# First Arrival Position in Molecular Communication Via Generator of Diffusion Semigroup

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*Abstract*—We consider the problem of characterizing the first arrival position (FAP) density in molecular communication (MC) with a diffusion-advection channel that permits a constant drift velocity pointed to arbitrary direction. The advantage of FAP modulation lies in the fact that it could encode more information into higher dimensional spatial variables, compared to other modulation techniques using time or molecule numbers. However, effective methods to characterize the FAP density in a general framework do not exist. In this paper, we devise a methodology that fully resolves the FAP density with planar absorbing receivers in arbitrary dimensions. Our work recovers existing results of FAP in 2D and 3D as special cases. The key insight of our approach is to remove the time dependence of the MC system evolution based on the generator of diffusion semigroups.

*Index Terms*—Molecular communication, diffusion, first arrival time (FAT), first arrival position (FAP), semigroup, generator.

#### I. INTRODUCTION

Since ancient times, the problem of conveying information over a distance has been an important issue in human history. Modern communication systems resolve this problem with electromagnetic (EM) signals. However, EM-based communication techniques are challenging for tiny (for instance, nanoscale) devices; if not feasible, due to the constraints such as the wavelength, antenna size, or energy issues [1], [2].

In molecular communication (MC) systems, small molecules<sup>1</sup> called message molecules (MMs) act as chemical signals conveying the information [3], [4]. After the information-carrying particles are released in the channel, a propagation mechanism is necessary for transporting them to the receiver. This mechanism can be diffusion-based [5], flow-based [6], or an engineered transport system such as molecular motors [7], [8]. Among these different propagation mechanisms, diffusion-based MC, sometimes in combination with advection and chemical reaction networks, has been the most prevalent approach for MC systems, and will be the main focus of study in this paper.

In order to transmit information in a diffusion-based MC system, we can modulate different physical properties of the MMs [9]–[12]. Signaling molecules that reach the vicinity of

the receiver can be observed and processed by the receiver to extract the information that is necessary for performing detection and decoding [13]. The reception mechanism of a MC receiver can be categorized into two classes: i) passive reception, and ii) active reception. The simplest active reception is the fully-absorbing receiver [14] which has the ability to measure the time and position of arrival of each molecule, and to remove the MM right after it is received. For MC systems with a fully-absorbing receiver, how to completely characterize the arrival time or the arrival position is no doubt a very important issue.

In Section I-A, we briefly review some important results concerning first arrival time (FAT) in MC literature. Until very recently, the first arrival position (FAP) information was also introduced into the MC realm, see [15], [16]. We will give a short introduction to the current status of FAP results in Section I-B.

#### A. First Arrival Time

When information is encoded on the time of release of MM, we refer to this subclass of MC channels as molecular timing channels (MTCs). The main difference between timing-based modulation and other modulations, such as the number or type modulation, is that: the channel input is continuous instead of discrete.

The MTC model was first proposed in [17]. In its simplest form, a MTC can be realized through a single MM released by the transmitter (Tx) at time  $t_{in}$  with information encoded on this release time. The MM goes through some random propagation and arrive at the receiver (Rx) at time  $t_{out}$ . We have

$$t_{\rm out} = t_{\rm in} + t_{\rm n},\tag{1}$$

where  $t_n$  is some random delay due to MM propagation mechanisms.

In [18], an MTC with additive inverse Gaussian noise (AIGN) was introduced into MC realm, where  $t_n$  in Eq. (1) is inverse Gaussian distributed. The authors of [18] derived upper and lower bounds on capacity per channel use. Later in [19], tighter bounds on capacity of the same MTC with AIGN noise were derived. The capacity-achieving MM input distribution was also characterized. In [20]–[22], single particle release is extended to multiple, say M MM releases. In this scenario,

<sup>&</sup>lt;sup>1</sup>We omit the shape of a message molecule and think of it as a mass point as most works in molecular communication do. Thus we use both terms "particle" and "molecular" interchangeably.

information is encoded in a vector  $\mathbf{t}$ , in which each component is the time of release of one of the M MMs. For multiple particle case, the channel model changes to:

$$\mathbf{t}_{\text{out}} = \text{sort}(\mathbf{t}_{\text{in}} + \mathbf{t}_{\text{n}}), \tag{2}$$

where  $\mathbf{t}_n$  is an  $\mathbb{R}^M$  vector of random delays associated with each MM. Notice that sort(t) is the sort operator that permutes the input vector into an ascending order. The sort operation is necessary when time information of each MM is considered since the MMs may arrive out of order.

## B. First Arrival Position

Apart from the first arrival time, there is another important degree of freedom to carry information: the first arrival position. The simplest FAP channel can be written as

$$\mathbf{x}_{\text{out}} = \mathbf{x}_{\text{in}} + \mathbf{x}_{\text{n}},\tag{3}$$

where  $\mathbf{x}_{in}$ ,  $\mathbf{x}_{out}$  and  $\mathbf{x}_n$  are all Euclidean vectors in  $\mathbb{R}^n$  with n being the dimension of the underlying space.

To the best of our knowledge, the first paper in MC society that mentions FAP as an information carrying property is [15], the density function of FAP is derived in closed-form for both pure diffusion and diffusion with a constant drift in 3D spaces. However, this approach is limited in scope when higher dimensional FAP is considered. Later, the authors in [16] use Green's function and the method of images to derive the FAP density function for 2D MC systems, where the fluid medium has a constant drift restricted to the longitudinal direction from the transmitter towards the receiver. However, the method of images in [16] cannot be generalized to the setting of arbitrary drift velocity field, which is commonly encountered in fluid environments, because it uses symmetry heavily, but an arbitrary direction of drift will break down the required symmetry. Finally, the capacity of molecular position channels remains completely unknown except some very specific cases, see [16] for capacity of *M*-ary modulation scheme.

## C. Our Contributions

Although most works in MC consider FAT modulation for absorbing receivers, there are at least two reasons why FAP is preferable.

- For each message particle, the FAT information is only one-dimensional, while the FAP could have higher dimensions to carry information. Hence, the capacity of FAP could be larger then FAT per single message particle.
- Practically, "guard intervals" between two consecutive transmissions are required to avoid cross-over effects, as described in Eq. (2). Due to these guard intervals, the total transmission time for FAT-type modulation will increase roughly proportional to the number of MMs to be transmitted. Consequently, for applications in which the time efficiency plays an important role, the FAP-type modulation is arguably a better solution.

The main contributions of this paper are two-fold. 1) We relax the constraint imposed on the drift direction in previous works. 2) We introduce the semigroup approach to facilitate

characterization of the FAP density for planar absorbing receivers in higher dimensional diffusion channels. Our methodology unifies the process toward finding FAP in 2D and 3D with a solid theoretical backup (see Section III for details). Technically, the semigroup approach avoids complicated time integration in finding FAP. We believe that our work opens the possibility toward general resolution of the capacity of molecular position channels.

#### D. Structure of this Paper

The remainder of this paper is structured as follows. Section II describes the system model we choose, and some related papers working on FAP. Section III presents the new methodology we proposed to find FAP. Finally, concluding remarks are made in Section IV.

# II. SYSTEM MODEL AND RELATED WORKS

## A. System Model

We consider a MC system located in an *n*-dimensional Euclidean space, consists of a point Tx and a planar absorbing Rx. The distance between Tx and Rx is *d*. Notice that we can always arrange the basis of  $\mathbb{R}^n$  so that the last vector in the basis set is parallel to the transmission direction. Without loss of generality, we consider that the transmitter is a point located at the Cartesian coordinate  $(0, \dots, 0, d)$ , and the receiver is an infinite large absorbing plane located at  $\{x \in \mathbb{R}^n : x_n = 0\}$ . Abstract MC system figures for 2D and 3D spaces are illustrated in Figure 1 and Figure 2, respectively. The physical channel of our MC model is composed of a diffusive fluid medium with a constant drift.

In theoretical MC literature, there are two different viewpoints to model diffusion channels. The macroscopic viewpoint uses *diffusion equation* (aka *heat equation*) to capture the evolution of the continuous distribution of concentration of MMs. While in the microscopic viewpoint, individual message molecule is monitored using its own trajectory. For the equivalence of these two viewpoints, readers can refer to classical potential theory as in [23], or a good review paper in MC such as [9] or [13].

In the macroscopic viewpoint, the physical channel is modeled by Eq. (4) below. The most important quantity in macroscopic MC system analysis is the concentration field<sup>2</sup>  $c(\mathbf{r}, t)$  of message molecules at spatial position  $\mathbf{r}$  and time t. By Fick's law of diffusion [13], the evolution of  $c(\mathbf{r}, t)$  can be captured by the diffusion-advection equation:

$$\partial_t c\left(\mathbf{r}, t; \mathbf{r}_0\right) + \mathbf{v}(\mathbf{r}, t) \cdot \nabla c\left(\mathbf{r}, t; \mathbf{r}_0\right) = D\nabla^2 c\left(\mathbf{r}, t; \mathbf{r}_0\right), \quad (4)$$

where  $\mathbf{r}_0$  is the point where the diffusion starts,  $\mathbf{v}$  is the velocity field of the fluid medium which is assumed to be incompressible,  $\nabla$  and  $\nabla^2$  are the gradient and the Laplace operators, respectively, and D is the diffusion coefficient. The value of D is determined by the temperature, the fluid viscosity, and the molecule's Stokes radius, see [9].

<sup>2</sup>Here we use the word "field" to mean a function of space and time.

On the other hand in the microscopic viewpoint, a common assumption is that the trajectory of each molecule can be well distinguished. A mainstream model in MC for the trajectory  $X_t$  of a MM is the Itô diffusion process. An Itô diffusion in Euclidean space  $\mathbb{R}^n$  is a stochastic process satisfying a stochastic differential equation (SDE) of the form

$$dX_t = b(X_t)dt + \sigma(X_t)dB_t,$$
(5)

where  $B_t$  is an *n* dimensional standard Brownian motion. Throughout this paper, we assume that  $b(\cdot)$  and  $\sigma(\cdot)$  are both constants and can be determined by the properties of fluid and MMs. We further assume that the receiver for our MC system is perfectly absorbing and has the ability to correctly measure the time and position at first-arrival for each individual molecule [16].

In the following, we denote the initial position of a MM by  $\mathbf{x}$ , the final (or received) position by  $\mathbf{y}$ , and the FAP distribution by a conditional density function  $f(\mathbf{y}|\mathbf{x})$ . The main problem is to characterize the function  $f(\mathbf{y}|\mathbf{x})$ .

## B. Related Works

1) 2D FAP density: The authors of [16] solved this problem in 2D partially<sup>3</sup>. In [16], a 2D MC system with a constant drift

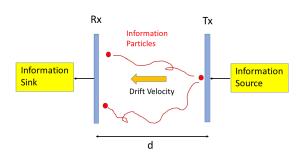


Fig. 1. System Model of 2D First Arrival Position Channels.

velocity **v** pointing precisely to the receiver is considered. The system model is illustrated in Figure 1. The authors of [16] adopt the method of images to construct Green's function for an absorbing boundary. The resulting FAP density function can be found as in [24, Eq. (42)] of Appendix A of the online version of this paper. Notice that we cannot recover the FAP expression as appeared in [16, Eq. (19)]. Instead, we have provided a self-contained proof in Appendix A of [24].

2) 3D FAP density: In [15], a 3D MC system with a constant drift velocity v pointing to arbitrary direction is considered. The system model is illustrated in Figure 2. The authors of [15] use Dynkin's formula to link the microscopic properties at first arrival time to the solution of macroscopic

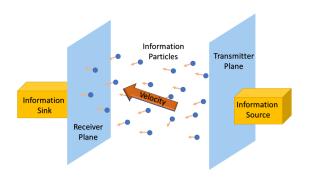


Fig. 2. System Model of 3D First Arrival Position Channels.

diffusion equation. A closed-form FAP density function in 3D is obtained in [15], which has the following form:

$$f_{Y|X}(\mathbf{y}|\mathbf{x}) = \frac{\lambda}{2\pi} \exp\left\{-\frac{v_3\lambda}{\sigma^2}\right\} \exp\left\{\frac{v_1}{\sigma^2}\left(\xi - x_1\right) + \frac{v_2}{\sigma^2}\left(\eta - x_2\right)\right\}$$
(6)  
$$\cdot \exp\left\{-\frac{|v|}{\sigma^2} \|\mathbf{y} - \mathbf{x}\|\right\} \left[\frac{1 + \frac{|v|}{\sigma^2} \|\mathbf{y} - \mathbf{x}\|}{\|\mathbf{y} - \mathbf{x}\|^3}\right],$$

where  $\sigma^2 = 2D$  is the microscopic diffusion coefficient,  $d = \lambda$ is the distance between transmitter plane and receiver plane,  $v_3$ is the component of drift velocity parallel (or longitudinal) to the information transmission direction, and  $v_1$  and  $v_2$  are the drift components perpendicular (or transverse) to the transmission. Here we use the symbol  $\|\cdot\|$  to represent the Euclidean norm. Namely,  $\|\mathbf{y} - \mathbf{x}\| = \sqrt{(\xi - x_1)^2 + (\eta - x_2)^2 + \lambda^2}$ , where  $\mathbf{x} = (x_1, x_2, \lambda)$ ,  $\mathbf{y} = (\xi, \eta, 0)$  are position vectors in  $\mathbb{R}^3$ .

# III. FINDING FAP VIA GENERATOR OF DIFFUSION SEMIGROUP

By suitably examine macroscopic and microscopic relations for the diffusion process, we come up with new ideas which can simplify the procedure towards finding FAP density. After a careful examination, one can realize that FAP density itself has no time dependency, so there must exist some redundant calculations in old methods playing with heat equations, for instance the method used in [16]. The key insight of our approach is to remove the time dependence of the MC system evolution based on the generator of diffusion semigroups.

Our proposed semigroup approach towards finding the FAP density can be summarized in three main steps:

- 1. By utilizing the generator of diffusion semigroup, we can remove the time variable from the very beginning. This can be done because of the Markov property of diffusion semigroup for our MC system.
- Look up representation formulas from partial differential equation (PDE) literature for the corresponding elliptic boundary value problems (BVP) we obtained in Step 1. Since there are plentiful well known results for solutions

<sup>&</sup>lt;sup>3</sup>Using the image method in [16], we can only tackle with drifts in longitudinal direction parallel to the direction of transmission, but not in arbitrary direction.

of elliptic PDEs (even in *high dimensional* cases, see [25], [26]), we do not need to derive representation formulas from scratch.

3. Via properly interpretating the Dynkin's formula, we claim that the FAP density can be obtained directly by the relation  $f_{Y|X}(\mathbf{y}|\mathbf{x}) = \left| \frac{\partial G(\mathbf{y}, \mathbf{x})}{\partial n_{\mathbf{y}}} \right|$ , once the elliptic Green's function  $G(\mathbf{y}, \mathbf{x})$  is known. Through this process, we can bypass the complicated integration step as appeared in [16, Eq. (17)].

The comparisons between the old and new methods are listed in Table I. For the sake of completeness, we present the old method concisely in Appendix B of [24] in a self-contained fashion.

TABLE I Comparison Between Old and New Methods for Finding FAP Density

	Old Method (with $t$ )	New Method (without t)
Step 1	Finding the free space Green's function for parabolic PDE.	Removing time $t$ from the beginning by considering the generator of diffusion.
Step 2	Solving for absorbing Green's function based on image method.	Looking up the solution forms for certain types of elliptic BVPs.
Step 3	Calculating FAP density flux and doing time integration.	Interpretating the Dynkin's formula and obtaining the FAP density directly.

# A. Infinitestimal Generator of Itô Diffusion

In physics, an Itô diffusion is used to describe the Brownian motion of a particle subjected to a potential in a fluid medium. In mathematics, an *n* dimensional Itô diffusion<sup>4</sup> is a stochastic process satisfying a specific type of SDE of the form  $dX_t = b(X_t)dt + \sigma(X_t)dB_t$ , as described in Eq. (5). Throughout this paper, we assume that  $b(\cdot)$  and  $\sigma(\cdot)$  are both constants.

To each Itô diffusion  $X_t$ , we can associate a corresponding operator called *infinitestimal generator*, or simply *generator*, which is defined as follows. Let  $\mathcal{D}(A)$  be the domain of the generator A. We define  $\mathbb{E}^{\mathbf{x}}[f(X_t)] := \mathbb{E}[f(X_t)|X_0 = \mathbf{x}]$ , where the notation  $\mathbb{E}^{\mathbf{x}}[\cdot]$  stands for taking expectation conditioned on  $X_0 = \mathbf{x}$ . The generator A of a process  $X_t$  can be then defined as

$$Af(\mathbf{x}) = \lim_{t \searrow 0} \frac{\mathbb{E}^{\mathbf{x}}[f(X_t)] - f(\mathbf{x})}{t} \quad \text{for} \quad f \in \mathcal{D}(A).$$
(7)

For time-homogeneous Itô process  $X_t$ , the time evolution is a Markov process. By letting  $T_t := \mathbb{E}^{\mathbf{x}}[f(X_t)]$ , we obtain a semigroup of operators:  $T = (T_t)_{t \ge 0}$ . Thinking from another perspective,  $Af = \lim_{t \searrow 0} \frac{T_t f - f}{t}$  can be regarded as the linear increment term (omitting all higher order terms) of the semigroup evolution. The next step is to calculate the generator A explicitly from the Itô diffusion SDE:  $dX_t = b(X_t)dt + \sigma(X_t)dB_t$ . Supposing f is of class  $C^2$ , by Taylor expansion and Itô's formula<sup>5</sup>, we have:

$$df(X_{t}) = f'(X_{t}) dX_{t} + \frac{1}{2} f''(X_{t}) d\langle X \rangle_{t} \\ = \left[ b(X_{t}) f'(X_{t}) + \frac{\sigma^{2}(X_{t})}{2} f''(X_{t}) \right] dt \quad ^{(8)} \\ + f'(X_{t}) \sigma(X_{t}) dB_{t}.$$

The notation  $d\langle X \rangle_t$  represents the quadrature variation of random process  $X_t$ , see [28]. Directly plugging Eq. (8) into Eq. (7) yields

$$Af(\mathbf{x}) = b(\mathbf{x})f'(\mathbf{x}) + \frac{\sigma^2(\mathbf{x})}{2}f''(\mathbf{x}).$$
 (9)

Eq. (9) is the generator of Itô diffusion corresponding to our MC system.

#### B. Boundary Value Problem for Elliptic PDE

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For MC systems located in a time-invariant and spatialhomogeneous fluid environment, we can restrict ourselves to the case that both  $b(\cdot)$  and  $\sigma(\cdot)$  are constants. Consider a PDE BVP with unknown function u:

$$\begin{cases} Au = 0 & \text{in } \Omega\\ u = g & \text{on } \partial\Omega \end{cases}$$
(10)

where g is some prescribed boundary data. Note that the right hand side of the first equation in (10) is zero. This means that there are no particle production and annihilation process in the fluid channel. For elliptic differential operators, BVPs are well studied, and the solution of (10) under common boundary conditions can be found in literature of PDE, for instance [25].

Let us discuss a simple example in more detail. Consider a half-space 3D domain with  $A = \nabla^2$  and a boundary condition:

$$u(x, y, z) = g(x, y)$$
 at  $z = 0.$  (11)

The solution of BVP (10) with (11) as boundary condition is well known and can be found in standard handbooks of PDE:

$$u(x,y,z) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{zg(\xi,\eta)d\xi d\eta}{\left[(x-\xi)^2 + (y-\eta)^2 + z^2\right]^{3/2}}.$$
(12)

Eq. (12) is called an integral representation formula in PDE language. Using Green's function, we can rewrite (12) as

$$u(x,y,z) = \int_{\partial\Omega} \left| \frac{\partial G(\xi,\eta,0;x,y,z)}{\partial \mathbf{n}} \right| g(\xi,\eta) d\xi d\eta, \quad (13)$$

where **n** is the normal unit vector of the boundary. We claim that the term  $\left|\frac{\partial G(\xi, \eta, 0; x, y, z)}{\partial \mathbf{n}}\right|$  is already the FAP density on the receiving plane. In this example, the BVP corresponds to no-drift pure diffusion. We will prove the above claim in Section III-C. The calculations for diffusion-with-drift case in 2D space are presented in Appendix A of [24].

<sup>&</sup>lt;sup>4</sup>We merely consider time-homogeneous Itô diffusion throughout this paper. That is,  $b(X_t)$  and  $\sigma(X_t)$  does not depend on t explicitly.

<sup>&</sup>lt;sup>5</sup>Itô's formula and Taylor expansion of an Itô process are standard results in stochastic analysis, see [27], [28].

## C. Dynkin's Formula and FAP Density

In this subsection, we will use the Dynkin's formula to clarify the relations between macroscopic and microscopic viewpoints of diffusion phenomena. During this clarification process, the FAP density is obtained incidentally.

Recall that the definition of an infinitestimal generator is  $Af(\mathbf{x}) = \lim_{t \searrow 0} \frac{\mathbb{E}^{\mathbf{x}}[f(X_t)] - f(\mathbf{x})}{t}$ . Rewriting the above equation into an integral form, we have

$$\mathbb{E}^{\mathbf{x}}\left[f\left(X_{t}\right)\right] = f(\mathbf{x}) + \mathbb{E}^{\mathbf{x}}\left[\int_{0}^{t} Af\left(X_{s}\right) ds\right].$$
 (14)

Note that the time t appeared in the above formula is a deterministic variable, not a random variable.

In stochastic analysis, Dynkin's formula is a theorem giving information about a diffusion process at a stopping time  $\tau$ (which is a random variable [28]). Let f be of class  $C^2$  with compact support and  $\tau$  be a stopping time with  $\mathbb{E}^{\mathbf{x}}[\tau] < +\infty$ . The Dynkin's formula can be stated as

$$\mathbb{E}^{\mathbf{x}}\left[f\left(X_{\tau}\right)\right] = f(\mathbf{x}) + \mathbb{E}^{\mathbf{x}}\left[\int_{0}^{\tau} Af\left(X_{s}\right) ds\right].$$
 (15)

With all these background materials at hand, we now show that how arbitrary FAP density is obtained by our newly proposed approach in principle. Let g be a smooth data defined on the boundary (i.e. the receiver plane) of the domain. We can write

$$\mathbb{E}^{\mathbf{x}}[g(X_{\tau})] = \mathbb{E}[g(X_{\tau}) \mid X_0 = \mathbf{x}] = \int_{\partial\Omega} f_{Y|X}(\mathbf{y}|\mathbf{x})g(\mathbf{y})d\mathbf{y}$$
(16)

by the definition of conditional probability density function (PDF). In Eq. (16),  $\mathbf{x} \in \Omega$  is the starting point of the diffusion; and since  $\tau$  is the hitting time, the hitting position  $\mathbf{y} \in \partial \Omega$ . Notice that the conditional PDF  $f_{Y|X}$  is exactly the desired FAP density distributed on the receiver boundary  $\partial \Omega$ .

Consider an Itô diffusion  $X_t$  and its corresponding generator A. Suppose we have a solution  $u(\mathbf{x})$  of the BVP problem (10) for some prescribed g. Then we plug  $f(\mathbf{x}) = u(\mathbf{x})$  into Eq. (15). The last term of Eq. (15) becomes

$$\int_0^\tau Au(X_s)ds = 0. \tag{17}$$

This is because  $0 < s < \tau$  and  $\tau$  is the first hitting time, so that  $X_s$  lies in  $\Omega$ , making  $u(X_s) = 0$ . On the other hand, the term on the left hand side of Eq. (15) becomes  $\mathbb{E}^{\mathbf{x}}[g(X_{\tau})]$  because  $u(\mathbf{x})$  coincides with  $g(\mathbf{x})$  on the boundary. Combining these two facts, we can get

$$\mathbb{E}^{\mathbf{x}}[g(X_{\tau})] = u(\mathbf{x}) = \int_{\partial\Omega} f_{Y|X}(\mathbf{y}|\mathbf{x})g(\mathbf{y})d\mathbf{y} \qquad (18)$$

for any  $\mathbf{x} \in \Omega$ .

Generically, for elliptic-type BVP defined in a domain V with boundary  $S = \partial V$ , we have

$$u(\mathbf{x}) = \int_{V} \Phi(\mathbf{y}) G(\mathbf{x}, \mathbf{y}) dV_{\mathbf{y}} + \int_{S} g(\mathbf{y}) H(\mathbf{x}, \mathbf{y}) dS_{\mathbf{y}} \quad (19)$$

where  $\Phi$  represents the source term,  $dV_{\mathbf{y}}$  is the volume element,  $dS_{\mathbf{y}}$  is the surface element, and the term  $H(\mathbf{x}, \mathbf{y})$ depends on which type of boundary conditions we are considering. If there is no molecule source reproducing MMs in the domain, we can set  $\Phi(\mathbf{y}) = 0$ . For the purpose of deriving FAP density, we consider the Dirichlet type boundary, which corresponds to

$$H(\mathbf{x}, \mathbf{y}) = -\frac{\partial G}{\partial \mathbf{n}_{\mathbf{y}}}(\mathbf{x}, \mathbf{y}).$$
 (20)

As a result, formula (19) reduces to

$$u(\mathbf{x}) = \int_{S} -\frac{\partial G}{\partial \mathbf{n}_{\mathbf{y}}}(\mathbf{x}, \mathbf{y}) g(\mathbf{y}) dS_{\mathbf{y}}.$$
 (21)

Finally, by comparing Eq. (18) and Eq. (21), we reveals an important relation between the FAP density and elliptic Green's function:

$$f_{Y|X}(\mathbf{y}|\mathbf{x}) = \left| \frac{\partial G}{\partial \mathbf{n}_{\mathbf{y}}}(\mathbf{x}, \mathbf{y}) \right|.$$
 (22)

Note that the left hand side of Eq. (22) always has a positive sign, so we add an absolute value on the right hand side for emphasis.

To conclude, Eq. (22) can be used to solve for FAP density as long as we know the Green's function. This method in principle works for higher n dimensional diffusion. By using generator of diffusion semigroup, we transform the original heat-type BVP (with time variable) into elliptic-type BVP (without time variable). Then we can look up solutions for the corresponding elliptic Green's functions in literature, such as [25], [26].

#### **IV. CONCLUSIONS**

In this paper, we fully resolve the FAP density problem for planar absorbing receivers in MC. Our approach is based on the theory of diffusion semigroups. The comparisons between the existing and our methods are listed in Table I. Through this semigroup approach, we integrate the existing FAP results in MC, and unified the process toward finding FAP in 2D and 3D.

Secondly, this is the first paper in MC to clarify in a rigorous way the mathematical link between the macroscopic and microscopic viewpoints for the diffusion mechanism in diffusion-based MC systems. Previous works in MC treat these two viewpoints separately. We hope this clarification could bring new insights into future theoretical MC system analysis.

Finally, we provided a self-contained proof for the formula proposed in [16] for 2D FAP density problem. We also make some improvements via relieving the restriction that the drift direction must point exactly toward the receiver. The calculation details are presented in Appendix A of [24].

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#### Appendix A

## CALCULATION OF FAP DENSITY IN 2D SPACE USING SEMIGROUP APPROACH

In this appendix section, we demonstrate how to calculate FAP density using semigroup approach proposed in Section III.

For two dimensional (2D) FAP density, we consider a 2D Itô diffusion  $X_t$  with its semigroup generator A as

$$A = \sum_{i=1}^{2} v_i \frac{\partial}{\partial x_i} + \frac{\sigma^2}{2} \sum_{i=1}^{2} \frac{\partial^2}{\partial x_i^2}.$$
 (23)

In the above equation, the term  $v_i$  stands for the *i*-th component of the drift velocity **v**. Let us denote the Laplacian operator in 2D by  $\Delta_2$  and consider the following BVP in Cartesian coordinate:

$$\begin{cases} A(u) = \sum_{i=1}^{2} v_i \frac{\partial u}{\partial x_i} + \frac{\sigma^2}{2} \Delta_2 u = 0 & \text{in } \Omega\\ u = g & \text{on } \partial \Omega \end{cases}, \quad (24)$$

where u is a (dummy) unknown function. Set the domain of BVP (24) to be

$$\Omega = \mathbb{R}^2 \cap \{x_2 > 0\}, \qquad (25)$$

and the boundary to be

$$\partial \Omega = \mathbb{R}^2 \cap \{x_2 = 0\}.$$
(26)

Here we use the notation  $x_j$  to denote the *j*-th component of the position vector  $\mathbf{x} = (x_1, \dots, x_n)$ . For the purpose of compatibility to higher dimensional cases, we arrange the basis order of the Cartesian coordinate so that the direction of the last component is parallel to the transmission direction.

The BVP (24) is not in a common resolved form in standard PDE solution tables such as [25]. However, we can use a change of variables to transform (24) into a Helmholtz equation. Before proceeding further, we temporarily set  $\sigma^2 = 1$  to avoid cumbersome calculations. After obtaining the final result, we will then replace  $v_i$  with  $\frac{v_i}{\sigma^2}$  to recover the solution for general  $\sigma^2$  which is not necessarily equal to 1.

Suppose u is the solution of BVP (24) with  $\sigma^2 = 1$ . That is, u satisfies  $\sum_{i=1}^{2} v_i \frac{\partial u}{\partial x_i} + \frac{1}{2}\Delta_2 u = 0$  in the domain  $\Omega$ , and coincides with the function g on the boundary  $\partial\Omega$ . We define a drift factor  $\gamma$  to facilitate later calculations; the drift factor is defined as follows:

$$\gamma(\mathbf{x}) := \exp\{\mathbf{v} \cdot \mathbf{x}\} = \exp\{v_1 x_1 + v_2 x_2\}, \qquad (27)$$

where  $\mathbf{v} \cdot \mathbf{x}$  denotes the standard inner product in  $\mathbb{R}^2$ . We consider an alternative function  $w(\mathbf{x}) = \gamma(\mathbf{x})u(\mathbf{x})$ . Plugging  $u(\mathbf{x}) = \frac{w(\mathbf{x})}{\gamma(\mathbf{x})}$  into BVP (24) yields

$$\frac{1}{\gamma(\mathbf{x})} \left[ \Delta_2 w(\mathbf{x}) - \left( v_1^2 + v_2^2 \right) w(\mathbf{x}) \right] = 0.$$
 (28)

Next, by letting

$$s = |\mathbf{v}| = \sqrt{v_1^2 + v_2^2},$$
 (29)

we can deduce that w satisfies the Helmholtz equation:

$$\Delta_2 w - s^2 w = 0 \quad (s \ge 0).$$
 (30)

The Helmholtz equation can be regarded as the eigenvalue problem of Laplacian operator; its solution form can be found in standard PDE books [25]. To solve w, we consider another BVP described by the Helmholtz equation:

$$\begin{cases} H(w) = \Delta_2 w - s^2 w = 0 & \text{in } \Omega\\ w = \tilde{g} & \text{on } \partial\Omega \end{cases}, \quad (31)$$

where  $H(\cdot)$  is the Helmholtz operator. Note that new boundary data  $\tilde{g}$  satisfies

$$\tilde{g}(\mathbf{y}) = e^{v_1 y_1} g(\mathbf{y}) \quad \text{for} \quad \mathbf{y} \in \partial\Omega$$
(32)

since  $y_2 = 0$  on the boundary.

The next step is to look up a representation formula of solution of BVP (31) in the literature. The following equations (33, 34, 35, 36) are all cited from [25]. Let the domain be  $-\infty < x_1 < \infty, 0 \leq x_2 < \infty$  and consider a first-type boundary condition<sup>6</sup> as:

$$w(x_1, 0) = g(x_1)$$
 at  $x_2 = 0.$  (33)

The solution of BVP (31) can be written down using the following representation formula:

$$w(x_1, x_2) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(\xi) \left[ \frac{\partial}{\partial \eta} G(x_1, x_2, \xi, \eta) \right]_{\eta=0} d\xi.$$
(34)

where the Green's function appeared in Eq. (34) has the form

$$G(x_1, x_2, \xi, \eta) = \frac{1}{2\pi} [K_0(s\rho_1) - K_0(s\rho_2)]$$
(35)

with

$$\rho_1 = \sqrt{(x_1 - \xi)^2 + (x_2 - \eta)^2},$$
  

$$\rho_2 = \sqrt{(x_2 - \xi)^2 + (x_2 + \eta)^2}.$$
(36)

Interested readers can refer to [29] for more details about the derivation of this Green's function.

Now we let  $\mathbf{x} = (x_1, x_2)$ ,  $\mathbf{y} = (\xi, \eta)$ . Based on the methodology presented in Section III, we know that

$$w(\mathbf{x}) = \int_{\partial\Omega} \left| \frac{\partial G(\mathbf{x}, \mathbf{y})}{\partial \mathbf{n}_{\mathbf{y}}} \right| \tilde{g}(\mathbf{y}) d\mathbf{y}.$$
 (37)

<sup>6</sup>First-type boundary condition, also known as Dirichlet boundary condition, means that we prescribe the values of the unknown function on the boundary. Here, the notation  $\left|\frac{\partial G(\mathbf{x},\mathbf{y})}{\partial \mathbf{n}_{\mathbf{y}}}\right|$  is the partial derivative of G with respect to the unit vector normal to the boundary  $\partial\Omega$ . Using the fact that  $K'_0(x) = -K_1(x)$ , we calculate

$$\begin{aligned} \frac{\partial G}{\partial \eta} \Big|_{\eta=0} \\ &= \left[ \frac{\partial G}{\partial \rho_1} \frac{\partial \rho_1}{\partial \eta} + \frac{\partial G}{\partial \rho_2} \frac{\partial \rho_2}{\partial \eta} \right]_{\eta=0} \\ &= \frac{-s}{2\pi} K_1 \left( s \sqrt{(x_1 - \xi)^2 + x_2^2} \right) \frac{-x_2}{\sqrt{(x_1 - \xi)^2 + x_2^2}} \qquad (38) \\ &+ \frac{s}{2\pi} K_1 \left( s \sqrt{(x_1 - \xi)^2 + x_2^2} \right) \frac{x_2}{\sqrt{(x_1 - \xi)^2 + x_2^2}} \\ &= \frac{|\mathbf{v}|_{x_2}}{\pi} \frac{K_1 \left( |\mathbf{v}| \sqrt{(x_1 - \xi)^2 + x_2^2} \right)}{\sqrt{(x_1 - \xi)^2 + x_2^2}}. \end{aligned}$$

To obtain a representation formula for the solution u of the original BVP (24), we substitute  $w(\mathbf{x}) = \gamma(\mathbf{x})u(\mathbf{x})$  into Eq. (37), yielding

$$u(\mathbf{x}) = \frac{w(\mathbf{x})}{\gamma(\mathbf{x})} = \exp\{-\mathbf{v} \cdot \mathbf{x}\} \int_{\partial\Omega} \left| \frac{\partial G(\mathbf{x}, \mathbf{y})}{\partial \mathbf{n}_{\mathbf{y}}} \right| \tilde{g}(\mathbf{y}) d\mathbf{y}$$
$$= \int_{\partial\Omega} \exp\{v_1 y_1 - v_1 x_1 - v_2 x_2\}$$
$$\left[ \frac{\partial G}{\partial \rho_1} \frac{\partial \rho_1}{\partial \eta} + \frac{\partial G}{\partial \rho_2} \frac{\partial \rho_2}{\partial \eta} \right]_{\eta=0} g(y_1) dy_1 , \quad (39)$$
$$= \int_{\partial\Omega} K_{\mathbf{v}}(\mathbf{x}, \xi) g(\xi) d\xi$$

where  $K_{\mathbf{v}}(\mathbf{x},\xi)$  is the integral kernel which we want to determine. Note that in the second equality of (39), we have used the relation  $\tilde{g}(\mathbf{y}) = e^{\mathbf{v} \cdot \mathbf{x}} g(\mathbf{y})$ .

Now we let  $x_2 = d > 0$  to be the transmission distance between Tx and Rx. By examining Eq. (38) and Eq. (39), we obtain an exact formula for the integral kernel  $K_{\mathbf{v}}(\mathbf{x}, \xi)$ :

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$$K_{\mathbf{v}}(\mathbf{x},\xi) = \exp\left\{v_{1}\xi - v_{1}x_{1} - v_{2}d\right\} \left[\frac{\partial G}{\partial\rho_{1}}\frac{\partial\rho_{1}}{\partial\eta} + \frac{\partial G}{\partial\rho_{2}}\frac{\partial\rho_{2}}{\partial\eta}\right]_{\eta=0}$$

$$= \frac{|v|d}{\pi}\exp\{-v_{2}d\}\exp\{-v_{1}(x_{1}-\xi)\}$$

$$\cdot \frac{K_{1}\left(|\mathbf{v}|\sqrt{(x_{1}-\xi)^{2}+d^{2}}\right)}{\sqrt{(x_{1}-\xi)^{2}+d^{2}}}.$$

$$(40)$$

To tackle with the general case  $\sigma^2 \neq 1$ , we can simply replace  $v_i$  with  $\frac{v_i}{\sigma^2}$ , yielding

$$f_{Y|X}(\mathbf{y}|\mathbf{x}) = \frac{|\mathbf{v}|d}{\sigma^2 \pi} \exp\left\{\frac{-v_2 d}{\sigma^2}\right\} \exp\left\{\frac{-v_1(x_1 - \xi)}{\sigma^2}\right\}$$
$$\cdot \frac{K_1\left(\frac{|\mathbf{v}|}{\sigma^2}\sqrt{(x_1 - \xi)^2 + d^2}\right)}{\sqrt{(x_1 - \xi)^2 + d^2}},$$
(41)

where  $\mathbf{x} = (x_1, d), \mathbf{y} = (\xi, 0)$ , and d is the distance between Tx and Rx. Eq. (41) is the desired conditional density function, allowing arbitrary drift directions, for 2D FAP problem.

In order to make a comparison to the restrictive version in [16, Eq. (19)], we can set  $v_1 = 0$  in Eq. (41), yielding

$$f_{Y|X}(\mathbf{y}|\mathbf{x}) = \frac{|\mathbf{v}|d}{\sigma^{2}\pi} \exp\left\{\frac{-v_{2}d}{\sigma^{2}}\right\} \frac{K_{1}\left(\frac{|\mathbf{v}|}{\sigma^{2}}\sqrt{(x_{1}-\xi)^{2}+d^{2}}\right)}{\sqrt{(x_{1}-\xi)^{2}+d^{2}}}$$
(42)
$$= \frac{|\mathbf{v}|d}{2\pi D} \exp\left\{\frac{-v_{2}d}{2D}\right\} \frac{K_{1}\left(\frac{|\mathbf{v}|}{2D}\sqrt{(x_{1}-\xi)^{2}+d^{2}}\right)}{\sqrt{(x_{1}-\xi)^{2}+d^{2}}},$$

where we use the relation  $\sigma^2 = 2D$ .

# Appendix B The Old Method: Separation of Variables and Method of Image

For the sake of completeness, we review in a self-contained fashion the original approach to finding FAP density function as proposed in [16]. Throughout this appendix section, we set the *x*-direction to be the direction of transmission, i.e. the direction pointing from Tx to Rx.

#### A. Finding the Green's Function for Free Space

For a 2-dimensional (2D) diffusion channel with a constant drift velocity  $\mathbf{v} = (v, 0)$  pointing from the transmitter to the receiver along the *x*-axis, equation (4) can be written explicitly as

$$\frac{\partial c(x,y,t)}{\partial t} + v \frac{\partial c(x,y,t)}{\partial x} = D\left(\frac{\partial^2 c(x,y,t)}{\partial x^2} + \frac{\partial^2 c(x,y,t)}{\partial y^2}\right)$$
(43)

where  $c(x, y, 0) = \delta(x - x_0) \delta(y - y_0)$  is the 2D Dirac delta function. The boundary condition is set to be:

$$c(x, y, t) = 0$$
 for  $x, y \in \partial\Omega$ , (44)

representing an absorbing receiver.

Using separation of variables, the concentration field c(x, y, t) can be written as

$$c(x, y, t) = c_1(x, t)c_2(y, t).$$
(45)

By plugging Eq. (45) back into Eq. (43), we get two separated equations

$$\frac{\partial c_1}{\partial t} + v \frac{\partial c_1}{\partial x} - D \frac{\partial^2 c_1}{\partial x^2} = 0, \tag{46}$$

$$\frac{\partial c_2}{\partial t} - D \frac{\partial^2 c_2}{\partial y^2} = 0.$$
(47)

The *fundamental solutions* (aka free space Green's function) of Eq. (46) and Eq. (47) are

$$c_1(x,t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{(x-x_0-vt)^2}{4Dt}\right)$$
 (48)

and

$$c_2(y,t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{(y-y_0)^2}{4Dt}\right)$$
 (49)

respectively. Hence, the free space Green's function of (43) can be written as the product of Eq. (48) and Eq. (49):

$$G(x, y, x_0, y_0, t) = \frac{1}{4\pi Dt} \exp\left(\frac{-(x - x_0 - vt)^2 - (y - y_0)^2}{4Dt}\right).$$
 (50)

## B. Finding the Green's Function for Absorbing Boundary

For Eq. (50), we have not yet taken the boundary conditions into account. Since the receiver is assume to be perfectly absorbing, we require the concentration to be zero on the boundary, as Eq. (44) shows.

There is one well-known method, originated in classical electrodynamics, that works well in problems of finding static distributions for flat boundaries, called *the method of image*, see [30]. Since we only care about the concentration function inside the domain, we can effectively put an "mirror image" of negative mass at the reflection point of the original releasing point. Using this method, the domain of the original unknown function is not extended, but the function is made to satisfy given boundary conditions, such as absorbing boundary in our case.

To use the method of image, we write

$$G_{abs}(x, y, x_0, y_0, t) = G(x, y, x_0, y_0, t) - a(x_0)G(x, y, -x_0, y_0, t)$$
(51)

and then solve for  $a(x_0)$ . Note that the subscript "abs" stands for absorbing. The absorbing boundary condition requires that

$$a(x_0) = \frac{G(0, y, x_0, y_0, t)}{G(0, y, -x_0, y_0, t)} = \exp\left(-\frac{x_0 v}{D}\right).$$
 (52)

We can now write down the Green's function for absorbing boundary as

$$G_{abs}(x, y, x_0, y_0, t) = \frac{1}{4\pi Dt} \left[ \exp\left(-\frac{(x - x_0 - vt)^2 + (y - y_0)^2}{4Dt}\right) \right] .$$
 (53)  
$$- \exp\left(-\frac{x_0 v}{D} - \frac{(x + x_0 - vt)^2 + (y - y_0)^2}{4Dt}\right) \right]$$

# C. From Green's function to FAP Density

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Consider a quantity called *diffusive flux* J(0, y, t) at x = 0 plane, which possesses a physical unit of particle density per unit length per unit time. By Fick's law, we know that

$$J(0, y, t) = -D \frac{\partial G_{abs}(x, y, x_0, y_0, t)}{\partial x}.$$
 (54)

Using the absorbing Green's function formula as shown in Eq. (53), we can calculate the flux explicitly, yielding

$$J(0, y, t) = -\frac{x_0}{4\pi Dt^2} \exp\left(-\frac{(x_0 + vt)^2 + (y - y_0)^2}{4Dt}\right).$$
(55)

Note that the original formula [16, Eq. (14)] has some calculation error, so we correct the formula herein.

Our goal is to find the FAP density  $f(\mathbf{y}|\mathbf{x})$ . Let  $\mathbf{x} = (x_0, y_0)$  denote the point of release of the information molecule and  $\mathbf{y} = (x, y)$  its arrival position at the receiver boundary. The conditional PDF of Y at a receiver located at x = 0 is given as

$$f_{Y|X}(0, y \mid x_0, y_0) = \int_0^\infty J(0, y, t) dt .$$
 (56)

Plugging the diffusion flux we just obtained in Eq. (55) into Eq. (56), we have

$$f_{Y|X}(0, y \mid x_0, y_0) = -\int_0^\infty \frac{x_0}{4\pi Dt^2} \exp\left(-\frac{(x_0 + vt)^2 + (y - y_0)^2}{4Dt}\right) \mathrm{d}t.$$
(57)

In order to calculate this integration explicitly, we rearrange the terms to get

$$f_{Y|X}(0, y \mid x_0, y_0) = \frac{-x_0}{4\pi D} \exp\left(-\frac{x_0 v}{2D}\right) \times \int_0^\infty \frac{1}{t^2} \exp\left(-\frac{x_0^2 + (y - y_0)^2}{4Dt} - \frac{v^2 t}{4D}\right) dt.$$
(58)

Letting  $K_s(z)$  be the modified Bessel function of the second kind of order s, for positive constants a and b, we have the relation [31]:

$$\int_{0} t^{-s-1} \exp\left(-\left(\frac{a}{t}+bt\right)\right) \mathrm{d}t = 2\left(\frac{b}{a}\right)^{s/2} K_s(2\sqrt{ab}),$$
(59)

where s and z are real and complex numbers respectively. Combining Eq. (58) and Eq. (59) with  $x_0 = d$ , we finally get

$$f(\mathbf{y}|\mathbf{x}) = f_{Y|X}(0, y \mid d, y_0)$$
  
=  $\frac{|v|d}{2\pi D} \exp\left(\frac{-dv}{2D}\right) \frac{1}{\sqrt{\left(d^2 + (y - y_0)^2\right)}}$ (60)  
 $\cdot K_1\left(\frac{|v|\sqrt{\left(d^2 + (y - y_0)^2\right)}}{2D}\right).$ 

It is worth noting that the conditional FAP density as shown in Eq. (60) depends only on  $y - y_0$ , but not on time variable t. We can conclude that the FAP channel is an additive timeinvariant channel.