Statistical Mechanics

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Lesson 1- What is Statistical Mechanics, a.k.a. Statistical Physics?

Complexity in Natural Systems

Many systems in nature, like a block of ice, a flock of birds, earthquake faults, an epidemic, or the internet structure, are **too complex** to analyze directly.

Analyzing every atom or component in these systems is **infeasible** due to their sheer number and interconnectedness.

Yet, these systems often display simple and predictable behavior despite their underlying complexity. **Statistical mechanics explains the simple behavior of complex systems.**

Simplifying Complexity with Statistical Mechanics

Statistical Mechanics is a powerful tool, and a **way of thinking**, that explains the simple behavior of these complex systems.

It provides methods to **understand and predict the macroscopic behavior of systems from their microscopic properties**.

The concepts of **ensembles, entropy, phases, fluctuations, and correlations**, among others, are central to this field.

Cross-Disciplinary Impact of Statistical Mechanics

Statistical Mechanics methods and concepts have permeated into **numerous fields**, including physics, chemistry, dynamical systems, communications, bioinformatics, and complexity studies.

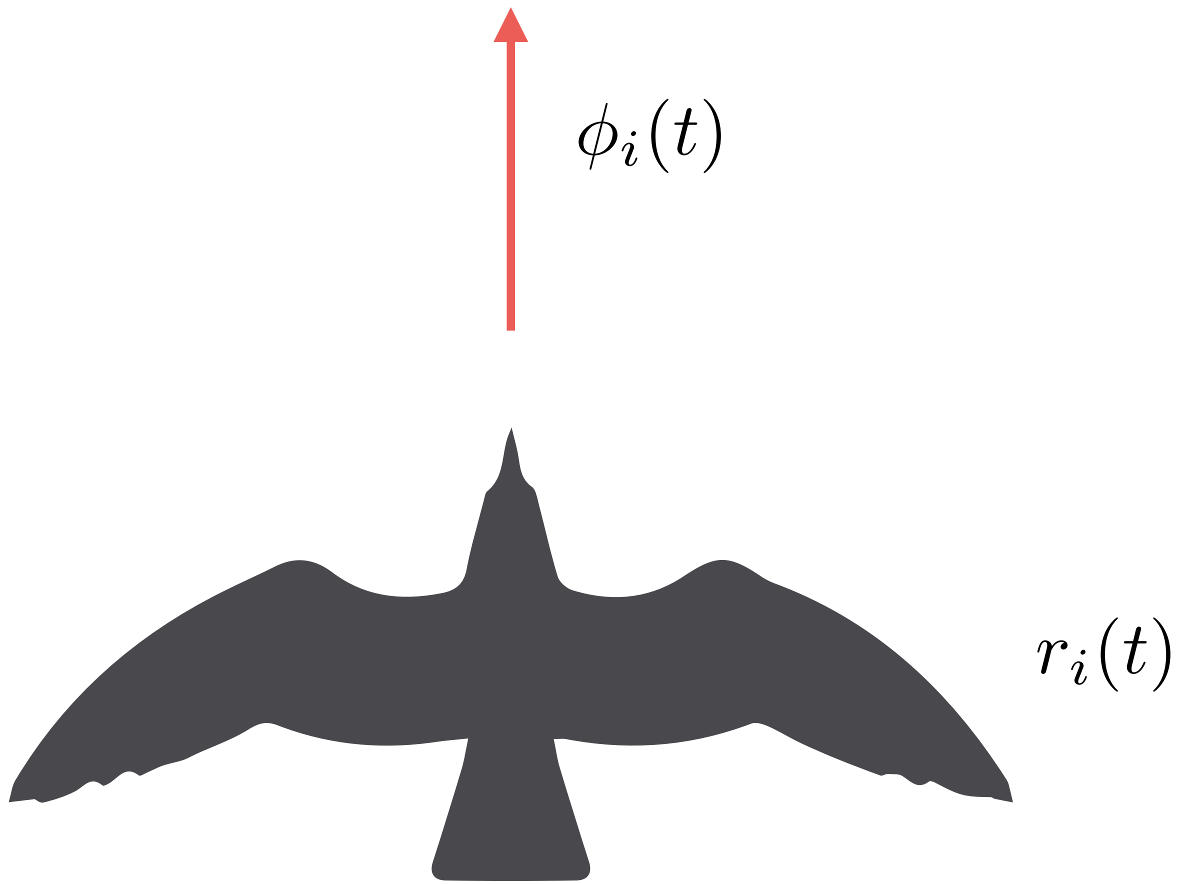
Quantum statistical mechanics, while more specific, forms the foundation of much of physics.

Through these methods, we can manage complexity and **gain insights** across a wide range of natural and engineered systems.

An illustrative example

1. Composed of **many equivalent parts**

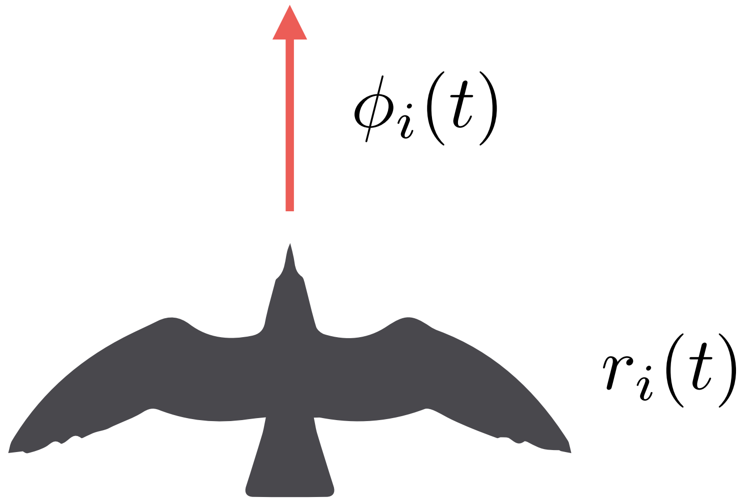
2. The parts **interact** following **simple rules**

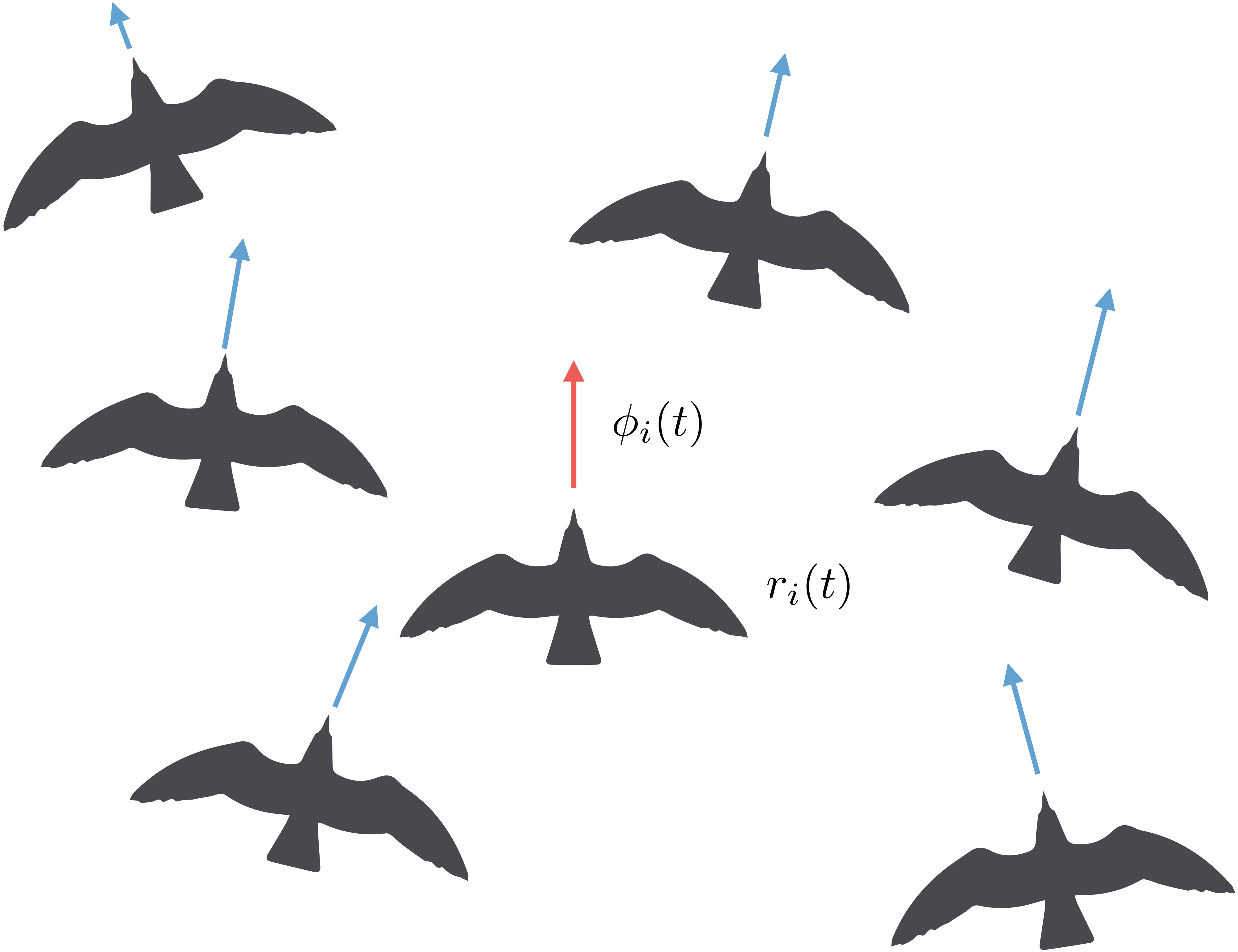


$$\phi_i(t + \Delta t) = \langle \phi_j \rangle_{|r_i - r_j| < r} + \eta_i(t)$$

$$r_i(t + \Delta t) = r_i(t) + v\Delta t(\cos \phi_i(t))$$

Vicsek, 1995


$\phi_i(t)$
$r_i(t)$


$\phi_i(t)$
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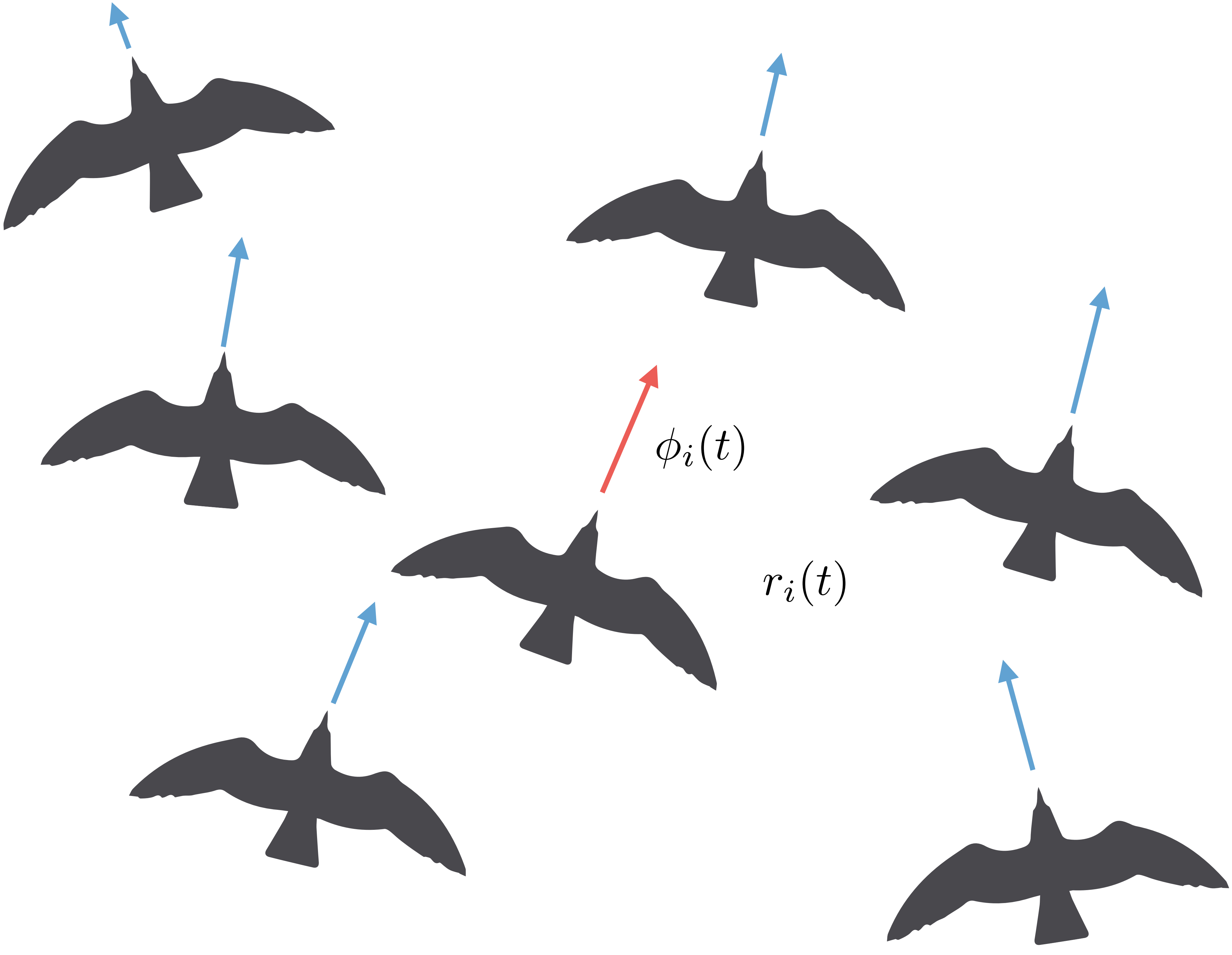
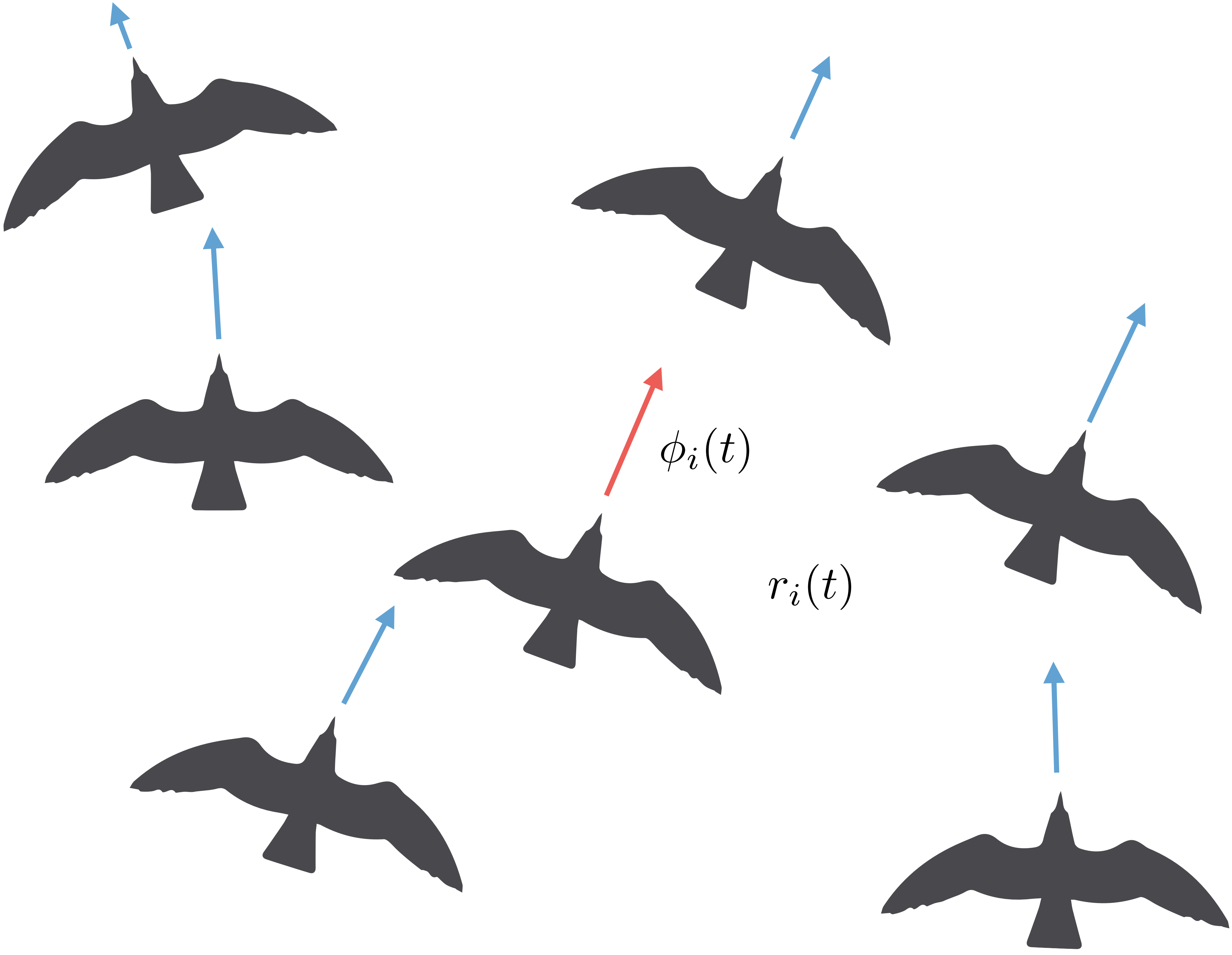
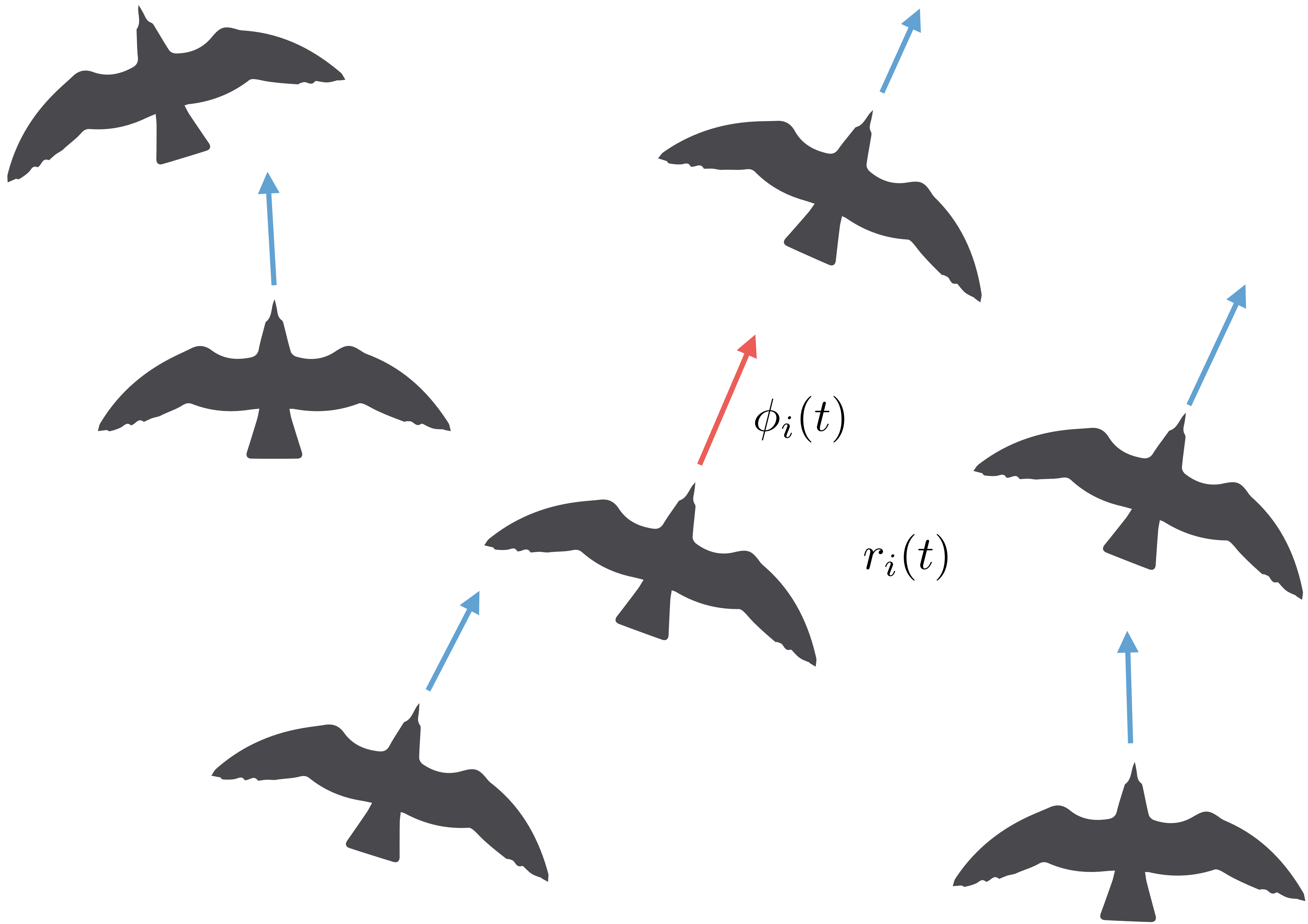
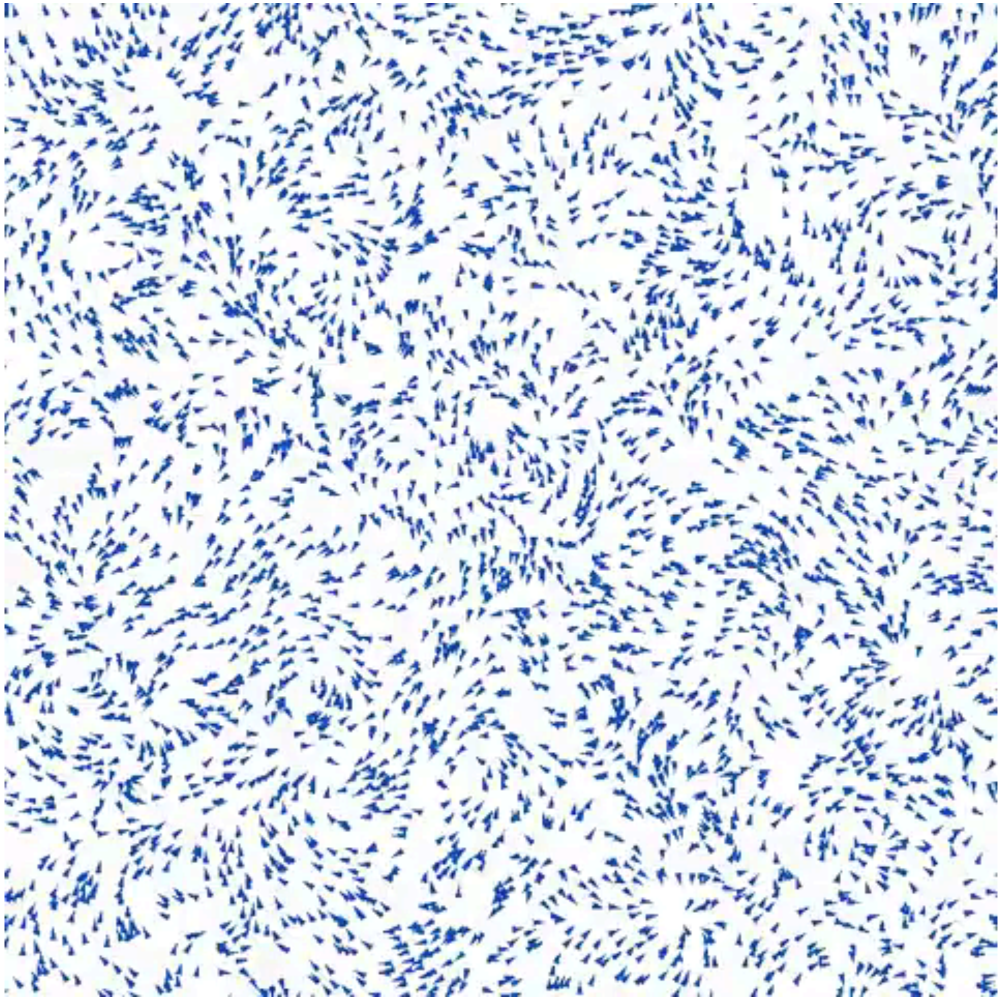


$\phi_i(t)$
$r_i(t)$


$\phi_i(t)$
$r_i(t)$

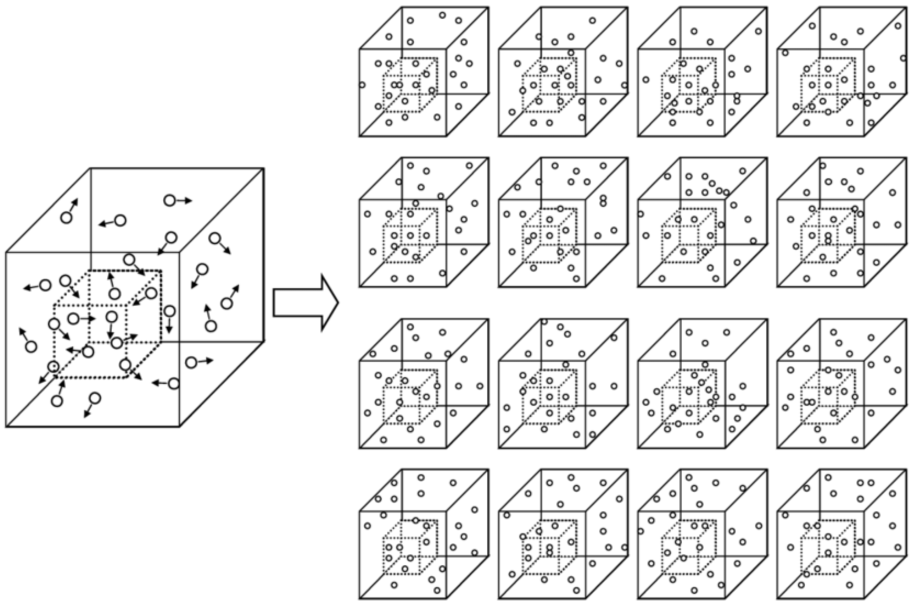

$\phi_i(t)$
$r_i(t)$

3. As a result of this interaction, **nonlinear emergent phenomena** are observed. Computational simulation of the **Vicsek model**



Key concepts in statistical physics

Ensembles. The **trick** of statistical mechanics is not to study a single system, but a large collection or ensemble of systems. Where understanding a single system is often impossible, one can often calculate the behavior of a large collection of similarly prepared systems.



Key concepts in statistical physics

Entropy. Entropy is the most influential concept arising from statistical mechanics. It was originally understood as a thermodynamic property of heat engines that inexorably increases with time. Entropy has become science's fundamental measure of **disorder and information**—quantifying everything from compressing pictures on the Internet to the heat death of the Universe.

Key concepts in statistical physics

Statistical Physics serves as a **bridge** between **microscopic and macroscopic** realms, offering a theoretical framework to understand macroscopic thermodynamic phenomena in terms of the statistical properties of a system's microscopic constituents.

Classical Statistical Physics: To describe a system of N particles, we often start with a Hamiltonian system (in 3D we will have 6N vars)

$$H(p_i, q_i) = T + V \qquad \dot{q}_i = \frac{\partial H}{\partial p_i}$$

$$\frac{\partial H}{\partial t} = 0 \quad \textbf{with} \quad \dot{p}_i = -\frac{\partial H}{\partial q_i} \quad \textbf{then} \quad \frac{\partial \dot{q}_i}{\partial q_i} + \frac{\partial \dot{p}_i}{\partial p_i} = 0$$

Key concepts in statistical physics

If we want to measure an observable $A(p_i, q_i, t)$:

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} + \sum_i \frac{\partial A}{\partial q_i}\dot{q}_i + \frac{\partial A}{\partial p_i}\dot{p}_i = \partial_t A + \{A, H\}_P$$

where we have used the Poisson bracket:

$$\{A, H\}_P = \sum_i \left(\frac{\partial A}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial H}{\partial q_i}\right)$$

The hamiltonian “makes things to move”.

Key concepts in statistical physics

Let us define the probability density $\rho(p, q, t)$. We call **phase space** to the space of all variables p_i, q_i , and **configuration space** to the space of all variables to the space of all variables q_i

We call **pure state** (or microscopic state) to the state of the system in which we know all $p_i(t), q_i(t)$

Then, we can define a **density** in the **phase space** as

$$\rho(\mathbf{p}, \mathbf{q}, t) = \prod_i \delta(q_i(t) - \mathbf{q}_i)\delta(p_i(t) - \mathbf{p}_i)$$

a function that quantifies the probability distribution of finding a system in a particular state defined by coordinates $(\mathbf{p}, \mathbf{q})$ in time t.

Key concepts in statistical physics

We call **mixed state** (or macroscopic state) to the mixture of pure states compatible with the same macroscopic observation

Using the **density** in the **phase space** we have a **weight** for every pure state, ad the macroscopic state can be defined as

$$\langle A(\mathbf{p}, \mathbf{q}, t) \rangle = \int_{\Delta\Gamma} A(\mathbf{p}, \mathbf{q}, t) \rho(\mathbf{p}, \mathbf{q}, t) d\Gamma$$

Liouville theorem

The **density** in the **phase space** evolves as

$$\frac{d\rho}{dt} = \frac{\partial\rho}{\partial t} + \{\rho, H\}_P$$

And here is the trick of statistical mechanics (geometric interpretation, the volume is constant $\frac{d\Delta\Gamma}{dt} = 0$)