Derivation of reaction-diffusion equations from kinetic systems for cell populations

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Structure of the talk

1. Introduction

Kinetic Theory
Boltzmann equation
Hydrodynamic limits
Extension to complex systems limits

2. Model for cell populations

Kinetic equations
Reaction diffusion equations
Turing instability

3. Numerical illustrations

Pattern formation
Self and cross diffusion

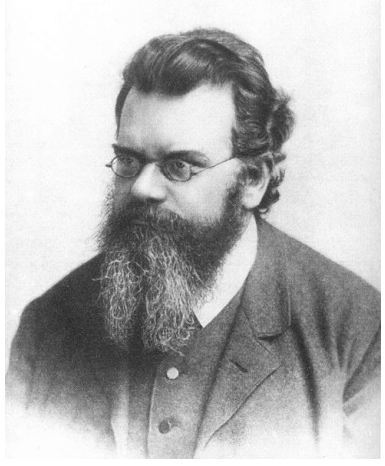
1. Introduction

Kinetic Theory og Gases

Description of **Maxwell-Boltzmann**

JC Maxwell

(1831-1879)



L Boltzmann

(1844-1906)

Kinetic Theory

a branch of **Statistical Mechanics**

Mesoscopic scale

in the between *macro-micro* scales

based on a **collisional dynamics**

Maxwell-Boltzmann description

rarefied or **moderate dense** gas

formed by a huge number of particles

which undergo **binary collisions**

Mesoscopic scale

Maxwell and Boltzmann introduce the

density function

$$f(x, v, t), \quad x, v \in \mathbb{R}^3, \quad t \in \mathbb{R}_0^+$$

of finding a molecule

at position x, with velocity v, at time t

Thus, the integral

$$\int_{\mathbb{R}^3} f(x, v, t)\, dv = n(x, t)$$

gives the density of particles

at position x and time t

Within the mesoscopic approach

Boltzmann equation

Changes in $f(x, v, t)$ are due to

- streaming (transport part)
- conservative binary collisions $(v, v_1) \leftrightarrow (v', v_1')$

General form of the BE

$$\frac{\partial f}{\partial t}(x, v, t) + \underbrace{v \cdot \nabla_x f(x, v, t)}_{\text{streaming}} = \underbrace{J(f, f)(x, v, t)}_{\text{collisions}}$$

Boltzmann equation

$$\frac{\partial f}{\partial t}(x,v,t) + \underbrace{v\cdot\nabla_x f(x,v,t)}_{\textbf{streaming part}} = \underbrace{J(f,f)(x,v,t)}_{\textbf{collisional part}}$$

$f(x,v,t) \geq 0,$ $\qquad f(x,v,t) \to 0 \quad \text{as} \quad \|v\| \to \infty$

$x, v \in \mathbb{R}^3, \quad t \in \mathbb{R}_0^+$

$J(f,f)$ is the collisional operator defined by

$$J(f,f) = \int_{\mathbb{R}^3}\int_{\mathbb{S}} B(v-v_1,\omega)\left(f'f_1' - ff_1\right)d\omega dv_1$$

which acts only on the velocity dependence of f

In the collision operator

$$J(f,f) = \int_{\mathbb{R}^3} \int_{\mathbb{S}} B(v - v_1, \omega)\left(f' f_1' - f f_1\right) d\omega dv_1$$

we use the **notation**

$$f = f(x,v,t) \qquad f_1 = f(x,v_1,t)$$
$$f' = f(x,v',t) \qquad f_1' = f(x,v_1',t)$$

where

v, v_1 are pre-collisional velocities (loss terms)

v', v_1' are post-collisional velocities (gain terms)

Moreover

ω is a unit vector (geometry of the collision)

$\mathbb{S}$ is the unit sphere in $\mathbb{R}^3$

In the collision operator

$$J(f,f) = \int_{\mathbb{R}^3}\int_{\mathbb{S}} B(v - v_1, \omega)\left(f' f_1' - f f_1\right) d\omega dv_1$$

we have that

$B(v - v_1, \omega)$ is the collision kernel, positive a.e.

and

$$v' = v - (v - v_1)\cdot\omega\,\omega$$
$$v_1' = v_1 + (v - v_1)\cdot\omega\,\omega$$

with

$$v' + v_1' = v + v_1 \qquad \text{(conservation of momentum)}$$
$$|v'|^2 + |v_1'|^2 = |v|^2 + |v_1|^2 \qquad \text{(conservation of kinetic energy)}$$

The most important result

about the structure of the Boltzmann equation

$\mathcal{H}$-Theorem The function $\mathcal{H}$ defined by

$$\mathcal{H}(t) = \int_\Omega \int_{\mathbb{R}^3} f(x,v,t) \log\Big[f(x,v,t)\Big] dvdx$$

is a Lyapunov function, such that

- $\dfrac{d\mathcal{H}}{dt} \leq 0$
- $\dfrac{d\mathcal{H}}{dt} = 0$ iff $J(f,f) = 0$ iff $f = f^M$ is **Maxwellian**

that is, there exist n, $T > 0$ and $u \in \mathbb{R}^3$ such that

$$f = f^M = n\Big(\frac{m}{2\pi k T}\Big)^{3/2} \exp\Big[-\frac{m(v-u)^2}{2kT}\Big]$$

It can be proven that

$$f = f^M = n\left(\frac{m}{2\pi k T}\right)^{3/2} \exp\left[-\frac{m(v-u)^2}{2kT}\right]$$

with n, T, u macroscopic observables given by

$$n(x,t) = \int_{\mathbb{R}^3} f(x,v,t)\,dv$$

number density

$$u(x,t) = \frac{1}{n}\int_{\mathbb{R}^3} v\, f(x,v,t)\,dv$$

mean velocity

$$T(x,t) = \frac{1}{3kn(x,t)}\int_{\mathbb{R}^3} m\big(v-u(x,t)\big)^2 f(x,v,t)\,dv$$

temperature

$\mathcal{H}$-Theorem

states that

function $\mathcal{H}$ is strictly decreasing until functions f are locally Maxwellians, that is, until there exist hydrodynamic (macroscopic) fields

$$n \text{ (scalar)}, \; u \text{ (vector)}, \; T \text{ (scalar)}$$

such that

$$f = f^M = n\Big(\frac{m}{2\pi k T}\Big)^{3/2} \exp\Big[-\frac{m(v-u)^2}{2kT}\Big]$$

$\mathcal{H}$-Theorem

Demonstrates

- the trend to equilibrium in the limit $t \to +\infty$
- the irreversibility character of the Boltzmann equation
- the evolution towards a hydrodynamic state characterized by density functions f univocally defined in terms of macroscopic fields n, u, T

Constitutes an important tool in studying hydrodynamic limits

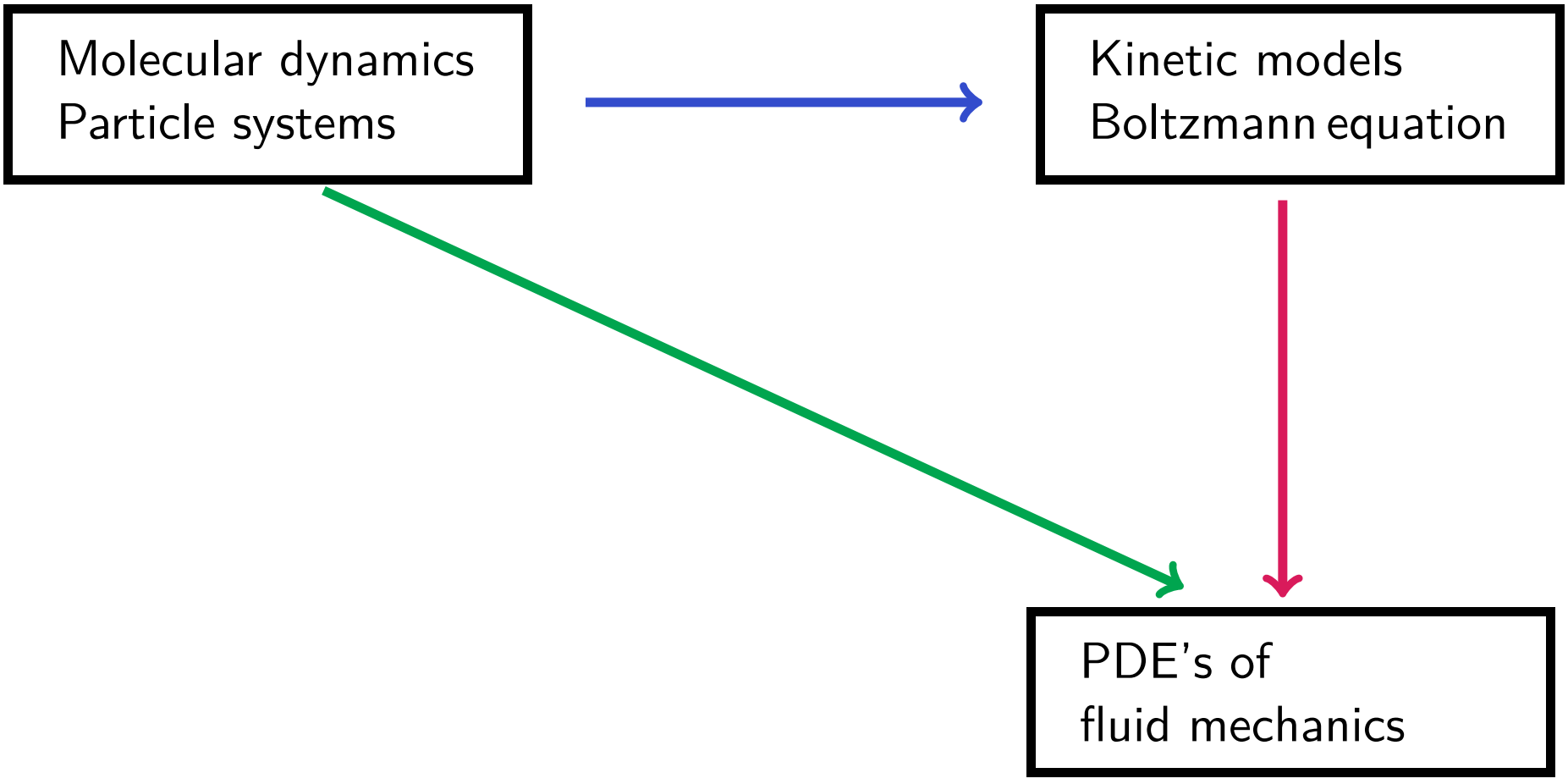
Hydrodynamic limits
Challenging problem

How can we pass
from a mesoscopic regime of Boltzmann equation
holding on a microscopic scale (time and space)
to a hydrodynamic regime

(Euler, Navier-Stokes, Diffusive, . . .),

holding on a macroscopic scale (time and space)?

The problem of hydrodynamic limits



- Lanford (1974), Gallagher & Collaborators (2016-2022)
- Varadhan (1993), Olla & Varadhan (1995)
- Bardos, Golse, Levermore (1991-93), Golse & Saint Raymond (2004-2009)

Hydrodynamic limit

The first attempt is due to **D. Hilbert**, who proposed to search a solution of the BE with small variations in time and space

D Hilbert

(1862-1943)

Hilbert's expansion (1912)

$$f(x,t,v) = f_\varepsilon(\varepsilon x, \varepsilon t, v) = f_\varepsilon(\hat{x},\hat{t},v)$$

$$f_\varepsilon(\hat{x},\hat{t},v) = \sum_{n\geq 0} \varepsilon^n f_n(\hat{x},\hat{t},v)$$

zero-order approximation $\longrightarrow$ **Euler equations**

first-order approximation $\longrightarrow$ **Navier-Stokes equations**

Hydrodynamic limits

Mathematical result

If the initial density f_0 is a **perturbation** of the Maxwellian equilibrium with fields n_0, u_0, T_0,

then, in the limit $\varepsilon \longrightarrow 0$,

the function f_ε tends to a Maxwellian equilibrium density whose fields $n(x,t), u(x,t), T(x,t)$ define a solution of the **hydrodynamic equations**

Euler equations

Navier Stokes equations

Diffusion equations

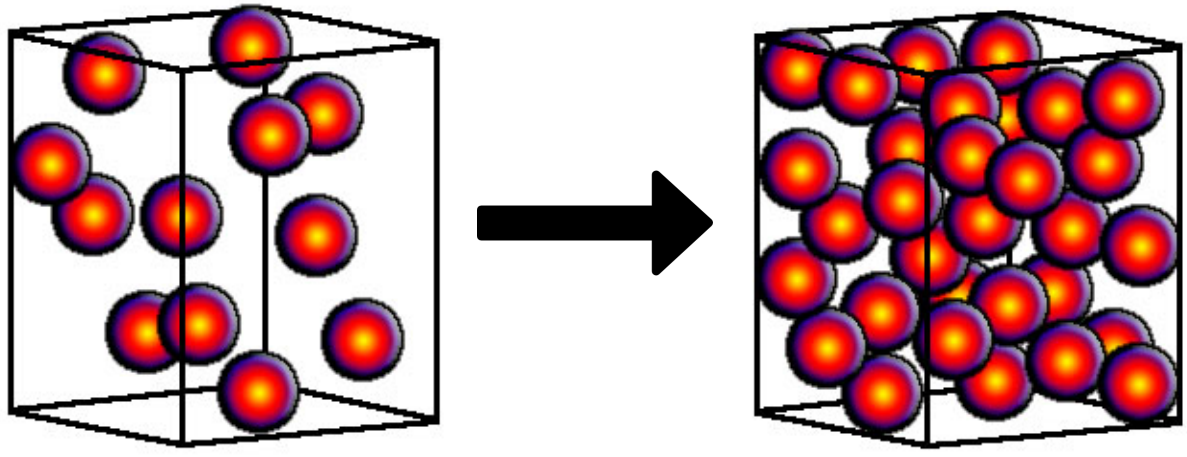
with initial data n_0, u_0, T_0

Complex systems

other relevant effects

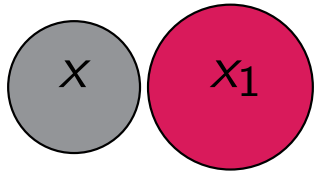
Modelling of more complex systems

Dense gas (Enskog equation,1922)



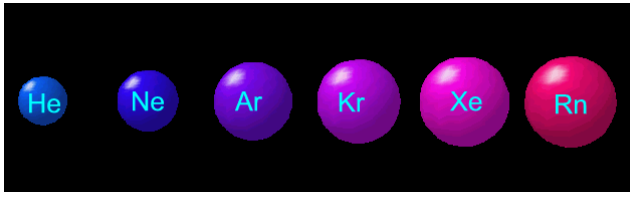
rarefied gas **dense gas**

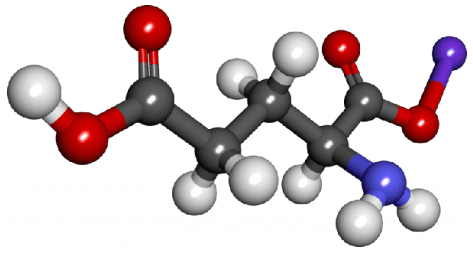
The two functions in the collisional term are evaluated at different points



$f(x, v, t)$ $f(x_1, v_1, t)$

Polyatomic gas





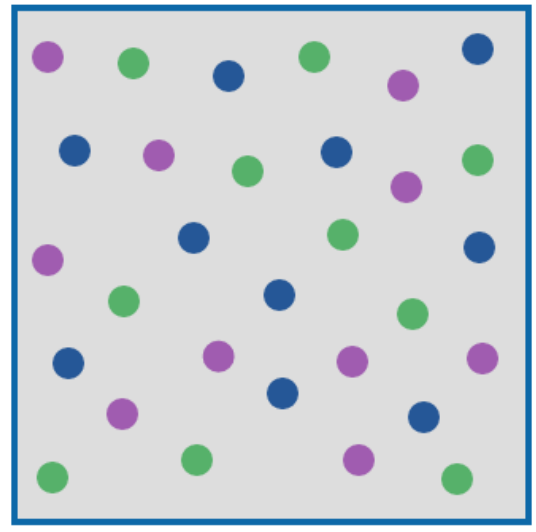
monatomic gases **polyatomic gases**

Function f depends on t, x, v, as before, **but also** on an **internal energy variable** $I \in [0, +\infty[$ $f(t, x, v, I)$

A **weight function** $\varphi_i(I)$ is introduced and ...

$$n(t, x) = \int_{\mathbb{R}^3} \int_0^{+\infty} f(t, \mathbf{x}, \mathbf{v}, I)\varphi(I)\, dI\, d\mathbf{v}$$

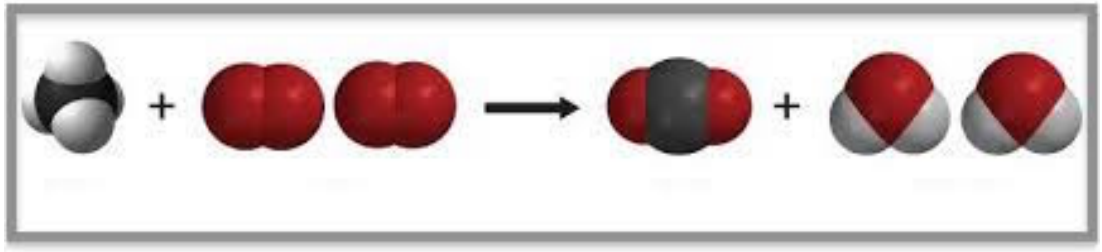
Mixtures



$$\frac{\partial f_i}{\partial t} + \boldsymbol{v}_i \cdot \nabla_x f_i = \sum_{s=1}^{N} J_{is}(\underline{f}, \underline{f}), \quad i = 1, 2, \ldots, N$$

collisions among all constituents of the mixture

Chemically reactive mixtures



four constituents A_i $\qquad A_1 + A_2 \leftrightharpoons A_3 + A_4$

$$\frac{\partial f_i}{\partial t} + \boldsymbol{v}\cdot\nabla_x f_i = \sum_{j=1}^{4} J_{ij}^{E}(\underline{f},\underline{f}) + J_i^{R}(\underline{f},\underline{f})$$

↙ ↓ ↘ ↘

streaming **inert** **mixture** **chem reaction**

Changing to a biological context

Kinetic theory of active particles

- cellular dynamics
- biological expression of cells (activity)
- cellular interactions

  conservative and non-conservative

  proliferation and destruction

  birth and death rates

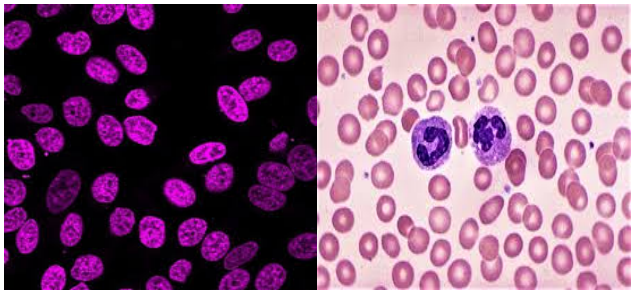
Crucial question

How the **cellular activity** and the **individual behaviour of cells** at the microscopic level **(kinetic)**

AFFECT

the **collective** behaviour of the **populations** at the *observable* level **(macroscopic)?**

kinetic (cellular) ⟷ **macro (global)**



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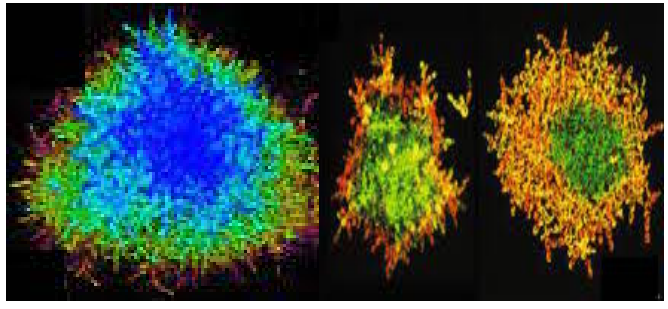


Biological context

Kinetic theory

Competing bacterial populations on a leaf surface

Hydrodynamic limit

Reaction-diffusion equations

Self and **cross diffusion** effects

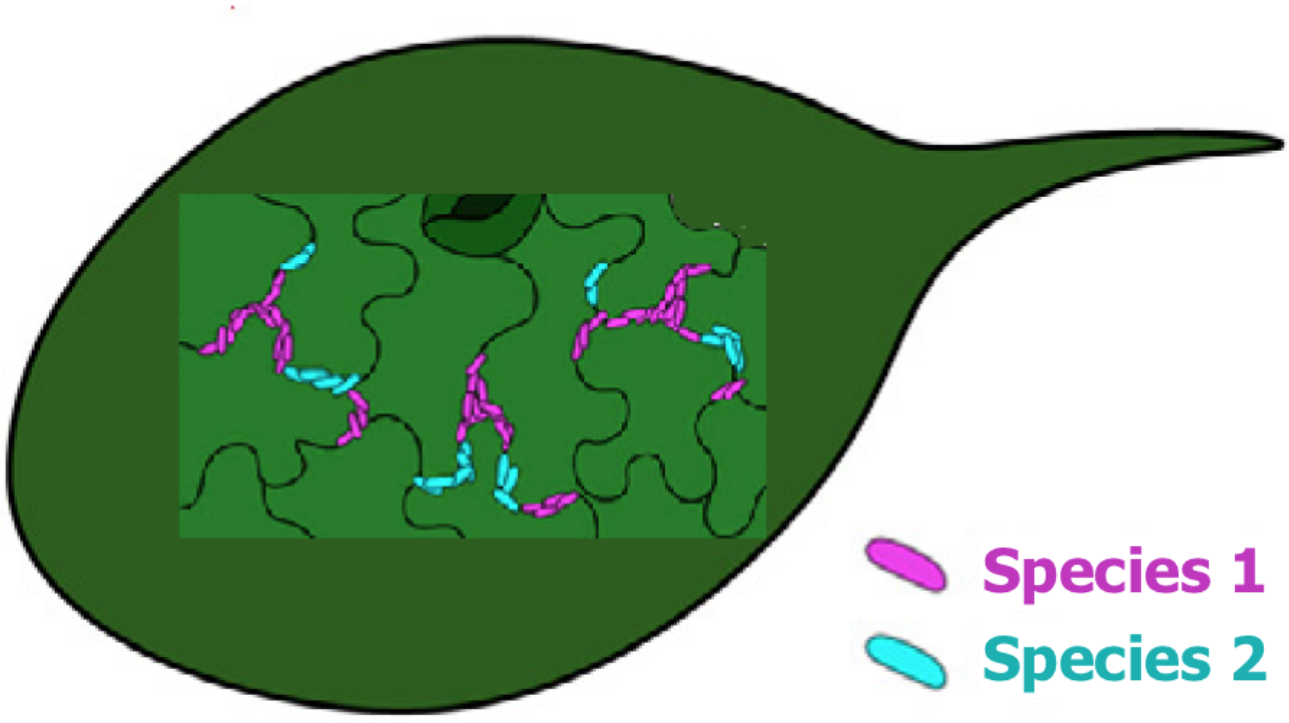
Turing instability

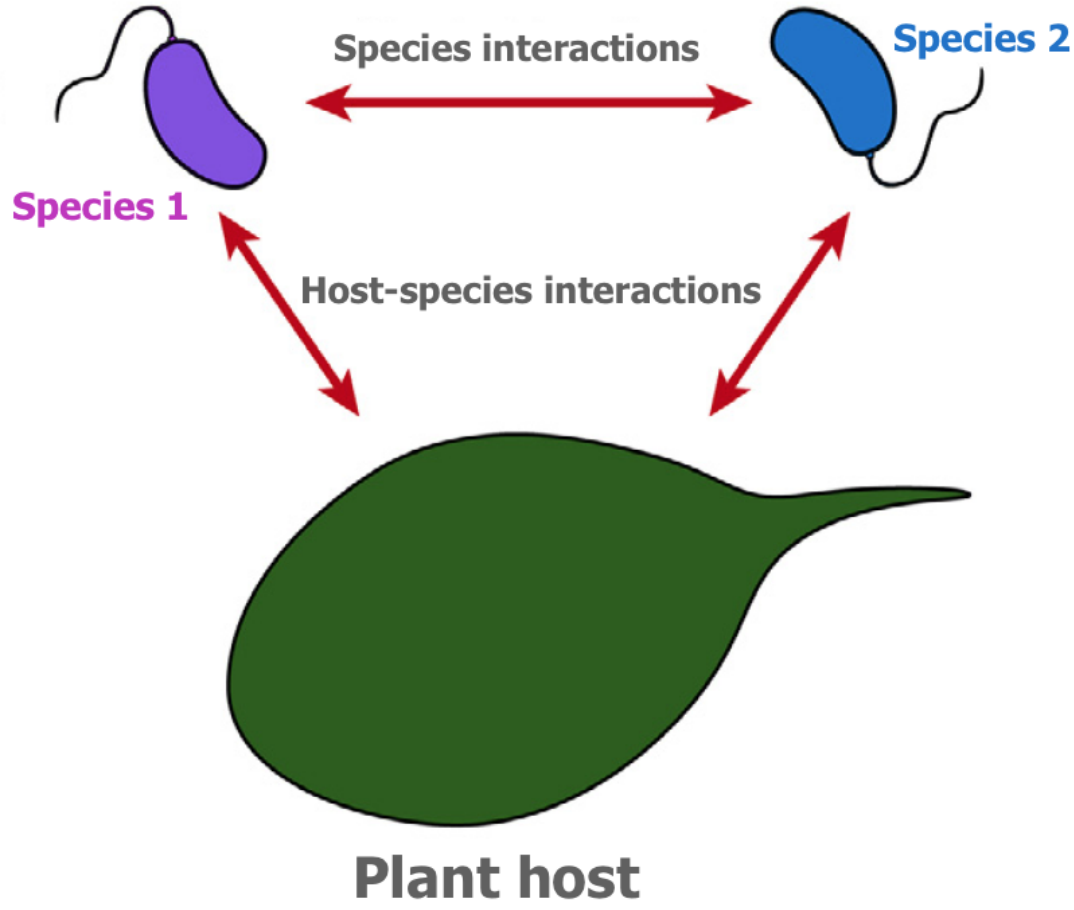
Formation of spatial patterns

2. Model for cell populations

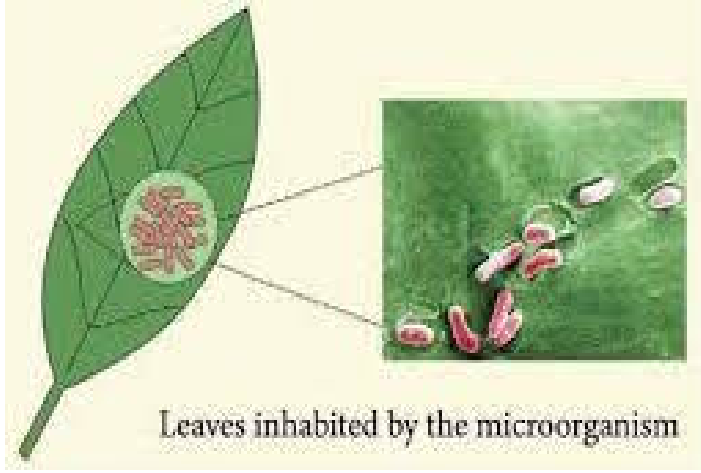
Problem | bacteria populations on a leaf surface

Two **bacterial strains** leave on a **leaf surface**





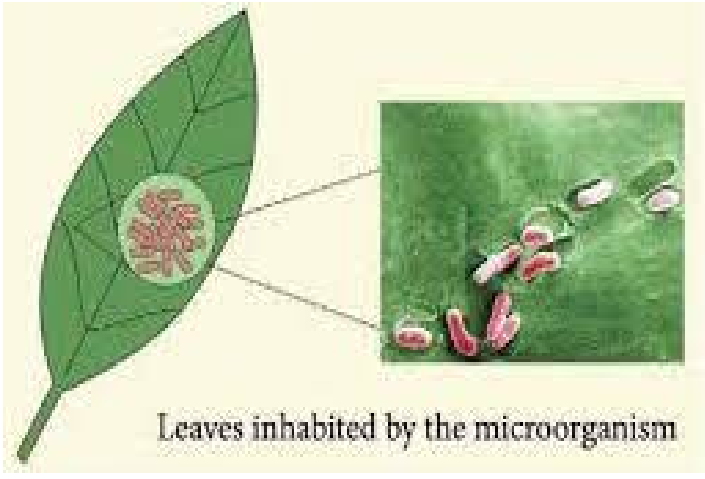
Bacteria **interact** one with each other and with **host**
They experience different **processes** with the **host**



Bacteria are exposed to **environmental stress** like **radiation**, temperature **oscillations**, **dryness**

They **interact** and **compete** with other **microbes**

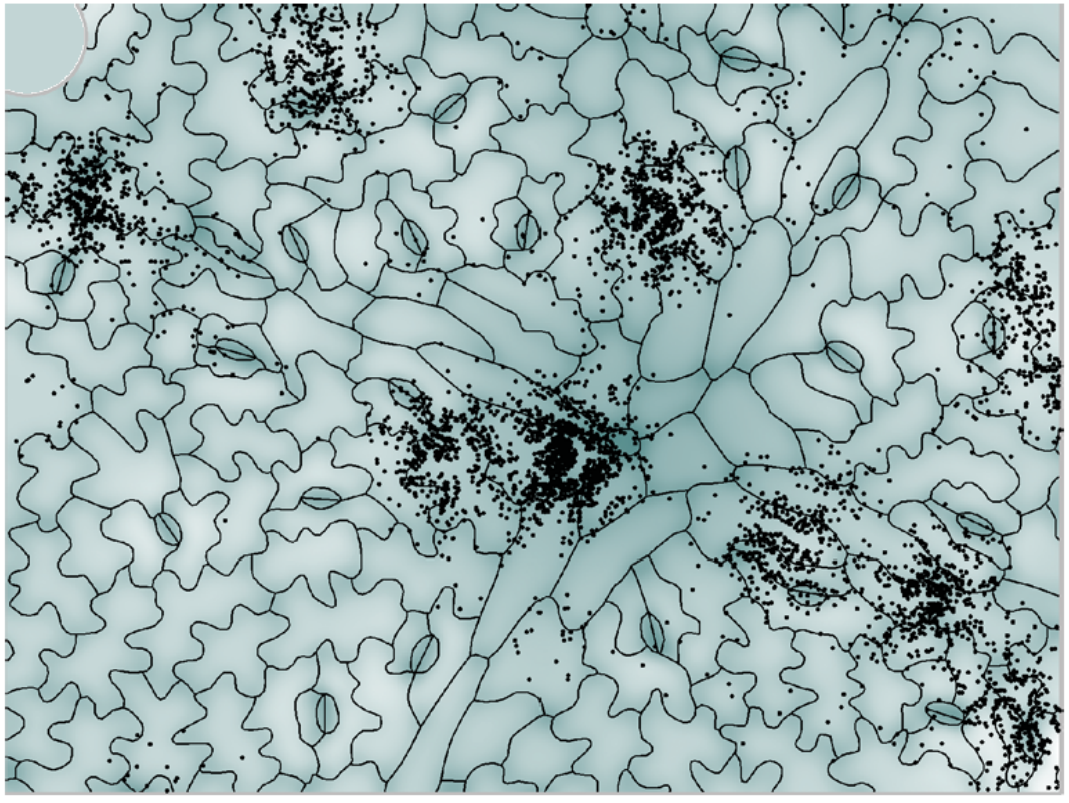
Their **survival** on the leaf surface depends on how many **nutrients are available**



Bacteria **compete for resources**
and the **resources availability** fluctuates

They **extract** the **nutrients** from the leaf surface
also by **cooperating**

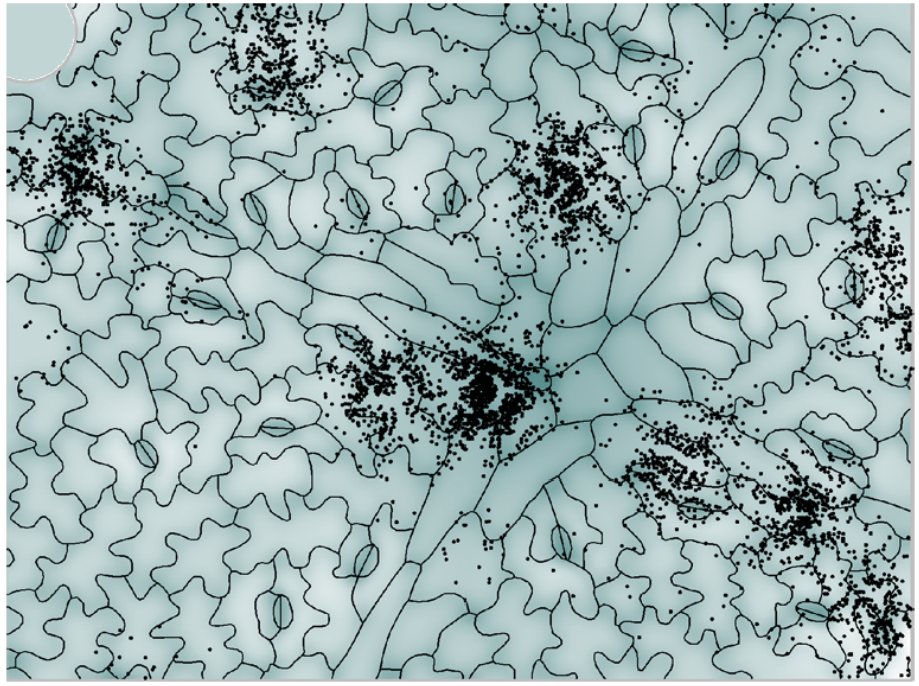
Bacteria form **clusters** in extracting nutrients



Esser, Leveau, Meyer, Wiegand, FEMS Microbiol Ecol, 91, 2015

Bacteria form **clusters** in extracting nutrients

Some **spatial patterns** appear



Esser, Leveau, Meyer, Wiegand, FEMS Microbiol Ecol, 91, 2015

These interactions occur at **different scales** of time and space

Understanding these scales is crucial for **interpreting** spatial microbial **collonization patterns**

[Esser, Leveau, Meyer, Wiegand, FEMS Microbiol Ecol, 91, 2015]

Kinetic Theory of Active Particles

- provides **powerful tools** to study this **biological process**

- is **able to describe** how **macroscopic phenomena** like

  observable patterns

  self organization

  collective motion

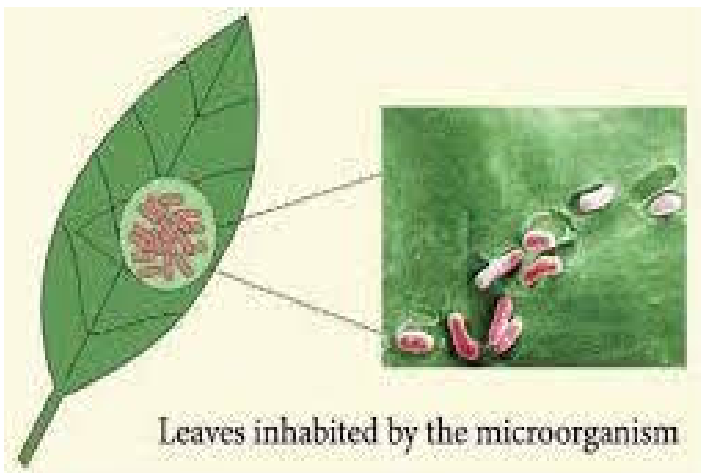
  emerge from the underlying **microscopic** dynamics and **individual** behaviour

The problem

Bacterial populations $\mathbf{C_1}$ and $\mathbf{C_2}$, with $\mathbf{C_2}$ being more competitive
Cells of $\mathbf{C_2}$ can **destroy** cells of $\mathbf{C_1}$

Host population **H** constituted by the cells of the leaf
Population **L** of cells of the leaf having disposable nutrient

The bacteria **proliferate** when extracting nutrient from the leaf



The kinetic description

The behaviour of cells is described by **distribution functions**

$$f_i : [0, \infty] \times \Gamma \times \mathbb{R}^2 \times [-1, 1] \to \mathbb{R}^+, \quad i = 1, 2, H, L$$

such that $f_i(t, x, v, u)$ gives the number of cells of i-population with activity $u \in [-1, 1]$ and velocity $v \in \mathbb{R}^2$ at time $t \geq 0$ and position $x \in \Gamma$

$i = 1, 2$ for bacteria $\quad i = H$ for Host $\quad i = L$ for Leaf nourishing cells

The number of cells of the i-population at time t and position x is

$$n_i(t, x) = \int_{-1}^{1} \int_{\mathbb{R}^2} f_i(t, x, v, u) \, \mathrm{d}v \, \mathrm{d}u, \quad i = 1, 2, H, L$$

Kinetic equations

We follow the behaviour of bacterial populations and population L

$$\frac{\partial f_1}{\partial t} + u\boldsymbol{c}_1(\boldsymbol{x},t)\cdot\nabla_{\boldsymbol{x}} f_1 = \mathcal{G}_1^H[f_1,f_H] + \mathcal{L}_{12}[f_1,f_2] + \Big(\mathcal{N}_{1L}[f_1,f_L] + \mathcal{N}_{12}[f_1,f_2]\Big)$$

$$\frac{\partial f_2}{\partial t} + u\boldsymbol{c}_2(\boldsymbol{x},t)\cdot\nabla_{\boldsymbol{x}} f_2 = \mathcal{G}_2^H[f_2,f_H] + \mathcal{L}_{21}[f_2,f_1] + \Big(\mathcal{N}_{2L}[f_2,f_L] + \mathcal{N}_{22}[f_2,f_2] + \mathcal{J}_2[f_2]\Big)$$

$$\frac{\partial f_L}{\partial t} = \Big(\mathcal{N}_{L1}[f_L,f_1] + \mathcal{N}_{L2}[f_L,f_2]\Big) + \mathcal{Q}_{12}^L[f_1,f_2]$$

The terms on the r.h.s are **non-linear integral operators**

Interacting operators

$$\frac{\partial f_1}{\partial t} + u\boldsymbol{c}_1(\boldsymbol{x},t)\cdot\nabla_{\boldsymbol{x}} f_1 = \mathcal{G}_1^H[f_1, f_H] + \mathcal{L}_{12}[f_1, f_2] + \Big(\mathcal{N}_{1L}[f_1, f_L] + \mathcal{N}_{12}[f_1, f_2]\Big)$$

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$$\frac{\partial f_L}{\partial t} = \Big(\mathcal{N}_{L1}[f_L, f_1] + \mathcal{N}_{L2}[f_L, f_2]\Big) + \mathcal{Q}_{12}^L[f_1, f_2]$$

$\mathcal{G}_i^H[f_i, f_H]$ conservative interactions between bacteria and host tissue

$$\mathcal{G}_i^H[f_i, f_H] = \overline{\eta}_i \overline{\beta}_i \int_{-1}^{1} \left[f_i(u') - f_i(u)\right] du', \quad i = 1, 2$$

where

$\overline{\eta}_i \geq 0$ is the **interaction frequency** between bacteria and host cell

$\overline{\beta}_i \in [0, 1]$ is a **transition probability** for a bacteria to pass from activity u to activity u' after interaction with a host cell

Interacting operators

$$\frac{\partial f_1}{\partial t} + u\boldsymbol{c}_1(\boldsymbol{x},t)\cdot\nabla_{\boldsymbol{x}} f_1 = \mathcal{G}_1^H[f_1, f_H] + \mathcal{L}_{12}[f_1, f_2] + \Big(\mathcal{N}_{1L}[f_1, f_L] + \mathcal{N}_{12}[f_1, f_2]\Big)$$

$$\frac{\partial f_2}{\partial t} + u\boldsymbol{c}_2(\boldsymbol{x},t)\cdot\nabla_{\boldsymbol{x}} f_2 = \mathcal{G}_2^H[f_2, f_H] + \mathcal{L}_{21}[f_2, f_1] + \Big(\mathcal{N}_{2L}[f_2, f_L] + \mathcal{N}_{22}[f_2, f_2] + \mathcal{J}_2[f_2]\Big)$$

$$\frac{\partial f_L}{\partial t} = \Big(\mathcal{N}_{L1}[f_L, f_1] + \mathcal{N}_{L2}[f_L, f_2]\Big) + \mathcal{Q}_{12}^L[f_1, f_2]$$

$\mathcal{L}_{ij}[f_i, f_j]$ turning operators that modify the re-orientation of bacteria

(they depend on densities n_1, n_2)

$$\mathcal{L}_{ij}[f_i, f_j] = \int_{\mathbb{S}^1} \lambda_{ij}\, \widehat{\boldsymbol{v}} \cdot \hat{\boldsymbol{v}}'(\hat{\boldsymbol{v}}' \cdot \nabla_{\boldsymbol{x}} n_j(t, \boldsymbol{x}))\, f_i(t, \boldsymbol{x}, \hat{\boldsymbol{v}}', u) d\hat{\boldsymbol{v}}'$$

where

λ_{ij} is a turning rate of type $\lambda_{ij}\Big(n_1(t, \boldsymbol{x}), n_2(t, \boldsymbol{x})\Big)$

Interacting operators

$$\frac{\partial f_1}{\partial t} + u\boldsymbol{c}_1(\boldsymbol{x},t)\cdot\nabla_{\boldsymbol{x}} f_1 = \mathcal{G}_1^H[f_1, f_H] + \mathcal{L}_{12}[f_1, f_2] + \Big(\mathcal{N}_{1L}[f_1, f_L] + \mathcal{N}_{12}[f_1, f_2]\Big)$$

$$\frac{\partial f_2}{\partial t} + u\boldsymbol{c}_2(\boldsymbol{x},t)\cdot\nabla_{\boldsymbol{x}} f_2 = \mathcal{G}_2^H[f_2, f_H] + \mathcal{L}_{21}[f_2, f_1] + \Big(\mathcal{N}_{2L}[f_2, f_L] + \mathcal{N}_{22}[f_2, f_2] + \mathcal{J}_2[f_2]\Big)$$

$$\frac{\partial f_L}{\partial t} = \Big(\mathcal{N}_{L1}[f_L, f_1] + \mathcal{N}_{L2}[f_L, f_2]\Big) + \mathcal{Q}_{12}^L[f_1, f_2]$$

Population C_2 is supposed to be more aggressive than C_1

$\mathcal{J}_2[f_2]$ natural decay $\mathcal{J}_2[f_2] = -\overline{\tau}_2\, f_2(\hat{\boldsymbol{v}}, u)$

$\mathcal{N}_{i2}[f_i, f_2]$ destructive interactions

$$\mathcal{N}_{i2}[f_i, f_2] = -\overline{\nu}_{i2}\, f_i(\hat{\boldsymbol{v}}, u) \int_{\mathbb{S}^1} \int_{-1}^{1} f_2(\hat{\boldsymbol{v}}', u')\, du'\, d\hat{\boldsymbol{v}}'$$

where $\mathcal{N}_{12}[f_1, f_2]$ describes **interspecific** competition

$\mathcal{N}_{22}[f_2, f_2]$ describes **intraspecific** competition

Interacting operators

$$\frac{\partial f_1}{\partial t} + u\boldsymbol{c}_1(\boldsymbol{x},t)\cdot\nabla_{\boldsymbol{x}} f_1 = \mathcal{G}_1^H[f_1, f_H] + \mathcal{L}_{12}[f_1, f_2] + \Big(\mathcal{N}_{1L}[f_1, f_L] + \mathcal{N}_{12}[f_1, f_2]\Big)$$

$$\frac{\partial f_2}{\partial t} + u\boldsymbol{c}_2(\boldsymbol{x},t)\cdot\nabla_{\boldsymbol{x}} f_2 = \mathcal{G}_2^H[f_2, f_H] + \mathcal{L}_{21}[f_2, f_1] + \Big(\mathcal{N}_{2L}[f_2, f_L] + \mathcal{N}_{22}[f_2, f_2] + \mathcal{J}_2[f_2]\Big)$$

$$\frac{\partial f_L}{\partial t} = \Big(\mathcal{N}_{L1}[f_L, f_1] + \mathcal{N}_{L2}[f_L, f_2]\Big) + \mathcal{Q}_{12}^L[f_1, f_2]$$

$\mathcal{N}_{iL}[f_i, f_L]$ proliferative for bacteria due the nutrient extracted from the leaf
$\mathcal{N}_{Li}[f_i, f_L]$ destructive for the leaf due the detriment of population L

$$\mathcal{N}_{iL}[f_i, f_L] = \overline{\mu}_{iL}\varphi_{iL}(\hat{\boldsymbol{v}}, u) \iint_{\mathbb{S}^1\times\mathbb{S}^1} \int_{-1}^{1}\int_{-1}^{1} f_i(\hat{\boldsymbol{v}}_*, u_*) f_L(\hat{\boldsymbol{v}}', u')\, du_*\, du'\, d\hat{\boldsymbol{v}}_*\, d\hat{\boldsymbol{v}}'$$

$$\mathcal{N}_{Li}[f_L, f_i] = -\overline{\nu}_{Li}\, f_L(\hat{\boldsymbol{v}}, u) \int_{\mathbb{S}^1} \int_{-1}^{1} f_j(\hat{\boldsymbol{v}}', u')\, du'\, d\hat{\boldsymbol{v}}'$$

where $\overline{\mu}_{iL}$ is a **proliferative** rate and $\overline{\nu}_{Li}$ a **consumption** rate

Interacting operators

$$\frac{\partial f_1}{\partial t} + u\boldsymbol{c}_1(\boldsymbol{x},t)\cdot\nabla_{\boldsymbol{x}} f_1 = \mathcal{G}_1^H[f_1, f_H] + \mathcal{L}_{12}[f_1, f_2] + \Big(\mathcal{N}_{1L}[f_1, f_L] + \mathcal{N}_{12}[f_1, f_2]\Big)$$

$$\frac{\partial f_2}{\partial t} + u\boldsymbol{c}_2(\boldsymbol{x},t)\cdot\nabla_{\boldsymbol{x}} f_2 = \mathcal{G}_2^H[f_2, f_H] + \mathcal{L}_{21}[f_2, f_1] + \Big(\mathcal{N}_{2L}[f_2, f_L] + \mathcal{N}_{22}[f_2, f_2] + \mathcal{J}_2[f_2]\Big)$$

$$\frac{\partial f_L}{\partial t} = \Big(\mathcal{N}_{L1}[f_L, f_1] + \mathcal{N}_{L2}[f_L, f_2]\Big) + \mathcal{Q}_{12}^L[f_1, f_2]$$

$\mathcal{Q}_{12}^L[f_i, f_L]$ cooperative operator

$$\mathcal{Q}_{12}^L[f_i, f_L] = \overline{\sigma}_{12}^L\, \psi_{12}^L(\hat{\boldsymbol{v}}, u) \iint_{\mathbb{S}^1\times\mathbb{S}^1} \int_{-1}^{1}\int_{-1}^{1} f_1(\hat{\boldsymbol{v}}_*, u_*) f_2(\hat{\boldsymbol{v}}', u')\, du_* du' d\hat{\boldsymbol{v}}_* d\hat{\boldsymbol{v}}'$$

where $\overline{\sigma}_{12}^L$ is an **interaction frequency**

ψ_{12}^L the **expected density** of newborn L-cells

Asymptotic analysis

- We perform a **time scaling** assuming that

  the **dominant process** is the
  interaction of bacteria with the host environment

  slow processes are
  proliferative interations and **destructive interations**

  moderate processes are
  re-orientation of bacteria
  movement of bacteria
  cooperation of bacteria

- We choose a **small parameter** ε and perform the
  the **scaling** of the equations
  the **expansion** of the unknown functions

Rescalled kinetic equations (diffusive limit)

$$\varepsilon \frac{\partial f_1}{\partial t} + u\boldsymbol{c}_1(\boldsymbol{x},t)\cdot\nabla_{\boldsymbol{x}} f_1 = \frac{1}{\varepsilon}\mathcal{G}_1^H[f_1,f_H] + \mathcal{L}_{12}[f_1,f_2] + \varepsilon\left(\mathcal{N}_{1L}[f_1,f_L] + \mathcal{N}_{12}[f_1,f_2]\right)$$

$$\varepsilon \frac{\partial f_2}{\partial t} + u\boldsymbol{c}_2(\boldsymbol{x},t)\cdot\nabla_{\boldsymbol{x}} f_2 = \frac{1}{\varepsilon}\mathcal{G}_2^H[f_2,f_H] + \mathcal{L}_{21}[f_2,f_1] + \varepsilon\left(\mathcal{N}_{2L}[f_2,f_L] + \mathcal{N}_{22}[f_2,f_2] + \mathcal{J}_2[f_2]\right)$$

$$\varepsilon \frac{\partial f_L}{\partial t} = \varepsilon\left(\mathcal{N}_{L1}[f_L,f_1] + \mathcal{N}_{L2}[f_L,f_2]\right) + \mathcal{Q}_{12}^L[f_1,f_2]$$

where the time is also rescaled as $\widetilde{t} = \varepsilon t$ and the tilde is omitted

Hilbert expansions of f_i in terms of ε

$$f_i(t, \boldsymbol{x}, \hat{\boldsymbol{v}}, u) = f_i^0(t, \boldsymbol{x}, \hat{\boldsymbol{v}}, u) + \varepsilon\, f_i^1(t, \boldsymbol{x}, \hat{\boldsymbol{v}}, u) + \varepsilon^2\, f_i^2(t, \boldsymbol{x}, \hat{\boldsymbol{v}}, u) + O(\varepsilon^3)$$

with the usual, convenient assumption that the total mass density is concentrated on the ε^0 term

$$\int_{\mathbb{S}^1} \int_{-1}^{1} f_i^0(t, \boldsymbol{x}, \hat{\boldsymbol{v}}, u)\, du\, d\hat{\boldsymbol{v}} = n_i(t, \boldsymbol{x})$$

$$\int_{\mathbb{S}^1} \int_{-1}^{1} f_i^k(t, \boldsymbol{x}, \hat{\boldsymbol{v}}, u)\, du\, d\hat{\boldsymbol{v}} = 0, \quad \text{for } k \geq 1$$

Solvability condition

about the **equilibrium** of the conservative operators

Assumption

• There exists an **equilibrium** distribution $M_i(u)$ of the **conservative** operator, uniform in $\hat{\boldsymbol{v}}$ and independent of x and t, satisfying a **detailed balance principle**, such that

$$\mathcal{G}_i^H[M_i, f_H] = 0$$

$$\int_{-1}^{1} M_i(u)\, du = 1 \qquad \text{and} \qquad \int_{-1}^{1} u\, M_i(u)\, du = 0$$

• There exists $\gamma > 0$ such that the following **bound condition** holds

$$\overline{\eta}_i \overline{\beta}_i \int_{-1}^{1} f_H(u_*)\, du_* \geq \gamma\, M_i(u)$$

Crucial result

about the **equilibrium** of the conservative operators

Theorem

Consider the previous Assumption.

Then, the equation

$$\mathcal{G}_i^H[h_i, f_H] = g_i \qquad \text{with} \qquad \int_{-1}^{1} g_i(u)\, du = 0$$

has a **unique solution** $h_i \in L^2\left([-1,1], \frac{du}{M_i}\right)$ satisfying

$$\int_{-1}^{1} h_i(u)\, du = 0$$

Macroscopic equations

Inserting **expansions** of f_i in the **scaled equations**

equating terms of the same order in ε

going from 0-order to 1-order and then to 2-order

using the properties of the operators

we obtain **global balance equations** for the time-space evolution of the densities of the bacterial populations

Theorem Reaction-diffusion equations (mac)

$$\frac{\partial n_1}{\partial t} = c_1 \nabla_{\boldsymbol{x}} \cdot \left(c_1 \mathcal{D}_1 \nabla_{\boldsymbol{x}} n_1 - \chi_1 \lambda_{12} \nabla_{\boldsymbol{x}} n_2 \right) + \frac{\zeta n_1^2 n_2}{n_1 + \beta n_2} - n_1 n_2$$

$$\frac{\partial n_2}{\partial t} = c_2 \nabla_{\boldsymbol{x}} \cdot \left(c_2 \mathcal{D}_2 \nabla_{\boldsymbol{x}} n_2 - \chi_2 \lambda_{21} \nabla_{\boldsymbol{x}} n_1 \right) + \frac{\zeta \beta n_1 n_2^2}{n_1 + \beta n_2} - \tau n_2 - \nu n_2^2$$

λ_{ij} turning rates $\mathcal{D}_i$ self diffusion coefficients

χ_i chemotaxis (cross diffusion) coefficients

they depend on **microscopic interaction rates**

The **cross-diffusion** terms come from the turning operators and re-orientation of bacteria

The kinetic equation for cells of the **leaf surface** is used to close the macroscopic equations for n_1, n_2

Turing instability

Homogeneous steady state (without diffusion)

$$(\overline{n}_1, \overline{n}_2) = \left(\frac{\beta\,\tau}{(\zeta-1)(\beta-\nu)}, \frac{\tau}{\beta-\nu} \right), \quad \zeta > 1,\ \beta > \nu$$

- It is **stable** if $\zeta > \dfrac{1-\beta}{1-\nu}$ and $\nu > 1$
- It is **unstable** if $\zeta < \dfrac{1-\beta}{1-\nu}$
- An **Hopf bifurcation** occurs if $\zeta = \dfrac{1-\beta}{1-\nu}$

Patterns formation and Turing instability

- a **Turing pattern** arises when a **stable equilibrium** state of the **spatial homogeneous** system **becomes unstable** in presence of **diffusion**

- This condition may lead to **spatial patterns** that can describe **relevant processes** in the **leaf flora** and **bacterial life**

Turing instability

This requires to linearize the **macroscopic system with diffusion around the equilibrium state**

We obtain

$$\frac{\partial \mathbf{w}}{\partial t}(t,x) = \mathbf{D}\Delta_{\mathbf{x}}\mathbf{w}(t,x) + \mathbf{J}\mathbf{w}(t,x) \quad \text{on } (0,+\infty)\times\Gamma$$

where **J** is the Jacobian matrix and **D** is the diffusion matrix

Turing instability is reached whenever the **steady state** becomes **unstable** to spatial perturbations.

Turing instability

We use **separation of variables** and consider a **normal mode** expansion in **Fourier series** to search solutions

$$\mathbf{w}(\mathbf{x}, t) = \sum_{k \in \mathbb{N}} c_k e^{\lambda_k t} \overline{\mathbf{w}}_k(\mathbf{x})$$

Eigenfunctions $\overline{\mathbf{w}}_k(\mathbf{x})$ represent independent **perturbation modes**

Eigenvaluess λ_k are the corresponding growth rates

Thus, **eigenfunctions** $\overline{\mathbf{w}}_k(\mathbf{x})$ solve the time-independent problem

$$\begin{cases} \Delta \overline{\mathbf{w}}_k + k^2 \overline{\mathbf{w}}_k = \mathbf{0} & \text{in } \Gamma \\ \boldsymbol{\nu} \cdot \nabla_{\mathbf{x}} \overline{\mathbf{w}}_k = 0 & \text{at } \partial\Gamma \end{cases}$$

and λ_k are **eigenvalues** of the matrix

$$\mathbf{J} - k^2 \mathbf{D}$$

Turing **instability** occurs if there exists an **eigenvalue** with **positive real part**

3. Numerical illustrations

Numerical simulations (cross diffusion)

Stability of the homogeneous steady state and **instability** of the equilibrium state in presence of **diffusion** leads to a suitable **parameter space**.

Bifurcation diagram ($\delta = \mathcal{D}_2/\mathcal{D}_1$)

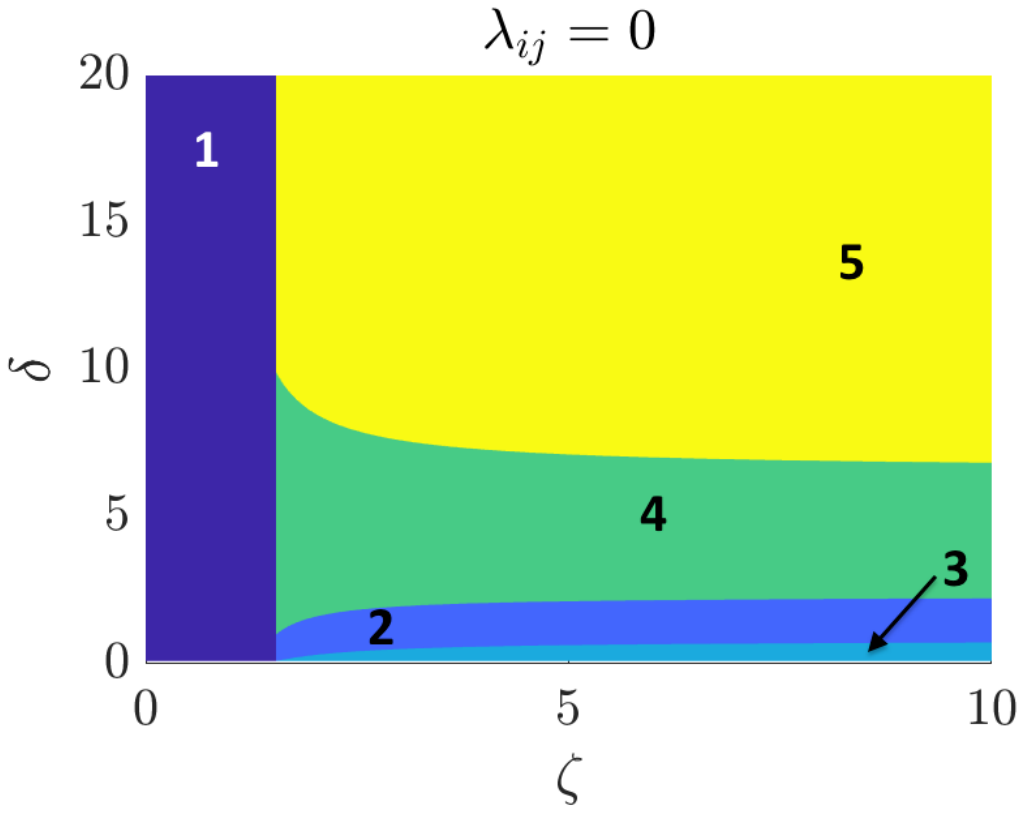
1 $(\overline{n}_1, \overline{n}_2)$ is not stable

2 no condition for Turing instab

3 only one condition holds

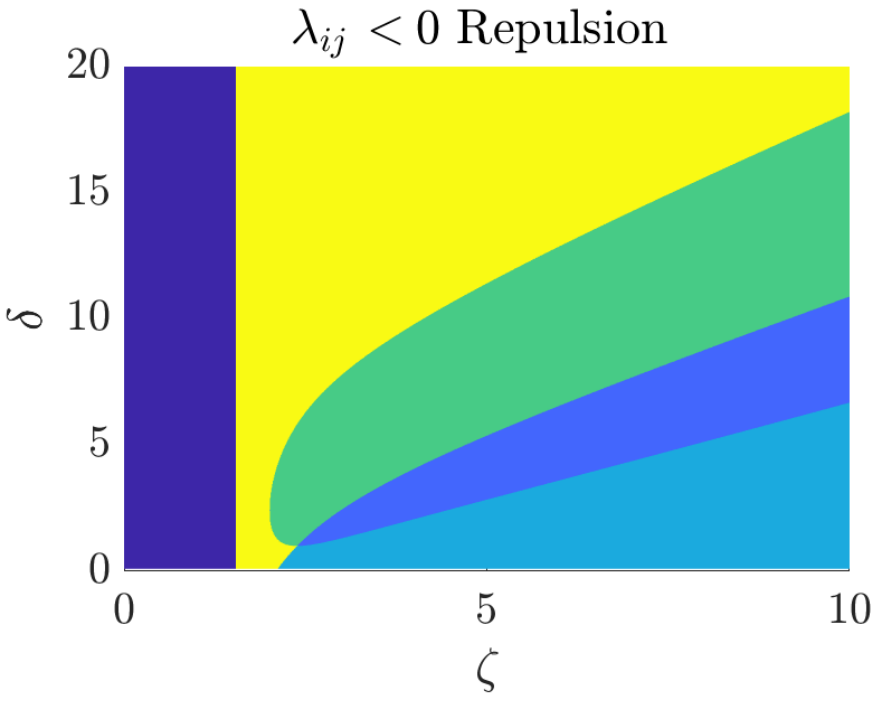
4 only other condition holds

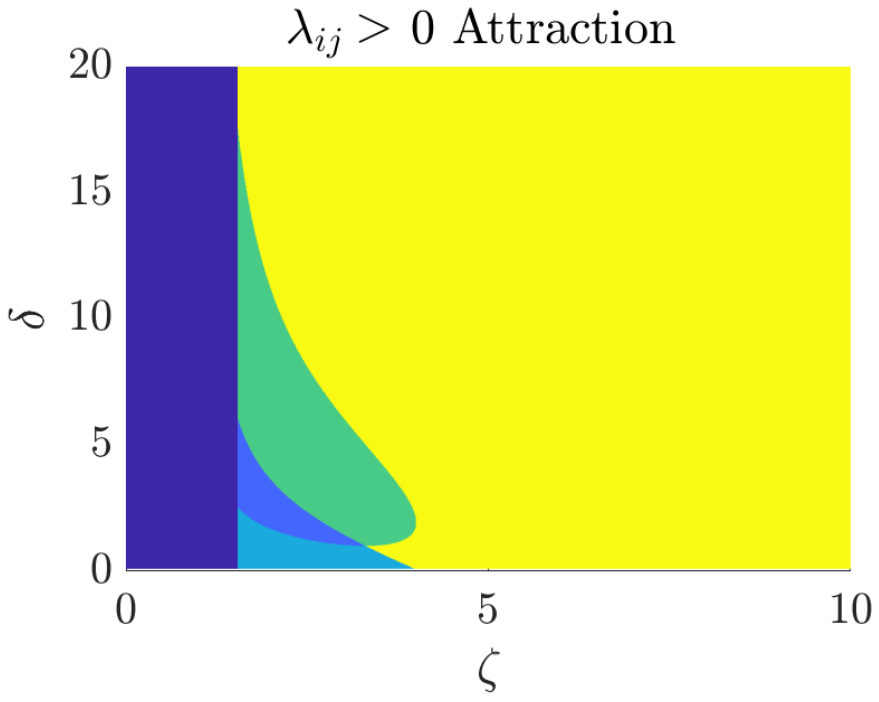
5 **Turing instability occurs**



no **cross-diffusion**

Bifurcation diagrams

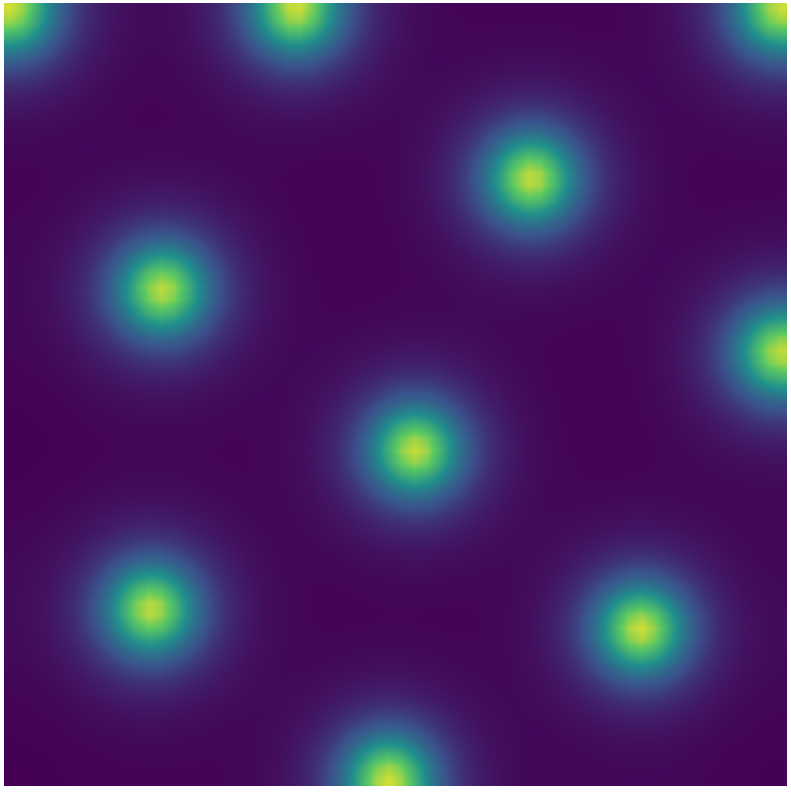




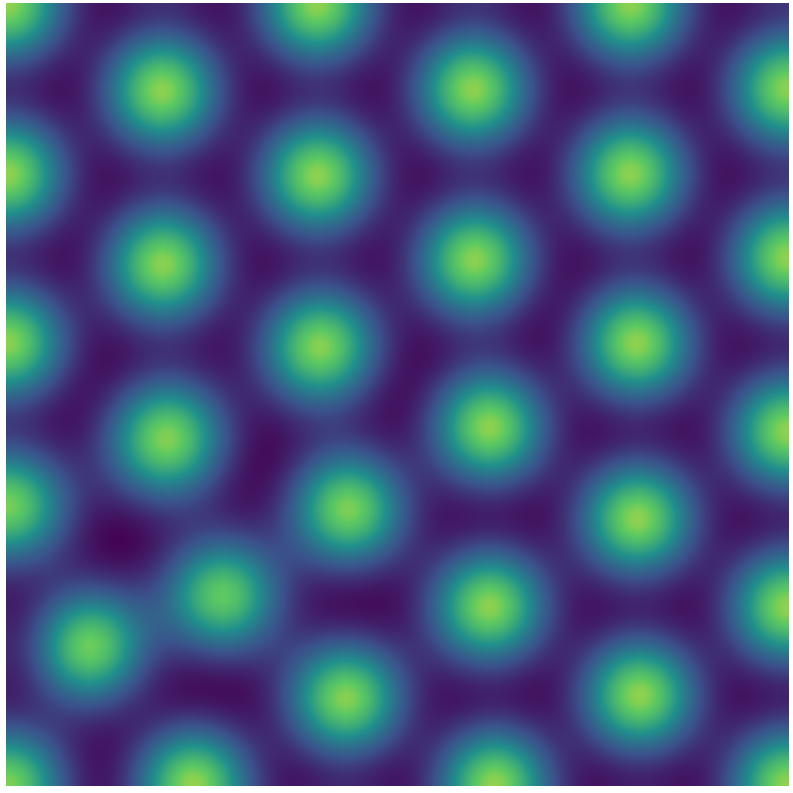
cross-diffusion
repulsive potential

cross-diffusion
attractive potential

Pattern formation (2D domain) for n_1

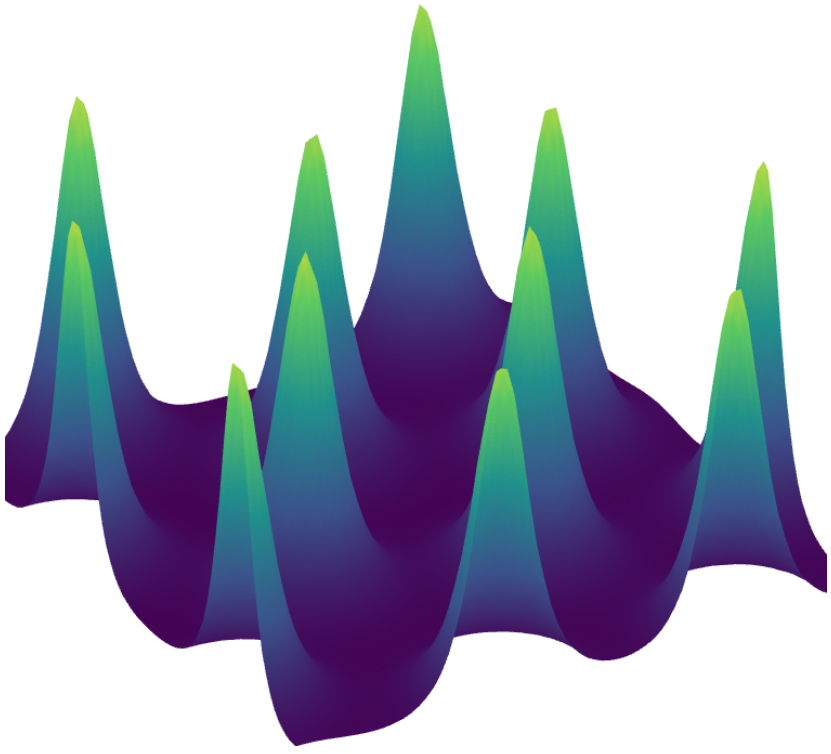


constant self-diffusion
cross-diffusion
repulsive potential

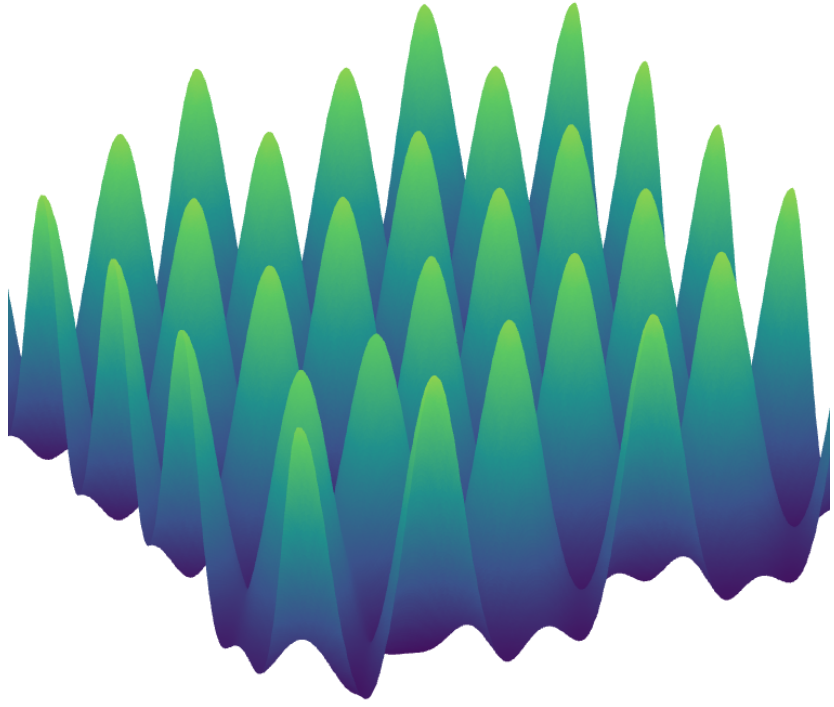


constant self-diffusion
cross-diffusion
attractive potential

Pattern formation (2D domain)



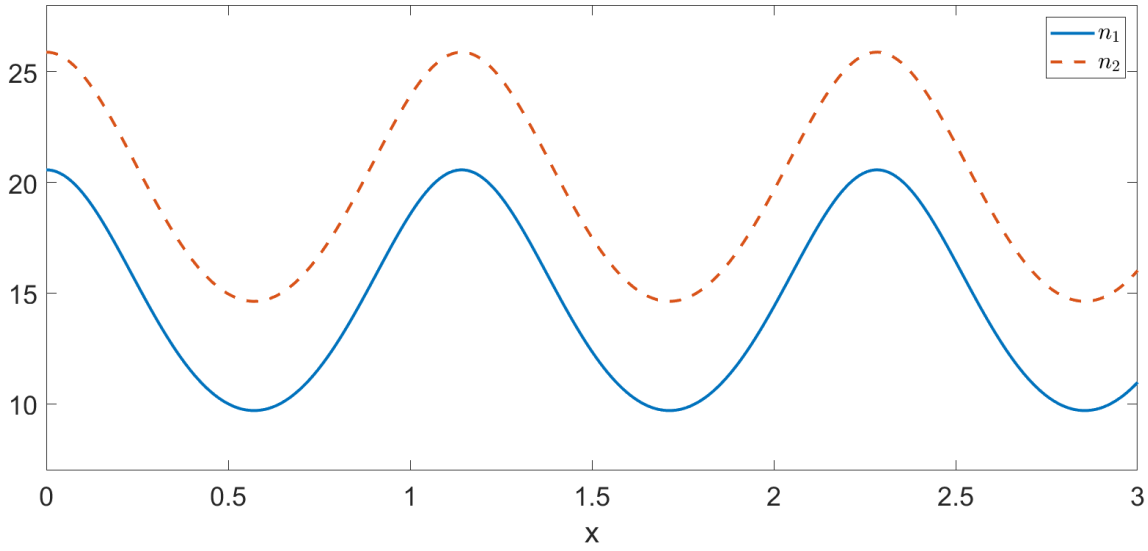
constant self-diffusion
cross-diffusion
repulsive potential



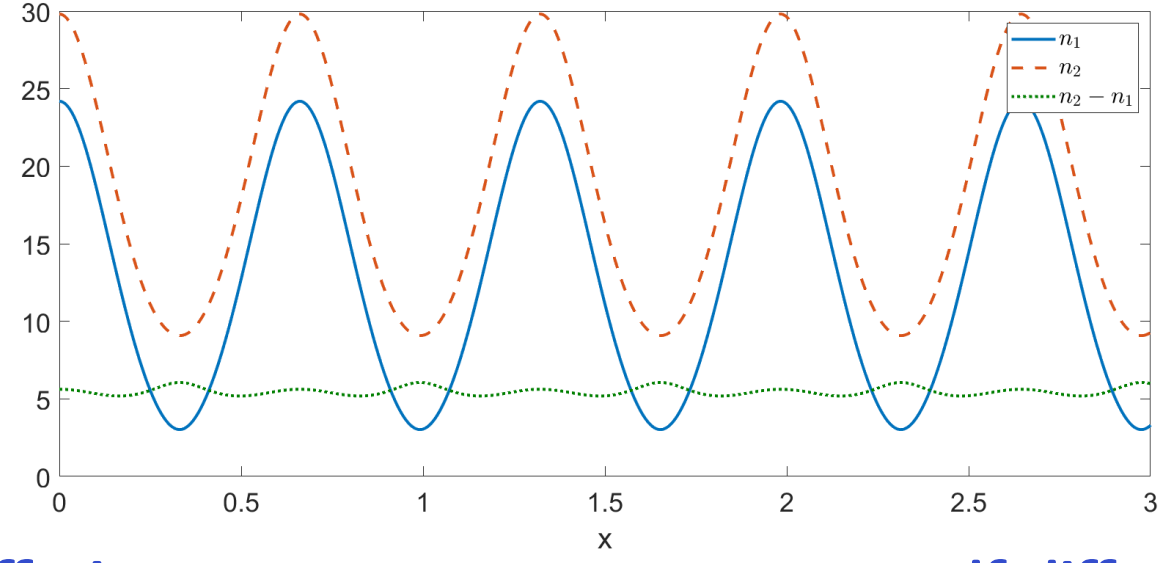
constant self-diffusion
cross-diffusion
attractive potential

Pattern formation (2D domain)

(A)



(B)



constant self-diffusion
cross-diffusion (repulsive)

constant self-diffusion
cross-diffusion (attractive)

Numerical method

- square domain $\Omega = [0, \pi] \times [0, \pi]$
- **initial conditions** correspond to a small perturbation of the steady state
- **Neumann boundary conditions** with no flux at the boundary
- **finite element method** in space **x**
- **finite difference method** in time t
- **non linear** system
- the **numerical scheme** is implemented in Python

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Obrigada pela vossa atenção!

Thank you for your attention!