Applied Partial Differential Equations

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Outline

- Nonlinear Schrödinger Equations
- Free Boundary Problems
- Reaction-Diffusion Systems
- A Chemotaxis-Fluid System
- Socio-Economics: Price Formation

Nonlinear Schrödinger Equations

Nonlinear partial differential equations:

$$i\partial_t \psi = -\frac{1}{2}\Delta\psi + V_{\text{ext}}(x)\psi + f(|\psi|^2)\psi,$$

where $\psi = \psi(t,x) \in \mathbb{C}$ for $x \in \mathbb{R}^d$ and $t \geq 0$. Moreover, V_{ext} models external potential forces and the nonlinear term describes particle interactions.

NLS equations are a generic description of nonlinear waves propagating in a dispersive medium, describing a large number of physical phenomena in:

- nonlinear optics (laser beams in fibres),
- quantum superfluids (Bose-Einstein condensates),
- plasma physics,
- water waves
- superconductivity.

Two prominent examples

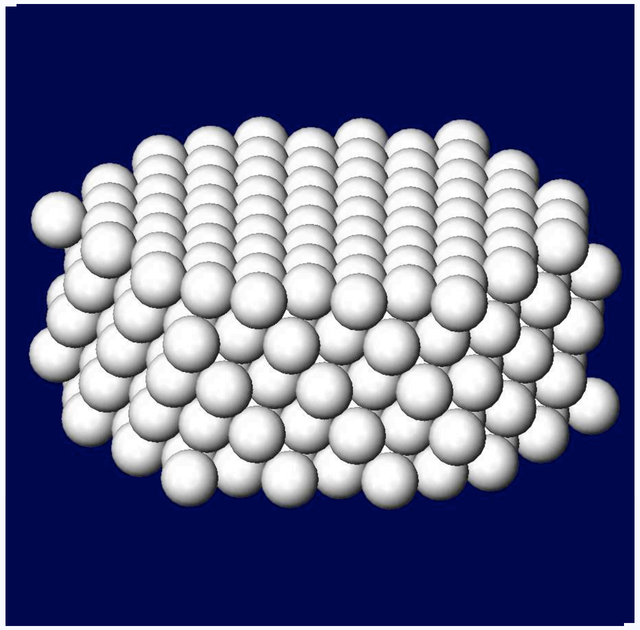
Example 1: The repulsive Schrödinger-Poisson system in $d = 3$:

$$i\partial_t \psi = -\frac{1}{2}\Delta\psi + V_{\text{ext}}(x)\psi + \left(\frac{1}{4\pi|x|} * |\psi|^2\right)\psi$$

describing the self-consistent transport of electrons in semiconductors.

In this case V_{ext} is periodic and models the crystalline lattice-structure of the ions, i.e.

$$V(x+L) = V(x), \quad L \in \Gamma \simeq \mathbb{Z}^d$$



Example 2:

The celebrated Gross- Pitaevskii equation (GP):

$$i\partial_t \psi = -\frac{1}{2}\Delta\psi + V_{\text{ext}}(x)\psi + g|\psi|^2\psi, \quad g \in \mathbb{R}.$$

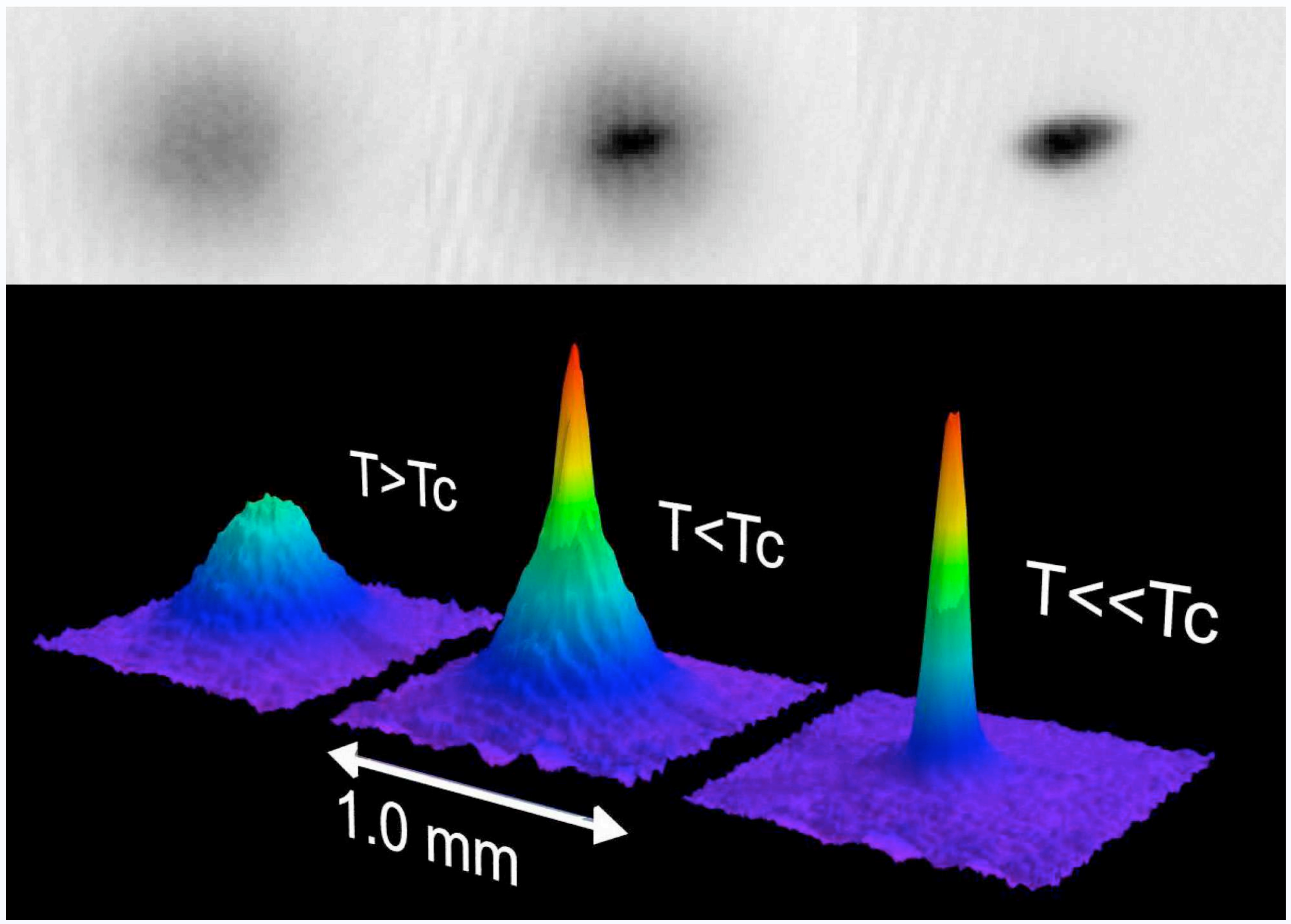
It describes the superfluid dynamics of Bose-Einstein condensates (BECs) in the mean-field limit.

BECs are ultra-cold gases of $N \simeq 10^3 - 10^6$ bosonic atoms (Rb, He,...) confined by laser traps. In this case

$$V_{\text{ext}} = \frac{|x|^2}{2},$$

modelling the electromagnetic trap needed in experiments and $g > 0$ (resp. $g < 0$) in the case of repulsive (resp. attractive) interactions.

Source: Group of W. Ketterle and D. Pritchard, MIT.



Basic Mathematical Questions

Existence of solutions and/or possible finite-time blow-up, i.e. in the focusing case $g < 0$,

$$\exists \; T < \infty : \lim_{t \to T} \|\nabla \psi(t)\|_{L^2} = \infty,$$

where T depends on the initial data. Notice that the total mass is preserved, i.e.

$$\|\psi(t)\|_{L^2} = \|\psi(0)\|_{L^2} \quad \forall \, t > 0.$$

Other mathematical questions:

- soliton dynamics,
- scattering of solutions,
- long-time asymptotics, ...

In the context of BECs blow-up indicates that new physical effects (three-body recombination) have to be taken into account. They can be described by a dissipative nonlinearity

$$i\partial_t\psi = -\frac{1}{2}\Delta\psi + V_{\text{ext}}(x)\psi + g|\psi|^2\psi - i\sigma|\psi|^4\psi, \quad g \in \mathbb{R}, \sigma > 0.$$

Mathematical difficulties:

- quintic nonlinearity is energy-critical;
- no Hamiltonian structure.

Uniform bounds on $\|\nabla\psi\|_{L_t^\infty L_x^2}$ and $\|\psi\|_{L_{t,x}^{10}}$ can be obtained from a-priori estimates on suitable energy-type functionals.

$$E(t) := \int_{\mathbb{R}^3} \frac{1}{2}|\nabla\psi|^2 + V_{\text{ext}}|\psi|^2 + \frac{g}{2}|\psi|^4 + c|\psi|^6 \mathrm{d}x, \quad \text{where } c = c(\sigma) > 0.$$

Multiscale analysis of NLS

Free Schrödinger equation:

$$i\varepsilon\partial_t\psi - \frac{\varepsilon^2}{2}\Delta\psi = 0, \quad \psi(0,x) = e^{ik\cdot x/\varepsilon}.$$

Then,

$$\psi(t,x) = e^{i(k\cdot x/\varepsilon - |k|^2 t/2\varepsilon)},$$

and hence $O(\varepsilon)$ oscillations are propagating in space-time. More generally, the asymptotic behaviour of

$$i\varepsilon\partial_t\psi = -\frac{\varepsilon^2}{2}\Delta\psi + V_{\text{ext}}^{\varepsilon}\psi + gf(|\psi|^2)\psi,$$

poses highly non-trivial multiscale problem even in the linear case $g = 0$. In particular, when

$$V_{\text{ext}}^{\varepsilon}(x) = V_1(x) + V_2(x/\varepsilon), \quad \text{(slow-fast coupling)}.$$

Physical applications:

- electron dynamics in crystals,
- BEC in optical lattices,...

Different analytic approaches in the linear and nonlinear case:

- Wigner measures (Bechouche, Gérard, Markowich, Mauser, Poupaud,....)
- double-scale convergence (Allaire '05)
- space adiabatic perturbation theory (Panati, Spohn, Teufel '02)
- (two-scale) WKB-expansion (Carles, Markowich, Sparber '04)

In the nonlinear case, only short-time results so far (caustics). For multi-scale potentials, only weak nonlinearities can be treated so far $g^\varepsilon = \pm\varepsilon$.

Numerical challenges due to high frequency oscillations:

- Finite-difference schemes require mesh size $\Delta x = o(1)$ and $\Delta t = o(1)$ (Markowich, Pietra, Pohl '00).
- Time-splitting schemes much better behaved (Bao, Jin, Markowich '01)
- Extension to the case of periodic potentials $V_{\text{ext}}(x/\varepsilon + L/\varepsilon) = V(x/\varepsilon)$ (Huang, Jin, Markowich, Sparber '07):

The basic idea is to split the NLS into

(Step 1) $$i\varepsilon\partial_t\psi = -\frac{\varepsilon^2}{2}\Delta\psi + V_{\text{ext}}(x/\varepsilon)\psi,$$

which can be solved exactly via Bloch decomposition, and a simple ODE

(Step 2) $$i\varepsilon\partial_t\psi = gf(|\psi|^2)\psi.$$

To this end, one first needs to solve Bloch's eigenvalue problem (numerical pre-processing)

$$(i\partial_y + k)^2 \varphi_n + V_{\text{ext}}(y)\varphi_n = \lambda_n \varphi_n,$$

subject to periodic boundary conditions. This yields the energy-eigenvalues $\lambda_n \in \mathbb{R}$ and Bloch-eigenfunctions φ_n required in Step 1.

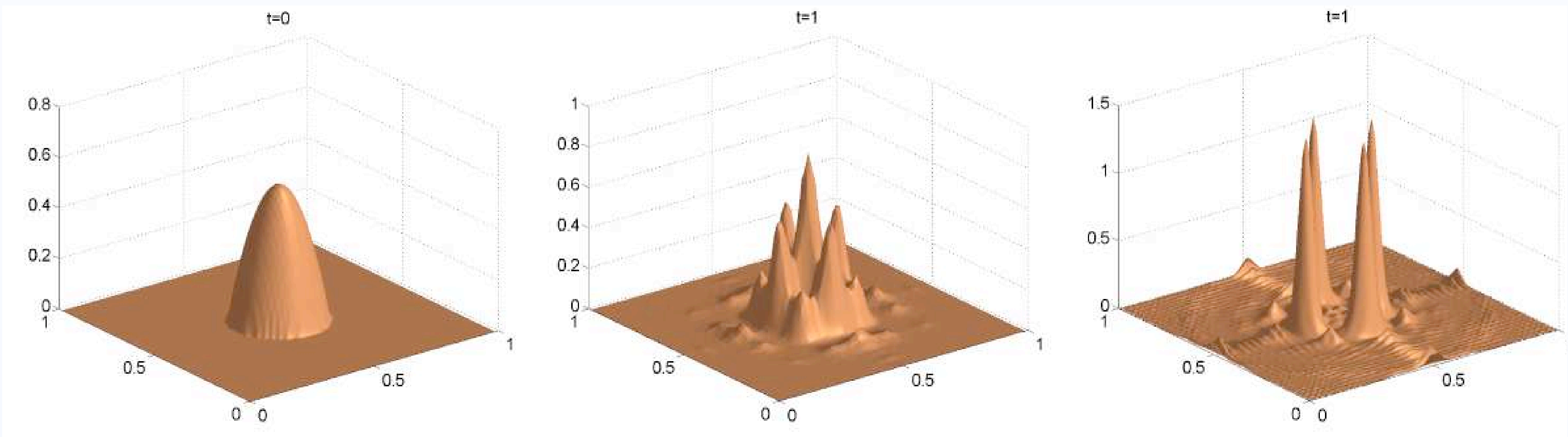
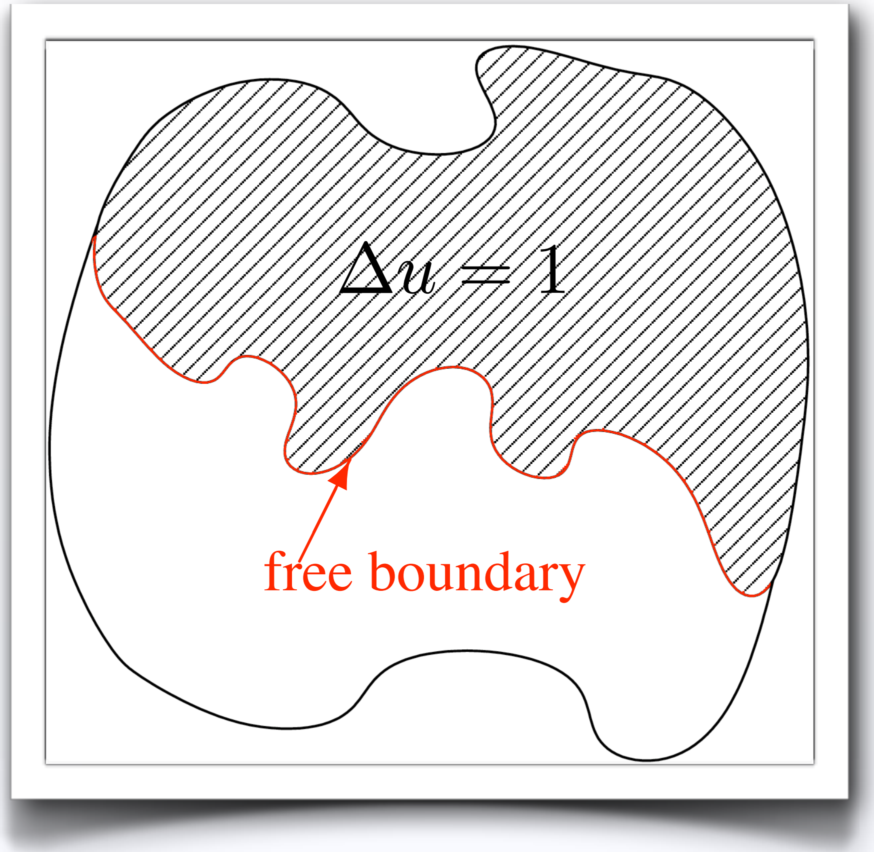


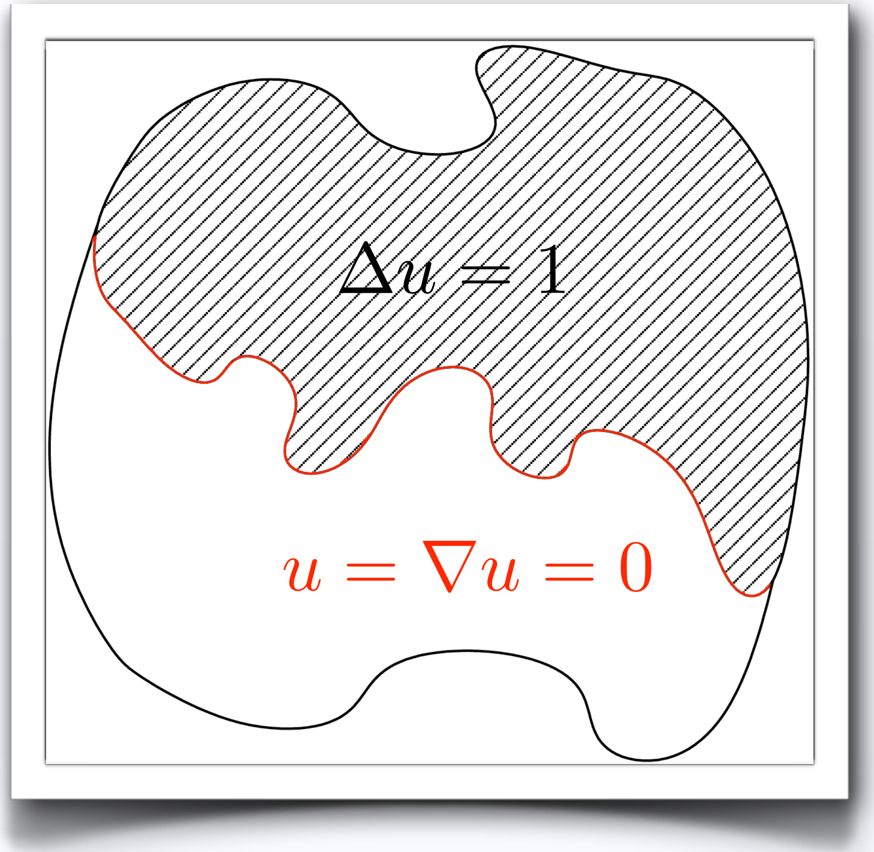
Figure: Computation of lattice BEC in 3D: $|\psi(t)|^2_{x_3=0}$ *for* $\lambda = -1$.

Free Boundary Problems



- PDEs is considered in domains with partially unknown (free) boundaries

Free Boundary Problems



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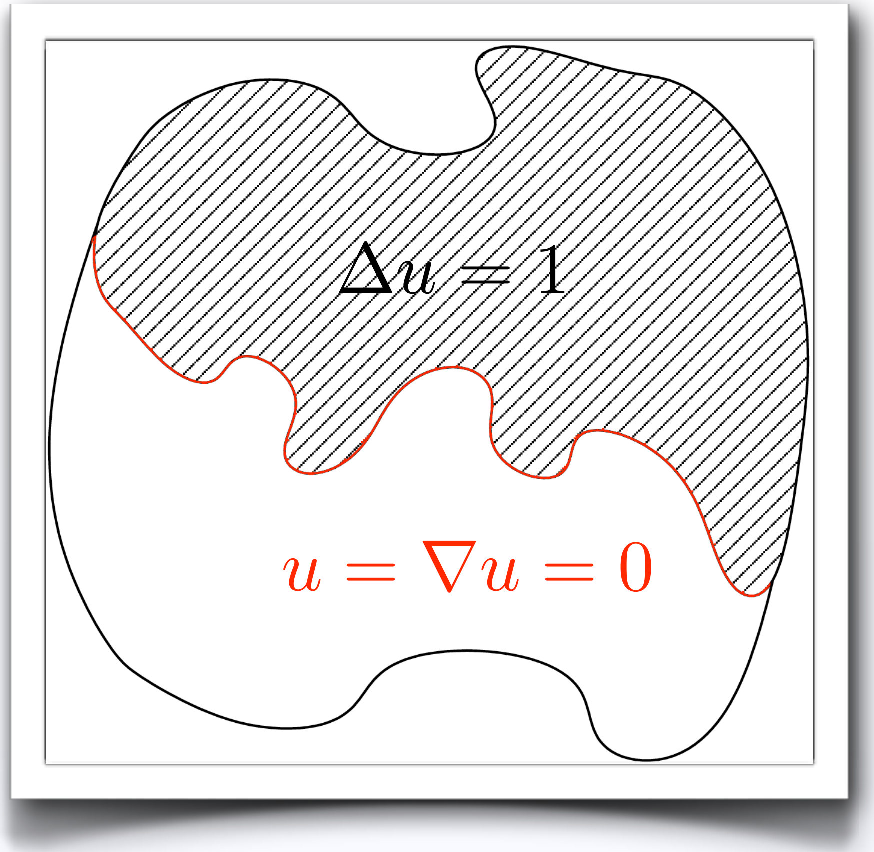
- Extra boundary condition on the unknown part of the boundary

Free Boundary Problems



- PDEs is considered in domains with partially unknown (free) boundaries
- Extra boundary condition on the unknown part of the boundary
- Suitable for modelling of phenomena in physics (superconductivity, solidification), finance (price formation, American put option), biology (tumour growth), chemistry (chemical vapour deposition)...

Superconductivity Modelling:

Conduction of electricity without resistance

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- The magnet is levitating above the superconductor (black disk), cooled below the critical temperature by liquid nitrogen. (Meissner Effect, 1933)

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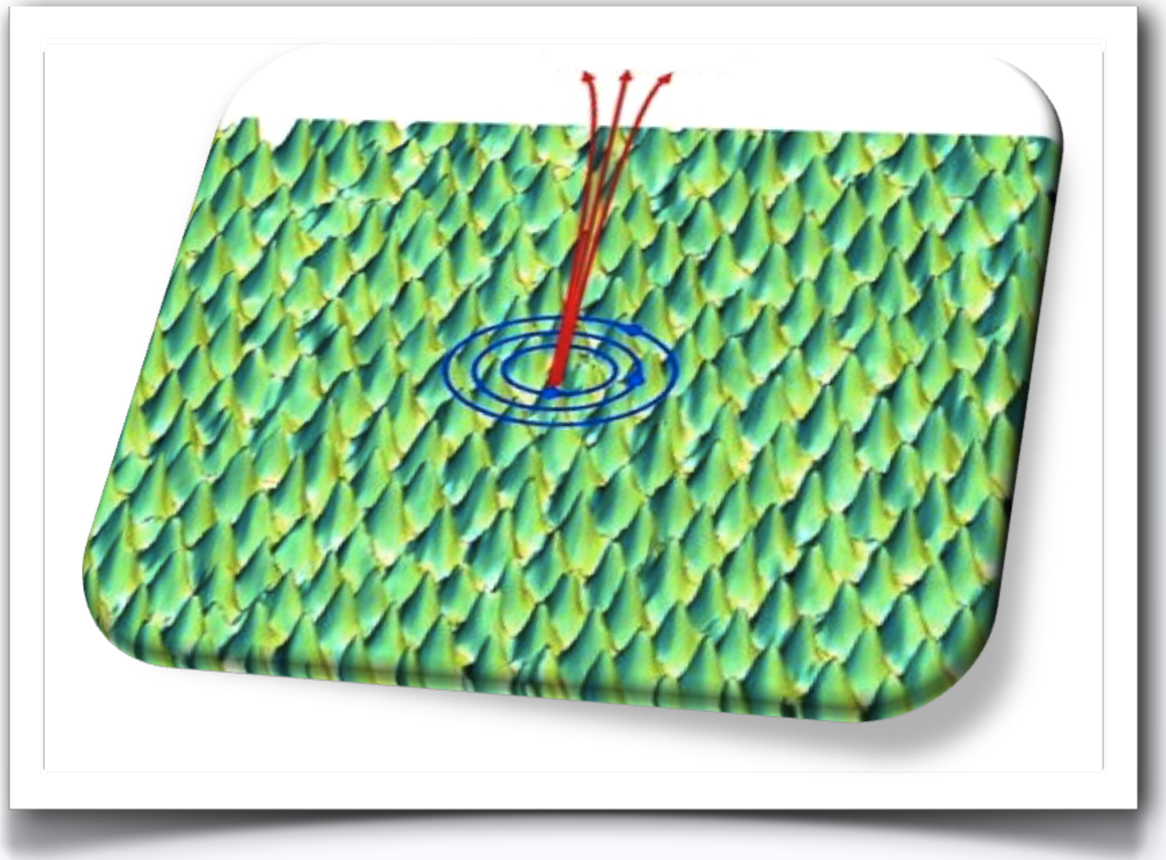
- Idea behind maglev trains and used in flywheel applications for energy storage.

Vortex Flux Lattice (500x500 Nm)



Vortex flux lattice in V3Si at H=3 T and T=2.3 K. The peaks indicate the location of a vortex with a single flux quantum of magnetic flux.

- The materials enter mixed mode, when vortices penetrate the superconductor
- The number of vortices is large

Mean Field Model

Ginzburg-Landau functional of superconductivity:

$$G(\psi, A) = \frac{1}{2}\int_\Omega \left|\left(\frac{1}{\kappa}\nabla - iA\right)\psi\right|^2 + \frac{1}{2}\left(1 - |\psi|^2\right)^2 + (curl A)^2 dx$$

where:

- ψ is a quantum mechanical order parameter
- A is the magnetic vector potential

- Individual vortices are averaged into vortex density (vorticity)
- Study the properties of vorticity regions such as regularity, geometry, etc...

Beresticky, Bonnet, Chapman

Magneto-Optical Imaging of Mesoscopic Dendritic Vortex Instability

Mathematical problems: free boundaries, fractal geometries, regularity

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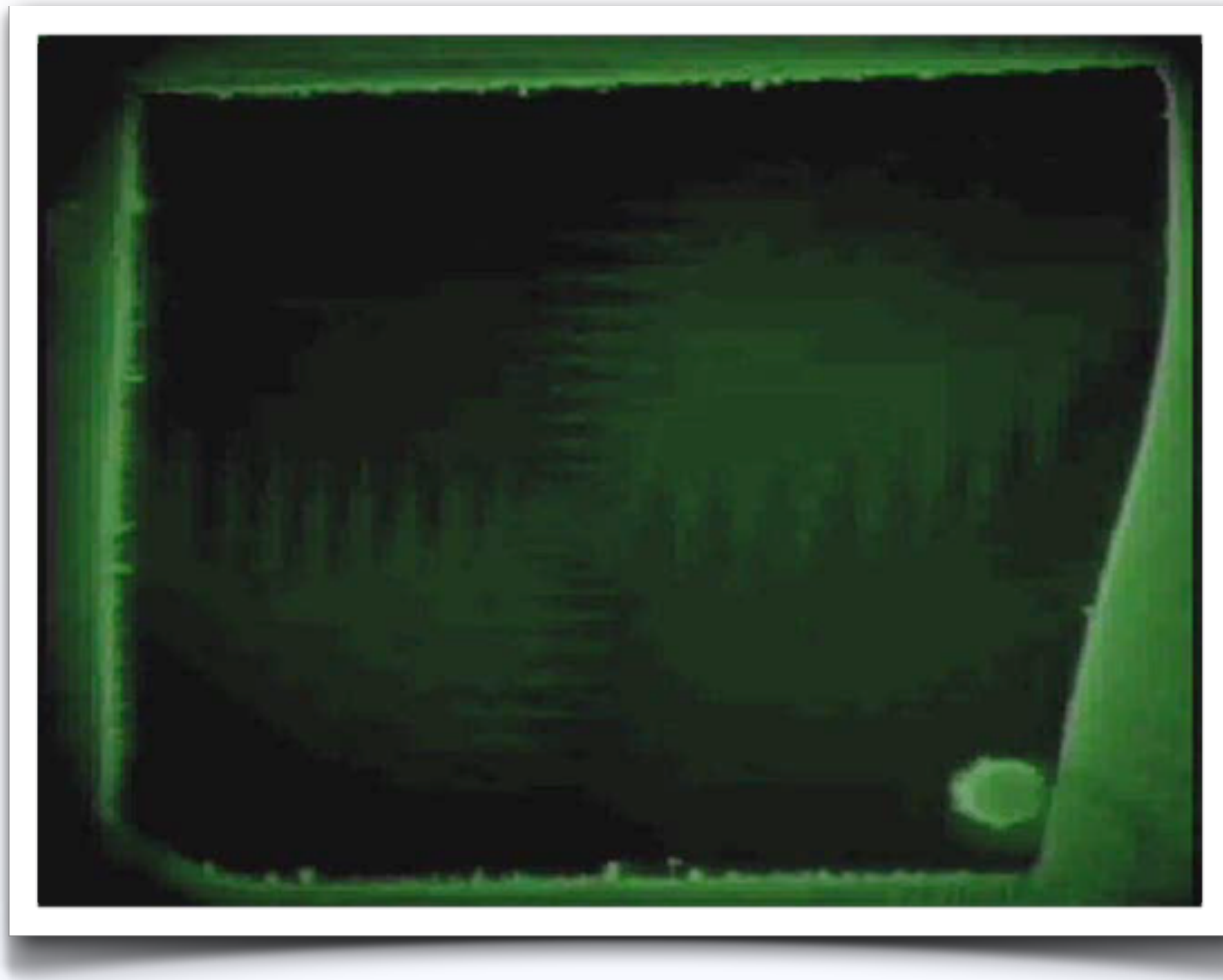


Mathematical problems: free boundaries, fractal geometries, regularity

The Free Boundary Problem

FBP with a non-linear operator in the divergence form:

$$\begin{cases} \operatorname{div}\left(F(|\nabla u|^2)\nabla u\right) = u\chi_\Omega \text{ in a domain } D \subset \mathbb{R}^n, \quad \Omega = \{|\nabla u| > 0\} \\ u \geq 0 \text{ in } D. \end{cases}$$

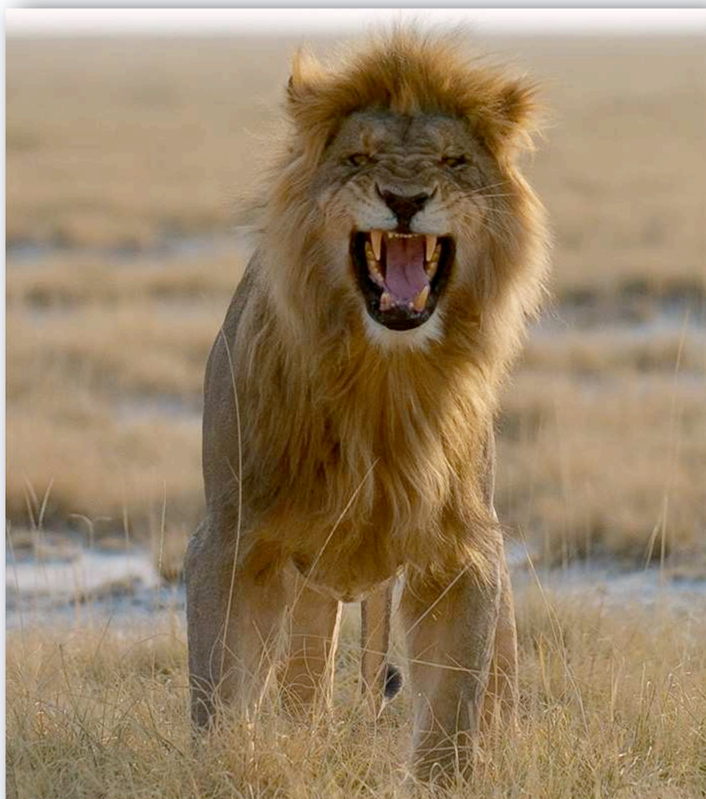
$F(s)$	is a nonlinear continuous nondecreasing function
$\chi(E)$	is the characteristic function of a set E
$\partial\Omega$	is the free boundary

- Optimal regularity of the solutions
- Classification of Global Solutions
- Regularity and geometric properties of the Free Boundary

Matevosyan, Petrosyan

Reaction-Diffusion Systems

Population dynamics: predator-prey systems



Reaction-Diffusion Systems

Pattern formation: Turing instability, Activator-Inhibitor systems

Reaction-Diffusion Systems

We consider the large time behaviour of systems of reaction-diffusion equations

$$U_t = \mathrm{div}(D(x,t,U)\,\nabla\, U) + F(x,t,U), \qquad U \in \mathbb{R}^N, \quad x \in \Omega.$$

with $\Omega \subset \mathbb{R}^d$ bounded (with zero flux boundary condition) or the whole space.

For the large time behaviour one expects the *conservation laws* to compensate the corresponding *degeneracy in the reaction rate* F.

Di Francesco, Fellner, Markowich - Proc. Royal Soc. A 2008

Reaction-Diffusion Systems

The entropy approach

- exploits an *entropy (Lyapunov, free-energy,...) functional* which dissipates monotonically in time.
- requires the conservation laws to identify an equilibrium state from the set of entropy minimising states.
- establishes a *quantitative entropy entropy-dissipation inequality* entailing
  a) convergence in entropy to an entropy minimising equilibrium state
  b) convergence in L^1 using Cziszár-Kullback-Pinsker type inequalities
  (cf. Otto, Carrillo et al., Markowich et al.)
- yields explicitly computable rates and constants of convergence.
- does not require any linearisation, smallness assumptions, ...

Arnold, Markowich, Toscani, Unterreiter 2000 – 2001

Reaction diffusion systems

An example from semiconductor device modelling

$$\begin{cases} n_t = \operatorname{div} J_n - R(n,p)\,, & J_n := \nabla n + n\nabla V_n \\ p_t = -\operatorname{div} J_p - R(n,p)\,, & J_p := -(\nabla p + p\nabla V_p) \end{cases}$$

where n and p model two densities of charged particles subject to diffusion, to *potentials* V_n and V_p and to a recombination–generation mechanism $R(n,p) = F(n,p,x)(np - e^{-V_n - V_p})$ (Shockley–Read–Hall).

Coupled chemotaxis-fluid system

Classical Keller-Segel system

elliptic-parabolic Keller-Segel system:

$$\begin{cases} -n = \Delta c \\ \partial_t n + \nabla \cdot (n \nabla c - \nabla n) = 0 \end{cases}$$

Global existence vs. blow-up:

Let $(1 + \log n(t=0) + |x|^2) n(t=0) \in L^1(\mathbb{R}^2)$, $M = \int n(t=0)\, dx$. Then

$M < 8\pi \Rightarrow$ global existence

$M > 8\pi \Rightarrow$ finite time blow-up

Proof based on the logarithmic Hardy-Littlewood-Sobolev inequality

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A. Blanchet, J. Dolbeault, B. Perthame, EJDE, 2005

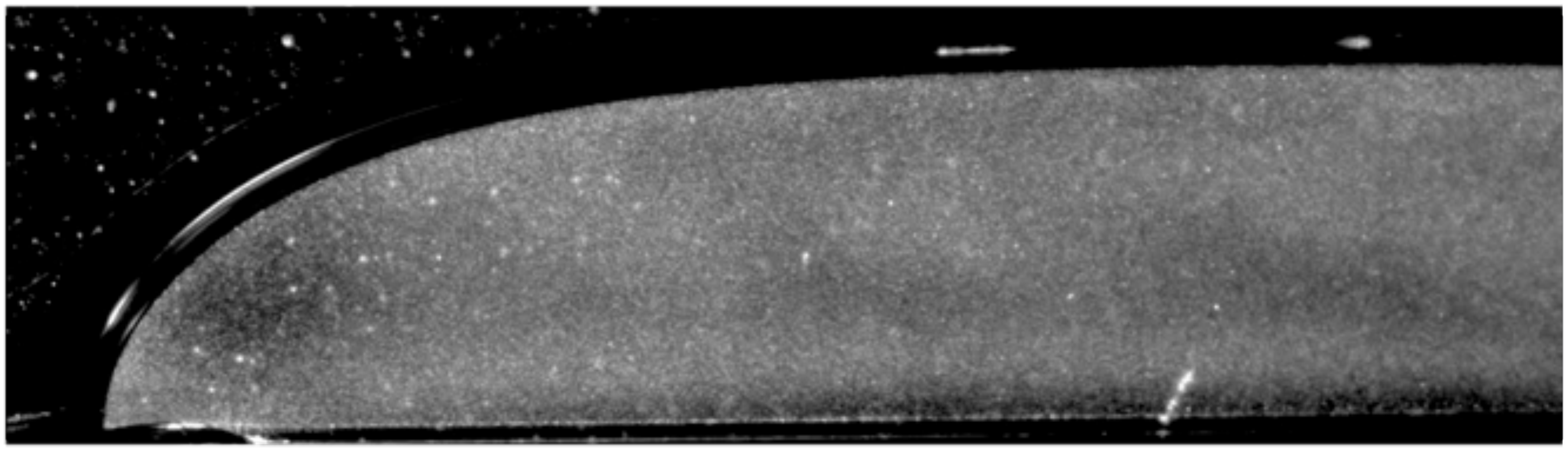
Coupled chemotaxis-fluid system

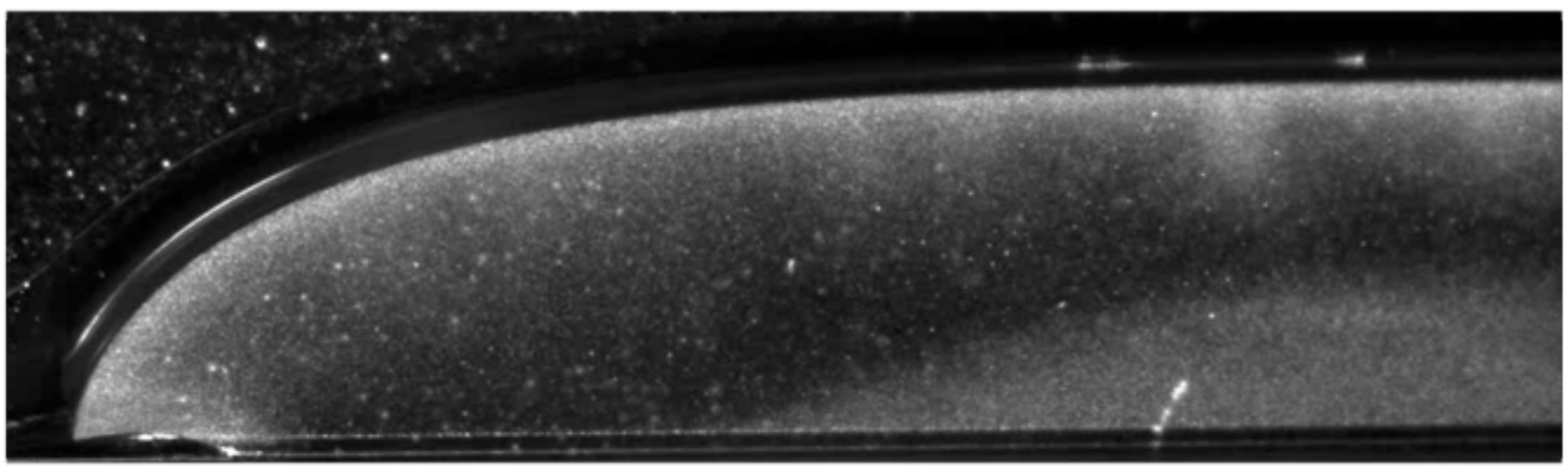
Motivation

movie courtesy of Goldstein Lab

Coupled chemotaxis-fluid system

Motivation

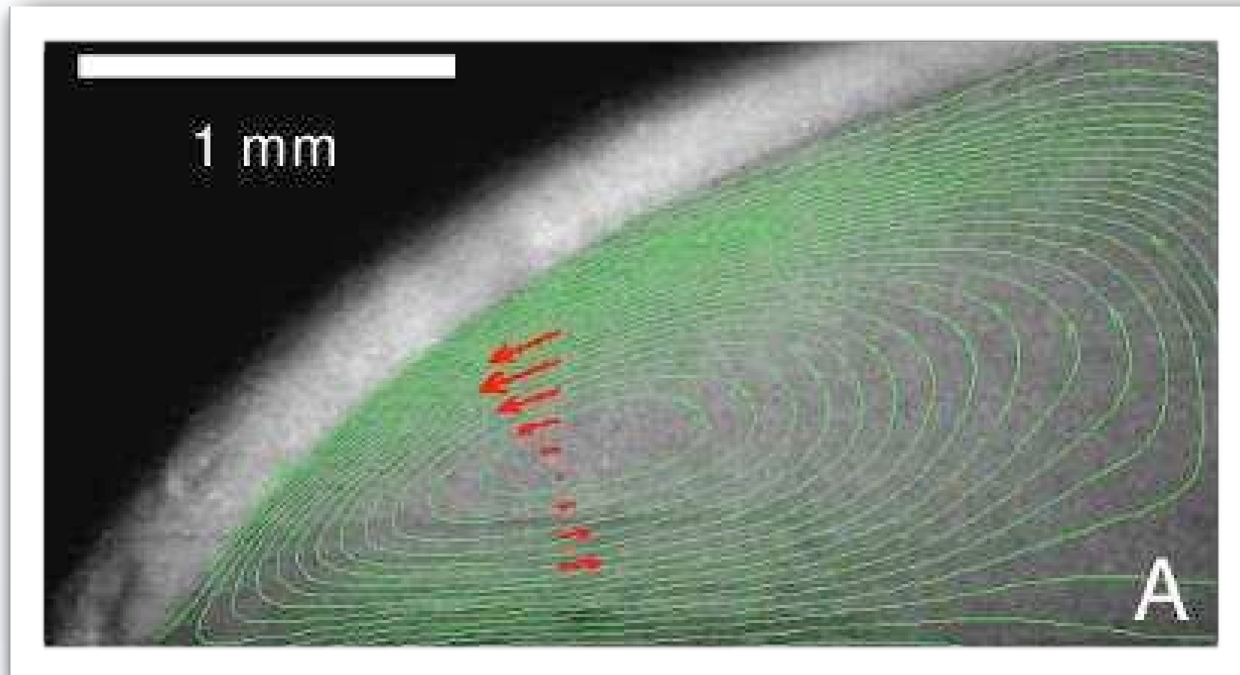




movie courtesy of Goldstein Lab

Coupled chemotaxis-fluid system

Flow pattern



$n = n(x,t) \geq 0$: bacteria density

$c = c(x,t) \geq 0$: oxygen concentration

$u = u(x,t) \in \mathbb{R}^3$: fluid velocity

$p = p(x,t)$: pressure, $\quad \rho$: (constant) fluid density

Coupled chemotaxis-fluid system

A combination of effects

$$\begin{cases} c_t + \mathbf{u} \cdot \nabla c = D_c \Delta c - n\kappa f(c) \\ n_t + \mathbf{u} \cdot \nabla n = D_n \Delta n - \chi \nabla \cdot [r(c) n \nabla c] \\ \rho(\mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u}) = -\nabla p + \eta \Delta \mathbf{u} - n \nabla \varphi \\ \nabla \cdot \mathbf{u} = 0. \end{cases}$$

The **bacteria** n *diffuse* with a constant diffusivity $D_n > 0$, are subject to *fluid convection* and are directed up to the gradient of the oxygen concentration in the *chemotaxis* term $-\chi \nabla \cdot [r(c) n \nabla c]$. The *chemotactic sensitivity* is given by $r(c)$. They are subject to *pure* transport (no reaction, i. e. no birth–death processes).
The **oxygen concentration** c is diffused with diffusivity D_c and subject to fluid convection. It *reacts* with the bacteria via the loss term $-n\kappa f(c)$.
The **fluid velocity u** obeys the incompressible viscous Navier–Stokes equations with a source term modelling *gravity*. φ models a gravitation potential.

Coupled chemotaxis-fluid system

What can we do?

$$\begin{cases} c_t + \mathbf{u} \cdot \nabla c = D_c \Delta c - n\kappa f(c) \\ n_t + \mathbf{u} \cdot \nabla n = D_n \Delta n - \chi \nabla \cdot [r(c) n \nabla c] \\ \rho \mathbf{u}_t = -\nabla p + \eta \Delta \mathbf{u} - n \nabla \varphi \\ \nabla \cdot \mathbf{u} = 0. \end{cases}$$

Domain: $\Omega \subset \mathbb{R}^d$, $d = 2, 3$ either bounded (with smooth boundary) or the whole space.

Stokes' approximation: we drop the nonlinear transport term $\mathbf{u} \cdot \nabla \mathbf{u}$ (justified for 'small' $\mathbf{u}$)

Boundary conditions: $\frac{\partial c}{\partial \nu}\big|_{\partial\Omega \times [0,T]} = \frac{\partial n}{\partial \nu}\big|_{\partial\Omega \times [0,T]} = 0$ and $u\big|_{\partial\Omega \times [0,T]} = 0$

Questions in analogy to classical Keller-Segel: do bacteria densities *concentrate* to singular measures (in finite or infinite time)? Or is it rather possible to prove their *global boundedness*? (cf. Jäger, Luckhaus, Herrero, Velazquez, Dolbeault, Perthame, Blanchet ...)

Coupled chemotaxis-fluid system

Local Existence

The above key question can be addressed with suitable local and global existence theorems. As a first basic step we can prove:

For $\Omega \subset \mathbb{R}^2, \mathbb{R}^3$, there exists $T > 0$ such that the system has a weak solution (c, n, u).

Global Existence for c_0 small

$\Omega = \mathbb{R}^3$, assumptions on $f, \varphi > 0$ and initial data. Then there exists a c_* depending only on $D_n, D_c, \eta, \varphi, f, \chi$ s.t. for $|c_0|_\infty \leq c_*$, there is a global-in-time weak solution.

$$\mathcal{E}(t) \quad := \quad \int_{\mathbb{R}^3} n(\ln n + \lambda\varphi)dx + \lambda(\|c\|_{H^1}^2 + \|u\|_2^2)$$

A. Lorz, M3AS, 2010

R.-J. Duan, A. Lorz, P. A. Markowich, CPDE, 2010

Coupled chemotaxis-fluid system

Global Existence without smallness assumptions

In $\Omega = \mathbb{R}^2$, under the assumptions on $\chi(c)$ and $f(c)$, $\frac{d^2}{dc^2}\left(\frac{f(c)}{\chi(c)}\right) < 0$, $\chi'(c)f(c) + \chi(c)f'(c) > 0$, the system has a global-in-time solution.

Nonlinear Diffusion in n

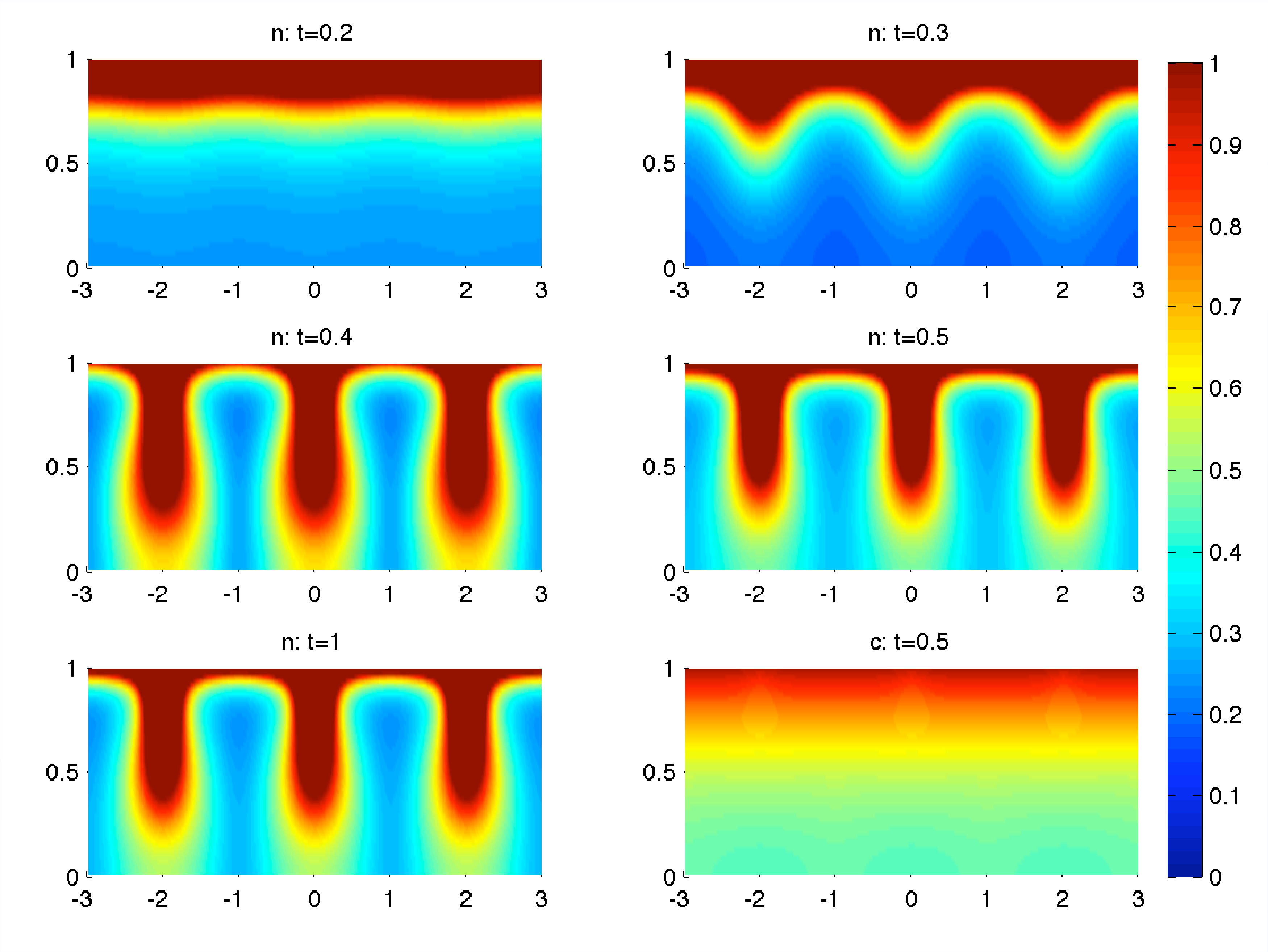
Replacing Δn by Δn^m: With weak assumptions, Ω bounded and $1.5 < m \leq 2$, we obtain a global-in-time solution.

J.-G. Liu, A. Lorz, Ann. IHP, 2011

M. Di Francesco, A. Lorz, P. A. Markowich, DCDS, 2010

Coupled chemotaxis-fluid system

Numerics: From falling plumes to a stationary state



Socio-Economics: Price Formation

- Consider a market
- Fixed number of goods to be traded
- Fixed number of buyers/vendors
- Question: How does the price of the good evolve in time?
- Assumption: Buyers/vendors do not take every single interaction into account, but make their decision based on the overall market outlook
- There is a fixed fee for every transaction

Price formation: J.-M. Lasry and P.-L. Lions

The state of each player satisfies the stochastic differential equation

$$dX_t^i = \sigma dW_t^i + \alpha^i dt,\; X_0^i = x^i,\; i = 1, \dots N$$

where W_t^i denote independent Brownian motions. Each agent tries to find the optimal strategy α such that his/her costs

$$\mathbb{E}\left[\int_0^T L(X^i, \alpha) + F(X^1, \dots, X^N) dt\right]$$

are minimal. Nash equilibrium and a mean-field limit ($N \to \infty$) give the Hamilton-Jacobi-Bellman equation

$$\frac{\partial u}{\partial t} - \nu \Delta u + H(x, \nabla u) = V(x, m),\;\; u(x,0) = V_0(x, m(x,0))$$

$$\frac{\partial m}{\partial t} + \nu \Delta m + \operatorname{div}\left(\frac{\partial H}{\partial p}(x, \nabla u)\, m\right) = 0,\; m(x,T) = m_0$$

Price formation - free boundary problem

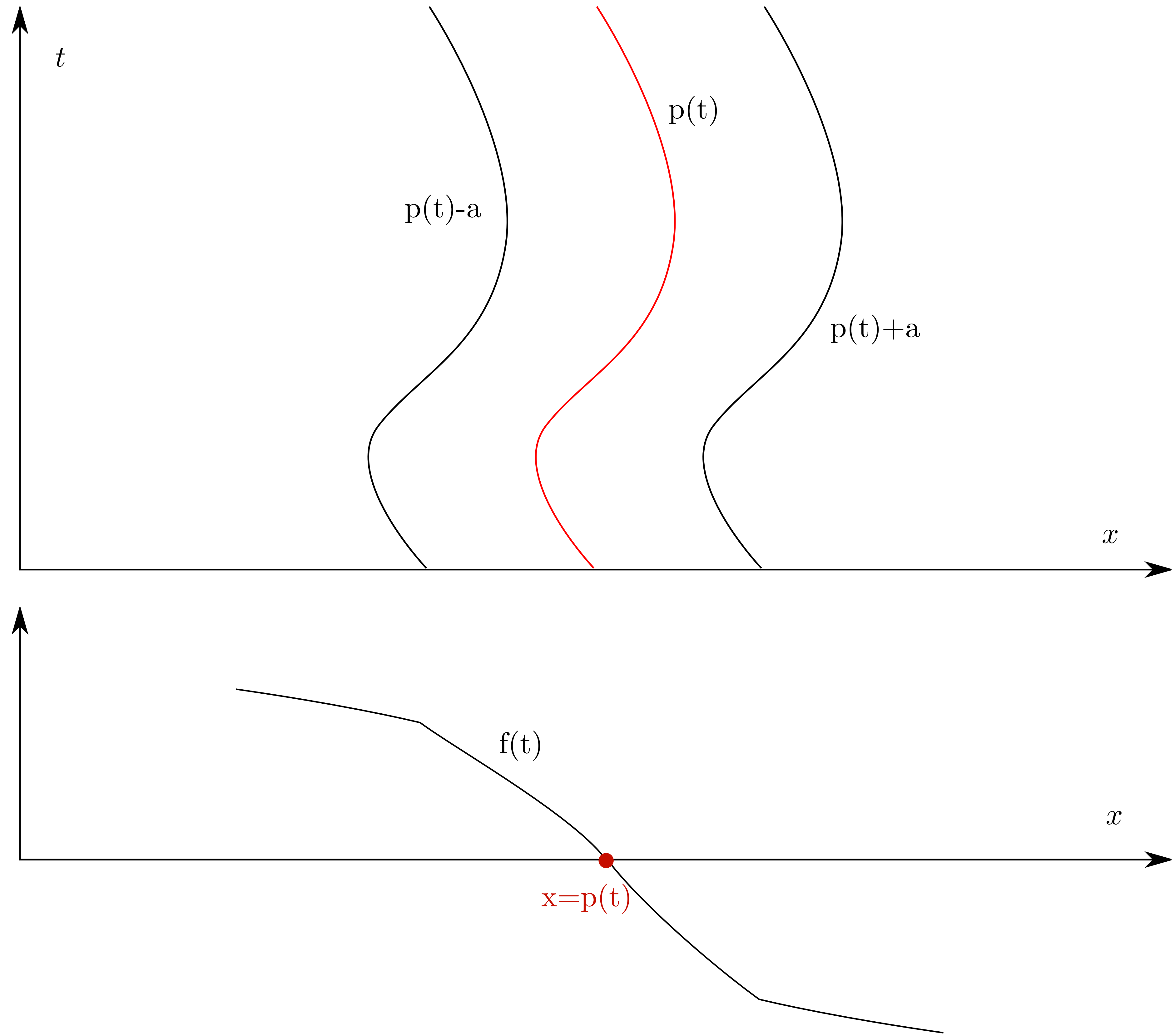
The signed density of buyers/vendors is denoted by f, the price $p(t)$ is the free boundary given by $f(p(t)) = 0$ and $\lambda(t) = -f(p(t),t)_x$ defines the transaction rate.

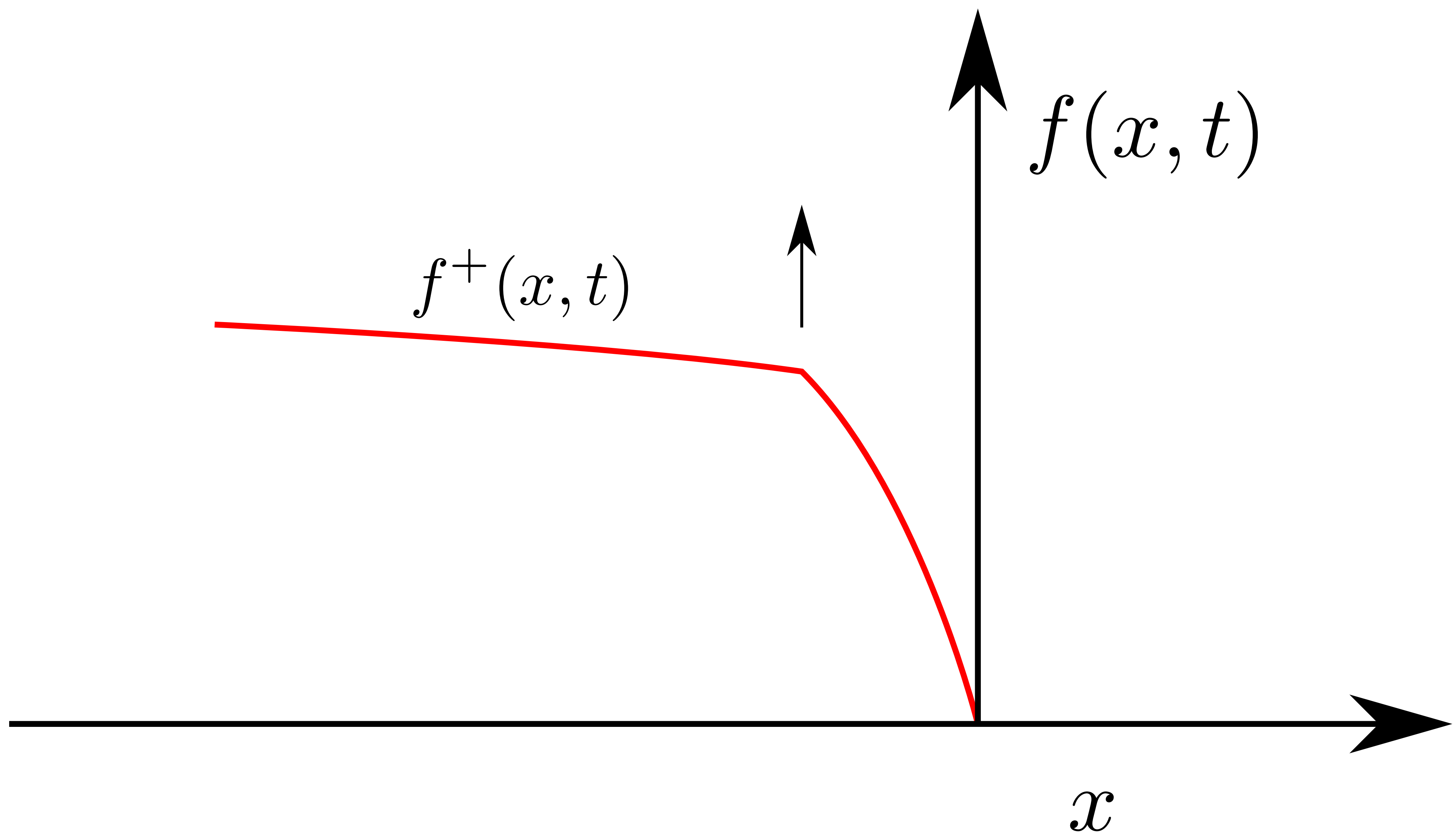
$$\frac{\partial f}{\partial t} - \frac{\sigma^2}{2}\frac{\partial^2 f}{\partial x^2} = \lambda(t)(\delta(x - p(t) + a) - \delta(x - p(t) - a))$$
$$f(x,t) > 0 \text{ if } x < p(t), \quad f(x,t) < 0 \text{ if } x > p(t).$$

References:

- L.A. Caffarelli, P.A. Markowich, M.-T. Wolfram, *On a price formation free boundary value model of Lasry & Lions: The Neumann Problem*, C. R. Acad. Sci. Paris, 349, 841-844,2011
- L.A. Caffarelli, P.A. Markowich, J.-F. Pietschmann, *On a price formation free boundary value model of Lasry & Lions*, C. R. Acad. Sci. Paris, 349, 621-624,2011
- P.A. Markowich, N. Matevosyan, J.-F. Pietschmann, M.-T. Wolfram, *On a parabolic free boundary equation modeling price formation*, M3AS, 11(19), 1929-1957,2009

Setup

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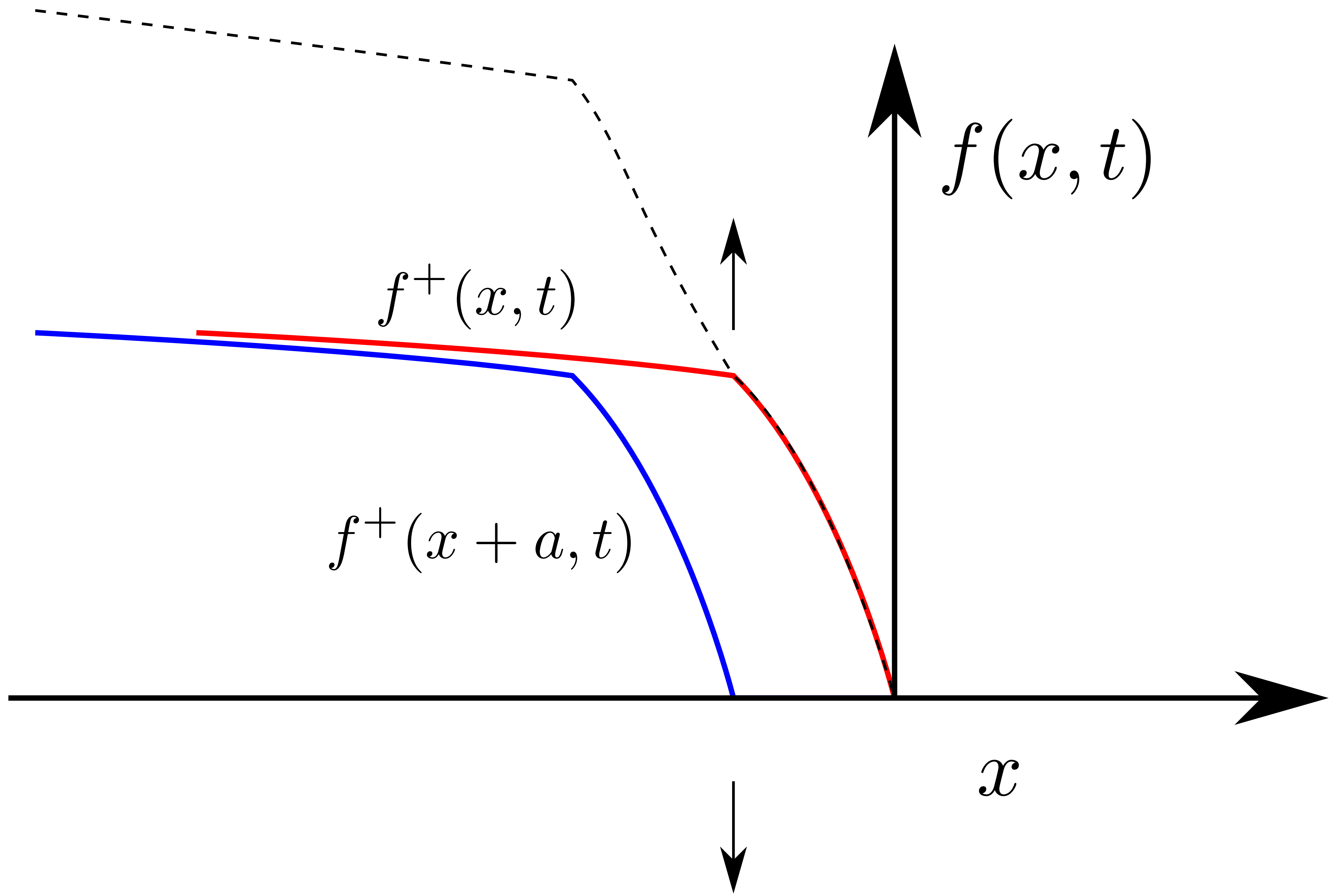
$f^+(x,t)$
x


$f(x,t)$
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$f^+(x+a,t)$
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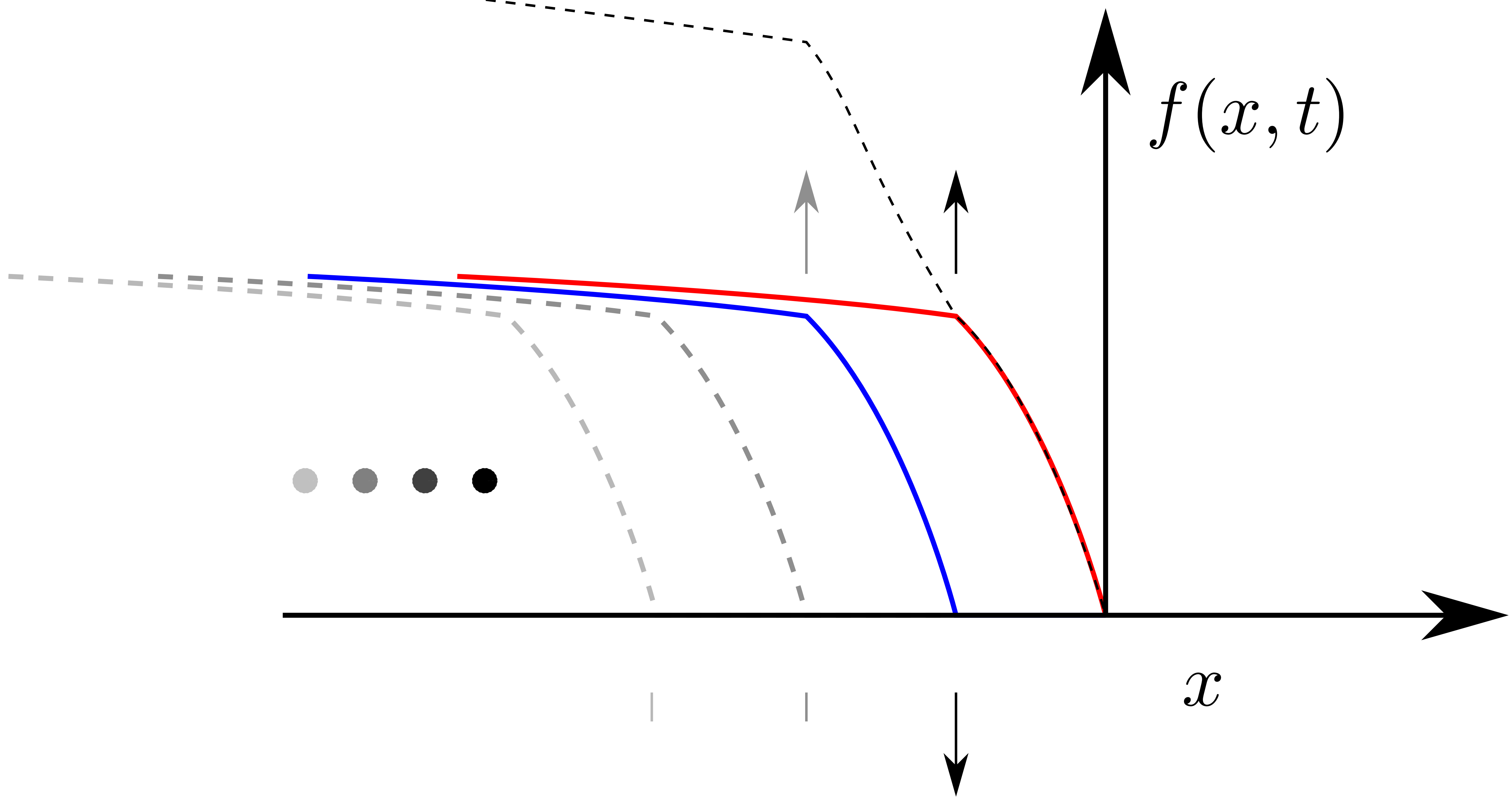

$f(x,t)$
x

Apply construction to positive and negative part, i.e.

$$F(x,t) = \begin{cases} \sum_{n=0}^{\infty} f^{+}(x+na,t), & x < p(t), \\ -\sum_{n=0}^{\infty} f^{-}(x-na,t), & x > p(t). \end{cases}$$

Then, F fulfils, in the sense of distributions

$$\frac{\partial F}{\partial t} = \frac{\partial^2 F}{\partial x^2}, \quad x \in \mathbb{R},\ t > 0,$$

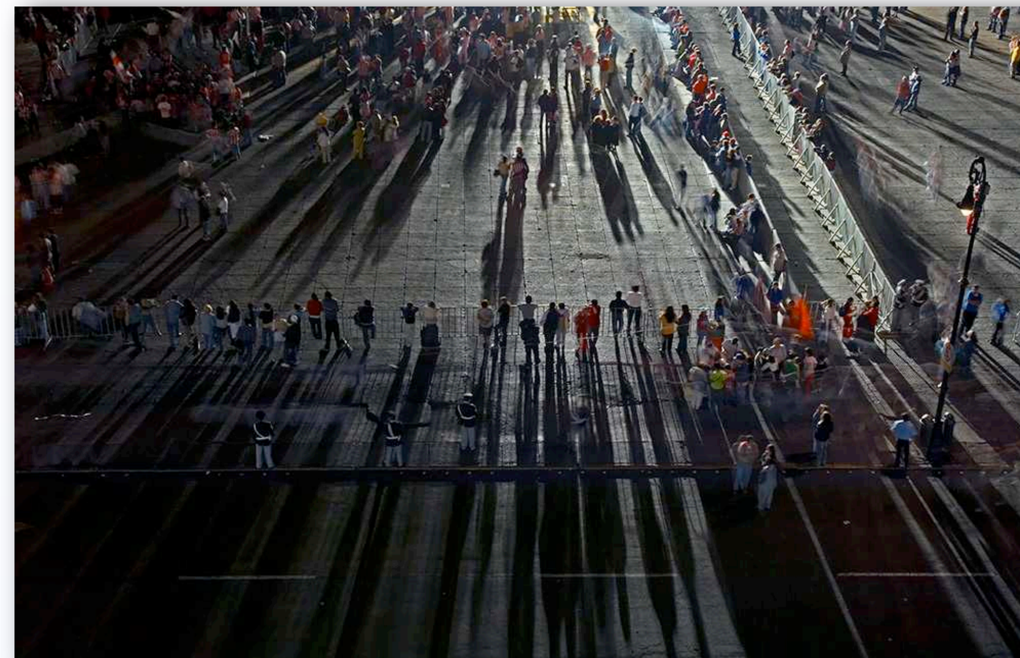
with initial datum

$$F_I(x) = \begin{cases} \sum_{n=0}^{\infty} f_I^{+}(x+na), & x < p_0, \\ -\sum_{n=0}^{\infty} f_I^{-}(x-na), & x > p_0, \end{cases}$$

The free boundary $p = p(t)$ is the zero-level set of the solution F of the heat equation.

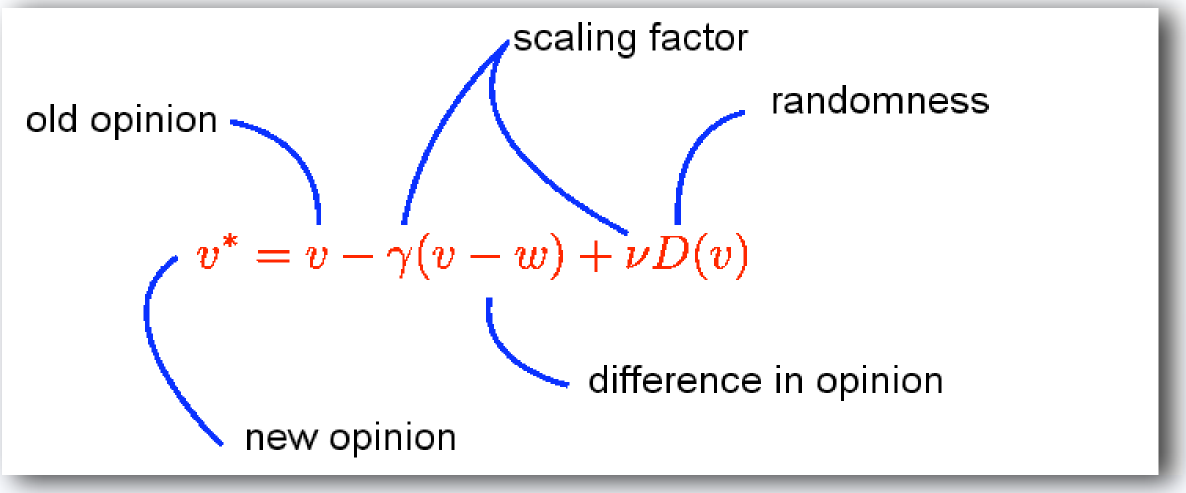
Socio-Economics: Opinion Formation

- Spread of a opinion in a society
- Question: How does the opinion evolve in time?
- Assumption: Opinion formation is determined by binary interactions with other people

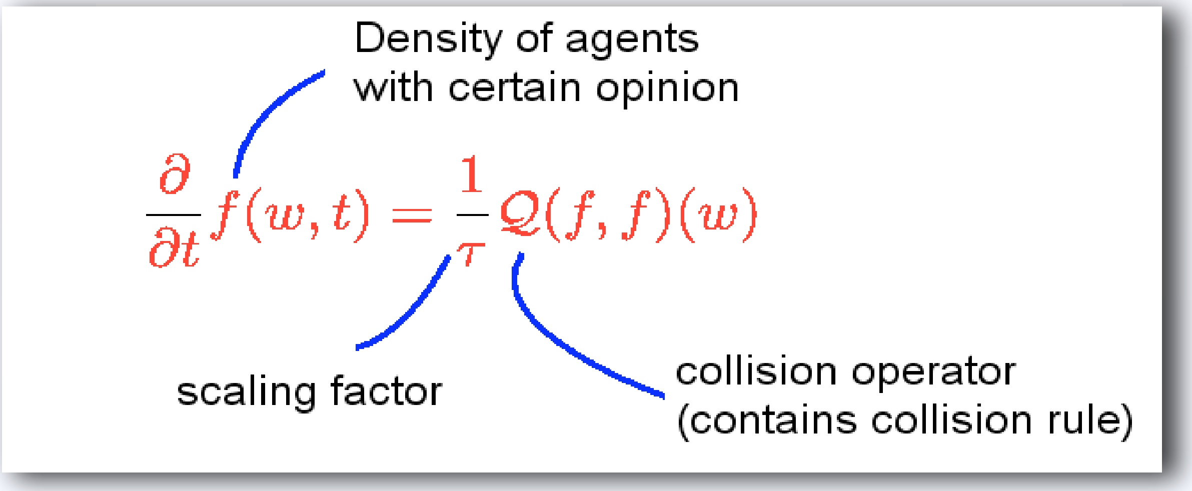


Opinion Formation: G. Toscani

The change of opinion is defined by collisional events



Time evolution of the distribution of opinion satisfies a Boltzmann equation

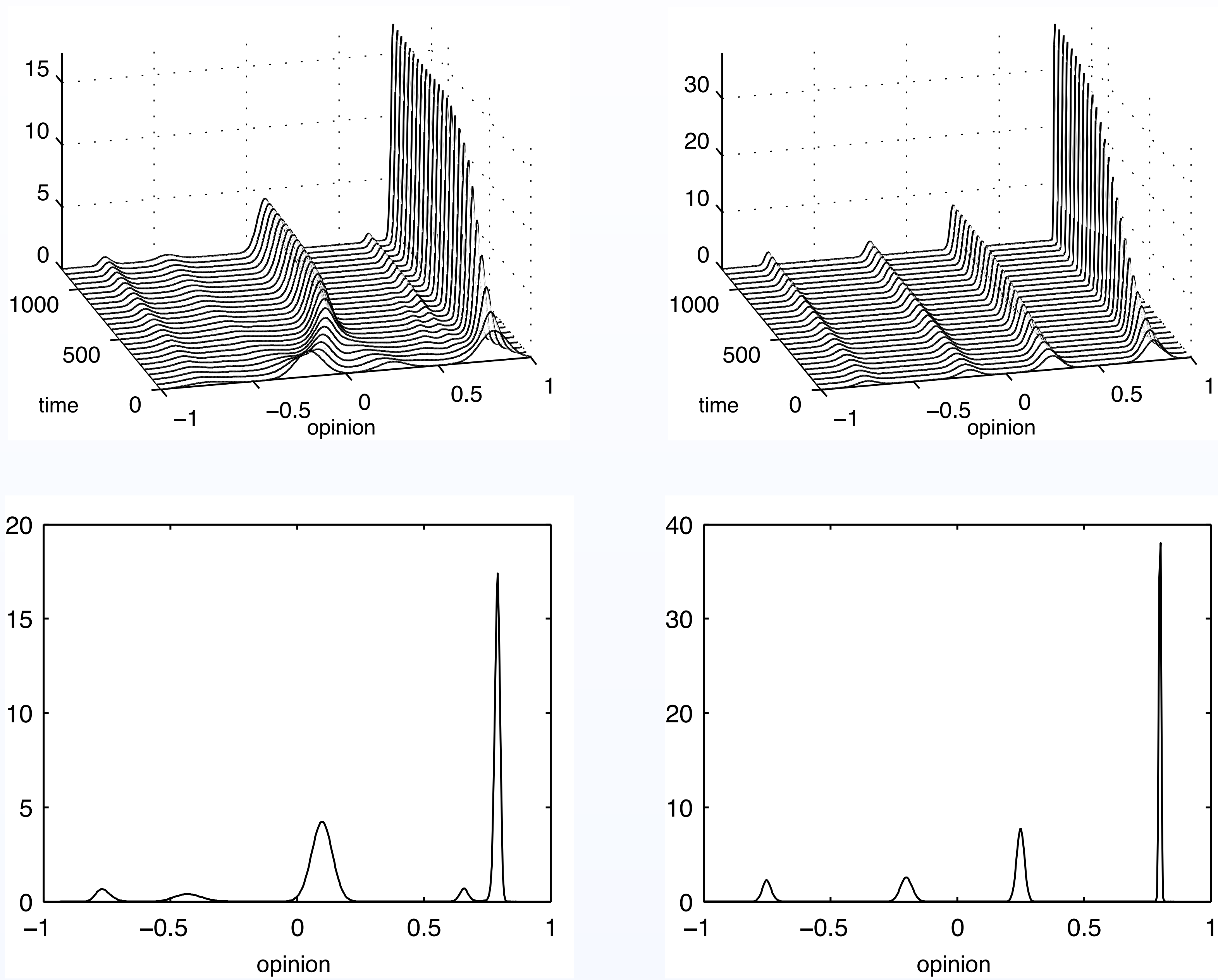


Understanding Carinthia

	Grüne	SPÖ	ÖVP	FPÖ	BZÖ
2004	6.7%	38.4 %	11.6 %	42.5 %	—
2009	5.2%	28.8 %	16.8 %	3.8 %	44.9 %

- Extreme opinions $v = \pm 1$ correspond to right/left wing of the political spectrum.
- Place parties according to their political views with weight that correspond to the results of the 2004 elections.

Understanding Carinthia



Thank You For Your Attention!