Nonequilibrium Field Theories and Stochastic Dynamics

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1 Biological background of bacterial chemotaxis

The movement pattern of *E. coli* is not a continuous, smooth swim, but rather consists of an alternation between two distinct behaviors:

- **Run:** During this phase, the bacterium's multiple flagella rotate **Counter-Clockwise (CCW)**. They gather into a bundle, pushing the bacterial body like a propeller, causing it to move approximately in a straight line.
- **Tumble:** During this phase, the rotation direction of the flagella switches to **Clockwise (CW)**. This causes the flagellar bundle to disperse, with each flagellum moving independently. This results in the bacterium randomly changing orientation in place, setting a new, random departure angle for the next "Run."

The core mechanism of chemotaxis does not lie in the bacterium's ability to "steer" a steering wheel for precise turning, but rather in its ability to **modulate the frequency of tumbling** based on changes in the concentration of beneficial or harmful chemicals in the environment.

When the bacterium senses that it is moving in a direction with a higher concentration of **chemoattractant**, it inhibits the occurrence of tumbling, thereby extending the duration of the current "Run." Conversely, if it discovers it is swimming in an unfavorable direction (e.g., attractant concentration is decreasing or repellent concentration is increasing), it increases the frequency of tumbling to more quickly attempt a new random direction.

Through this simple strategy of **if better, continue; if worse, change**, the bacterium's random walk acquires a statistical bias, ultimately achieving macroscopic migration toward areas of high attractant concentration.

To understand why bacteria adopt this seemingly clumsy Run-Tumble strategy, we must examine the physical environment they inhabit. The dimensionless number describing the relative importance of inertial forces versus viscous forces in fluid dynamics is the **Reynolds number**, defined as:

$$Re = \frac{\rho L v}{\eta}$$

Where L is the characteristic length (approximately a few micrometers for bacteria), v is the velocity (approx. 20-30 μm/s), ρ is the fluid density (density of water), and η is the fluid viscosity. For a typical *E. coli*, the calculated Reynolds number is extremely low, approximately 10^{-6}.

Such a low Reynolds number implies that viscous forces play an absolutely dominant role in the bacterium's movement, while inertial forces can be completely neglected. This leads to several crucial physical consequences. **First, there is no "coasting" or "inertia".** Once the bacterium's flagella stop providing thrust, viscous drag brings it to an almost instantaneous halt. This explains why the transition between "Run" (with thrust) and "Tumble" (reorientation) is so sharp and distinct. Secondly, strategies of continuous turning through body undulation, like fish in the macroscopic world, are not feasible in a viscosity-dominated world. Therefore, bacteria had to evolve a unique movement strategy adapted to this "high damping" environment, i.e., the random Run-Tumble motion. This is not a suboptimal choice, but rather an efficient and necessary navigation mode at the physical scale in which they exist.

2 Simplified model of motion: two-state process

To understand the nature of chemotaxis from a physical perspective, we need to construct a mathematical model. We will start with a simplified model, abstracting the complex three-dimensional running-rolling motion into a two-state process in a one-dimensional space.

We assume that bacteria can only move along a one-dimensional straight line. Their state is determined not only by their position x but also by their internal direction of motion σ.

- $\sigma = 1$: represents that the bacteria are moving to the right.
- $\sigma = -1$: represents that the bacteria are moving to the left.

Bacteria maintain a fixed direction while "running," while "rolling" corresponds to a change in orientation σ. We model this state transition (i.e., rolling) as a stochastic process controlled by two rate parameters.

- $a_+(x)$: on the postion x, a Bacteria which is moving to the right ($\sigma = 1$:) rolls and change its orientation
- $a_-(x)$: on the postion x, a Bacteria which is moving to the left ($\sigma = -1$:) rolls and change its orientation

Now, we introduce two core variables to describe this system:

- $p_+(x,t)$: The probability density of finding a bacterium moving to the right at time t, position x.
- $p_-(x,t)$: The probability density of finding a bacterium moving to the left at time t, position x.

We can derive their evolution equations, namely the Master Equations, by considering the changes in these two probability densities over time within a microscopic interval $[x, x+dx]$.
For $p_+(x,t)$, the change over time is contributed by three parts:

1. **Advection Term:** Since bacteria move to the right with velocity v_0, this represents the probability flux flowing into the interval from the left x and flowing out of the interval from the right $x+dx$ per unit time.
2. **Loss Term:** Right-moving bacteria at position x tumble with rate $\alpha_+(x)$, turning into left-moving bacteria, resulting in a decrease of p_+.
3. **Gain Term:** Left-moving bacteria at position x tumble with rate $\alpha_-(x)$, turning into right-moving bacteria, resulting in an increase of p_+.

Combining these three terms, we obtain the Master Equation for p_+:

$$\partial_t p_+(x,t) = -v_0 \partial_x p_+(x,t) - \alpha_+(x) p_+(x,t) + \alpha_-(x) p_-(x,t)$$

Similarly, for $p_-(x,t)$, where bacteria move to the left with velocity $-v_0$, the Master Equation is:

$$\partial_t p_-(x,t) = +v_0 \partial_x p_-(x,t) - \alpha_-(x) p_-(x,t) + \alpha_+(x) p_+(x,t)$$

These two coupled partial differential equations constitute our minimal theoretical model for describing one-dimensional chemotactic movement. The master equation describes the probabilistic evolution of microscopic directional states, but we are more concerned with the macroscopic behavior of the entire bacterial community, such as the total bacterial density distribution and net flow. For this, we need to construct macroscopic physical quantities from p_+ and p_-.

We define two macroscopic quantities:

- **Total Probability Density:**

$$p(x,t) := p_+(x,t) + p_-(x,t)$$

This represents the total probability of finding a bacterium at time t, position x, regardless of its direction of motion.

- **Probability Current:**

$$J(x,t) := v_0[p_+(x,t) - p_-(x,t)]$$

This quantity describes the net flow of probability at point x. If there are more bacteria moving to the right than to the left ($p_+ > p_-$), then there is a net rightward flow, $J > 0$. Vice versa.

With these two definitions, we can combine the two Master Equations using simple algebraic operations. Adding the two Master Equations describing p_+ and p_-:

$$\partial_t(p_+ + p_-) = -v_0\partial_x(p_+ - p_-) - (\alpha_+ p_+ - \alpha_- p_-) + (-\alpha_- p_- + \alpha_+ p_+)$$

We observe that the terms related to the tumbling rates $\alpha_\pm$ cancel out perfectly. Substituting the definitions of p and J, we immediately obtain:

$$\partial_t p(x,t) = -\partial_x J(x,t)$$

This is an extremely important equation, the **Continuity Equation**, which is a universal conservation law. This derivation reveals a profound physical implication: tumbling (state switching) is an **internal process**. It only redistributes particles between the right-moving and left-moving populations, but does not create or destroy particles in space out of nothing. The only reason the total particle number (or total probability) at a location changes is that particles swim in or out from neighboring regions. Mathematically, the perfect cancellation of the tumbling terms precisely reflects the fundamental physical principle of **local conservation of particle number (probability)**.

Now, instead of adding the two master equations, we subtract the second equation from the first to examine the dynamics of the probability difference ($p_+ - p_-$), which is directly proportional to the probability current J.

$$\partial_t(p_+ - p_-) = -v_0\partial_x(p_+ + p_-) - (\alpha_+ p_+ - \alpha_- p_-) + (\alpha_- p_- - \alpha_+ p_+)$$

To express this equation using the macroscopic quantities p and J, we need to use the relations:

$$p_\pm = \frac{1}{2}\left(p \pm \frac{J}{v_0}\right)$$

Substituting this in and rearranging, we obtain the evolution equation for the probability current J itself:

$$\partial_t J(x,t) = -v_0^2\partial_x p(x,t) - (\alpha_+ + \alpha_-)J(x,t) + v_0(\alpha_- - \alpha_+)p(x,t)$$

The structure of this equation is remarkably rich, with each term having a clear physical significance:

- $-v_0^2\partial_x p$: **Diffusion Term**. It indicates that the gradient of the total density ($\partial_x p$) acts like pressure to drive the generation of probability current.
- $-(\alpha_+ + \alpha_-)J$: **Persistence Damping Term**. Any existing net probability current J will decay at a total rate of $\alpha_+ + \alpha_-$. This is because the tumbling process randomizes the direction of bacterial motion, thereby destroying directional *persistence* and causing the net flow to tend towards zero.
- $v_0(\alpha_- - \alpha_+)p$: **Drift Term**. This is the core term that enables chemotaxis. If there is an asymmetry in the switching rates ($\alpha_- \neq \alpha_+$), a net drift current proportional to the total density p will be generated even in the absence of a density gradient. This is precisely the source of directed motion.

We have obtained two coupled equations describing the macroscopic quantities and their evolution. However, in many cases, we can further simplify the model to obtain an efficient equation that only includes the total density. We have obtained two coupled equations describing the macroscopic quantities p and J their evolution. However, in many cases, we can further simplify the model to obtain an efficient equation that only includes the total density.

Let us examine the time scales involved in the system:

- **Run time:** $\tau_{run} \sim 1/\alpha \sim 1\,\text{s}$. This is the characteristic time for direction changes at the microscopic level, determined by the tumbling rate.
- **Diffusion time:** $\tau_D \sim L^2/D_{eff}$. This is the characteristic time for significant changes in the macroscopic density distribution $p(x,t)$. For a scale of $L \sim 100\,\mu\text{m}$, this time is approximately $25\,\text{s}$.

We find that $\tau_D \gg \tau_{run}$. This significant separation in time scales is the key to making approximations. It tells us that the dynamics of the probability current J (dominated by the rapid tumbling process) are much faster than the dynamics of the total density p. This means that for the slowly evolving p, we can assume that J is always able to instantaneously adjust to a quasi-steady state corresponding to the current p and its gradient. This is known in physics as "Adiabatic Elimination" or the "Slave Principle": the fast-changing variable (J) is "slaved" by the slow-changing variable (p). Therefore, we can make a powerful approximation: $\partial_t J \approx 0$.

Applying the adiabatic approximation $\partial_t J \approx 0$ to the dynamical equation for the probability current, we can directly solve for the effective probability current J_{eff} in the quasi-steady state:

$$J_{eff}(x,t) = -\frac{v_0^2}{\alpha_+ + \alpha_-}\partial_x p + v_0\frac{\alpha_- - \alpha_+}{\alpha_+ + \alpha_-}p$$

This expression clearly demonstrates that the effective probability current is composed of two parts: one driven by the density gradient (diffusion), and the other driven by the asymmetry of the switching rates (drift).

Next, we substitute this expression for J_{eff} back into the exact continuity equation derived earlier, $\partial_t p = -\partial_x J$. In this way, we obtain a closed equation containing only the total density p:

$$\partial_t p = \partial_x\left[\frac{v_0^2}{\alpha_+ + \alpha_-}\partial_x p - v_0\frac{\alpha_- - \alpha_+}{\alpha_+ + \alpha_-}p\right]$$

This equation is the standard form describing the evolution of particles under the combined action of drift and diffusion, known as the **Fokker-Planck Equation (FPE)**. We can write it in a more compact form:

$$\partial_t p(x,t) = \partial_x[D_{eff}(x)\partial_x p - v_{eff}(x)p]$$

Where we defined two effective transport coefficients dependent on the local tumbling rates:

- **Effective Diffusion Coefficient:**

$$D_{eff}(x) = \frac{v_0^2}{\alpha_+(x) + \alpha_-(x)}$$

- **Effective Drift Velocity:**

$$v_{eff}(x) = v_0\frac{\alpha_+(x) - \alpha_-(x)}{\alpha_+(x) + \alpha_-(x)}$$

This result is significant: starting from a complex model describing microscopic state switching, through a reasonable physical approximation (time scale separation), we successfully derived a continuous medium model describing macroscopic population behavior with a simpler form.

3 Python Simulation I: Biased Run-Roll Model

4 Closed loops: the biological basis of perception

So far, we have established the mathematical connection from the microscopic switching rate $\alpha_\pm(x)$ to the macroscopic drift velocity $v_{eff}(x)$. However, a key question remains unanswered: **How do bacteria, through their biochemical networks, transform the sensing of the external chemical field $c(x)$ into the modulation of the spatially dependent switching rate $\alpha_\pm(x)$?**

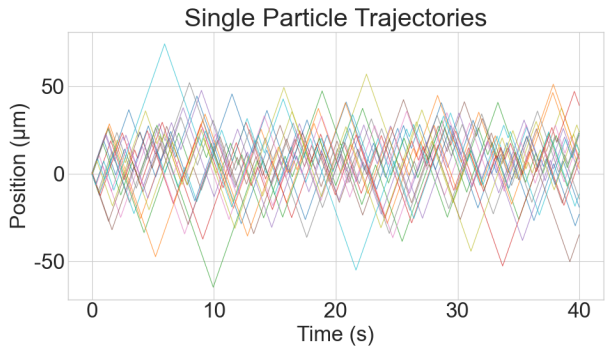

Figure 1: The trajectory diagram shows that the motion of individual particles is random, but overall they are "pulled" towards the central region (0), exhibiting biased characteristics.

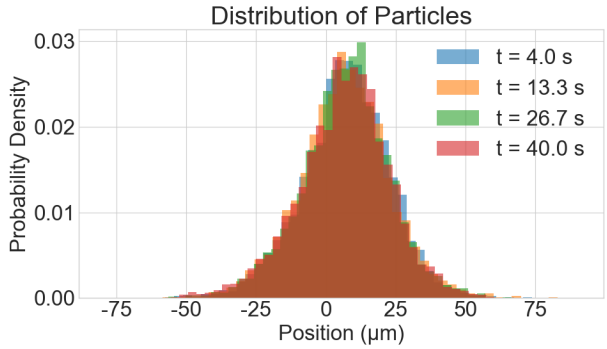

Figure 2: The distribution histogram shows that the particle ensemble gradually aggregates towards the center from an initial uniform distribution, forming a stable distribution. This confirms the existence of macroscopic drift.

A bacterium with a size of only a few micrometers cannot directly measure the minute concentration difference across its body to determine the spatial gradient $\partial_x c$. It adopts a more ingenious strategy: Temporal Sensing. When a bacterium swims in space, it continuously monitors the chemical concentration in its surroundings. What it actually measures is the rate of change of concentration with respect to time, $\frac{dc}{dt}$. Using the chain rule, we can relate this time derivative to the spatial gradient:

$$\frac{dc}{dt} = \frac{\partial c}{\partial t} + \frac{\partial c}{\partial x}\frac{dx}{dt} \tag{1}$$

Assuming the chemical field $c(x)$ is static ($\frac{\partial c}{\partial t} = 0$), and the bacterium moves with velocity $v_0\sigma(t)$, then the rate of concentration change it experiences is:

$$\frac{dc}{dt} = v_0\sigma(t)\partial_x c \tag{2}$$

It is this time derivative $\frac{dc}{dt}$ acting as the input signal that is processed by the chemical sensory system described in the first section. If the bacterium is moving in the direction of increasing attractant concentration (e.g., $\sigma = +1$ and $\partial_x c > 0$), then $\frac{dc}{dt} > 0$. This positive signal will inhibit CheA activity through the signaling pathway, reduce CheY-P levels, thereby decreasing the tumbling probability and extending the current "run". Conversely, if $\frac{dc}{dt} < 0$, the tumbling probability will increase.

We can describe the aforementioned biological mechanism using a simple **linear response model**. Assuming the tumbling rate is a linear response to the sensed rate of concentration change $\frac{dc}{dt}$, fluctuating around a basal rate α_0:

$$\alpha(\text{sensed change}) = \alpha_0\left(1 - \chi'\frac{dc}{dt}\right) \tag{3}$$

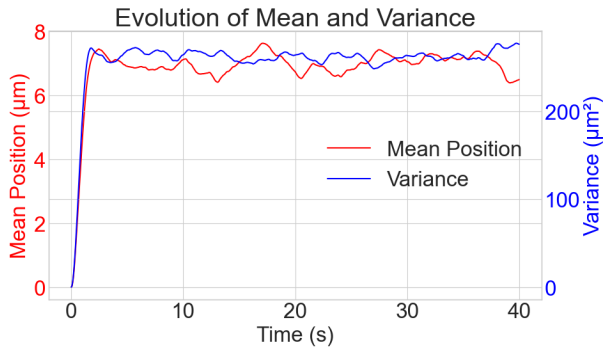

Figure 3: The mean and variance plots quantitatively illustrate the behavior of the ensemble. In this example, the mean position of the ensemble tends to 0 as the drift points towards the center. The variance, on the other hand, increases initially and then reaches a stable value, reflecting the balance between drift and diffusion. If the drift field is constant (e.g., and are constant and unequal), we observe that the mean changes linearly over time, and the variance also increases linearly over time, which is perfectly consistent with the predictions of FPE.

where χ' is a coefficient measuring the sensitivity of chemotaxis. For a particle moving to the right ($\sigma = +1$), the sensed rate of change is $v_0 \partial_x c$; for a particle moving to the left ($\sigma = -1$), the sensed rate of change is $-v_0 \partial_x c$. Therefore, we can obtain the specific expressions for α_+ and α_-:

$$\alpha_+(x) = \alpha_0(1 - \chi v_0 \partial_x c) \tag{4}$$
$$\alpha_-(x) = \alpha_0(1 + \chi v_0 \partial_x c) \tag{5}$$

Here, we have combined $\chi' \alpha_0$ into a new chemotactic coefficient χ.

Now, we can substitute these two expressions into the formulas for the **effective drift velocity** v_{eff} and the **effective diffusion coefficient** D_{eff} that we derived previously, thereby directly linking the transport coefficients to the chemical field gradient.

Derivation of Effective Drift Velocity:

$$\begin{aligned} v_{eff} &= v_0 \frac{\alpha_+(x) - \alpha_-(x)}{\alpha_+(x) + \alpha_-(x)} = v_0 \frac{\alpha_0(1 - \chi v_0 \partial_x c) - \alpha_0(1 + \chi v_0 \partial_x c)}{\alpha_0(1 - \chi v_0 \partial_x c) + \alpha_0(1 + \chi v_0 \partial_x c)} \\ v_{eff} &= v_0 \frac{-2\chi v_0 \partial_x c}{2\alpha_0(1 - (\chi v_0 \partial_x c)^2)} \approx -\frac{\chi v_0^2}{\alpha_0} \partial_x c \end{aligned} \tag{6}$$

In the common case of a **shallow gradient** ($\chi v_0 \partial_x c \ll 1$), we arrive at a core conclusion: The effective drift velocity is proportional to the negative gradient of the chemical attractant concentration. This means the bacterial population will drift towards the direction of increasing attractant concentration (if $\chi > 0$).

$$D_{eff} = \frac{v_0^2}{\alpha_+(x) + \alpha_-(x)} = \frac{v_0^2}{2\alpha_0(1 - (\chi v_0 \partial_x c)^2)} \approx \frac{v_0^2}{2\alpha_0} \tag{7}$$

Under the same shallow gradient approximation, the effective diffusion coefficient approximates to a constant.

Thus far, we have completely constructed the theoretical chain from the external chemical field to the macroscopic motion of the bacterial population.

The previous discussions assumed that the chemical field $c(x)$ is a fixed background field determined by the external environment. However, in many biological scenarios, organisms themselves alter their chemical environment through metabolic activities (such as consuming nutrients or secreting signaling molecules). This introduces a crucial **feedback loop**: bacterial motion responds to chemical gradients, while their aggregation and metabolic activities, in turn, modify the chemical gradients.

This dynamic coupling between cells and the environment is the root cause of complex collective behaviors and pattern formation.

The **Keller-Segel model** was co-proposed by Evelyn F. Keller and Lee A. Segel in the early 1970s. It was originally intended to describe the aggregation process of slime molds (*Dictyostelium discoideum*) guided by cyclic adenosine monophosphate (cAMP) concentration gradients under starvation conditions via a system of coupled partial differential equations. This pioneering work laid the foundation for mathematical biology research on cell **chemotaxis**. The core of the model lies in capturing the key biophysical phenomenon that cell populations not only diffuse randomly but also migrate directionally along the concentration gradient of chemical signaling agents. Its specific applications have expanded vastly from the initial slime mold research to numerous fields, including explaining bacterial colony pattern formation, the guided migration of endothelial cells in **angiogenesis**, tumor cell invasion and metastasis processes, the recruitment of leukocytes to inflammation sites in the immune system, and even **morphogenesis** in the embryonic development of multicellular organisms, becoming a paradigmatic mathematical model linking cell self-organization behavior with the emergence of macroscopic patterns.

One of the most famous models describing this coupled system is the **Keller-Segel (KS) Model**. It consists of two coupled partial differential equations:

1. **The evolution equation for cell density $\rho(x,t)$:**

   This is essentially the Fokker-Planck equation we derived earlier, but now the drift term depends explicitly on the dynamically changing chemical field $c(x,t)$. The drift term $v_{eff}\rho$ is usually written in the form of a **chemotactic flux**, i.e., $-\chi(\rho,c)\rho\nabla c$. Furthermore, a reaction term describing cell growth or death can be added.

   $$\partial_t \rho = \nabla \cdot [D\nabla\rho - \chi(\rho,c)\rho\nabla c] + f_{growth}(\rho) \tag{8}$$

   (Here we use ρ to represent cell density and use the gradient operator ∇ to facilitate generalization to higher-dimensional spaces.)

   Physical Interpretation of the Equation: The change in the number of cells within a region equals the random diffusion entering minus diffusing out, plus the chemotactic migration entering minus migrating out, and finally adding the quantity of local net growth.

2. **The evolution equation for chemical concentration $c(x,t)$:**

   This is a standard **reaction-diffusion equation**, describing the diffusion of the chemical substance, the process of production by bacteria, and its own degradation process.

   $$\partial_t c = D_c\nabla^2 c + f_{prod}(\rho) - f_{degrad}(c) \tag{9}$$

   Physical Interpretation of the Equation: The change in the concentration of the signaling substance within a region equals the diffusion entering minus diffusing out, plus the production by cells, minus the natural degradation.

The lecture cites and provides a link to a visualized KS model, which has the specific form:

$$\frac{\partial u}{\partial t} = \nabla^2 u - \nabla\cdot(\chi(u)\nabla v) + u(1-u)$$
$$\frac{\partial v}{\partial t} = D\nabla^2 v + u - av$$

Here, u represents cell density, and v represents the concentration of the chemical substance. Let us analyze this model term by term:

- $\nabla^2 u$: **Random motion of cells**, corresponding to the effective diffusion D_{eff} we derived earlier (here set to 1).
- $-\nabla\cdot(\chi(u)\nabla v)$: **Chemotactic flux**. Cells move at a velocity proportional to ∇v (i.e., moving towards areas of high v concentration). The chemotactic sensitivity $\chi(u) = \frac{cu}{1+u^2}$ is density-dependent, which can simulate **saturation effects** at high densities.

- $u(1-u)$: **Logistic growth of cells**. When the density u is small, cells grow at a rate proportional to u; when u approaches the carrying capacity of 1, growth stops.
- $D\nabla^2 v$: **Diffusion of the chemical substance**.
- $u - av$: **Production and degradation of the chemical substance**. The production rate is proportional to the cell density u, while the degradation rate is a simple linear decay $-av$.

What are the core dynamics of this coupled system? Consider a minute fluctuation within a uniform cell distribution, that is, a slightly higher cell density in a certain local region. According to the second equation, these cells will produce more chemical substances, thereby creating a weak concentration peak at this location. This concentration peak generates a gradient ∇v pointing towards itself. According to the chemotactic term in the first equation, this gradient will attract more surrounding cells to aggregate towards this peak. The newly aggregated cells will produce even more chemicals, further reinforcing the concentration peak and thereby attracting even more cells.

This is a powerful **Positive Feedback Loop**. If the effect of chemotactic attraction (controlled by coefficient χ) is strong enough to overwhelm the effect of the cells' own random diffusion (controlled by coefficient D), then this positive feedback will become unstable. The initial minute density fluctuation will be amplified exponentially, leading to massive aggregation of cells at certain points and forming sharp peaks. This phenomenon is known as **Chemotactic Collapse**. It perfectly demonstrates how simple local interaction rules can lead to the **emergence** of complex spatial structures and patterns at the macroscopic level, which is a hallmark feature of complex systems. Mathematical **Linear Instability Analysis** can provide the precise conditions for pattern formation.

5 Python Simulation II: Finite Difference Solution of a One-Dimensional Keller-Segel Model

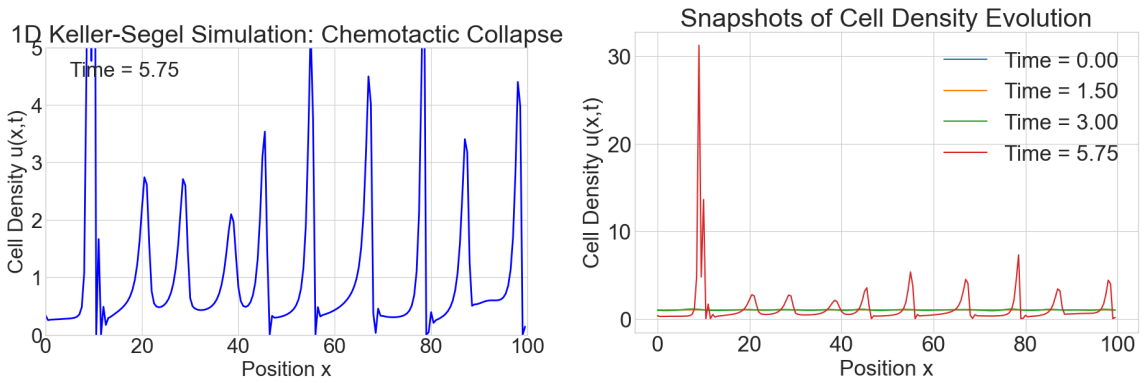

Figure 4:

The simulation results vividly reproduce the chemotactic collapse process. Starting from an almost uniform initial state with tiny random perturbations, we can see the density in certain regions begin to slowly increase. Over time, these tiny "hills" become higher and narrower, eventually forming very sharp, stable density peaks. This clearly demonstrates that intercellular (chemically mediated) interactions can spontaneously disrupt the homogeneity of a system, forming a highly ordered macroscopic structure.

6 Schnitzer model: A microscopic description of running-rolling dynamics

This discussion will revolve around this issue, exploring a novel pattern formation mechanism. We will see that the intrinsic properties of particle motion—particularly how its velocity is affected by the

surrounding environment (e.g., particle density)—are sufficient to drive phase separation in a system. This phenomenon is known as Motility-Induced Phase Separation (MIPS). This marks a shift from studying specific biological behaviors driven by external signals to exploring self-organizing phenomena governed by more general physical principles.

The Schnitzer model was developed in the late 1990s and early 21st century by Martin J. Schnitzer, George Oster, Howard C. Berg, and others. Its historical context was to establish a rigorous statistical mechanics framework for the chemotactic behavior of bacteria such as Escherichia coli, based on first principles. The core essence of this model is to couple microscopic "running-tumbling" random motion with intracellular chemical signal transduction pathways. Using mathematical tools such as the master equation and the Fokker-Planck equation, it derives the macroscopic diffusion and drift behaviors of cell populations in a chemical concentration field from the random motion patterns of individual bacteria. Its applications extend far beyond explaining chemotaxis; it has become a standard paradigm for studying microbial movement, widely used to quantify bacterial search strategies in complex environments, optimize models for pathogen invasion and immune cell tracking, and inspire algorithm design for micro/nano robot swarms.

We consider a simplified one-dimensional system. In this system, there are two types of particles:

- Particles with density $P_+(x,t)$, which move to the right ($+x$ direction) with velocity $v(x)$.
- Particles with density $P_-(x,t)$, which move to the left ($-x$ direction) with velocity $v(x)$.

Here, both the velocity $v(x)$ and the tumbling rate $\alpha(x)$ may depend on the spatial position x. "Tumble" refers to particles randomly changing their direction of motion at a certain rate $\alpha(x)$. In the one-dimensional case, this means that particles moving to the right will switch to moving to the left, and vice versa.

Based on the definitions above, we can write down the **Master Equations** describing the evolution of the densities P_+ and P_-. This is a system of coupled partial differential equations.

For the density of right-moving particles P_+, the evolution equation is:

$$\partial_t P_+ = -\partial_x[v(x)P_+] - \frac{1}{2}\alpha(x)P_+ + \frac{1}{2}\alpha(x)P_- \tag{10}$$

The physical meaning of this equation can be decomposed into three parts:

1. **Advection Term** (Advection): $-\partial_x[v(x)P_+]$. This is the flux term of a continuity equation, describing the density change caused by P_+ particles moving with velocity $v(x)$.
2. **Loss Term** (Loss): $-\frac{1}{2}\alpha(x)P_+$. Right-moving particles tumble at a rate $\alpha(x)$. In a one-dimensional model, we assume the direction after tumbling is completely random, so there is a 50% probability (here simplified as deterministic) that they switch to moving left. Therefore, this term describes the rate of decrease in the P_+ population due to tumbling.
3. **Gain Term** (Gain): $+\frac{1}{2}\alpha(x)P_-$. Similarly, left-moving particles P_- also tumble, and have a certain probability of switching to move right, thereby replenishing the P_+ population.

For the density of left-moving particles P_-, the evolution equation takes a symmetric form:

$$\partial_t P_- = +\partial_x[v(x)P_-] - \frac{1}{2}\alpha(x)P_- + \frac{1}{2}\alpha(x)P_+ \tag{11}$$

Note: The sign before the advection term $\partial_x[v(x)P_-]$ is positive here, because it describes particles moving to the left ($-x$ direction). The physical interpretation of the loss and gain terms is similar to that of the P_+ equation.

P_+ and P_- are descriptions of the microscopic state. In experiments or macroscopic theory, we are more interested in some macroscopic observables, such as total particle density and particle flux. They can be defined by P_+ and P_- as follows:

- **Total Density**: $g(x,t) = P_+(x,t) + P_-(x,t)$
- **Particle Flux** (Particle Flux/Current): $J(x,t) = v(x)[P_+(x,t) - P_-(x,t)]$

Our ultimate goal is to derive a closed evolution equation containing only the macroscopic quantity $g(x,t)$, without needing to concern ourselves with the microscopic P_+ and P_-. This process is called "**coarse-graining**".

7 Coarsening: Eliminating the transition from microscopic rules to macroscopic laws through adiabatic processes

To obtain the equation describing the macroscopic density (g) from the Schnitzer model, which describes the microscopic states (P_+, P_-), we need a systematic simplification method. Here, we will use a very powerful technique in physics — **Adiabatic Elimination**.

The core idea of adiabatic elimination is that when a dynamical system contains variables with vastly different evolution rates, we can simplify the system. Specifically, variables in the system can be divided into "fast variables" and "slow variables". Fast variables have a very short evolution time scale (fast relaxation rate), while slow variables have a very long evolution time scale (slow relaxation rate). Adiabatic elimination assumes that fast variables can "instantaneously" adapt to any changes in slow variables, and always remain in a **quasi-steady state** determined by the current values of the slow variables. By solving for the quasi-steady state of the fast variables and substituting it into the dynamic equations of the slow variables, we can "eliminate" the fast variables, thereby obtaining a simpler, effective dynamic equation describing only the evolution of the slow variables.

In our Schnitzer model:

- **Slow Variable**: Total density $g = P_+ + P_-$. Its change depends on the transport of particles in space, which is a relatively slow process.
- **Fast Variable**: The density difference $P_+ - P_-$ associated with the particle flux J. Particles switch rapidly between left-moving and right-moving states via tumbling (controlled by rate α). We assume the tumbling process is much faster than the process of particle movement on the macroscopic scale, i.e., α is very large.

1. Add and Subtract the Master Equations for P_+ and P_-.

Add:

$$\partial_t(P_+ + P_-) = -\partial_x[v(P_+ - P_-)] \implies \partial_t g = -\partial_x J$$

This result is an exact particle number conservation law, indicating that the rate of change of the total density is equal to the negative divergence of the particle flux.

Subtract:

$$\partial_t(P_+ - P_-) = -\partial_x[v(P_+ + P_-)] - \alpha(P_+ - P_-)$$

2. Apply Adiabatic Approximation.

We assume the fast variable $(P_+ - P_-)$ relaxes very quickly, such that its time derivative can be approximated as zero, i.e., $\partial_t(P_+ - P_-) \approx 0$.

3. Solve for the Quasi-Steady State of the fast variable.

Under the condition $\partial_t(P_+ - P_-) \approx 0$, the second equation becomes:

$$0 \approx -\partial_x[v(P_+ + P_-)] - \alpha(P_+ - P_-) = -\partial_x[vg] - \alpha(P_+ - P_-)$$

Solving for $(P_+ - P_-)$:

$$(P_+ - P_-) \approx -\frac{1}{\alpha(x)}\partial_x[v(x)g(x,t)]$$

4. Substitute the Quasi-Steady Expression back into the macroscopic definitions.

First, substitute into the definition of particle flux J:

$$J = v(x)(P_+ - P_-) \approx -\frac{v(x)}{\alpha(x)}\partial_x[v(x)g(x,t)]$$

Then, substitute this expression for the effective particle flux into the particle number conservation law $\partial_t g = -\partial_x J$:

$$\partial_t g(x,t) = \partial_x\left(\frac{v(x)}{\alpha(x)}\partial_x[v(x)g(x,t)]\right)$$

In the Master Equation, α implicitly contained a factor of $\frac{1}{2}$ (loss term was $\frac{1}{2}\alpha P_+$). For rigor, the final equation requires the explicit addition of $\frac{1}{2}$:

$$\partial_t g(x,t) = \partial_x \left(\frac{v(x)}{2\alpha(x)} \partial_x [v(x) g(x,t)] \right)$$

Through this series of steps, we have successfully eliminated the microscopic variables P_+ and P_-, obtaining a closed partial differential equation describing only the evolution of the macroscopic total density g. This equation is formally a **Fokker-Planck Equation**.

To gain a deeper understanding of the physical meaning of this macroscopic equation, we can expand the expression for the effective particle flux J:

$$J = -\frac{v(x)}{\alpha(x)} \left(g(x,t) \frac{\partial v(x)}{\partial x} + v(x) \frac{\partial g(x,t)}{\partial x} \right)$$

Rearranging gives:

$$J = -\underbrace{\frac{v^2(x)}{\alpha(x)}}_{D_{\text{eff}}(x)} \frac{\partial g}{\partial x} - \underbrace{\frac{g(x,t)v(x)}{\alpha(x)} \frac{\partial v(x)}{\partial x}}_{\text{Drift Term}}$$

This expression reveals two components of the macroscopic particle motion:

- **Effective Diffusion Term**: The form of the first term is identical to Fick's Law of Diffusion, where $D_{\text{eff}}(x) = \frac{v^2(x)}{\alpha(x)}$ plays the role of the **effective diffusion coefficient**. It indicates that even if the microscopic motion is deterministic running, macroscopically, due to frequent tumbling, it will exhibit diffusion-like behavior.
- **Effective Drift Term**: The second term is a drift term. Its magnitude is proportional to the particle density g and the velocity gradient $\partial_x v(x)$. This term implies that particles will experience an equivalent "force", driving them towards directions with lower velocity $v(x)$.

The macroscopic equations we just derived contain a core principle of active matter physics. To reveal this, let's analyze the steady-state solution of the system. We consider a closed system, which means that in the steady state, the net particle flux J_{ss} must be zero everywhere. To simplify the analysis, we assume the tumbling rate $\alpha(x)$ is a constant α_0.

The steady-state condition $J_{ss} = 0$ implies:

$$-\alpha_0 v(x) \partial_x [v(x) g_{ss}(x)] = 0$$

This requires the term inside the square brackets to be a constant:

$$v(x) g_{ss}(x) = \text{constant}$$

Therefore, we obtain a very concise and profound conclusion:

$$g_{ss}(x) \propto \frac{1}{v(x)}$$

The steady-state particle density $g_{ss}(x)$ is inversely proportional to the local particle velocity $v(x)$.

This relationship $g \propto 1/v$ is one of the cornerstones that distinguishes active matter physics from equilibrium statistical physics.

In **equilibrium systems**, the steady-state distribution of particles is determined by the Boltzmann distribution, $g \propto \exp(-U/k_B T)$, where U is the potential energy. The distribution of particles depends only on the energy landscape and is independent of their kinematic parameters (such as velocity).

However, in **active systems**, the system is in a non-equilibrium state, and its steady-state distribution is determined by dynamical processes. The physical picture of $g \propto 1/v$ is very intuitive: it can be thought of as a "traffic jam" effect. When particles move into a region where their speed slows down, they take longer to leave that region. Conversely, when particles are in a high-speed region, they pass through quickly. Over time, this dynamical difference leads to a net accumulation of particles in

low-speed regions. This simple dynamical "traffic jam" argument is precisely the profound physical principle behind $g \propto 1/v$.

We assume that the particle's motion velocity is no longer an *a priori* function of spatial coordinates, but instead depends on the **local particle density**, i.e., $v = v(g)$. This is a very reasonable assumption. In many real systems, such as dense cell clusters or colloidal suspensions, when particle density rises, they hinder each other due to steric hindrance or "crowding" effects, leading to a decrease in motion speed (10). Furthermore, biochemical signaling mechanisms (such as quorum sensing) may exist, causing particles to actively slow down at high densities (10). In this lecture, we primarily consider the case where velocity decreases as density increases, i.e.,

$$v'(g) = \frac{dv}{dg} < 0$$

After introducing $v(g)$, we re-examine the expression for the effective particle flux J. For simplicity, we adopt the setting from the lecture and let the tumbling rate $\alpha = 1$.

$$J = -v(g)\partial_x[gv(g)]$$

Expand the derivative term using the chain rule:

$$J = -v(g)\left[v(g)\frac{\partial g}{\partial x} + g\frac{dv(g)}{dg}\frac{\partial g}{\partial x}\right]$$

Rearranging gives:

$$J = -\left[v(g)^2 + gv(g)v'(g)\right]\frac{\partial g}{\partial x}$$

The form of this expression is still Fick's Law $J = -D_{\text{eff}}(g)\frac{\partial g}{\partial x}$, but now the effective diffusion coefficient $D_{\text{eff}}(g)$ itself also depends on the density:

$$D_{\text{eff}}(g) = v(g)^2 + gv(g)v'(g)$$

The behavior of this density-dependent effective diffusion coefficient $D_{\text{eff}}(g)$ determines the macroscopic dynamics of the system.

- **Normal Diffusion**: If $D_{\text{eff}}(g) > 0$, the direction of the particle flux is opposite to the density gradient (flowing from high density to low density). This smoothes out any inhomogeneities, tending the system towards a uniform steady state.
- **Anti-Diffusion**: If $D_{\text{eff}}(g) < 0$, the situation reverses dramatically! The sign of the particle flux becomes positive, meaning particles will flow **up the density gradient**, i.e., flowing from low-density regions to high-density regions (1). This behavior amplifies any tiny density fluctuations, leading to spontaneous particle aggregation and ultimately forming clusters and patterns.

Therefore, the condition for the system to become unstable is $D_{\text{eff}}(g) < 0$. Since $v(g)$ is always positive, this condition can be simplified to:

$$v(g) + gv'(g) < 0$$

This condition is equivalent to the form given in the lecture notes:

$$\frac{d}{dg}[gv(g)] < 0$$

Behind this mathematical condition lies a **Positive Feedback Loop**, which is the core mechanism of MIPS.

1. **Initial Fluctuation**: Assume the system is initially in a uniform density state. Due to thermal noise or other random factors, a tiny positive density fluctuation appears in a local region.
2. **Deceleration**: Since we assume $v'(g) < 0$, the movement speed of particles within this slightly higher density region will decrease.

3. **Aggregation**: Based on the principle we established in Section 4 ($g \propto 1/v$), active particles tend to accumulate in places where they move slowly. Therefore, more particles are attracted to this already slightly denser region.

4. **Amplification**: The further aggregation of particles makes the density in this region even higher, leading to a further decrease in particle speed, which in turn attracts even more particles...

This is a runaway process. Initially insignificant density fluctuations are continuously amplified, eventually leading to the collapse of the uniform state. The system spontaneously separates into a high-density, low-mobility "liquid phase" and a low-density, high-mobility "gas phase". This is **Motility-Induced Phase Separation**. It is worth emphasizing that this is a purely non-equilibrium phenomenon driven by the motility characteristics of the particles, unlike equilibrium phase transitions driven by attractive forces between particles.

To delve into the rich details of motion-induced phase separation (MIPS) in the spatial self-organization process, we will directly build and solve a two-dimensional model. While a one-dimensional model can reveal the nature of instability, a two-dimensional simulation can more intuitively demonstrate the formation, competition, and coarsening of patterns, which are core characteristics of phase separation phenomena.

In two-dimensional space, the most general and robust equation describing phase separation is the **Cahn-Hilliard Equation**. It elegantly captures the competition between the "anti-diffusion" effect driving phase separation and the "surface tension" effect suppressing infinitely sharp interfaces.

This equation describes the evolution of particle density $g(\vec{x}, t)$ over time, and its form is as follows:

$$\frac{\partial g}{\partial t} = M\nabla^2\mu$$

This is a continuity equation, where M is a constant called *mobility*, and μ is the *effective chemical potential*. The equation indicates that particles flow from regions of high chemical potential to regions of low chemical potential. The chemical potential μ itself consists of two contributions, given by the functional derivative of an effective free energy functional $F[g]$ with respect to density:

$$\mu = \frac{\delta F}{\delta g} = \underbrace{f'(g)}_{\text{Bulk Energy Term}} - \underbrace{\kappa\nabla^2 g}_{\text{Interfacial Energy Term}}$$

- **Bulk Energy Term** $f'(g)$: This term originates from the effective interactions between particles. In the context of MIPS, it is directly related to the effective diffusion coefficient $D_{\text{eff}}(g)$ derived earlier (specifically, $f''(g) \propto D_{\text{eff}}(g)$). Its function is to drive the system to separate into two phases with different densities when the density falls within the unstable region. For the $v(g) = v_0(1 - g/g^*)$ model we use, the specific form of this term is:

$$f'(g) = v_0^2\left(g - \frac{3}{2g^*}g^2 + \frac{2}{3(g^*)^2}g^3\right)$$

- **Interfacial Energy Term** $-\kappa\nabla^2 g$: This term is a key modification to the model. κ is a positive constant representing the strength of surface tension. $\nabla^2 g$ is the Laplacian of the density, which measures the "curvature" of the density field. The function of this term is to penalize regions with high curvature or sharp density gradients, thereby preventing the non-physical sharp peaks observed in our primary model and assigning a characteristic width and energy cost to the phase separation interface.

Combining these two formulas gives us the complete fourth-order nonlinear partial differential equation to be solved.

Many types of bacteria, such as *E. coli* or *Myxococcus xanthus*, form high-density "swarms" or biofilms on nutrient-rich culture surfaces. In these dense groups, bacterial movement is hindered by frequent physical collisions. This fits the core rule of **"crowding-induced deceleration"**, leading to spontaneous separation into high-density, nearly static bacterial clusters (droplets) and low-density, fast-moving "gas" regions.

A macroscopic intuitive analogy is the crowded crowd (Shopping Window Effect), which is an excellent analogy mentioned by Prof. Frey in his lecture. Imagine a busy commercial street; when an

interesting window display attracts some people to stop and watch, their deceleration forces people behind them to slow down or detour. This leads to an instantaneous increase in the density of people in this area, forming a spontaneous "traffic jam". There is no "attraction" here, only the motion rule (deceleration) leading to aggregation.

We will use the **Finite Difference Method** on an $N_x \times N_y$ two-dimensional orthogonal grid to numerically solve the Cahn-Hilliard equation. The index for spatial points is (i, j), and the index for time steps is n.

Spatial Discretization: 2D Laplacian Operator

The core of the equation is the **Laplacian Operator** $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$. We use the second-order central difference (also known as the **five-point stencil**) to approximate it. For any function U at grid point (i, j), its Laplacian can be discretized as:

$$(\nabla^2 U)_{i,j} \approx \frac{U_{i+1,j} + U_{i-1,j} + U_{i,j+1} + U_{i,j-1} - 4U_{i,j}}{(\Delta x)^2}$$

Here we assume the grid lengths in the x and y directions are the same, i.e., $\Delta x = \Delta y$. $U_{i+1,j}$ represents the value at the next grid point in the x-direction, $U_{i,j+1}$ represents the value at the next grid point in the y-direction, and so on.

Temporal Discretization: Forward Euler Method

For the time derivative $\frac{\partial g}{\partial t}$, we use the simplest **Forward Euler Method**:

$$\left.\frac{\partial g}{\partial t}\right|_{t=t_n} \approx \frac{g_{i,j}^{n+1} - g_{i,j}^{n}}{\Delta t}$$

Where $g_{i,j}^n$ is the density value at point (i, j) at time n, and $g_{i,j}^{n+1}$ is the value at the next time step.

Complete Update Algorithm

Combining the discretization methods above, we can calculate the density field g^{n+1} at time $n+1$ from the density field g^n at time n. The complete algorithm is:

1. **Step 1: Calculate the Laplacian of g^n** for every point (i, j) on the grid, using the five-point stencil formula to calculate $(\nabla^2 g)_{i,j}^n$.
2. **Step 2: Calculate the Chemical Potential μ^n** using the result from the previous step. Calculate the chemical potential for each point:
$$\mu_{i,j}^n = f'(g_{i,j}^n) - \kappa(\nabla^2 g)_{i,j}^n$$
3. **Step 3: Calculate the Laplacian of μ^n**. Again, use the five-point stencil formula. Apply it to the chemical potential field μ^n just obtained to get $(\nabla^2 \mu)_{i,j}^n$.
4. **Step 4: Update the Density Field g^{n+1}** using the Forward Euler method:
$$g_{i,j}^{n+1} = g_{i,j}^n + M \cdot \Delta t \cdot (\nabla^2 \mu)_{i,j}^n$$

By repeating these four steps for the entire grid, we can complete the evolution for one time step. By iterating continuously, we can simulate the complete phase separation process.

The lecture points out that the effective particle flux J_{eff} can be rewritten in a form commonly found in equilibrium transport theory:

$$J_{\text{eff}}(x, t) = -M(g)\partial_x \mu_{\text{eff}}(g)$$

By comparing with the expression for J we derived earlier, we can identify the following two terms:

- **Mobility**: $M(g) = gv(g)^2$. It describes the ease with which particles move when subjected to an equivalent "force" (generated by the chemical potential gradient).

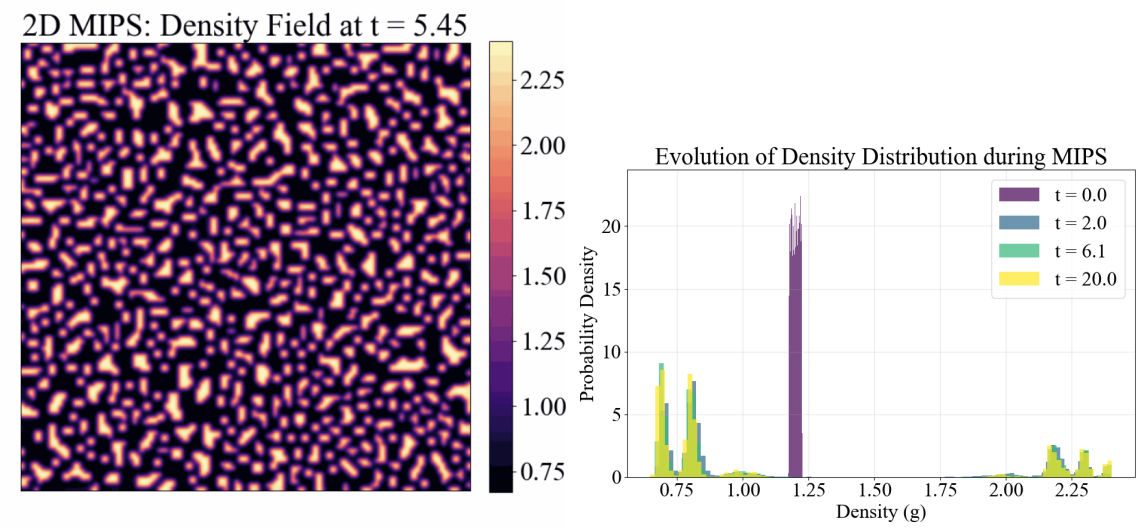

Figure 5: The animation clearly demonstrates the initiation process of phase separation: the system starts from an almost uniform state, and the inherent instability rapidly amplifies tiny random noises, forming an interwoven, maze-like "helix" structure. Soon, these slender structures break and contract due to surface tension, forming well-defined "droplet"-shaped high-density regions that float in a low-density "gas" background. t = 0.0 (purple): The distribution is a single narrow peak at the average density, representing the initial homogeneous state of the system. t = 2.0 (blue): The distribution rapidly broadens and collapses to both sides, indicating that the homogeneous state is disintegrating, and regions above and below the average density have appeared simultaneously. t = 6.1 (green): A bimodal structure appears! This signifies that phase separation has occurred, and two distinct phases have clearly formed in the system: a low-density phase and a high-density phase. t = 20.0 (yellow): The bimodal structure is fully mature. The two sharp peaks represent the stable "gas" phase (density approximately 0.7) and the "liquid" phase (density approximately 2.25), respectively.

- **Effective Chemical Potential**: $\mu_{\text{eff}}(g) = \log g + \log v(g)$. In equilibrium thermodynamics, differences in chemical potential drive particles to flow from regions of high chemical potential to regions of low chemical potential. Here, μ_{eff} plays a similar role.

Chemical potential is usually obtained by taking the derivative of a free energy function with respect to the number of particles. Similarly, the effective chemical potential $\mu_{\text{eff}}(g)$ here can be viewed as the functional derivative of an **Effective Free Energy Functional** $F_{\text{eff}}[g]$ with respect to density g. This functional $F_{\text{eff}}[g]$ is also called a **Lyapunov Functional**.

Its definition is as follows:

$$F_{\text{eff}}[g] = \int dx \left[g(x) \log g(x) - g(x) + \int_0^g ds \log v(s) \right]$$

We can verify that taking the functional derivative of this functional with respect to g indeed yields the effective chemical potential we defined earlier:

$$\mu_{\text{eff}}(g) = \frac{\delta F_{\text{eff}}}{\delta g} = \frac{\partial}{\partial g} \left(g \log g - g + \int_0^g ds \log v(s) \right) = (\log g + 1) - 1 + \log v(g) = \log g + \log v(g)$$

This verifies the self-consistency of the entire mathematical framework. With the effective free energy functional, the dynamic equation of the entire system can be elegantly written in the form of a **Gradient Flow**:

$$\partial_t g = \partial_x \left[M(g) \partial_x \frac{\delta F_{\text{eff}}}{\delta g} \right]$$

This form has an extremely important corollary: during the evolution of the system, its effective free energy F_{eff} always decreases continuously. We can prove this:

$$\frac{dF_{\text{eff}}}{dt} = \int dx \frac{\delta F_{\text{eff}}}{\delta g} \frac{\partial g}{\partial t} = \int dx \, \mu_{\text{eff}} \partial_t g$$

Substitute the expression for $\partial_t g$:

$$\frac{dF_{\text{eff}}}{dt} = \int dx \, \mu_{\text{eff}} \partial_x [M(g) \partial_x \mu_{\text{eff}}]$$

Using integration by parts (assuming periodic boundary conditions):

$$\frac{dF_{\text{eff}}}{dt} = -\int dx (\partial_x \mu_{\text{eff}}) [M(g) \partial_x \mu_{\text{eff}}] = -\int dx M(g) (\partial_x \mu_{\text{eff}})^2$$

Since the mobility $M(g) = gv(g)^2$ is always non-negative, and $(\partial_x \mu_{\text{eff}})^2$ is also always non-negative, the entire integral term is non-negative. Therefore, we have proved:

$$\frac{dF_{\text{eff}}}{dt} \leq 0$$

This result tells us that although MIPS is a complex non-equilibrium dynamic process, its evolution direction can be viewed as a process of sliding down an effective "**Energy Landscape**" defined by F_{eff}. The system will constantly adjust its configuration to find and eventually reach the minimum value of this effective free energy. The state corresponding to this minimum value is the stable, phase-separated steady state we observe. This also explains the "coarsening" phenomenon observed in simulations: small droplets merge into large droplets to reduce the total "interface" and thus lower the system's total effective free energy, which is very similar to the Ostwald ripening process in equilibrium systems.

8 Summary

This lecture starts from a **microscopic model** (Schnitzer model) describing the "run-and-tumble" motion of a single particle. Through **coarse-graining techniques** (adiabatic elimination), we derived the **macroscopic dynamic equation** (effective Fokker-Planck equation) describing the density of the particle population.

By introducing a physically reasonable **feedback mechanism** (crowding-induced deceleration), this macroscopic equation predicted a **dynamic instability** (anti-diffusion), and ultimately led to a spectacular **collective phenomenon** (Motility-Induced Phase Separation). Finally, we discovered that this entire complex non-equilibrium process can be described by an elegant **effective thermodynamic framework** (Lyapunov functional), where the system's evolution is like finding the lowest point on an energy landscape.

Motility-Induced Phase Separation is one of the most fundamental and universal self-organization mechanisms in active matter physics. It exists widely in various systems ranging from bacterial colonies and synthetic active colloids to robot swarms. The theoretical tools introduced in this lecture provide a solid foundation for understanding these fascinating self-organization phenomena.

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