Graphical Abstract

Fractionation by persistent random walk and two-component diffusion law

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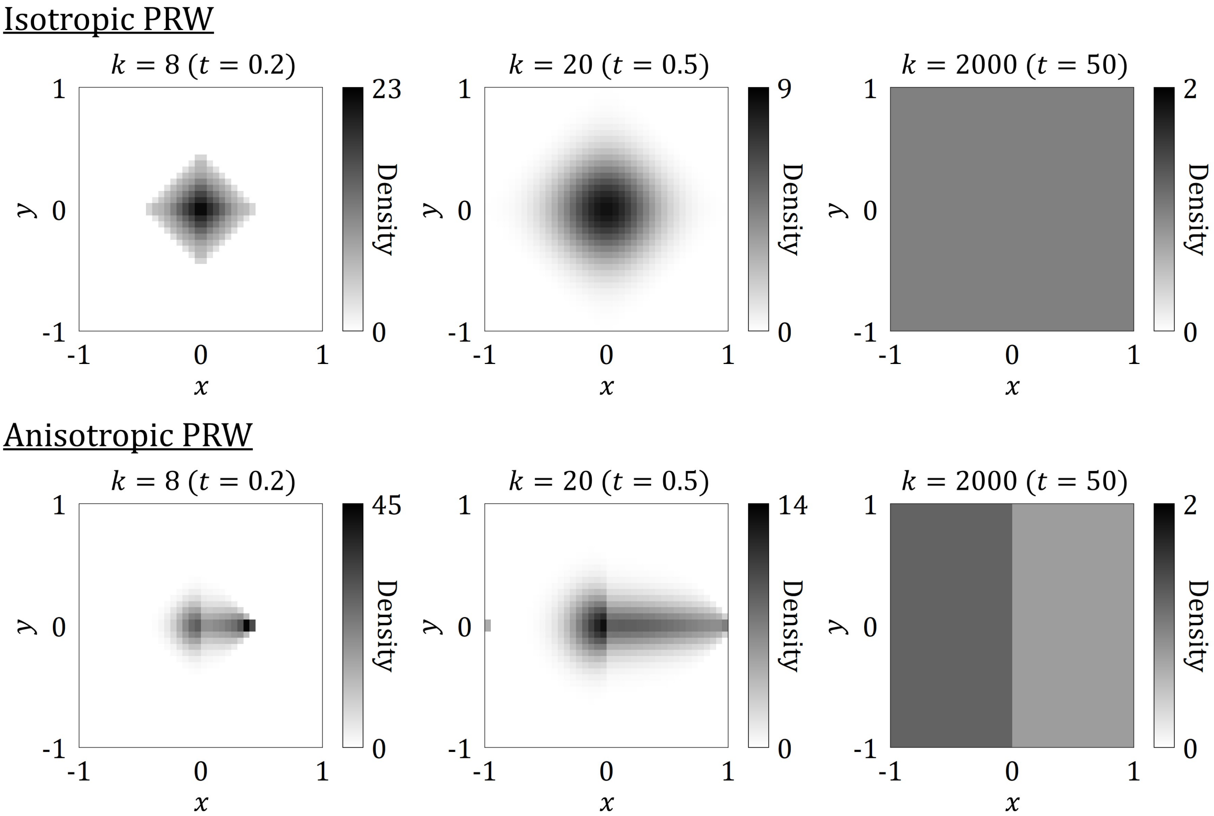

Highlights

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- A recursive relation for a spatially heterogeneous anisotropic PRW is introduced.
- The anisotropic diffusion equation for the PRW is derived.
- We show that isotropic persistence gives homogeneous steady states, but anisotropic persistence gives inhomogeneous ones in a heterogeneous environment.
- Numerical simulations for PRW, PDE, and Monte Carlo method are compared.

Fractionation by persistent random walk and two-component diffusion law

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Abstract

Random movement of microscopic particles in heterogeneous environments leads to fractionation phenomena, with the Soret effect being one of the most representative examples. This raises a fundamental question: what characteristics of random movement give rise to such fractionation phenomena? We investigate whether the persistence of a random-walk system has such a property and show that fractionation occurs only when the persistence is anisotropic. This is shown by investigating the convergence of a heterogeneous persistence random-walk system to a resulting anisotropic diffusion equation. Numerical simulations of the diffusion equation are compared with a Monte Carlo method and solutions to the recursive relations.

Keywords: persistent random walk, heterogeneous diffusion, fractionation, anisotropic diffusion

1. Introduction

Many random-walk systems are designed to understand how the behavior of individual microscopic particles affects the diffusivity. To achieve this, individual movement has been analyzed by breaking it down into various components, including particle speed, turning frequency, sojourn time, walk length, viscosity, anisotropy, persistence, permeability, etc. These components are the features of various random-walk systems, which are designed to study their specific impacts on diffusivity. The parameters for these components, which are mathematical quantities defining their characteristics in the model, are taken as constants—meaning they do not vary with position— under the assumption that the environment is spatially homogeneous. Then, the diffusion equation satisfied by the random walk system is

$$\frac{\partial u}{\partial t} = \nabla \cdot (D\nabla u), \tag{1}$$

where $\frac{\partial u}{\partial t}$ is the partial derivative of the mass density u with respect to the time variable t, ∇u is the gradient of u with respect to space variable $\mathbf{x} \in \mathbb{R}^n$, and $\nabla\cdot$ is for the divergence. The coefficient D is a constant diffusivity, which is a scalar in an isotropic diffusion or a matrix in an anisotropic diffusion. The steady state of this problem is constant with respect to $\mathbf{x}$, and the solution of (1) converges to the steady state as $t \to \infty$.

For a long time, the diffusion process has been considered as a homogenization process of the initial disturbance. However, this is a property of a homogeneous environment. When the environment is spatially heterogeneous, fractionation phenomena are observed, where a previously uniform distribution transitions into a non-uniform state. In 1856, Ludwig [1] discovered that salt particles, under diffusion, were distributed unevenly in water with an uneven temperature. Later, Soret[2] discovered the separation of two liquid mixtures under a temperature gradient, and Darken[3] observed the uneven distribution of carbon particles in a non-uniform metal rod. Similar phenomena are widespread, and fractionation is a common phenomenon that occurs due to diffusion in non-homogeneous environments. However, the diffusion equation (1) cannot explain this fractionation phenomenon.

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It has been unclear for a long time whether fractionation phenomena occur due to diffusion or whether other mass transfer processes are involved. Recently, Kim *et al.* [4] showed that experimentally measured dynamical patterns of a fractionation phenomenon match completely to the predicted patterns by the two-component diffusion law,

$$\frac{\partial u}{\partial t} = \nabla \cdot (K\nabla(Mu)), \quad D = KM, \tag{2}$$

where K is called the conductivity, M the motility, and the diffusivity D is the product of the two. In other words, two coefficients are needed to explain the diffusion phenomenon in a heterogeneous environment, and by doing so, the fractionation phenomena can be fully predicted by diffusion alone without the need for additional advection dynamics. If the environment is homogeneous, the coefficients are constant, and (1) and (2) become equivalent. However, if M is not constant, we obtain a non-constant steady state, which is the cause of a fractionation phenomenon.

Diffusion laws so far have been one-coefficient laws, which are determined solely by the diffusivity D. For example, Equation (2) is referred to as Fick's diffusion law when $K = D$ and $M = 1$, which gives (1) and is the most widely known case. Equation (2) is called the Fokker-Planck, Chapman [5], or Ito type when $K = 1$ and $M = D$. If $K = M = \sqrt{D}$, (2) is called Wereide or Stratonovich type. These diffusion laws require the diffusivity D only and hence, traditional random walk models are designed to estimate D assuming all the parameters of the system to be constant. Note that models with constant parameters are enough to decide the diffusivity, which is the random-walk models used so far. However, if one wants to see how the two parameters, K and M, are decided, the parameters should be assumed to vary in space. Then, their contribution to K and M are separated. The authors and their collaborators have studied different roles of random walk components, walk length[6], velocity[7, 8], sojourn time[9], and jumping rate[10] in deciding K and M. We will see later that the heterogeneous persistence also has its unique way of deciding K and M.

The purpose of this paper is to understand how the two coefficients K and M are decided by a PRW system, which explains how persistence gives a fractionation phenomenon. In this paper, we construct a PRW system with spatial heterogeneity and directional anisotropy. The theory of random-walk systems has evolved in various directions since its introduction by Einstein [11] and Pearson [12] in 1905. The correlated or persistent random walk model, which is influenced by the movement of the previous step, was introduced by R. Fürth [13] and Taylor [14], and the term "persistence" has been used since the work of Patlak [15]. These models are widely used to describe particle movements in various media in physics and are frequently employed in ecology to explain animal movement paths, as reviewed in Codling's (2008) paper[16]. Persistent random walks converge to solutions of the Telegrapher's equation through a hyperbolic limit [17, 18, 19, 20, 21]. However, the focus of this paper is on the convergence to diffusion equations through the diffusion limit. The influence of persistence on diffusivity is well known [22, 23]. Lenci (2007) addresses anisotropic PRW, where persistence varies depending on the direction, from a probabilistic perspective [24]. Lutscher and Hillen [25] introduced heterogeneous PRW.

To obtain a spatially heterogeneous and directionally anisotropic PRW in the simplest way, we consider a two-dimensional lattice system where particles move in one of four directions:

$$V := \{\mathbf{v}_1 = (1,0), \mathbf{v}_2 = (0,1), \mathbf{v}_3 = (-1,0), \mathbf{v}_4 = (0,-1)\},$$

and the persistence at position $\mathbf{x}$ in the direction $\mathbf{v}_\ell \in V$ is $0 \le \mu_\ell(\mathbf{x}) < 1$ (see Figure 1). The persistence μ_ℓ is the probability of keeping the previous movement direction $\mathbf{v}_\ell$ for the next step. More specifically, if the previous direction was $\mathbf{v}_\ell$, the probability of continuing in the same direction $\mathbf{v}_\ell$ from the current position $\mathbf{x}$ is $\mu_\ell(\mathbf{x}) + \frac{1-\mu_\ell(\mathbf{x})}{4}$, while the probability of moving in a different direction $\mathbf{v}_j$ for $j \ne i$ is $\frac{1-\mu_\ell}{4}$. Thus, if $\mu_\ell = 0$ for all i, the particles move with probability $\frac{1}{4}$ in all four directions, regardless of their previous movement, and persistence disappears. If $\mu_\ell(\mathbf{x}) = c_0$ is constant for all directions, the persistence becomes isotropic and homogeneous. In this case, it is known well that the diffusivity is given by

$$D = \frac{1 + c_0}{1 - c_0} D_0, \tag{3}$$

where D_0 is the diffusivity in the absence of persistence. [22]

We assume $\mu_1 = \mu_3$ and $\mu_2 = \mu_4$, which are necessary conditions to produce a diffusion phenomenon. Using the PRW, we derive the two-component diffusion law

$$\frac{\partial u}{\partial t} = D_0 \nabla \cdot \Big(K\nabla(Mu)\Big), \tag{4}$$

where the conductivity K and the motility M are

$$K = \begin{bmatrix} \frac{1+\mu_1}{1-\mu_1} & 0 \\ 0 & \frac{1+\mu_2}{1-\mu_2} \end{bmatrix}, \qquad M = \begin{bmatrix} \frac{2-2\mu_2}{2-\mu_1-\mu_2} & 0 \\ 0 & \frac{2-2\mu_1}{2-\mu_1-\mu_2} \end{bmatrix}. \tag{5}$$

In this anisotropic diffusion case, Mu is a matrix, where its gradient vector $\nabla(Mu)$ is defined in the Appendix. See Lemma 1 for its basic properties. If $\mu_1 = \mu_2$, the persistence in both x and y directions are identical, and there is no direction dependence in the persistence. Hence, the problem becomes isotropic. In this case, the motility M becomes the identity matrix I_2, where I_n denotes $n \times n$ identity matrix. The conductivity K becomes a scalar matrix $\frac{1+\mu_1}{1-\mu_1} I_2$. Hence, (4) is written as

$$\frac{\partial u}{\partial t} = \nabla \cdot \Big(\frac{1+\mu_1}{1-\mu_1} D_0 \nabla u \Big). \tag{6}$$

We may conclude that the spatial heterogeneity in persistence affects only the conductivity K in the isotropic persistence case, whereas it influences both K and M in the anisotropic case. The diffusivity in (6) is the same as the one in (3). If $\mu_1 \neq \mu_2$, the problem becomes anisotropic and the motility M is a non-constant matrix. In other words, the motility matrix M represents the anisotropy of PRW. If ϕ is a steady state, then it satisfies

$$\partial_x \Big(\frac{2-2\mu_2}{2-\mu_1-\mu_2} \phi \Big) = 0, \quad \partial_y \Big(\frac{2-2\mu_1}{2-\mu_1-\mu_2} \phi \Big) = 0. \tag{7}$$

In conclusion, the spatial heterogeneity in persistence can make a fractionation phenomenon only when it is anisotropic.

The paper is organized as follows. In Section 2, a random walk system with anisotropic persistence is constructed. We make a recursive relation satisfied by the particle density function. In Section 3, the anisotropic diffusion equation (4) is derived formally using Taylor expansion. We show the validity of the derived equation in two ways. First, in Section 4, the convergence of discrete solutions of the recursive relation is proved mathematically. Then, we provide Monte-Carlo simulations that show the convergence individual-based model to a nonconstant steady-state satisfying (4). A discussion is given in Section 6, and notations used in the paper are given in the Appendices.

2. Random walk with heterogeneous persistence

In this section, we construct a PRW in the simplest form that is spatially heterogeneous and directionally anisotropic. Details are as follows. We take a bounded domain in the two space dimensions,

$$\Omega = [0,1] \times [0,1] \subset \mathbb{R}^2,$$

where the periodic boundary condition is taken. The domain is divided into $N \times N$ lattice cells. Each cell has horizontal and vertical edges of the length,

$$\Delta x = \Delta y = \epsilon,$$

where $\epsilon = \frac{1}{N}$ for an integer $N > 0$. The lattice cells are denoted by C_{ij} for $1 \le i, j \le N$, and their centers by

$$\mathbf{x}_{ij} = (x_i, y_j) = ((i-0.5)\epsilon, (j-0.5)\epsilon), \quad i, j \in \{1, \cdots, N\}.$$

Then, cells are of area $\Delta C_{ij} = \epsilon^2$ and specifically given by

$$C_{ij} = \{(x,y) \in \mathbb{R}^2 : |x - x_i| < \frac{\epsilon}{2} \text{ and } |y - y_j|) < \frac{\epsilon}{2}\}.$$

We may extend the indices to the whole integer set $\mathbb{Z}$, by taking $\mathbf{x}_{i'j'} = \mathbf{x}_{ij}$ if $i' - i$ and $j' - j$ are multiples of N. This notation imposes periodic boundary conditions.

Particles walk at the moment $t_k := k\tau$ for each natural number $k \in \mathbb{N}$ with a constant time interval $\Delta t = \tau$. We assume each particle walks to one of the four neighbor cells instantaneously at the moment t_k. The four possible walking directions are denoted as

$$V := \{\mathbf{v}_1 = (1,0), \mathbf{v}_2 = (0,1), \mathbf{v}_3 = (-1,0), \mathbf{v}_4 = (0,-1)\}.$$

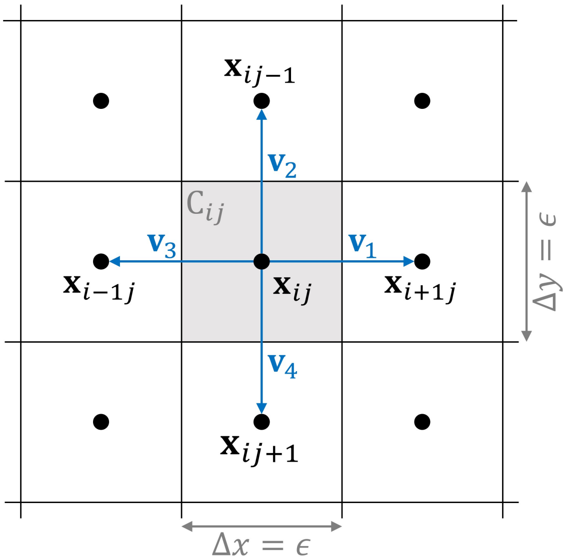

Figure 1: Lattice diagram for the random walk. Particles in a cell may move to one of the four adjacent cells.

The particle population in cell C_{ij} is divided into four sub-groups using their next walking direction. Let $U_k^{\mathbf{v}}(\mathbf{x}_{ij})$ be the number of particles that have arrived at cell C_{ij} at time t_k and will move in direction $\mathbf{v} \in V$ at the next time step t_{k+1}. To construct the model explicitly, we assume all particles are located at the center $\mathbf{x}_{ij}$ and that they immediately decide their new direction upon arrival at this spot. Let $\mu_{\mathbf{v}}(\mathbf{x}_{ij})$ be the persistence at the position $\mathbf{x}_{ij}$ in direction $\mathbf{v}$ and μ_ℓ denote $\mu_{\mathbf{v}_\ell}$ for $\ell \in \{1, 2, 3, 4\}$. Then, these population sub-groups satisfy a recursive relation,

$$U_{k+1}^{\mathbf{v}}(\mathbf{x}_{ij}) = \mu_{\mathbf{v}}(\mathbf{x}_{ij}) U_k^{\mathbf{v}}(\mathbf{x}_{ij} - \epsilon\mathbf{v}) + \sum_{\mathbf{v}' \in V} \frac{1}{4}(1 - \mu_{\mathbf{v}'}(\mathbf{x}_{ij})) U_k^{\mathbf{v}'}(\mathbf{x}_{ij} - \epsilon\mathbf{v}'). \tag{8}$$

This recursive relation is isotropic if the persistence $\mu_\ell(\mathbf{x})$ is identical for all ℓ. The relation is homogeneous if $\mu_\ell(\mathbf{x})$ are independent of $\mathbf{x}$.

Since the particle number $U_k^{\mathbf{v}}(\mathbf{x}_{ij})$ approaches zero as $\epsilon \to 0$, we work with mass density given by

$$u_k^{\mathbf{v}}(\mathbf{x}_{ij}) := \rho \frac{U_k^{\mathbf{v}}(\mathbf{x}_{ij})}{\epsilon^2},$$

where ρ denotes the molar mass of the particle. Then, (8) is rewritten as

$$u_{k+1}^{\mathbf{v}}(\mathbf{x}_{ij}) = \mu_{\mathbf{v}}(\mathbf{x}_{ij}) u_k^{\mathbf{v}}(\mathbf{x}_{ij} - \epsilon\mathbf{v}) + \sum_{\mathbf{v}' \in V} \frac{1}{4} \left(1 - \mu_{\mathbf{v}'}(\mathbf{x}_{ij})\right) u_k^{\mathbf{v}'}(\mathbf{x}_{ij} - \epsilon\mathbf{v}'). \tag{9}$$

We similarly denote $u^{\mathbf{v}_\ell}$ by u^ℓ. Since the mesh size is identical to each other, we obtain the same equation as (8). The effect of using the mass density is in the initialization step,

$$u_0^\ell(\mathbf{x}_{ij}) = \frac{1}{4\epsilon^2} \int_{C_{ij}} u_0(\mathbf{x})\, d\mathbf{x}, \quad \ell \in \{1, 2, 3, 4\}. \tag{10}$$

comment (7) the upper script ℓ is missing on the right hand side. - 이 식은 주어진 u_0를 4개의 방향에 대한 particle density가 똑같이 나누어가진다는 뜻인데 설명을 추가하거나 아니면 $u_0^\ell(\mathbf{x})$가 주어지고 $u_0^\ell(\mathbf{x}_{ij}) = \frac{1}{\epsilon^2} \int_{C_{ij}} u_0^\ell(\mathbf{x})\, d\mathbf{x}$라고 쓰는 것이 더 좋을 수도?

The (total) mass density at time t_k and cell C_{ij} is denoted as $u_k(\mathbf{x}_{ij})$ and given by

$$u_k(\mathbf{x}_{ij}) = \sum_{\ell=1}^{4} u_k^\ell(\mathbf{x}_{ij}).$$

In summary, we take three hypotheses on the persistence $\mu_{\mathbf{v}}(\mathbf{x})$:

(H_1) $V = \{\mathbf{v}_1 = (1,0), \mathbf{v}_2 = (0,1), \mathbf{v}_3 = (-1,0), \mathbf{v}_4 = (0,-1)\}$.
(H_2) $0 \le \mu_\ell(\mathbf{x}) < 1$ for $\ell \in \{1,2,3,4\}$ and $\mathbf{x} \in \Omega$.
(H_3) $\mu_1 = \mu_3$ and $\mu_2 = \mu_4$.

Persistence $\mu_{\mathbf{v}}(\mathbf{x}_{ij})$ is a probability and thus is less than 1 as in (H_2). If it is zero, then there is no persistence in the direction. Note that the summation in (8) includes $\mathbf{v}$. If $\mu_{\mathbf{v}} = 0$, the probability of taking the direction $\mathbf{v}$ is $1/4$. Hypothesis (H_3) is to make the process random and is needed to obtain the diffusion limit. The two directions $\mathbf{v}_1$ and $\mathbf{v}_3$ are of the opposite direction parallel to the x-axis. If the two are different, the obtained phenomenon is not diffusion, and the diffusion limit will blow up. If the four persistences are all identical, we will obtain an isotropic model. Hence, the hypothesis (H_2) together with $\mu_1 \neq \mu_2$ will give an anisotropic phenomenon.

3. Heterogeneous Diffusion Equation

In this section, we derive the diffusion equation satisfied by the discrete solution $u_k^{\mathbf{v}}(\mathbf{x}_{ij})$ of the recursive relation (9) after taking the limit as $\epsilon \to 0$. To achieve this, we first interpolate the sequence of discrete solutions with a continuous function in both space and time. Then, we demonstrate that this continuous function satisfies the mass conservation property, and its limit as $\epsilon \to 0$ satisfies (4).

3.1. Interpolation

We construct the interpolated solution u as follows. The discrete function sequences $u_k^{\mathbf{v}}(\mathbf{x}_{ij})$ obtained from the recursive relations (9) and (10) are for the four movement directions $\mathbf{v} \in V$. We construct a space-time function $u^{\mathbf{v}}(\mathbf{x}, t)$ in two steps. First, we set the fractional density as

$$u^{\mathbf{v}}(\mathbf{x}, t_k) = u_k^{\mathbf{v}}(\mathbf{x}_{ij}), \quad \mathbf{x} \in C_{ij},$$

which gives piecewise constant functions in space. Then, for $t_k < t < t_{k+1}$, we take the linear interpolation in time, i.e., for $t = (1-\alpha)t_k + \alpha t_{k+1}$,

$$u^{\mathbf{v}}(\mathbf{x}, t) = (1-\alpha)u^{\mathbf{v}}(\mathbf{x}, t_k) + \alpha u^{\mathbf{v}}(\mathbf{x}, t_{k+1}). \tag{11}$$

Then, for $t_k < t < t_{k+1}$,

$$\frac{\partial u^{\mathbf{v}}(\mathbf{x}, t)}{\partial t} = \frac{u^{\mathbf{v}}(\mathbf{x}, t_{k+1}) - u^{\mathbf{v}}(\mathbf{x}, t_k)}{\Delta t}. \tag{12}$$

The full density is given by

$$u(\mathbf{x}, t) = \sum_{\mathbf{v} \in V} u^{\mathbf{v}}(\mathbf{x}, t).$$

We observe that u is nonnegative and preserves the initial mass, i.e.,

$$\int_\Omega u(\mathbf{x}, t) d\mathbf{x} = \int_\Omega u_0(\mathbf{x}) d\mathbf{x}, \quad t \ge 0.$$

This can be easily proved by showing $\sum_{i,j=1}^N u_{k+1}(\mathbf{x}_{ij}) = \sum_{i,j=1}^N u_k(\mathbf{x}_{ij})$ using the recursive relation (9).

3.2. Derivation

We now derive the diffusion equation. We assume $u^{\mathbf{v}}$ and $\mu_{\mathbf{v}}$ are smooth enough so we can apply Taylor's theorem. In order to obtain the diffusion limit, we set the constant time step as $\tau = \frac{\epsilon^2}{4D_0}$. This will give diffusivity D_0 when persistence is absent. For $t_k < t < t_{k+1}$,

$$\frac{\partial u}{\partial t}(\mathbf{x}_{ij}, t) = \frac{u_{k+1}(\mathbf{x}_{ij}) - u_k(\mathbf{x}_{ij})}{\Delta t}.$$

Taylor's theorem gives

$$u_k^{\mathbf{v}}(\mathbf{x}_{ij} - \epsilon\mathbf{v}) = u^{\mathbf{v}}(\mathbf{x}_{ij}, t_k) - \epsilon\mathbf{v} \cdot \nabla u^{\mathbf{v}}(\mathbf{x}_{ij}, t_k) + \frac{\epsilon^2}{2}\nabla \cdot ((\mathbf{v} \otimes \mathbf{v})\nabla u^{\mathbf{v}}(\mathbf{x}_{ij}, t_k)) + o(\epsilon^2) \quad \text{as} \quad \epsilon \to 0.$$

Comment (8) The Taylor expansion with respect to ϵ includes the term $o(\epsilon^2)$ in the mathematical expressions, including Eq. (13) on page 6. Please verify the accuracy of this expression. If it is correct, please specify the terms that are neglected and whether they are eligible for neglect. - remainder term을 써주고 이걸 $o(\epsilon^2)$라고 써줄 수 있다고 언급?

Here, the symbol $\otimes$ denotes the tensor product, where $\mathbf{v} \otimes \mathbf{v}$ is defined as $\mathbf{v}\mathbf{v}^T$. Then note that $\nabla \cdot ((\mathbf{v}_1 \otimes \mathbf{v}_1)\nabla u)$ is equal to $\frac{\partial^2 u}{\partial x^2}$. By substituting this into the recursive relation (9) and summing it over $\mathbf{v} \in V$, we obtain

$$u_{k+1}(\mathbf{x}_{ij}) - u_k(\mathbf{x}_{ij}) = -\epsilon \sum_{\mathbf{v} \in V} \mathbf{v} \cdot \nabla u^{\mathbf{v}}(\mathbf{x}_{ij}, t_k) + \frac{\epsilon^2}{2} \sum_{\mathbf{v} \in V} \nabla \cdot ((\mathbf{v} \otimes \mathbf{v})\nabla u^{\mathbf{v}}(\mathbf{x}_{ij}, t_k)) + o(\epsilon^2). \tag{13}$$

For the first term, we need to calculate $u^1 - u^3$ and $u^2 - u^4$. From the recursive relation (9) and Taylor's theorem of first order,

$$\begin{aligned} u_k^1(\mathbf{x}_{ij}) - u_k^3(\mathbf{x}_{ij}) &= u_{k+1}^1(\mathbf{x}_{ij}) - u_{k+1}^3(\mathbf{x}_{ij}) + o(\epsilon) \\ &= \mu_1(\mathbf{x}_{ij})(u_k^1(\mathbf{x}_{i-1,j}) - u_k^3(\mathbf{x}_{i+1,j})) + o(\epsilon) \\ &= \mu_1(\mathbf{x}_{ij})\left((u_k^1 - u_k^3)(\mathbf{x}_{ij}) - \epsilon\frac{\partial}{\partial x}(u_k^1 + u_k^3)(\mathbf{x}_{ij})\right) + o(\epsilon). \end{aligned}$$

By subtracting $\mu_1(u_k^1 - u_k^3)(\mathbf{x}_{ij})$ from both sides, we obtain

$$u_k^1(\mathbf{x}_{ij}) - u_k^3(\mathbf{x}_{ij}) = -\epsilon\frac{\mu_1(\mathbf{x}_{ij})}{1 - \mu_1(\mathbf{x}_{ij})}\frac{\partial}{\partial x}(u^1 + u^3)(\mathbf{x}_{ij}, t_k) + o(\epsilon).$$

By the same calculation for $u^2 - u^4$ and putting them into (13), we obtain

$$u_{k+1}(\mathbf{x}_{ij}) - u_k(\mathbf{x}_{ij}) = \frac{\epsilon^2}{2}\sum_{\mathbf{v} \in V} \nabla \cdot \left(\frac{1 + \mu_{\mathbf{v}}(\mathbf{x}_{ij})}{1 - \mu_{\mathbf{v}}(\mathbf{x}_{ij})}(\mathbf{v} \otimes \mathbf{v})\nabla u^{\mathbf{v}}(\mathbf{x}_{ij}, t_k)\right) + o(\epsilon^2). \tag{14}$$

The recursive relation (9) and the smoothness of $u^{\mathbf{v}}$ give

$$u^{\mathbf{v}}(\mathbf{x}_{ij}, t_k) = u_{k+1}^{\mathbf{v}}(\mathbf{x}_{ij}) + o(1) = \left(\mu_{\mathbf{v}} u^{\mathbf{v}} + \sum_{\mathbf{v}' \in V}\frac{1}{4}(1 - \mu_{\mathbf{v}'})u^{\mathbf{v}'}\right)(\mathbf{x}_{ij}, t_k) + o(1).$$

By subtracting $\mu_{\mathbf{v}} u^{\mathbf{v}}$ from both sides, we can observe that the difference in the left side, $((1 - \mu_{\mathbf{v}})u^{\mathbf{v}})(\mathbf{x}_{ij}, t_k)$, is order $o(1)$. In other words, the number of particles moving in the direction $\mathbf{v}$ is approximately proportional to $1/(1 - \mu_{\mathbf{v}})$. Hence, we have

$$u^{\mathbf{v}}(\mathbf{x}_{ij}, t_k) = \frac{1/(1 - \mu_{\mathbf{v}}(\mathbf{x}_{ij}))}{\sum_{\mathbf{v}' \in V} 1/(1 - \mu_{\mathbf{v}'}(\mathbf{x}_{ij}))} u(\mathbf{x}_{ij}, t_k) + o(1).$$

Putting this into the above, we finally obtain

$$\frac{\partial u}{\partial t} = 2D_0 \sum_{\mathbf{v} \in V} \nabla \cdot \left(\frac{1 + \mu_{\mathbf{v}}}{1 - \mu_{\mathbf{v}}}(\mathbf{v} \otimes \mathbf{v})\nabla\left(\frac{1/(1 - \mu_{\mathbf{v}})}{\sum_{\mathbf{v}' \in V} 1/(1 - \mu_{\mathbf{v}'})}u\right)\right) + o(1), \tag{15}$$

at $\mathbf{x} = \mathbf{x}_{ij}$, $t = t_k$ as $\epsilon \to 0$. After taking $\epsilon \to 0$ limit of (15), we formally obtain a heterogeneous diffusion equation:

$$\begin{cases} \dfrac{\partial u}{\partial t} = 2D_0 \displaystyle\sum_{\mathbf{v} \in V} \nabla \cdot \left(\frac{1 + \mu_{\mathbf{v}}}{1 - \mu_{\mathbf{v}}}(\mathbf{v} \otimes \mathbf{v})\nabla\left(\frac{1/(1 - \mu_{\mathbf{v}})}{\sum_{\mathbf{v}' \in V} 1/(1 - \mu_{\mathbf{v}'})}u\right)\right) & \text{in } \Omega \times (0, T) \\ u(\mathbf{x}, 0) = u_0(\mathbf{x}) & \text{on } \Omega. \end{cases} \tag{16}$$

Finally, if Lemma 1(4) in Appendix is used, we can rewrite (16) as

$$\frac{\partial u}{\partial t}(\mathbf{x},t) = D_0 \nabla \cdot \Big(K(\mathbf{x}) \nabla (M(\mathbf{x}) u(\mathbf{x},t)) \Big),$$

where

$$K(\mathbf{x}) = \begin{bmatrix} \frac{1+\mu_1(\mathbf{x})}{1-\mu_1(\mathbf{x})} & 0 \\ 0 & \frac{1+\mu_2(\mathbf{x})}{1-\mu_2(\mathbf{x})} \end{bmatrix}, \quad M(\mathbf{x}) = \begin{bmatrix} \frac{2-2\mu_2(\mathbf{x})}{2-\mu_1(\mathbf{x})-\mu_2(\mathbf{x})} & 0 \\ 0 & \frac{2-2\mu_1(\mathbf{x})}{2-\mu_1(\mathbf{x})-\mu_2(\mathbf{x})} \end{bmatrix}.$$

Remark. *For a isotropic PRW case, $\mu_\mathbf{v}(\mathbf{x})$ is independent of the direction $\mathbf{v}$, and we may denote $\mu(\mathbf{x}) = \mu_\mathbf{v}(\mathbf{x})$. Then, the diffusion equation becomes*

$$\begin{cases} \frac{\partial u}{\partial t}(\mathbf{x},t) = \frac{1}{2} D_0 \sum\limits_{\mathbf{v}\in V} \nabla \cdot \Big(\frac{1+\mu(\mathbf{x})}{1-\mu(\mathbf{x})} (\mathbf{v}\otimes\mathbf{v}) \nabla u(\mathbf{x},t) \Big) & \text{in } \Omega \times (0,T) \\ u(\mathbf{x},t) = u_0(\mathbf{x}) & \text{on } \Omega \times \{t=0\}. \end{cases}$$

In this case, there is no fractionation phenomenon, and the steady state of the solution is constant.

4. Numerical Simulation

In this section, we test the property of heterogeneous anisotropic PRW numerically. First, we test the behavior of persistent random walk for four cases using the recursive relation (9). We will observe asymptotic convergence to constant or non-constant steady states starting from an initial value concentrated at the center of the domain. Then, we compare the behavior of the recursive relation with Monte Carlo simulation and the solution of the diffusion equation (4)–(5). These three give the same fractionation phenomenon, which confirms the anisotropic diffusion equation gives the phenomenon correctly.

4.1. Four scenarios of persistent random walk

We test fractionation phenomena by numerically computing the recursive relation (9). We selected four scenarios that illustrate the differences between isotropic and anisotropic persistence, and between heterogeneous and homogeneous persistence. The space domain is $\Omega = [-1,1]\times[-1,1]$ and divided two sub-domains $\Omega_1 = \{(x,y)\in\Omega : x<0\}$ and $\Omega_2 = \{(x,y)\in\Omega : x>0\}$. The persistence parameters μ_1 and μ_2 are constant in each sub-domain as given in Table 1. Note that the parameters are constant in the y variable and discontinuous in the x variable for each fixed y. For the numerical simulation, the space domain Ω is discretized into 40×40 cells with space mesh size $\Delta x = 0.05$. We take the time step $\Delta t = 0.025$. In this case, if $\mu_\mathbf{v} = 0$ for all $\mathbf{v}\in V$, the diffusivity is

	Case 1		Case 2		Case 3		Case 4	
	$x<0$	$x>0$	$x<0$	$x>0$	$x<0$	$x>0$	$x<0$	$x>0$
μ_1	0.6	0.6	0.2	0.8	0.2	0.2	0.2	0.8
μ_2	0.6	0.6	0.2	0.8	0.2	0.8	0.2	0.2

Table 1: Persistence of the four tested cases

$$D_0 = \frac{|\Delta x|^2}{4\Delta t} = 0.025.$$

The initial value is 400 in the central four cells and 0 in others, which makes the average of the initial value to be 1. We assume the periodic boundary condition.

After taking a diffusion limit $(\Delta x, \Delta t)\to(0,0)$ with D_0 unchanged, the limit satisfies the diffusion equation (4)–(5):

$$\frac{\partial u}{\partial t} = D_0 \nabla\cdot(K\nabla(Mu)), \quad K = \begin{bmatrix} k_{11} & 0 \\ 0 & k_{22} \end{bmatrix}, \ M = \begin{bmatrix} m_{11} & 0 \\ 0 & m_{22} \end{bmatrix}, \tag{17}$$

where the conductivity K and the motility M in (5) are

$$k_{11} = \frac{1+\mu_1(\mathbf{x})}{1-\mu_1(\mathbf{x})}, \quad k_{22} = \frac{1+\mu_2(\mathbf{x})}{1-\mu_2(\mathbf{x})},$$

$$m_{11} = \frac{2-2\mu_2(\mathbf{x})}{2-\mu_1(\mathbf{x})-\mu_2(\mathbf{x})}, \quad \text{and} \quad m_{22} = \frac{2-2\mu_1(\mathbf{x})}{2-\mu_1(\mathbf{x})-\mu_2(\mathbf{x})}.$$

Using k_ℓ's and m_ℓ's, (17) is written as

$$\frac{\partial u}{\partial t} = D_0((k_{11}(m_{11}u)_x)_x + (k_{22}(m_{22}u)_y)_y). \tag{18}$$

We compare the solution of the recursive relation with the diffusion equation. We also do a Monte Carlo simulation for comparison.

Case 1: Spatially homogeneous and directionally isotropic persistence

The persistence coefficient in the first case is $\mu = 0.6$ in all directions and at all locations. Then,

$$k_{11} = k_{22} = \frac{1+\mu}{1-\mu} = 4 \quad \text{and} \quad m_{11} = m_{22} = 1.$$

The diffusion equation (17) becomes an isotropic diffusion with diffusivity $D = \frac{1+\mu}{1-\mu}D_0$. Three snapshots of the recursive relation (9) are given in Figure 2. The effect of persistence is clearly observed in the early stage ($k = 8$). However, it is eventually forgotten, and the solution converges to a constant steady state.

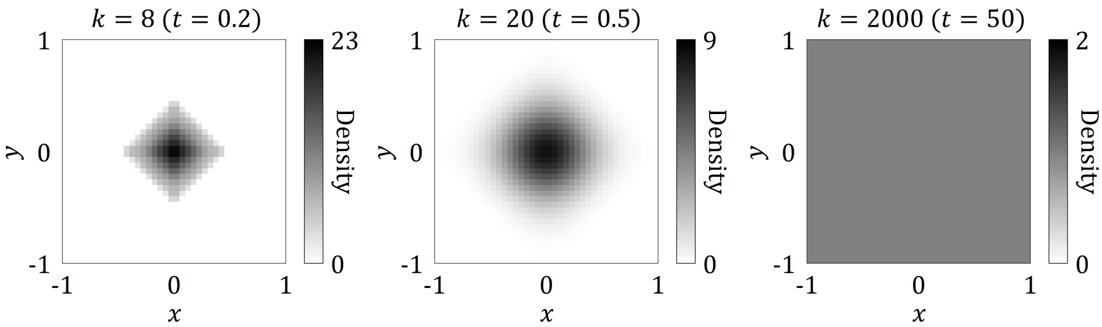

Figure 2: Three snapshots of Case 1 at $k = 8, 20,$ and 2000.

Case 2: Spatially heterogeneous and directionally isotropic persistence

The persistence coefficients of the second case are $\mu_1 = \mu_2 = 0.2$ in Ω_1, and $\mu_1 = \mu_2 = 0.8$ in Ω_2. Then, we have

$$k_{11} = k_{22} = \begin{cases} 1.5 & \text{if } x < 0, \\ 9.0 & \text{if } x > 0. \end{cases}, \quad m_{11} = m_{22} = 1.$$

In this case, the motility M is a constant, and the conductivity K is a variable. The corresponding diffusion equation is Fick's law diffusion. Three snapshots of the recursive relation (9) are given in Figure 3. We can observe that the initial propagation pattern is different in the two subdomains. However, the solution eventually converges to a constant state.

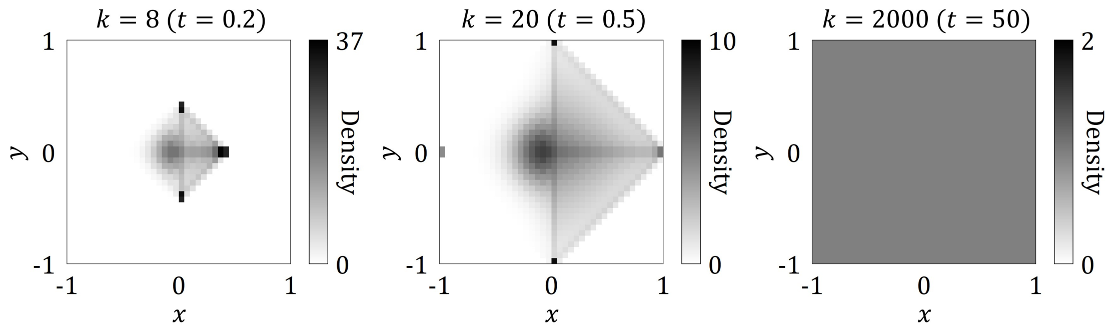

Figure 3: Three snapshots of Case 2 at $k = 8, 20$, and 2000.

Case 3: Spatially heterogeneous and directionally anisotropic persistence

In the third case, the persistence coefficients are $\mu_1 = \mu_2 = 0.2$ in Ω_1, while in Ω_2, they are $\mu_1 = 0.2$ and $\mu_2 = 0.8$. Persistence is isotropic in Ω_1. However, in Ω_2, persistence along the y-axis is significantly greater than in other directions. This scenario clearly illustrates the impact of heterogeneous persistence.

The conductivity and motility are

$$k_{11} = \begin{cases} 1.5, \\ 1.5, \end{cases} \quad k_{22} = \begin{cases} 1.5, \\ 9.0, \end{cases} \quad m_{11} = \begin{cases} 1.0, \\ 0.4, \end{cases} \quad m_{22} = \begin{cases} 1.0, & x < 0, \\ 1.6, & x > 0, \end{cases}$$

This is a case when both K and M are non-constant matrices. Note that if $(m_{11}u)_x = 0$ and $(m_{22}u)_y = 0$, then u is a steady-state solution of (18). Since m_{22} is independent of the y variable, $(m_{22}u)_y = 0$ if u is independent of the y variable. Therefore, since m_{11} is constant in Ω_1 and Ω_2 and jumps from 0.5 to 0.2 across $x = 0$,

$$u(x, y) = \begin{cases} u_-, & x < 0, \\ u_+, & x > 0, \end{cases} \tag{19}$$

is a steady-state solution when

$$\frac{u_-}{u_+} = \frac{0.4}{1.0} = 0.4.$$

Three snapshots of the recursive relation (9) are shown in Figure 4. The pictures show an anisotropic evolution

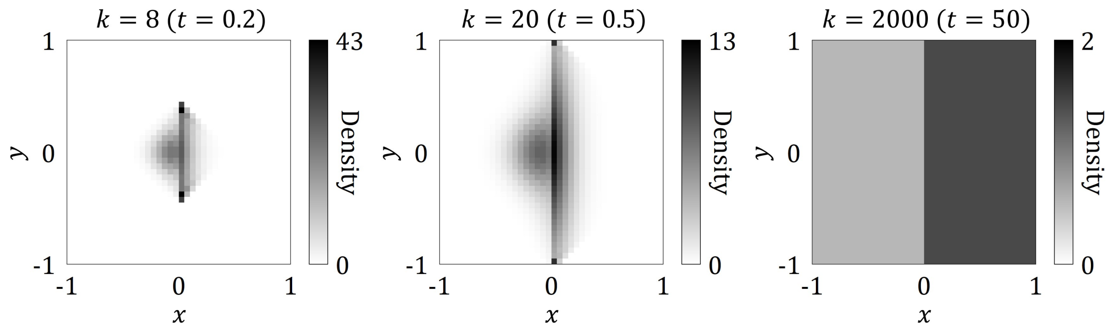

Figure 4: Three snapshots of Case 3 at $k = 8, 20$, and 2000.

in Ω_2. Particles in Ω_2 diffuse fast in the y direction and slow in the x direction. On the other hand, the particles in Ω_1 diffuse equally in both directions. This makes the final steady state heterogeneous. We observe that the solution converges to a piecewise constant state where $u_- = 0.5714$ and $u_+ = 1.4286$. This jump satisfies the ratio $\frac{u_-}{u_+} = 0.4$.

Case 4: Heterogeneous anisotropic persistence #2

We consider another case of heterogeneous anisotropy, which shows aggregation in the other region. The persistence coefficients of the fourth case are $\mu_1 = \mu_2 = 0.2$ in Ω_1 and $\mu_1 = 0.8$ and $\mu_2 = 0.2$ in Ω_2. Hence, the persistence is isotropic in Ω_1 and anisotropic in Ω_2. The conductivity and the motility are

$$k_{11} = \begin{cases} 1.5, \\ 1.5, \end{cases} \quad k_{22} = \begin{cases} 9.0, \\ 1.5, \end{cases} \quad m_{11} = \begin{cases} 1.0, \\ 1.6, \end{cases} \quad m_{22} = \begin{cases} 1.0, & x < 0, \\ 0.4, & x > 0, \end{cases}$$

In this case m_{11} jumps from 0.5 to 0.8 across $x = 0$, and $u(x, y)$ given by (19) is a steady-state solution if $\frac{u_-}{u_+} = 1.6$.

Three snapshots of the recursive relation (9) are given in Figure 5. Particles in Ω_2 diffuse rapidly in the x direction

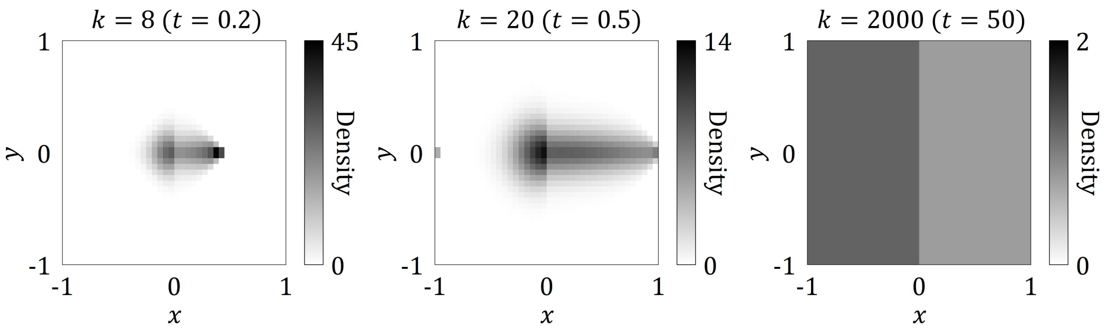

Figure 5: Three snapshots of Case 4 at $k = 8, 20$, and 2000.

and slow in the y direction. The particles in Ω_1 diffuse equally in both directions. This makes particles stay more in Ω_1 and the final steady state heterogeneous. We can observe that the solution converges to a piecewise constant state where $u_- = 1.2308$ and $u_+ = 0.7692$. This jump satisfies the ratio $\frac{u_-}{u_+} = 1.6$.

4.2. Simulations of the recursive relation, Monte Carlo, and PDE

We compare the solutions of the recursive relation (9), diffusion equation (17), and Monte Carlo method. In these comparisons, we will numerically compute the fractionation phenomenon corresponding to the scenario of Case 3. The three simulations start with the uniform distribution and show the convergence to a non-constant steady state.

Two snapshots of simulations based on the recursive relation (9) are presented in Figure 6a. The initial value is set to a constant 1. The left two images show two-dimensional representations of the evolution, which primarily exhibit a one-dimensional phenomenon. The right two images illustrate cross-sections with a fixed y value. As time progresses, the fractionation phenomenon becomes evident. These results clearly demonstrate that anisotropic persistence can lead to fractionation. It is important to note that periodic boundary conditions are applied, resulting in two interfaces located at $x = 0$ and $x = \pm 1$. The final equilibrium state matches the one shown in Figure 4.

In Figure 6b, two snapshots of a Monte Carlo simulation are given that correspond to the previous ones. In this simulation, the same spatial and temporal mesh is used as the one used in the recursion model. Initially, the total of 50×1600 particles are uniformly distributed in each cell. Hence, the average is 50. Particles move to one of the four neighboring cells at each time step using the same parameters in Case 3. We can see how it converges to a non-constant equilibrium state. The left two show the two-dimensional evolution which is simply the version of Figure 6a with stochastic nature. The right two are the average of each column (not a cross-section).

The two snapshots in Figure 6care numerical solutions of the PDE model (17). Note that the PDE model is obtained from the recursion model after taking a diffusion limit as $(\Delta x, \Delta t) \to (0, 0)$. Therefore, we may consider the case where the mesh size approaches an infinitesimally small value. On the other hand, the previous two simulations are with fixed mesh size $\Delta x = 0.05$. Due to this difference, we observe that the initial stage is a little bit different. The peaks at the interface in the early stage ($t = 0.5$) are sharper in comparison with the previous two cases. However, the fractionation phenomenon of the PDE model is of the same equilibrium state.

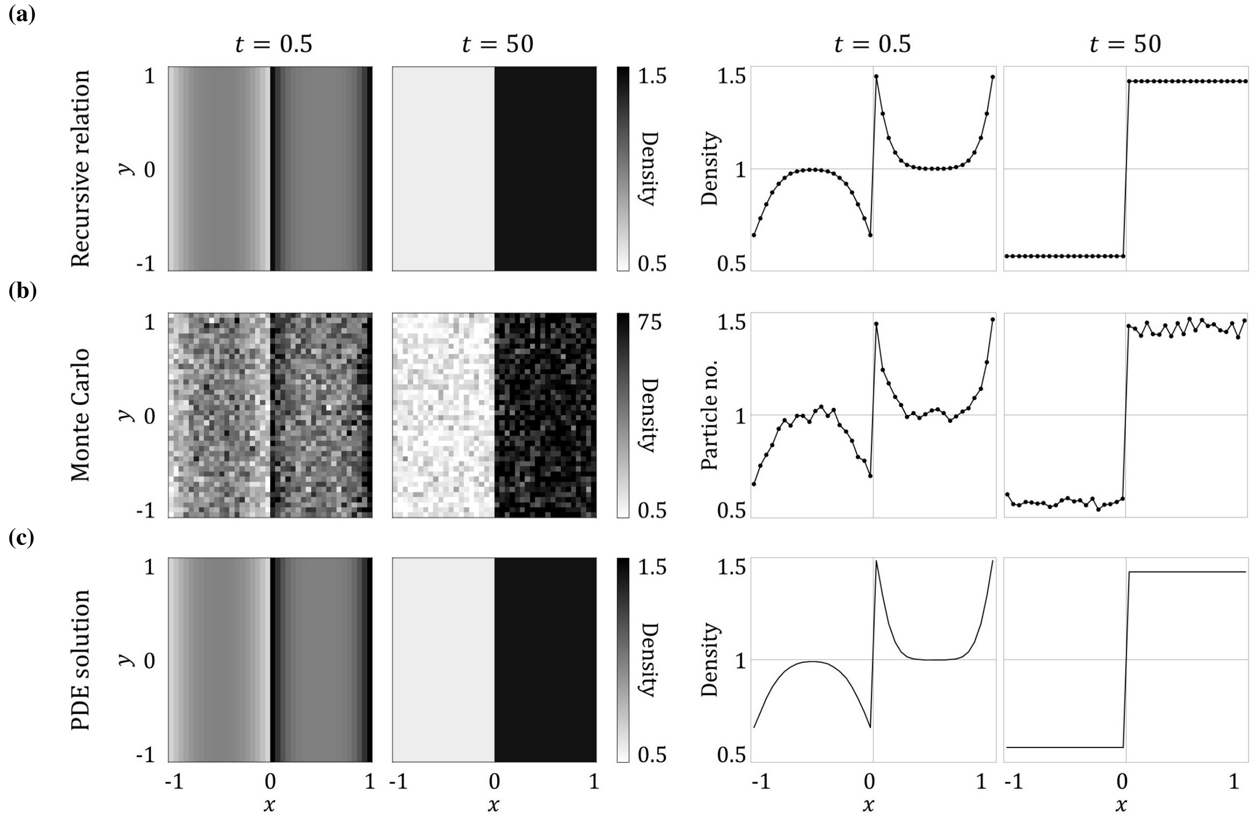

Figure 6: Snapshots of the recursive relation (9), Monte Carlo method, and PDE solution for Case 3 at $t = 0.5, 50$.

5. Discussion

Diffusion is a mass transfer phenomenon driven by random microscopic movements and involves various dynamic components, such as mean free path, collision time, jumping rate, temperature, permeability, and persistence. However, for homogeneous diffusion phenomena, the detailed dynamics of these components are not critical since their use is to determine the diffusivity. Measuring the diffusivity D is sufficient, which allows us to use the diffusion equation (1).

In contrast, diffusion in a heterogeneous environment differs significantly from that in a homogeneous one. One key difference is that in a homogeneous environment, the diffusion-induced equilibrium state is constant, whereas in a heterogeneous environment, it is not. There are so many examples as discussed in Introduction. This arises because the diffusion equation (1) is invalid when the diffusivity D depends on the spatial variable. In such cases, rendering equation (1) meaningless. Instead, the two-component diffusion law,

$$\frac{\partial u}{\partial t} = \nabla \cdot (K\nabla(Mu)), \quad D = KM,$$

can be used for a heterogeneous environment. When the conductivity K and motility M are constant, this equation reduces to (1). However, if M is non-constant, steady-state solutions become non-constant. To effectively work with this diffusion model in heterogeneous environments, it is essential to understand how D is split into K and M. Analyzing the dynamics of each component contributing to the diffusion phenomenon is crucial in such cases, as it reveals how these components influence K and M.

In this paper, we investigate how heterogeneous persistence contributes to conductivity and motility. If persistence is isotropic, heterogeneity in persistence affects K, while M remains the identity matrix. On the other hand, if persistence is anisotropic, both K and M become non-constant matrices, leading to non-constant steady-state solutions. In this study, we propose a recursive relation for a persistent random walk (PRW), formally derive the diffusion equation from the PRW, and validate these findings numerically. The numerical simulations of the PDE, PRW, and Monte Carlo method are shown to agree with one another.

Through this research, we confirm that a persistent random walk exhibits intriguing properties in heterogeneous and anisotropic environments. A particularly unexpected and interesting finding is that isotropic heterogeneity is reflected in K, while anisotropic heterogeneity appears in M.

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Appendix A. Gradient vector for a matrix field.

Anisotropic diffusion theory requires a proper definition for the gradient vector of a matrix field $U : \mathbb{R}^n \to \mathbb{R}^{n\times n}$. Let u_{ij} be the component of U at the ith row and jth column. We define the gradient vector of this matrix U as a column vector,

$$\nabla U = \begin{pmatrix} \sum_{j=1}^n \partial_j u_{1j} \\ \vdots \\ \sum_{j=1}^n \partial_j u_{nj} \end{pmatrix} \in \mathbb{R}^n, \tag{A.1}$$

which takes its ith element as the divergence of the ith row of U, i.e.

$$\text{the } i\text{th component of column vector } \nabla U \text{ is } \quad \sum_{j=1}^n \partial_j u_{ij}.$$

This definition makes the differentiation of anisotropic quantities compatible with existing conventions and notation as follows.

Lemma 1. *Let I_n be the identity matrix, C be a constant matrix, M be a differentiable matrix, $\mathbf{v}$ be a constant unit vector, and u be a differentiable scalar function. Then, (1) $\nabla(Mu) = (\nabla M)u + M\nabla u$, (2) $\nabla u = \nabla(I_n u)$, (3) $\nabla(Cu) = C\nabla u$, and (4) $\mathbf{v}\otimes\mathbf{v}\nabla u = \mathbf{v}\otimes\mathbf{v}\nabla(\mathbf{v}\otimes\mathbf{v}u)$.*

Proof. The vector $\nabla(Mu)$ is a column vector, and the ith component is

$$\sum_{j=1}^n \partial_j(m_{ij}u) = \sum_{j=1}^n \partial_j(m_{ij})u + \sum_{j=1}^n m_{ij}\partial_j u,$$

where the product rule is used. Therefore, (1) holds. Equalities in (2) and (3) are from (1). Since $\mathbf{v}\otimes\mathbf{v}$ is a constant matrix, we have

$$(\mathbf{v}\otimes\mathbf{v})\nabla(\mathbf{v}\otimes\mathbf{v}u) = (\mathbf{v}\otimes\mathbf{v})(\mathbf{v}\otimes\mathbf{v})\nabla u.$$

Since $\mathbf{v}$ is a unit vector, we have

$$(\mathbf{v}\otimes\mathbf{v})(\mathbf{v}\otimes\mathbf{v}) = \mathbf{v}(\mathbf{v}^t\mathbf{v})\mathbf{v}^t = \mathbf{v}\mathbf{v}^t = \mathbf{v}\otimes\mathbf{v},$$

which gives (4) and completes the lemma. □

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