forcing* $S_\varepsilon = 0$.

1D finite difference scheme for ρ

Equation for ρ

With standard finite difference notations

$$\delta_t^+ \rho_j^n + \langle v_k \delta_x (q(\bar{\rho}_*^n) g_{*,k}^{n+1})_j \rangle_h + D_h \delta_x (\bar{\rho}_*^n q'(\bar{\rho}_*^n) \delta_x \rho_*^{n+1})_j = r_0 \rho_j^n \left(1 - \frac{\rho_j^n}{\rho_{\max}}\right)_+$$

where $\langle \eta_{j,k}^n \rangle_h := \Delta v \sum_k \eta_{j,k}^n$, $D_h := \langle v_k^2 \psi_0(v_k) \rangle_h$ *and*

$$\delta_x (q(\bar{\rho}_*^n) g_{*,k}^n)_j = \frac{q(\bar{\rho}_{j+\frac{1}{2}}^n) g_{j+\frac{1}{2},k}^n - q(\bar{\rho}_{j-\frac{1}{2}}^n) g_{j-\frac{1}{2},k}^n}{\Delta x},$$

Upwind discretization for chemotaxis

- Cells aggregate to form patterns in regions where chemoattractant is highly concentrated
- To avoid instability issues and inspired by [4], we discretize $q(\rho)\rho\psi_1(\mathbf{v}, \nabla c)$ in an upwind manner as follows

$$\Phi^{n_1,n}_{j+\frac{1}{2}} = \begin{cases} \rho_j^{n_1} q(\rho^n_{j+1}) \ , & \text{if } \delta_x c^n_{j+\frac{1}{2}} \geq 0 \ , \\ \rho_{j+1}^{n_1} q(\rho^n_j) \ , & \text{if } \delta_x c^n_{j+\frac{1}{2}} < 0 \ , \end{cases}$$

where $n_1 = n$ or $n+1$.

[4] L. Almeida, F. Bubba, B. Perthame, and C. Pouchol. (2018)

1D finite difference scheme for g

Equation for g

$$\delta_t^+ g^n_{j+\frac{1}{2},k} + \frac{1}{\varepsilon}(I-\Pi_h)K^n_{j+\frac{1}{2},k} = \frac{1}{\varepsilon^2}S^{n,n+1}_{j+\frac{1}{2},k} + r_0 g^n_{j+\frac{1}{2},k}\left(1-\frac{\rho^n_{j+\frac{1}{2}}}{\rho_{\max}}\right)_+$$

where $\Pi_h \eta^n_{j,k} = \langle \eta^n_{j,k}\rangle_h \psi_0(v_k)$ *for some general* η *and*

$$\begin{aligned}
K^n_{j+\frac{1}{2},k} &= v_k^+ \delta_x (q(\bar\rho^n_*) g^n_{*,k})_j - v_k^- \delta_x (q(\bar\rho^n_*) g^n_{*,k})_{j+1} \\
&\quad + v_k^2 \psi_0(v_k) \delta_x (\bar\rho^n_* q'(\bar\rho^n_*) \delta_x \rho^n_*)_{j+\frac{1}{2}} \\
S^{n,n+1}_{j+\frac{1}{2},k} &= -v_k \psi_0(v_k) q(\bar\rho^n_{j+\frac{1}{2}}) \delta_x \rho^{n+1}_{j+\frac{1}{2}} + \psi_1(v_k, \delta_x c^n_{j+\frac{1}{2}}) \Phi^{n+1,n}_{j+\frac{1}{2}} \\
&\quad - q(\bar\rho^n_{j+\frac{1}{2}}) g^{n+1}_{j+\frac{1}{2},k}
\end{aligned}$$

Decoupling of ρ and g

To decouple ρ and g, we define

$$\frac{\tilde{g}^{n+1}_{j+\frac{1}{2},k} - g^{n}_{j+\frac{1}{2},k}}{\Delta t} + \cdots = \frac{1}{\varepsilon^2}\tilde{S}^{n,n+1}_{j+\frac{1}{2},k} + \cdots,$$

where

$$\tilde{S}^{n,n+1}_{j+\frac{1}{2},k} = -v_k\psi_0(v_k)q(\bar{\rho}^{n}_{j+\frac{1}{2}})\delta_x\rho^{n}_{j+\frac{1}{2}} + \psi_1(v_k, \delta_x c^{n}_{j+\frac{1}{2}})\Phi^{n,n}_{j+\frac{1}{2}} - q(\bar{\rho}^{n}_{j+\frac{1}{2}})\tilde{g}^{n+1}_{j+\frac{1}{2},k}\,.$$

Remark

$\tilde{g}^{n+1}_{j+\frac{1}{2},k}$ *can be computed explicitly*

Decoupling of ρ and g

To decouple ρ and g, we define

$$\frac{\tilde{g}^{n+1}_{j+\frac{1}{2},k} - g^{n}_{j+\frac{1}{2},k}}{\Delta t} + \cdots = \frac{1}{\varepsilon^2}\tilde{S}^{n,n+1}_{j+\frac{1}{2},k} + \cdots,$$

where

$$\tilde{S}^{n,n+1}_{j+\frac{1}{2},k} = -v_k\psi_0(v_k)q(\bar{\rho}^n_{j+\frac{1}{2}})\delta_x\rho^n_{j+\frac{1}{2}} + \psi_1(v_k,\delta_x c^n_{j+\frac{1}{2}})\Phi^{n,n}_{j+\frac{1}{2}} - q(\bar{\rho}^n_{j+\frac{1}{2}})\tilde{g}^{n+1}_{j+\frac{1}{2},k}\,.$$

Remark

$\tilde{g}^{n+1}_{j+\frac{1}{2},k}$ *can be computed explicitly*

The equation for ρ can be reformulated as

$$\frac{\rho^{n+1}_j}{\Delta t} - \delta_x(a^n_*\delta_x\rho^{n+1}_*)_j + \delta_x(b^n_*\Phi^{n+1,n}_*)_j + D_h\delta_x(\rho^n_* q'(\rho^n_*)\delta_x\rho^{n+1}_*)_j = r^n_j,$$

where $a^n_{j+\frac{1}{2}}$, $b^n_{j+\frac{1}{2}}$ and r^n_j can be explicitly computed using $\tilde{g}^{n+1}_{j+\frac{1}{2},k}$

Asymptotic preserving property

Checking the order of ε in the equation for g, we should have $S^{n,n+1}_{j+\frac{1}{2},k} = 0$ as $\varepsilon \to 0$, namely

$$q(\bar{\rho}^n_{j+\frac{1}{2}})g^{n+1}_{j+\frac{1}{2},k} = -v_k\psi_0(v_k)q(\bar{\rho}^n_{j+\frac{1}{2}})\delta_x\rho^{n+1}_{j+\frac{1}{2}} + \psi_1(v_k, \delta_x c^n_{j+\frac{1}{2}})\Phi^{n+1,n}_{j+\frac{1}{2}} \ .$$

A direct computation shows that

$$\langle v_k\delta_x(q(\bar{\rho}^n_*)g^{n+1}_{*,k})_j\rangle_h = \delta_x(-D_h q(\bar{\rho}^n_*)\delta_x\rho^{n+1}_* + \langle v_k\psi_1(v_k, \delta_x c^n_*)\rangle_h\Phi^{n+1,n}_*)_j \ .$$

Substituting into the equation for ρ, we recovered

$$\delta^+_t\rho^n_j - \delta_x\left[D_h d(\bar{\rho}^n_*)\delta_x\rho^{n+1}_* - \langle v_k\psi_1(v_k, \delta_x c^n_*)\rangle_h\Phi^{n+1,n}_*\right]_j = r_0\rho^n_j\left(1 - \frac{\rho^n_j}{\rho_{\max}}\right)$$

the finite difference scheme for the volume-exclusion PKS model.

Positive preserving in the limit

Considering $q(\rho) = 1 - \rho/\bar{\rho}$ and $f(\rho) = r_0\rho\left(1 - \frac{\rho}{\rho_{\max}}\right)_+$

Proposition

- *If* $\rho_0^n \geq 0$ *for all* j*, then, for whatever* $\Delta t > 0$*, we have*

$$\rho_j^n \geq 0$$

for all j *and* $n \geq 1$*.*

- *If we use a modified implicit scheme by changing* $d(\bar{\rho}_*^n)$ *to* $d(\bar{\rho}_*^{n+1})$*, where* $d(\rho) = q(\rho) - \rho q'(\rho)$*, it can be further proved that if* $\rho_j^0 < \overline{\rho}$ *for all* j *and* $(1 + r_0\Delta t)\rho_{\max} < \bar{\rho}$*, then*

$$\rho_j^n \leq \overline{\rho}$$

for all j*, and* $n \geq 1$ *.*

Generalization to 2D

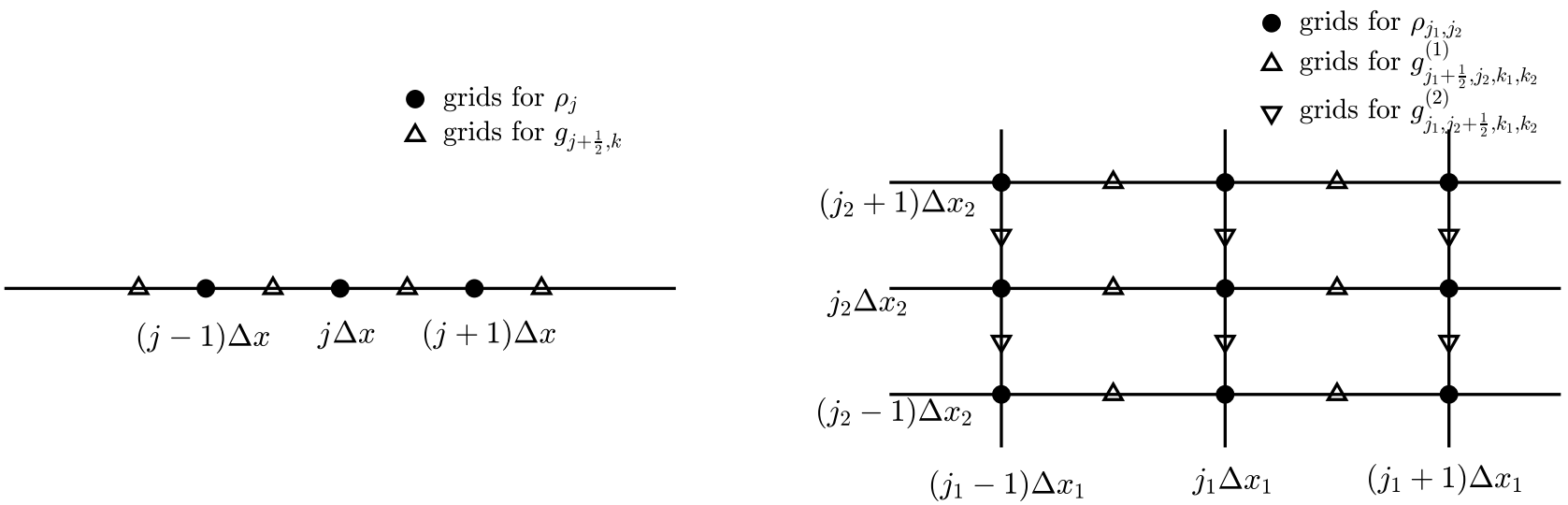

Figure: Grids in $\mathbf{x}$-space for computing $\rho(t,\mathbf{x})$ and $g(t,\mathbf{x},\mathbf{v})$ in 1D and 2D.

Outline

Numerical setup for 1D tests

- Domain $(x, v) \in (-20, 20)^2$ with a uniform mesh $\Delta x = 0.1, \Delta v = 0.2$
- Periodic boundary condition in x and the zero boundary condition in v
- Parameters: $r_0 = 0.1$, $\rho_{\max} = 0.5$, $\bar{\rho} = 1$ and

$$\psi_0(v) = \frac{1}{\sqrt{2\pi}} e^{-\frac{v^2}{2}} , \quad \psi_1(v, \nabla c) = \frac{v}{\sqrt{2\pi}} e^{-\frac{v^2}{2}} \nabla c .$$

- Initial data

$$\rho_0(x) = 0.5 + u(x) , \quad c_0(x) = 0.5 , \quad g_0^\varepsilon(x, v) = 0 ,$$

where $u(x) \in (-0.1, 0.1)$ is a uniformly distributed random function

Comparison of 1D solutions

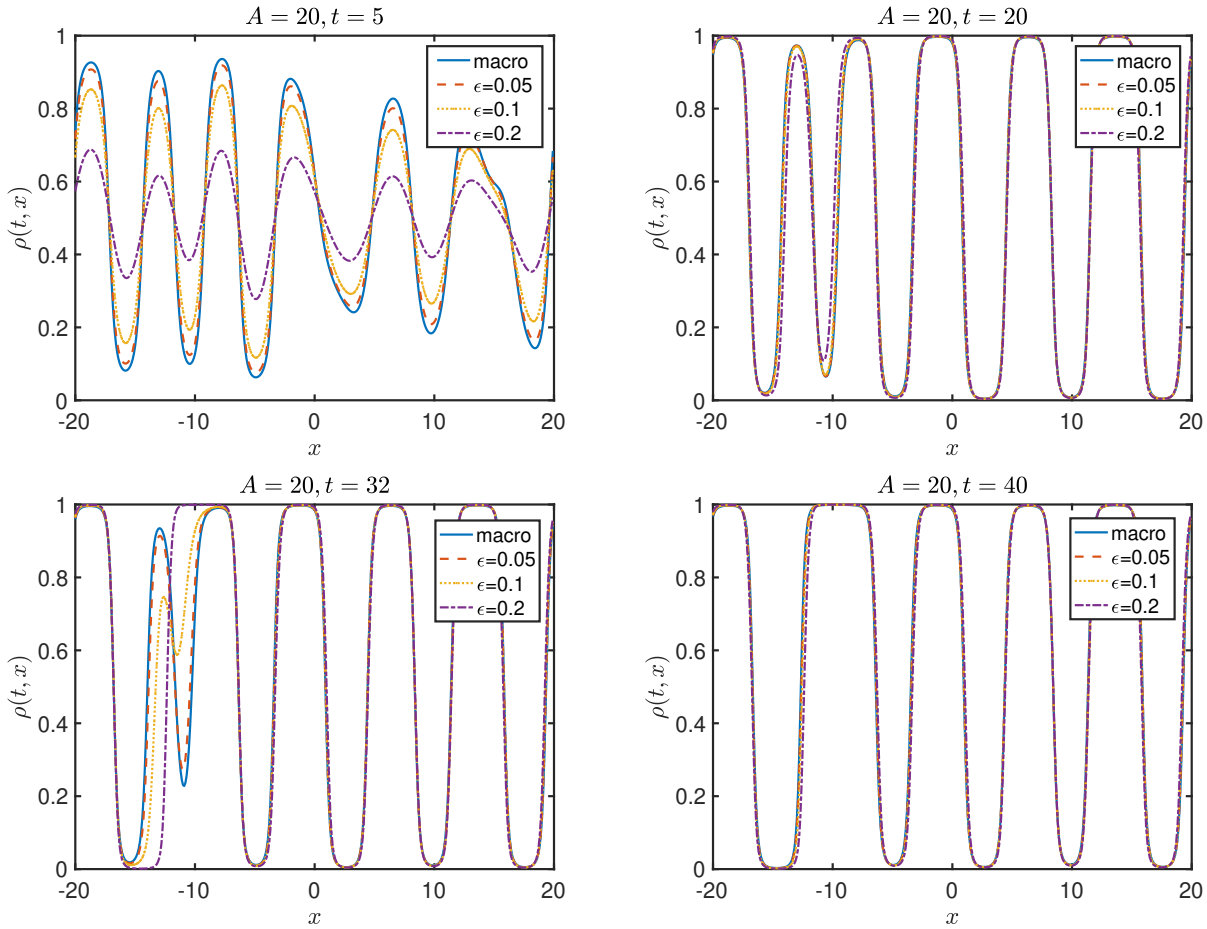

Figure: Comparison of ρ_{macro} and $\rho^{\varepsilon}_{\text{kinetic}}$ for $A = 20$ and different ε's. Here A is the chemotactic sensitivity.

Energy dissipation

Proposition

Define the energy

$$\mathcal{E}(t) = \int \Phi(\rho)\,\mathrm{d}x - \frac{1}{2}\int \rho c\,\mathrm{d}x\ ,$$

where

$$\Phi'(\rho) = H(\rho) := \frac{D_0}{\beta}\ln\left(\frac{\rho}{q(\rho)}\right)\ ,$$

we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(t) = -\int \rho\chi(\rho)|\nabla(H-c)|^2\,\mathrm{d}x \le 0\ ,$$

when $r_0 = 0$ *or* $r_0 > 0$ *but* $\rho_{\max} + \rho_{\max}/\bar{\rho} \le 1$

Numerical test of energy dissipation

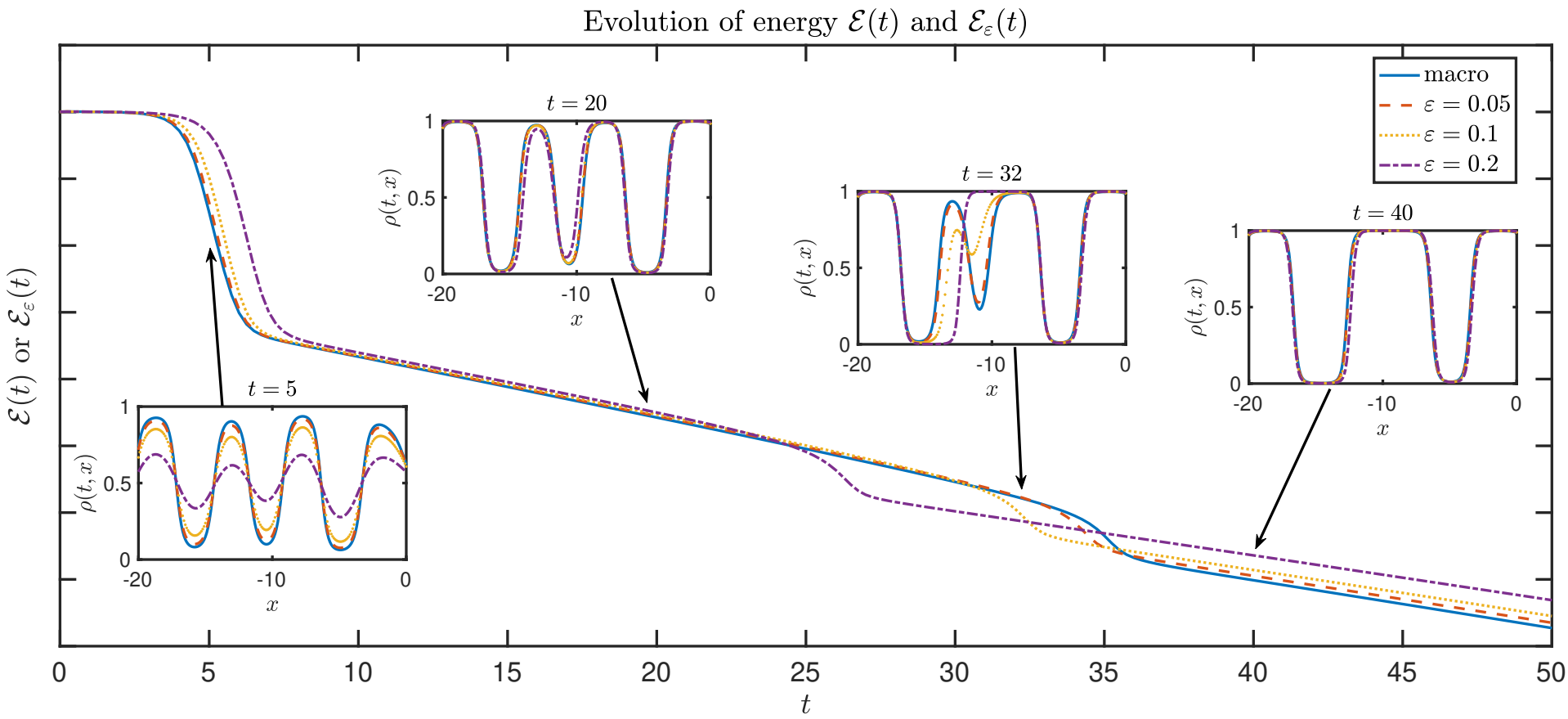

Figure: Evolution of $\mathcal{E}(t)$ and $\mathcal{E}_\varepsilon(t)$ along with the comparison between the kinetic solutions $\rho^\varepsilon_{\text{kinetic}}$ and the macroscopic solutions $\rho_{\text{macro}}(t,x)$ at $t = 5,\ 20,\ 32,\ 40$ for $A = 20$.

Convergence test in ε

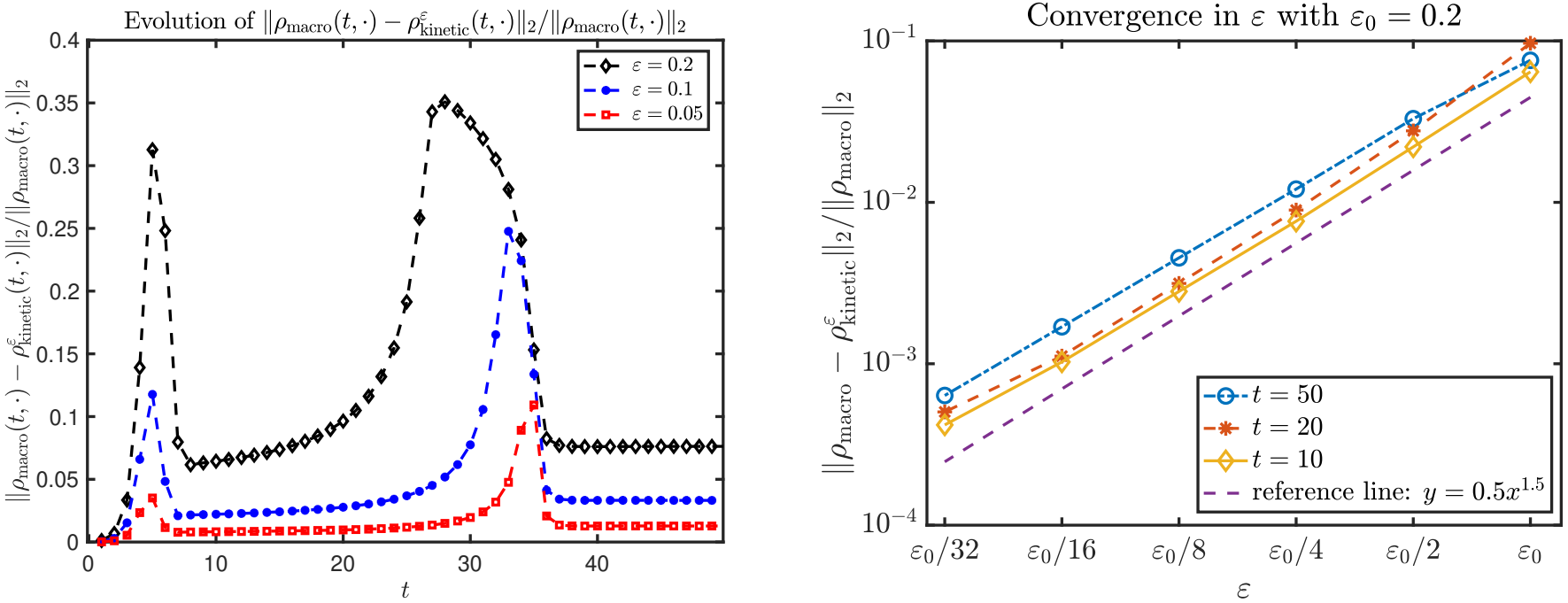

Figure: Left: Evolution of the relative L_2-error $\frac{\|\rho_{\text{macro}}(t,\cdot)-\rho_{\text{kinetic}}(t,\cdot)\|_2}{\|\rho_{\text{macro}}(t,\cdot)\|}$ over time with $A = 20$. Right: Convergence of the relative L_2-error in ε at $t = 10,\ 20,\ 50$.

Pattern formation from a perturbed initial data

- With a randomly perturbed initial data

$$\rho(t=0,x) = 0.5 + u(x) \ ,$$

where $\rho \equiv 0.5$ is an equilibrium solution when $\rho_{\max} = 0.5$, a linear stability analysis [5] will give an analytical prediction of the pattern size.

- To numerically compute the pattern sizes, we consider using $1/k_{\max}$, where

$$k_{\max} = \text{argmax}_{\lambda}(|\hat{\rho}(\lambda)|).$$

and $\hat{\rho}(\lambda) = \mathcal{F}(\rho)(t,x)$ is the Fourier transform of $\rho(t,x)$.

[5] L. Almeida, G. Estrada-Rodriguez, L. Oliver, D. Peurichard, A. Poulain, and F. Vallette (2020)

Numerical verification of pattern size

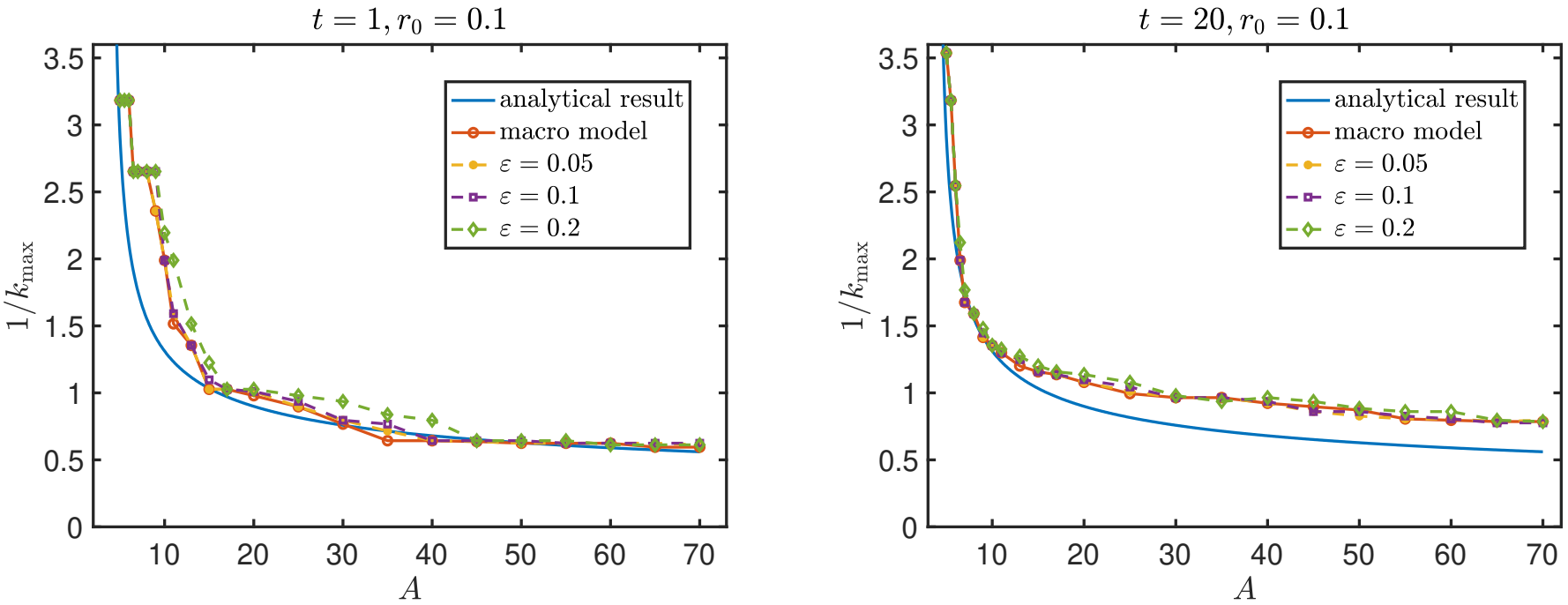

Figure: Comparison of $\frac{1}{k_{\max}}$ between the analytical, the numerical results of the macro and the kinetic model. The numerical result is computed by averaging 10 solutions, each evolved from a random initial data around 0.5. Here A is the chemotactic sensitivity.

Numerical setup for 2D tests

- Domain $\mathbf{x} \in (-20, 20)^2$, $\mathbf{v} \in (-10, 10)^2$ with a uniform mesh
- Periodic boundary condition in $\mathbf{x}$ and the zero boundary condition in $\mathbf{v}$
- Parameters: $r_0 = 0.1$, $\rho_{\max} = 0.5$, $\bar{\rho} = 1$ and

$$\psi_0(\mathbf{v}) = \frac{1}{2\pi} e^{-\frac{|\mathbf{v}|^2}{2}}, \quad \psi_1(\mathbf{v}\ , \nabla_{\mathbf{x}} c) = \frac{\mathbf{v}}{2\pi} e^{-\frac{|\mathbf{v}|^2}{2}} \cdot \nabla_{\mathbf{x}} c\ .$$

- Initial data

$$\rho_0(\mathbf{x}) = 0.5 + u(\mathbf{x})\ , \quad c_0(\mathbf{x}) = 0.5, \quad g_0^{\varepsilon}(\mathbf{x}, \mathbf{v}) = 0\ ,$$

where $u(\mathbf{x}) \in (-0.1, 0.1)$ is a uniformly distributed random function

Chemotactic sensitivity and patterns

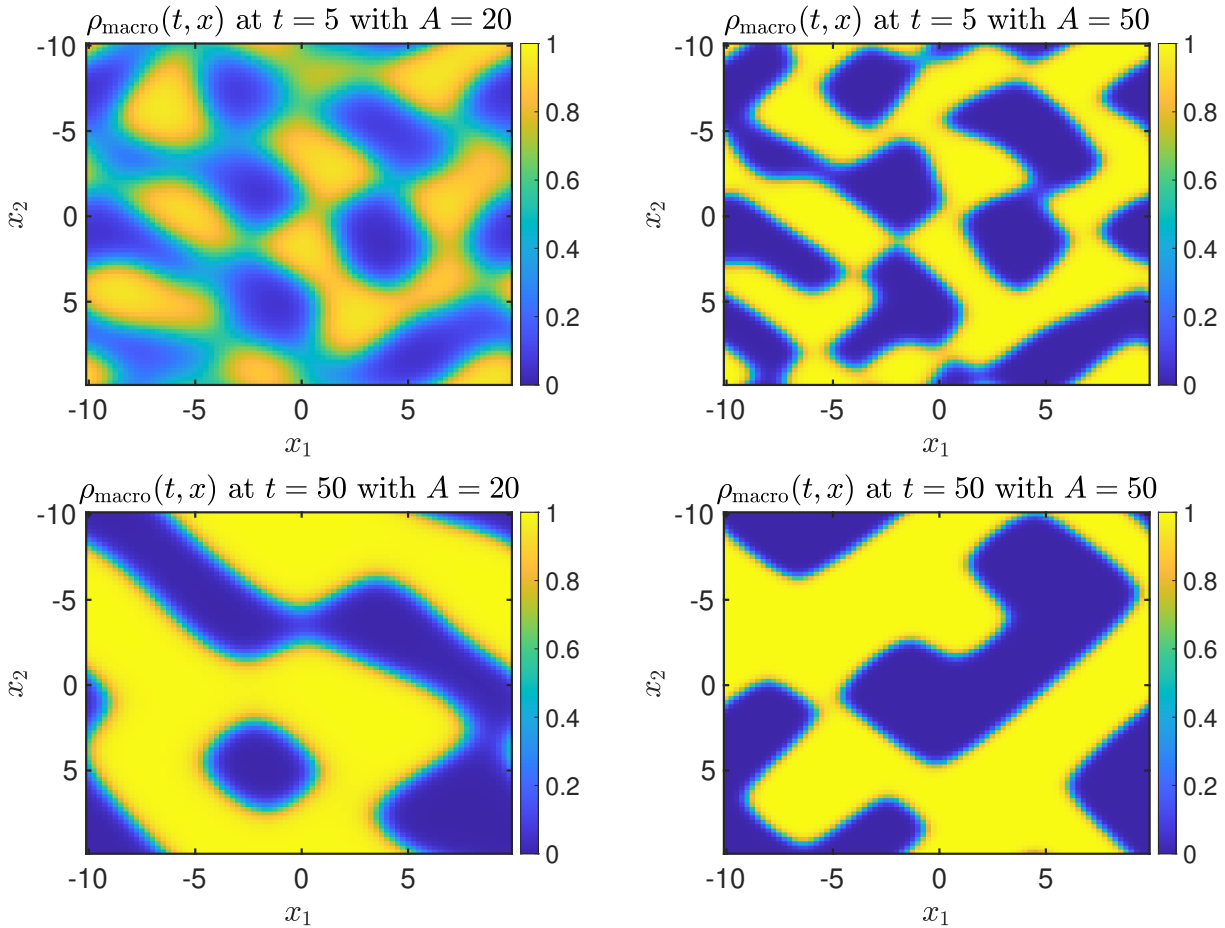

Figure: Plots of density $\rho_{\text{macro}}(t,\mathbf{x})$ at $t=5,\ 50$ (from top to bottom) with $A=20,\ 50$ (from left to right), respectively.

Patterns for different initial data

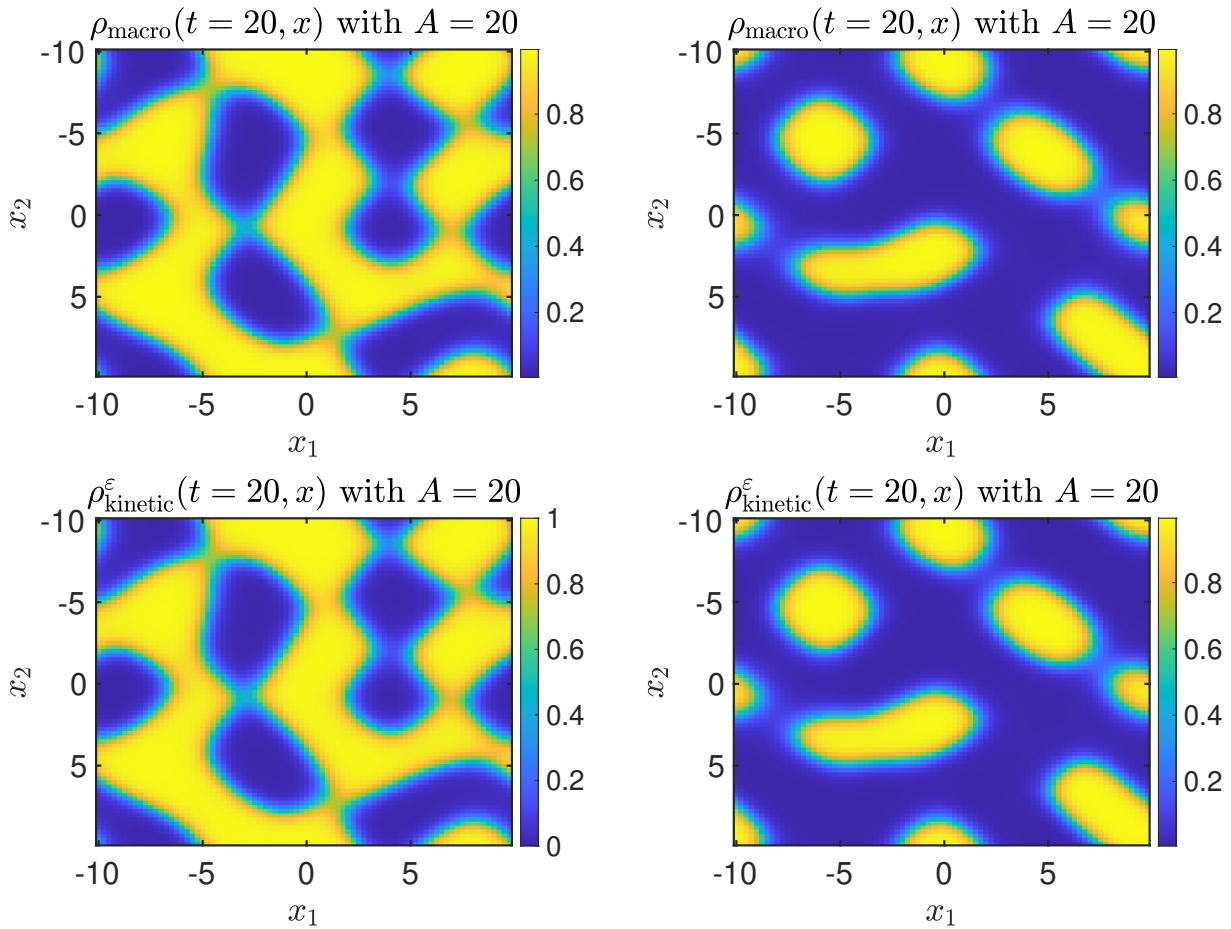

Figure: Comparison between $\rho_{\text{macro}}(t,\mathbf{x})$ (first row) and $\rho^{\varepsilon}_{\text{kinetic}}(t,\mathbf{x})$ with $\varepsilon = 10^{-2}$ (second row) for different initial conditions $\rho_0 \approx 0.5$ (first column) and $\rho_0 \approx 0.1$ (last column) and different values of the chemotactic sensitivity $A = 20$.

Convergence test of 2D model

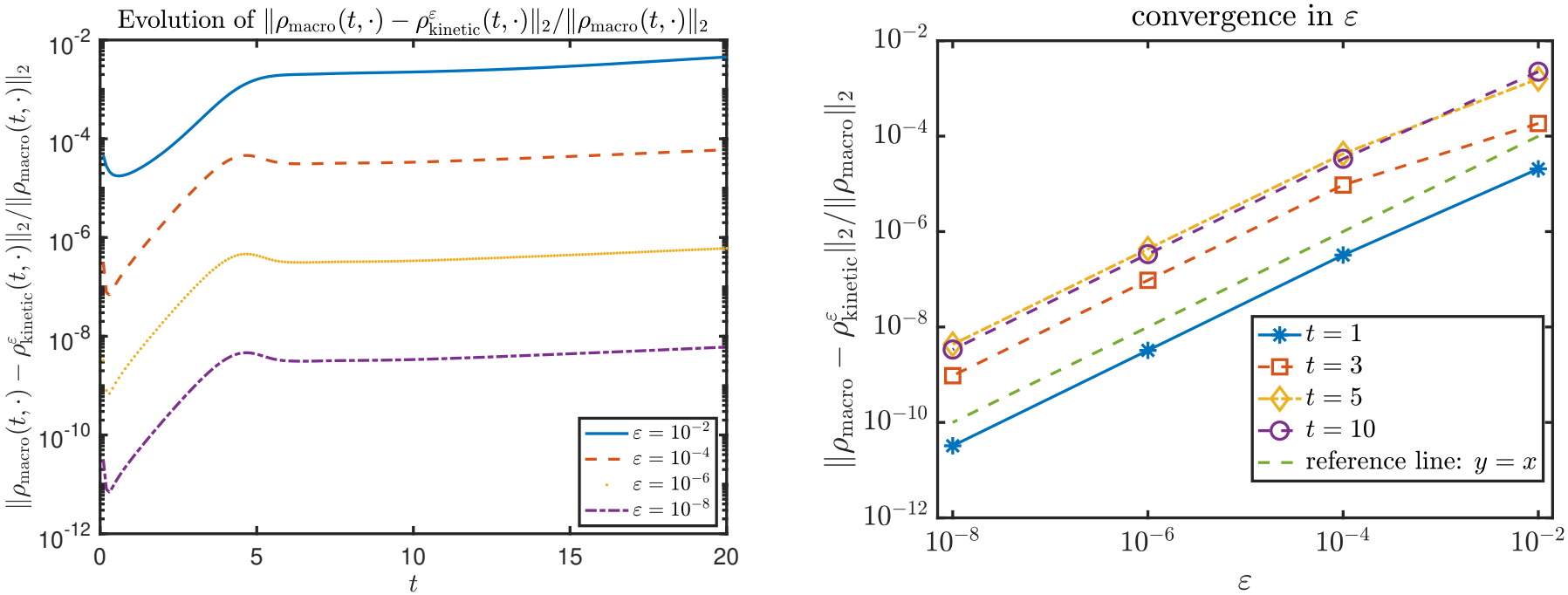

Figure: Left: Evolution of the relative L_2-error. Right: Convergence of the relative L_2-error in ε at $t = 1,\ 3,\ 5,\ 10$ with $A = 20$ and $\Delta t = 10^{-2}$.

Conclusions

- A kinetic model for chemotaxis incorporating a density dependence is derived.
- The volume-exclusion PKS model can be formally proved as the diffusion limit of the kinetic 'velocity-jump' model.
- An IMEX asymptotic preserving finite difference scheme based on a micro-macro decomposition is proposed for the kinetic model.
- In numerical experiments, we verified the convergence of the kinetic model, yet observed some differences, such as a delay in the aggregation process.

Future work:

- To extend the derivation to consider different turning kernels, to take into account cell-cell adhesion, etc.
- To construct numerical schemes for related cases.
- To connect with stochastic processes of interacting populations.

Reference: arXiv:2211.01415 [math.AP]

Thank you all for your attention!