

Mathematical modeling of complex systems

Part 2. Morphogenesis driven by non-overlapping

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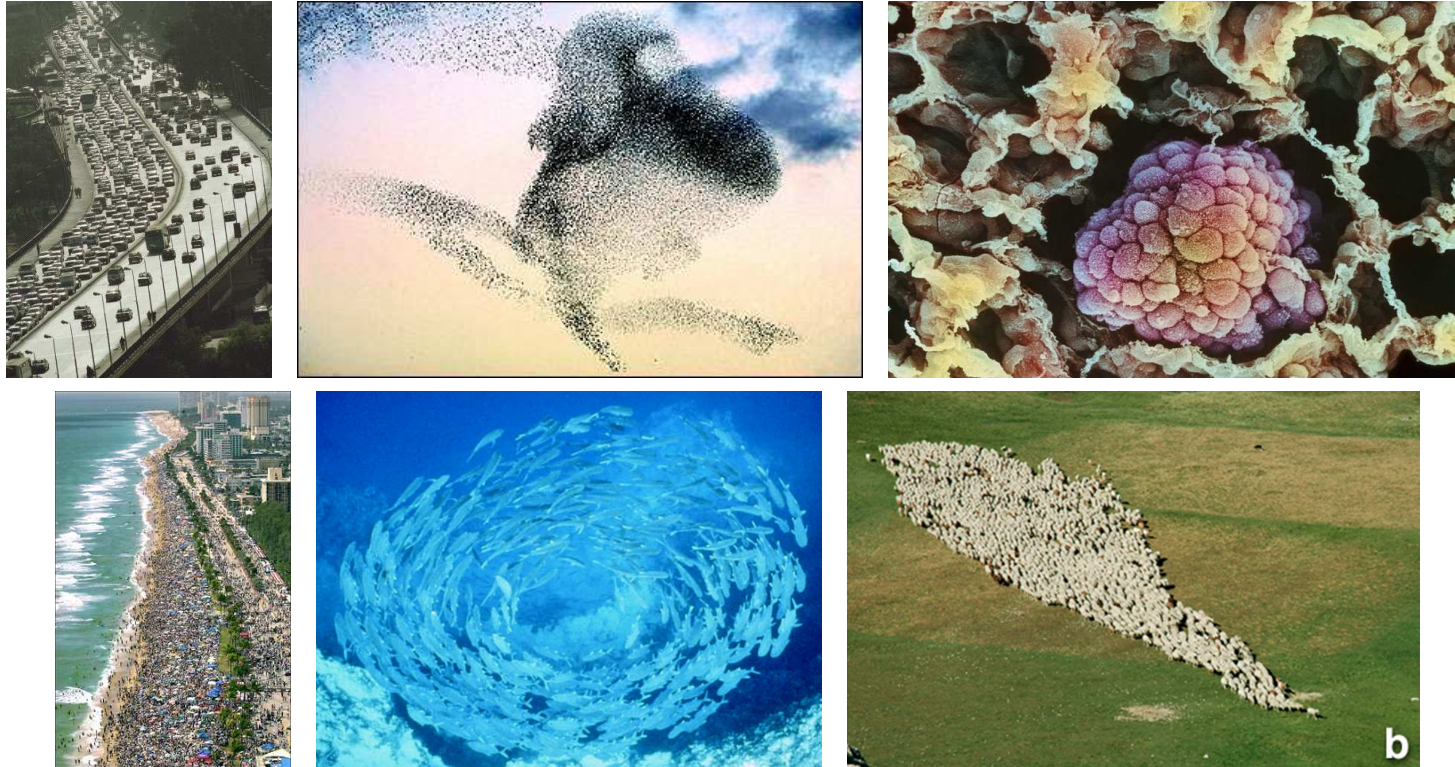
Joint work with J. Hua, L. Navoret, D. Sanchez (IMT)

& R. Bon (CRCA)

1. Introduction
2. Phase transitions driven by non-overlapping constraint
3. Numerical treatment of phase transition
4. Conclusion

1. Introduction

Non-overlapping constraint in complex systems⁴



➤ Well-defined patterns

➤ phase transition: Free / Congested

➤ non-overlapping (steric) constraint \Rightarrow incompressible

2. Phase transitions driven by non-overlapping constraint

Ex 1: Compressible Euler

$$\partial_t \rho + \nabla \cdot (\rho u) = 0$$

$$\partial_t(\rho u) + \nabla \cdot (\rho u \otimes u) + \nabla p(\rho) = 0$$

Ex 2: Vicsek Hydrodynamics & nonlinear pressure

$$\partial_t \rho + \nabla \cdot (\rho u) = 0$$

$$\rho(\partial_t u + c(u \cdot \nabla)u) + (\text{Id} - u \otimes u)\nabla p(\rho) = 0$$

$$|u| = 1$$

→ Normalization condition $|u| = 1$

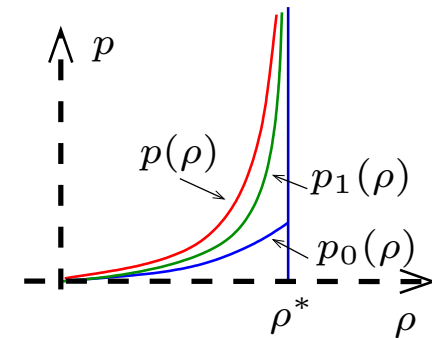
→ Speed of 'velocity waves' $c \neq 1$

→ [D. & Motsch, M3AS 2008]

➤ $p(\rho) \rightarrow \infty$ as $\rho \rightarrow \rho^* =$ congestion density

➤ Ex: $p(\rho) = p_0(\rho) + p_1(\rho)$

$$p_0(\rho) = K\rho^k, \quad p_1(\rho) = \frac{1}{\left(\frac{1}{\rho} - \frac{1}{\rho^*}\right)^\gamma}$$



➤ Two phases of motion:

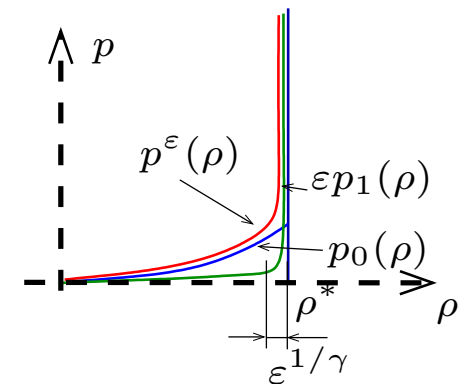
➤ Uncongested: $\rho < \rho^*$

➤ Congested: $\rho \sim \rho^*$

➤ Sharp transition of width $= O(\varepsilon)$

➤ Rescale p_1 into εp_1

➤ Pressure: $p^\varepsilon = p_0(\rho) + \varepsilon p_1$



➤ After rescaling: perturbation problem \mathcal{P}^ε

$$\partial_t \rho^\varepsilon + \nabla \cdot (\rho^\varepsilon u^\varepsilon) = 0$$

$$\partial_t (\rho^\varepsilon u^\varepsilon) + \nabla \cdot (\rho^\varepsilon u^\varepsilon \otimes u^\varepsilon) + \nabla p_0(\rho^\varepsilon) + \varepsilon \nabla p_1(\rho^\varepsilon) = 0$$

➤ Limit $\varepsilon \rightarrow 0$ (formal)

➤ leads to a limit problem \mathcal{P}^0

➤ associated to a two-phase model:

➤ Free: $\rho < \rho^*$, $\varepsilon p_1(\rho^\varepsilon) \rightarrow 0$

➤ Congested: $\rho = \rho^*$, $\varepsilon p_1(\rho^\varepsilon) \rightarrow \bar{p}_1 > 0$

➤ and abrupt transitions between the 2 phases

Free phase: $\rho < \rho^*$, $\varepsilon p_1(\rho^\varepsilon) \rightarrow 0$

limit model is standard Euler with pressure p_0

$$\partial_t \rho + \nabla \cdot (\rho u) = 0,$$

$$\partial_t(\rho u) + \nabla \cdot (\rho u \otimes u) + \nabla p_0(\rho) = 0$$

Congested phase: $\rho = \rho^*$, $\varepsilon p_1(\rho^\varepsilon) \rightarrow \bar{p}_1 > 0$

limit model is incompressible Euler

$$\nabla \cdot u = 0, \quad \rho = \rho^*$$

$$\partial_t(\rho^* u) + \nabla \cdot (\rho^* u \otimes u) + \nabla \bar{p} = 0$$

➤ Computation of \bar{p} in problem \mathcal{P}^0 :

➤ Take $\nabla \cdot$ of vel. eq.

$$-\Delta \bar{p} = \nabla^2 : \cdot (\rho^* u \otimes u)$$

➤ elliptic eq.

➤ requires boundary conditions

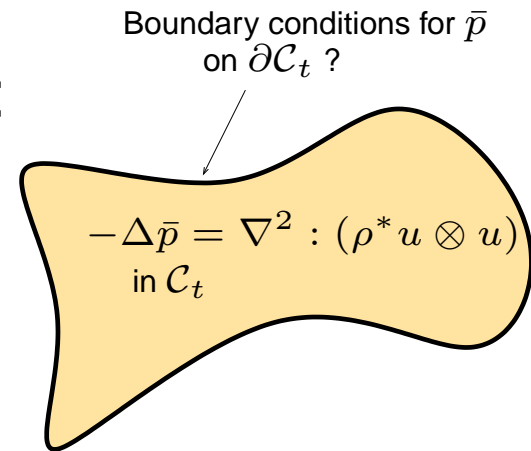
➔ at boundary $\partial \mathcal{C}_t$ of congestion region \mathcal{C}_t

➤ not given by formal asymptotics

➤ depends on the microscopic scales ε

➤ Find these boundary conditions

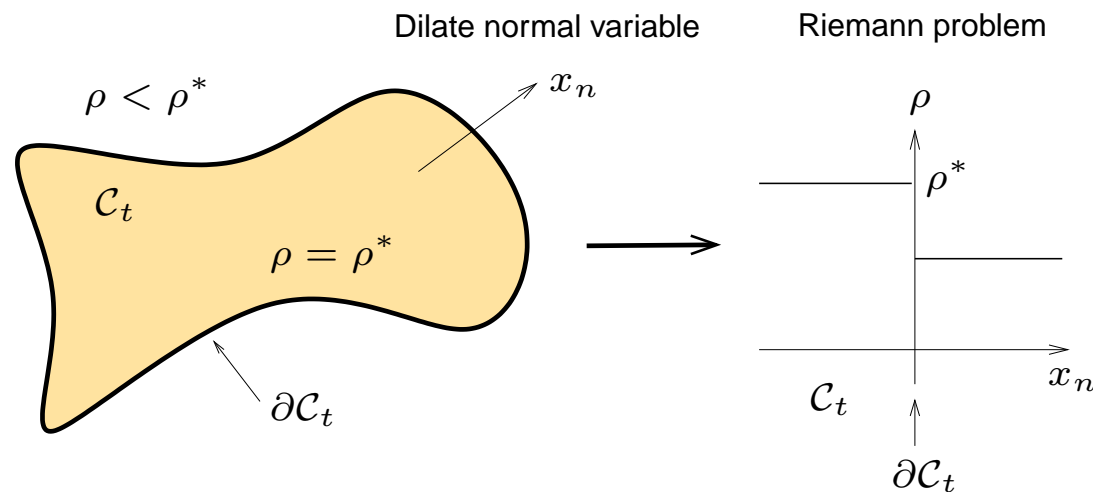
➤ by analyzing perturbation problem \mathcal{P}^ε



1D Riemann problem in dilated variables

for the perturbation problem \mathcal{P}^ε

in the normal direction to boundary $\partial\mathcal{C}_t$



$\varepsilon \rightarrow 0$ in Riemann problem solutions of \mathcal{P}^ε

analytic forms can be found

deduce boundary conditions on $\partial\mathcal{C}_t$

Extrapolate result to general solutions (formal)

➤ Congestion / Uncongested transition

$$\bar{p}|_{\partial\mathcal{C}_t} = \frac{[(u \cdot n)]^2}{\left[\frac{1}{\rho}\right]}, \quad \sigma = \frac{[\rho u \cdot n]}{[\rho]} = \text{interface velocity}$$

➤ Congestion / Vacuum transition

$$\bar{p}|_{\partial\mathcal{C}_t} = 0, \quad \sigma = u \cdot n$$

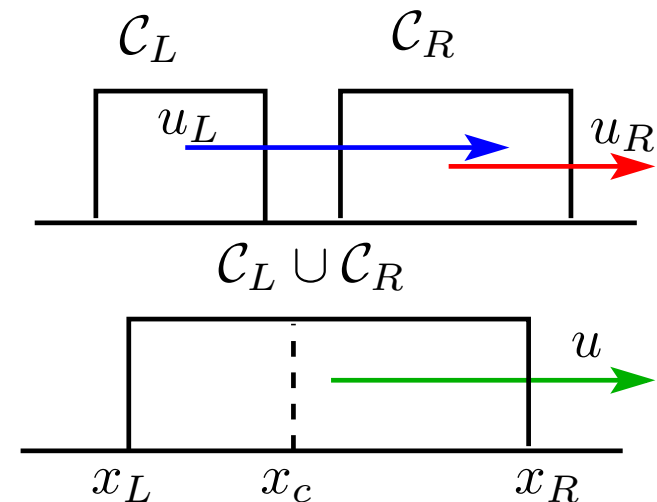
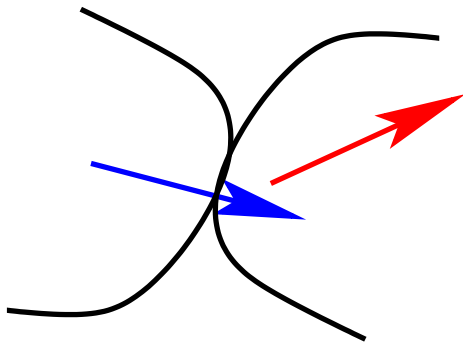
➤ Similar analysis for Vicsek-Hydrodynamic

➤ Additional difficulty $|u| = 1$

➤ Non-conservative model

➤ [D., Navoret, Bon, Sanchez, JSP'10]

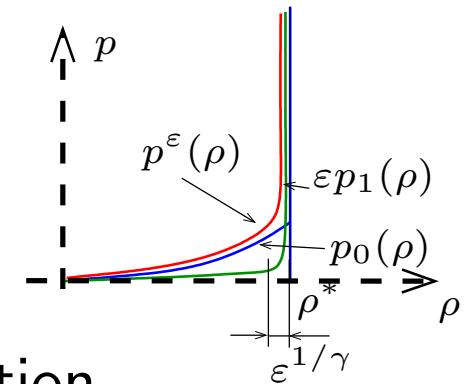
- Problem: what when two clusters collide ?
- Not given by the Riemann pb analysis (delta pressure)
- Solved in 1D in [Bouchut et al, J Nonlinear Sci. 2000]
- 2D case depends on cluster geometry. Open ?



- To resolve the cluster-collision problem:
- Only possibility is numerical simulation of problem \mathcal{P}^ε

3. Numerical treatment of phase transition

- Numerical simulation of perturbation problem \mathcal{P}^ε
 - Only way to access the true physics or the $\varepsilon \rightarrow 0$ limit
 - Requires simulations with $\varepsilon \ll 1$



- Stiff problem
 - Because of stiff pressure p^ε
 - Acoustic wave-speed $\rightarrow \infty$ near congestion
 - CFL condition breaks down: $\Delta t = O(\varepsilon) \rightarrow 0$

- Requires special numerical treatment
 - Asymptotic-Preserving [D., Hua, Navoret, subm.]
 - Based on [D., Tang, CICP, to appear] for low-Mach
 - See also [Haack, Jin & Liu, subm.]

➡ Semi-implicit discretization

$$\frac{\rho^{n+1} - \rho^n}{\Delta t} + \nabla_{\mathbf{x}} \cdot \mathbf{q}^{n+1} = 0, \quad \mathbf{q} = \rho \mathbf{u}$$

$$\frac{\mathbf{q}^{n+1} - \mathbf{q}^n}{\Delta t} + \nabla_{\mathbf{x}} \cdot \left(\frac{\mathbf{q}^n \otimes \mathbf{q}^n}{\rho^n} \right) + \nabla_{\mathbf{x}} p_0(\rho^n) + \varepsilon \nabla_{\mathbf{x}} p_1(\rho^{n+1}) = 0$$

➡ Reformulate into an elliptic eq. for p :

➡ Insert \mathbf{q}^{n+1} into first eq.

$$\begin{aligned} \rho^{n+1} - \varepsilon \Delta t^2 \Delta_{\mathbf{x}} p_1(\rho^{n+1}) &= \\ &= \rho^n - \Delta t \nabla_{\mathbf{x}} \cdot \mathbf{q}^n + \Delta t^2 \nabla_{\mathbf{x}}^2 : \left(\frac{\mathbf{q}^n \otimes \mathbf{q}^n}{\rho^n} \right) + \Delta t^2 \Delta_{\mathbf{x}} p_0(\rho^n) \end{aligned}$$

➡ Can be shown to be AP

➡ consistent with limit problem \mathcal{P}^0 when $\varepsilon \rightarrow 0$

4. Conclusion

- ▶ Phase transitions by non-overlapping constraint
 - ▶ Within macroscopic models
 - ▶ Compressible Euler / Vicsek hydrodynamics ($|u| = 1$)
- ▶ Singular pressure
 - ▶ Tends to ∞ as ρ tends to congestion density ρ^*
 - ▶ Limit problem as $\varepsilon \rightarrow 0$ is 2-phase model
 - ▶ Compressible (free) / Incompressible (congested)
- ▶ Interface conditions
 - ▶ Recovered for smooth interface from Riemann pb
 - ▶ Unknown in case of cluster collision
 - ▶ Numerical methodology but stiff problem
 - ▶ Asymptotic-Preserving methodology

- ▶▶▶ Enrich the physics of the model
 - ▶▶ Swarming systems
 - ▶ Fish, birds, ...
 - ▶▶ Pedestrians
 - ▶ Lane formation
 - ▶ Fluctuations at congestion: crowd turbulence

- ▶▶▶ Investigate other kinds of constraints
 - ▶▶ Flux constraints
 - ▶ Supply chain models

- ▶▶▶ Investigate different morphogenetic forces
 - ▶▶ Dissipative structures
 - ▶ Turing instability