Statistical Science
2013, Vol. 28, No. 4, 487–509
DOI: 10.1214/13-STS442

Advection–Dispersion Across Interfaces

Jorge M. Ramirez, Enrique A. Thomann and Edward C. Waymire

Abstract. This article concerns a systemic manifestation of small scale interfacial heterogeneities in large scale quantities of interest to a variety of diverse applications spanning the earth, biological and ecological sciences. Beginning with formulations in terms of partial differential equations governing the conservative, advective-dispersive transport of mass concentrations in divergence form, the specific interfacial heterogeneities are introduced in terms of (spatial) discontinuities in the diffusion coefficient across a lower-dimensional hypersurface. A pathway to an equivalent stochastic formulation is then developed with special attention to the interfacial effects in various functionals such as first passage times, occupation times and local times. That an appreciable theory is achievable within a framework of applications involving one-dimensional models having piecewise constant coefficients greatly facilitates our goal of a gentle introduction to some rather dramatic mathematical consequences of interfacial effects that can be used to predict structure and to inform modeling.

Key words and phrases: Skew Brownian motion, heterogeneous dispersion, interface, local time, occupation time, breakthrough curve, ocean upwelling, mathematical ecology, solute transport, river network dispersion, insect dispersion.

1. INTRODUCTION

To set the perspective of this article, let us first consider classic advection–dispersion phenomena in $\mathbb{R}^k$ of a concentration of particles immersed in a fluid as described by the following partial differential equation for $\mathbf{x} \in \mathbb{R}^k$ and $t \geq 0$:

$$\begin{aligned}\frac{\partial u}{\partial t} &= \frac{1}{2}\nabla \cdot \bigl(\mathbf{D}(\mathbf{x})\nabla u(t,\mathbf{x})\bigr)\\ &\quad - \nabla \cdot \bigl(\mathbf{v}(\mathbf{x})u(t,\mathbf{x})\bigr), \qquad (1.1)\\ u\bigl(0^+,\mathbf{x}\bigr) &= u_0(\mathbf{x}).\end{aligned}$$

In particular, assume that the coefficients $\mathbf{D}$ and $\mathbf{v}$ are smooth (matrix/vector-valued) functions[1] on $\mathbb{R}^k$, $\nabla = \sum_{j=1}^k \frac{\partial}{\partial x_j}$. Such an equation describes the evolution of an initial (scalar) mass concentration u_0 evolving at a temporal rate assumed to be locally controlled by spatial fluxes $\frac{1}{2}\mathbf{D}(\mathbf{x})\nabla u(t,\mathbf{x}) - \mathbf{v}(\mathbf{x})u(t,\mathbf{x})$. The first term expresses Fick's law of flux as being proportional to the concentration gradient, and the second term being the advection of mass by fluid velocity. Many physical as well as biological/ecological problems take this form, perhaps on a spatial domain $\mathbf{G} \subseteq \mathbb{R}^k$, with appropriate boundary conditions, such as Dirichlet or Neumann boundary conditions. The success of nineteenth- and twentieth-century mathematical developments in analysis, geometry and numerical computation continues to guide research into the 21st century. In particular, this single linear partial differential equation has inspired a body of mathematical research that is likely unmatched in diversity and scope.

Jorge M. Ramirez is Associate Professor of Mathematics, Escuela de Matemáticas, Universidad Nacional de Colombia Sede Medellín, Medellín, Colombia (e-mail: jmramirezo@unalmed.edu.co). Enrique A. Thomann and Edward C. Waymire are Professors of Mathematics, Department of Mathematics, Oregon State University, Corvallis, Oregon, USA (e-mail: thomann@math.oregonstate.edu; waymire@math.oregonstate.edu).

[1]Throughout this article we restrict attention to time homogeneous equations.

The pervasive role of (1.1) in the development of probability and statistical theory is therefore no surprise. The recognition of the fundamental role of standard Brownian motion $\mathbf{B} = \{\mathbf{B}(t) : t \geq 0\}$ and the corresponding Itô's stochastic calculus opened the door to a more natural reformulation of advective-dispersive phenomena in terms of the stochastic differential equation

$$\mathrm{d}\mathbf{X}(t) = \tilde{\mathbf{v}}(\mathbf{X}(t))\,\mathrm{d}t + \sqrt{\mathbf{D}(\mathbf{X}(t))}\,\mathrm{d}\mathbf{B}(t), \quad t > 0, \mathbf{X}(0) = \mathbf{x}, \tag{1.2}$$

relating the conditional distribution $p(t, \mathbf{x}, \mathrm{d}\mathbf{y})$ of $\mathbf{X}(t)$ given $\mathbf{X}(0) = \mathbf{x}$, that is, the transition probabilities, to the fundamental solution of (1.1) via the basic semigroup formula

$$u(t, \mathbf{x}) = \int_{\mathbb{R}^k} u_0(\mathbf{y}) p(t, \mathbf{x}, \mathrm{d}\mathbf{y}). \tag{1.3}$$

In (1.2), $\sqrt{\mathbf{D}}$ is the matrix square root of the molecular dispersion tensor $\mathbf{D}$, which augments the macroscopic advection $\mathbf{v}$ via

$$\tilde{\mathbf{v}}(\mathbf{x}) = \left(-\sum_j \frac{1}{2} \frac{\partial D_{ji}}{\partial x_j}(\mathbf{x}) + v_i(\mathbf{x})\right)_{1 \leq i \leq k}. \tag{1.4}$$

The Markov process $\mathbf{X}$ so determined becomes the probabilistic representation of the object of interest in relation to the p.d.e. (1.1), be it physical, biological or perhaps financial.

Not only does a stochastic framework enable new approaches to the analysis of problems related to (1.1), but it inspires still more diverse ways in which to model, analyze and measure naturally occurring phenomena. After all, the coefficients $\mathbf{v}$ and $\mathbf{D}$ now admit a statistical interpretation! The significance of this fact was made manifestly clear through the observations and measurements of Perrin (1913) in his historic determination of Avogadro's constant, following up Einstein's 1905 theory of the molecular structure of matter. In addition, new models that may be a priori less obvious to formulate at the scale of (1.1) emerge to describe phenomena at the scale of particle trajectories as observed in certain financial data or biological experiments (see, e.g., Decamps, Goovaerts and Schoutens, 2006; Fagan, Cantrell and Cosner, 1999). Moreover, in the context of particle trajectories, a wide variety of sample path functionals, such as first passage times, escape and occupation times, and local times also emerge naturally in both theory and applications.

From a probabilistic perspective, the smoothness of the coefficients in (1.1) goes a long way toward the alternative view expressed through (1.2) of particle trajectories being (approximately) shifts and rescalings of a standard Brownian motion when observed locally (infinitesimally) in time. In particular, if the coefficients are in fact constant, then the solution to (1.2) is a Brownian motion

$$\mathbf{X}(t) = \mathbf{x} + \mathbf{v}t + \sqrt{\mathbf{D}}\mathbf{B}(t), \quad t \geq 0, \tag{1.5}$$

with *drift coefficient* $\tilde{\mathbf{v}} \equiv \mathbf{v}$, and *diffusion coefficient* $\mathbf{D}$, whose transition probabilities $p(t, \mathbf{x}, \mathbf{y})$, assuming nonsingularity ($\det \mathbf{D} \neq 0$), provide the fundamental solution to

$$\frac{\partial u}{\partial t} = \frac{1}{2}\mathbf{D}\Delta u + \mathbf{v} \cdot \nabla u \tag{1.6}$$

with Laplacian $\Delta \equiv \nabla \cdot \nabla = \sum_{j=1}^k \frac{\partial^2}{\partial {x_j}^2}$, that is, differentiation with respect to the backward variable $\mathbf{x}$. More generally, assuming sufficient smoothness of coefficients, (1.1) may be directly recast after relabeling $\mathbf{x}$ as $\mathbf{y}$, in the form of *Kolmogorov's forward equation*, or the *Fokker–Planck equation* as it is called in the physical sciences,

$$\frac{\partial u}{\partial t}(t, \mathbf{y}) = \frac{1}{2} \sum_{i,j} \frac{\partial^2 (D_{ij}(\mathbf{y}) u(t, \mathbf{y}))}{\partial y_i\, \partial y_j} - \sum_i \frac{\partial (\tilde{v}_i(\mathbf{y}) u(t, \mathbf{y}))}{\partial y_i}, \tag{1.7}$$

where $\tilde{\mathbf{v}}$ already appeared in (1.4). Note that this is merely an equivalent way in which to express the equation (1.1), with the relabeling of variables suggested by their respective roles as backward and forward variables in the transition probabilities $p(t, \mathbf{x}, d\mathbf{y})$. On the other hand, *Kolmogorov's backward equation*, with (1.6) as a special case, is obtained from (1.7) by integration by parts as the adjoint

$$\frac{\partial u}{\partial t}(t, \mathbf{x}) = \frac{1}{2} \sum_{i,j} D_{ij}(\mathbf{x}) \frac{\partial^2 u}{\partial x_i\, \partial x_j}(t, \mathbf{x}) + \sum_i \tilde{v}_i(\mathbf{x}) \frac{\partial u}{\partial x_i}(t, \mathbf{x}). \tag{1.8}$$

As will be discussed as the primary point of the present article, there are phenomena for which the smoothness of the coefficients is untenable. The particular "nonsmoothness" of focus here can most generally be framed as a discontinuity, of otherwise (piecewise) continuous coefficients, on a hypersurface of co-dimension one. This includes discontinuities at (0-dimensional) points in one dimension or across a curve in two dimensions.

Advection–dispersion was framed in terms of the k-dimensional model (1.1) in an effort to frame the *big* problems for continued research. However, there is much yet to be learned about interfacial problems in dimensions greater than one. Perhaps surprisingly, but indeed fortunately, the applications involving one-dimensional processes are already extensive enough to provide a rich source of examples with features of both mathematical and empirical interest, especially as manifested in the behavior of the functionals noted earlier. One may also expect that some results in one dimension will at least partially inform higher-dimensional problems.

Just as standard Brownian motion plays a basic, albeit secondary, role in constructing the Markov process X associated with (1.1) in the case of smooth coefficients via (1.2), a class of *skew Brownian motions* will emerge in the construction of the Markov processes (termed *skew diffusions*) associated with one-dimensional advection–dispersion across an interface. *Skew Brownian motion* $B^{(\alpha)} = \{B^{(\alpha)}(t) : t \geq 0\}, 0 < \alpha < 1$ is a continuous semimartingale introduced by Itô and McKean (1963). Fundamental papers on skew Brownian motion by Harrison and Shepp (1981), Walsh (1978), Ouknine (1990) and Le Gall (1984) are summarized in a mathematically comprehensive survey article by Lejay (2006). Interesting fresh ideas on some of the foundational questions about skew Brownian motion continue to emerge, for example, Hairer and Manson (2010), Prokaj (2011) and Fernholz, Ichiba and Karatzas (2013). These provide a number of equivalent ways in which to view skew Brownian motion on which the present survey article will build. It is not our intention to provide a mathematically comprehensive survey of skew Brownian motion.[2] Indeed, the primary focus here is on the Markov process (skew diffusion) associated with advection–dispersion across an interface in one dimension. Our goal is to provide a simple, focused mathematical framework of skew diffusion in which to then illustrate rather dramatic consequences of *interfacial effects* pertaining to specific physical and biological phenomena.

Just as with the case of smooth coefficients, the analysis, in terms of both partial differential and stochastic differential equations, the numeric computational schemes, and the statistical aspects of advection–dispersion across an interface, relate to each other in an interesting mathematical interplay. Accordingly, as will be illustrated by examples, empirical observations in this context often point to new and interesting phenomena amenable to mathematical explanation or prediction.

Therein lies the overarching goal of this article. Namely, within the context of the Mathematics of Planet Earth and International Year of Statistics 2013 initiatives, we seek to illustrate some of the mathematical structure reflected in observed and predicted large scale properties of advection–dispersion as a consequence of locally defined *interfacial discontinuities* of the type described above. For example, results are described that quantify the dramatic effect of a (small scale) point discontinuity on the behavior of occupation times of large scale regions in one dimension. This is achieved by identification and analysis of the basic Markov process associated with the given coefficients. That this is in fact achievable within a framework of one-dimensional models with piecewise constant coefficients facilitates our goal of a gentle introduction to results that are also relevant to a diverse range of applications to be described herein.

The organization of the paper is as follows: in Section 1 skew Brownian motion and its properties are introduced in a broader context of dispersion of a solute in the presence of a so-called *conservative interface condition*, that is, physical skew diffusion. This is followed by subsequent sections to provide illustrations of some more general (nonconservative) interface conditions that arise naturally in the physical and biological sciences, including free surface heights in ocean upwellings, animal movement models in ecology and dispersion in a river network. Building on these examples, a summary of complementary results and open problems inspired by these examples is provided in the closing section.

2. ONE-DIMENSIONAL PHYSICAL SKEW DIFFUSION AND SKEW BROWNIAN MOTION

Building on the theme laid out in the Introduction, the Markov process to be referred to as one-dimensional *physical skew diffusion* with parameters $D^+ > 0$, $D^- > 0$ $(v = 0)$ will be defined in relation to the following continuity equation for a solute immersed in fluid medium separated by a point interface at the origin:

$$\frac{\partial u}{\partial t}(t, x) = \frac{1}{2} D(x) \frac{\partial^2 u}{\partial x^2}(t, x) \quad (x \neq 0), \tag{2.1}$$

[2] The survey article Lejay (2006) in fact fills this need quite thoroughly and is recommended as follow-up to the present article.

$$D^+ \frac{\partial u}{\partial x}(t, 0^+) = D^- \frac{\partial u}{\partial x}(t, 0^-),$$
$$u(t, 0^+) = u(t, 0^-), t > 0,$$

where

(2.2) $$D(x) = \begin{cases} D^+, & \text{if } x > 0, \\ D^-, & \text{if } x \le 0. \end{cases}$$

The particular interface condition

(2.3) $$D^+ \frac{\partial u}{\partial x}(t, 0^+) = D^- \frac{\partial u}{\partial x}(t, 0^-)$$

ensures that the diffusive *flux* $D(x)\frac{\partial u}{\partial x}(t, x)$ is continuous at all $x \in \mathbb{R}$ and for all $t > 0$. Moreover, it yields "conservation of mass" $\int_{-\infty}^{\infty} u(t, x)\,\mathrm{d}x = \int_{-\infty}^{\infty} u(0, x)\,\mathrm{d}x$, $t > 0$, since after integration by parts, one has

(2.4) $$\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty} u(t, x)\,\mathrm{d}x = 0.$$

In particular, this interface condition makes the spatial operator in (2.1) formally self-adjoint.

The simplest approach to identify the corresponding physical skew diffusion process is perhaps by explicitly solving (2.1). Indeed, for any initial condition $u(0, x) = u_0(x)$, equation (2.1) has solution $u(t, y) = \int_{-\infty}^{\infty} p^*(t, x, y)u_0(x)\,\mathrm{d}x$ where the fundamental solution $p^*(t, x, y)$ can be simply checked to be (see Ramirez et al., 2006)

(2.5)
$$p^*(t, x, y) = \begin{cases} \frac{1}{\sqrt{2\pi D^+ t}}\left[\exp\left\{\frac{-(y-x)^2}{2D^+ t}\right\} + \frac{\sqrt{D^+}-\sqrt{D^-}}{\sqrt{D^-}+\sqrt{D^+}}\exp\left\{\frac{-(y+x)^2}{2D^+ t}\right\}\right], \\ \quad x > 0, y > 0, \\ \frac{1}{\sqrt{2\pi D^- t}}\left[\exp\left\{\frac{-(y-x)^2}{2D^- t}\right\} - \frac{\sqrt{D^+}-\sqrt{D^-}}{\sqrt{D^+}+\sqrt{D^-}}\exp\left\{\frac{-(y+x)^2}{2D^- t}\right\}\right], \\ \quad x < 0, y < 0, \\ \frac{2}{\sqrt{D^+}+\sqrt{D^-}}\frac{1}{\sqrt{2\pi t}} \cdot \exp\left\{-\frac{(y\sqrt{D^-}-x\sqrt{D^+})^2}{2D^-D^+ t}\right\}, \\ \quad x \le 0, y \ge 0, \\ \frac{2}{\sqrt{D^+}+\sqrt{D^-}}\frac{1}{\sqrt{2\pi t}} \cdot \exp\left\{-\frac{(y\sqrt{D^+}-x\sqrt{D^-})^2}{2D^-D^+ t}\right\}, \\ \quad x \ge 0, y \le 0. \end{cases}$$

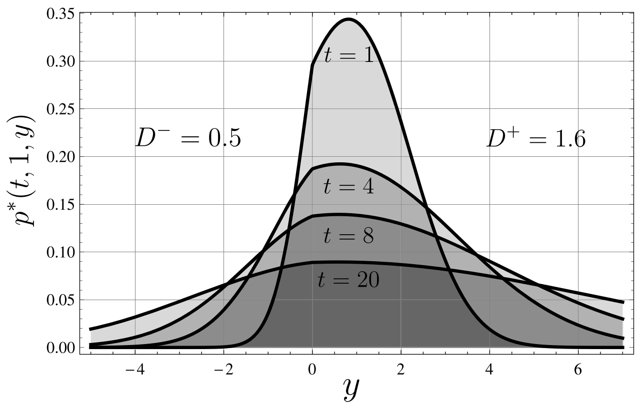

FIG. 1. *Plots of $p^*(t, x, y)$ for $x = 1$, several values of tk and fixed $D^+ > D^-$.*

See Figure 1. Observe that while

(2.6) $$p^*(t, x, y) = p^*(t, y, x), \quad x, y \in \mathbb{R}, t > 0,$$

there is nonetheless a "skewness asymmetry" around the interface exhibited in the calculation

(2.7) $$\int_{[0,\infty)} p^*(t, 0, y)\,\mathrm{d}y = \frac{\sqrt{D^+}}{\sqrt{D^+}+\sqrt{D^-}}.$$

To prepare for the definition of skew Brownian motion, let $B = \{B(t): t \ge 0\}$ denote standard Brownian motion started at $B(0) = 0$, and let $A = \{A_n : n = 1, 2, \ldots\}$ be an i.i.d. sequence of ± 1-valued Bernoulli random variables with $\alpha = P(A_n = 1)$, independent of B, defined on a common probability space $(\Omega, \mathcal{F}, P)$. Since the paths $t \to B(t)$ are continuous, the complement to the closed subset $B^{-1}(\{0\})$ is a countable disjoint union of (random) open intervals of $[0, \infty)$ enumerated as $J_1, J_2, \ldots$; see Figure 2.

DEFINITION 2.1 (α-skew Brownian motion). Let $\alpha \in [0, 1]$. The stochastic process given by

$$B^{(\alpha)}(t) = \sum_{n=1}^{\infty} A_n \mathbb{1}_{J_n}(t)|B(t)|, \quad t \ge 0,$$

is referred to as *skew Brownian motion with transmission parameter* α starting at 0.

REMARK 2.1. The cases $\alpha = 0, 1$ correspond to reflecting Brownian motion $B^{(0)} = -|B|$, and $B^{(1)} = |B|$ and will not be considered further.

It is not difficult to see from this definition that skew Brownian paths inherit almost sure continuity from that of Brownian motion B. Moreover, let $\mathcal{F}_t := \sigma\{|B(s)| : 0 \le s \le t\} \vee \sigma\{A_1, A_2, \ldots\}$, therefore, $\mathcal{F}_t \supseteq \sigma(B^{(\alpha)}(s) : s \le t)$. For $0 \le s < t$ and a nonnegative,

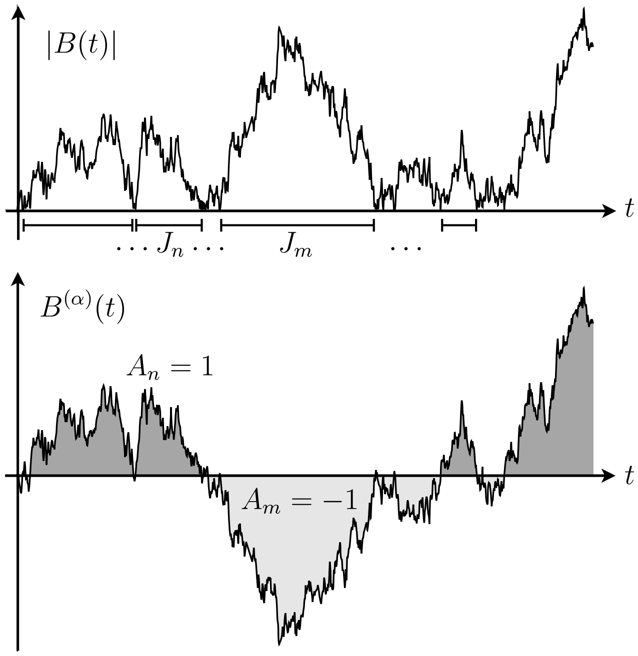

FIG. 2. *Skew Brownian motion construction.*

measurable function g, one may use the Markov property of $|B|$, and the independence of $|B|$ from the i.i.d. sign changes $A_1, A_2, \dots$, to check that

$$\mathbb{E}\{g(B^{(\alpha)}(t))|\mathcal{F}_s\} = \mathbb{E}\{g(B^{(\alpha)}(t))|B^{(\alpha)}(s)\}.$$

The Markov property of $B^{(\alpha)}$ follows since $\mathcal{F}_s \supseteq \sigma(B^{(\alpha)}(u) : u \le s)$.

Using the strong Markov property for Brownian motion, Walsh (1978) calculated the transition probabilities $p^{(\alpha)}(t, x, y)$ for α-skew Brownian motion as given by

$$\begin{aligned} p^{(\alpha)}&(t, x, y) \\ &= \begin{cases} \dfrac{1}{\sqrt{2\pi t}} e^{-(y-x)^2/(2t)} + \dfrac{(2\alpha - 1)}{\sqrt{2\pi t}} e^{-(y+x)^2/(2t)}, & \text{if } x > 0, y > 0, \\ \dfrac{1}{\sqrt{2\pi t}} e^{-(y-x)^2/(2t)} - \dfrac{(2\alpha - 1)}{\sqrt{2\pi t}} e^{-(y+x)^2/(2t)}, & \text{if } x < 0, y < 0, \\ \dfrac{2\alpha}{\sqrt{2\pi t}} e^{-(y-x)^2/(2t)}, & \text{if } x \le 0, y > 0, \\ \dfrac{2(1-\alpha)}{\sqrt{2\pi t}} e^{-(y-x)^2/(2t)}, & \text{if } x \ge 0, y < 0. \end{cases} \end{aligned} \tag{2.8}$$

Now, since a Markov process is uniquely determined by its transition probabilities and initial distribution, it is a simple matter to use a change of variable transformation to check that the physical skew diffusion X^* is a particular (rescaling) function of a skew Brownian motion with a particular transmission coefficient $\alpha = \alpha^*$. In particular, the above may be summarized as the following:

THEOREM 2.1. *Define the physical skew diffusion process* $X^* = \{X^*(t) : t \ge 0\}$ *by*

$$X^*(t) = s_{\sqrt{D}}(B^{(\alpha^*)}(t)), \quad t \ge 0, \alpha^* = \frac{\sqrt{D^+}}{\sqrt{D^+} + \sqrt{D^-}}, \tag{2.9}$$

where

$$s_{\sqrt{D}}(x) = \begin{cases} \sqrt{D^+}x, & \text{if } x > 0, \\ \sqrt{D^-}x, & \text{if } x \le 0. \end{cases} \tag{2.10}$$

Then X^* *is the diffusion on* $\mathbb{R}$ *with transition probabilities given by* (2.5) *started at zero.*

REMARK 2.2. As previously noted, the self-adjointness property that results from the conservative interface condition (2.3) may be viewed as a symmetry of the transition probabilities (2.5) of the physical skew diffusion. Although one sees by inspection that the transition probabilities (2.8) of skew Brownian motion are *not* symmetric in the sense of (2.5), using the strong Markov property of skew Brownian motion,[3] one has that $r_\alpha(B^{(\alpha)})$ is a martingale, where $r_\alpha(x) = \alpha x \mathbf{1}_{(-\infty,0]}(x) + (1-\alpha)x\mathbf{1}_{[0,\infty)}(x)$, $x \in \mathbb{R}$; see Walsh (1978).

REMARK 2.3. A similar, albeit somewhat more technical, procedure may be developed for

$$\begin{aligned} \frac{\partial u}{\partial t}(t, x) &= \frac{1}{2} D(x) \frac{\partial^2 u}{\partial x^2}(t, x) - v \frac{\partial u}{\partial x}(t, x) \quad (x \ne 0), \\ D^+ \frac{\partial u}{\partial x}(t, 0^+) &= D^- \frac{\partial u}{\partial x}(t, 0^-), \\ u(t, 0^+) &= u(t, 0^-), t > 0, \end{aligned} \tag{2.11}$$

[3]One may check that for fixed y, the transition probabilities of the skew Brownian motion are continuous in the backward variable x, that is, a *Feller property* holds. As a consequence of this and the sample path continuity, the *strong Markov property* for skew Brownian motion also follows.

for a constant drift v by a change of measure that converts the problem into one of an elastic skew Brownian motion; see Appuhamillage et al. (2011b) for details.

While we have perhaps traced the most direct route from the p.d.e. model (2.1) to probability theory, several others naturally emerge. Some of these are summarized in the next section.

3. ALTERNATIVE MATHEMATICAL DESCRIPTIONS OF PHYSICAL SKEW DIFFUSION

In this section four equivalent approaches to represent the Markov process associated with (2.1) are provided as alternatives to the construction in terms of excursions of reflected Brownian motion paths. Each of these provides additional mathematical tools in which to gainfully address diverse problems involving dispersion in the presence of the conservative interface condition (2.3). We begin with perhaps the most mathematically technical framework, that of Dirichlet forms, which can be useful for existence theory and for weak formulations used in developing numerical methods. This subsection can certainly be skimmed on first reading. The overall section progresses to the least technical framework of skew random walks and is followed by a subsection addressing a more general class of (nonconservative) interface conditions that will be seen to arise naturally in certain physical, biological and ecological dispersion contexts.

Dirichlet Forms

Below we outline the procedure leading to a semigroup framework for X^* via Dirichlet forms theory, and refer the reader to the more comprehensive references by Fukushima, Ōshima and Takeda (1994), Ma and Röckner (1992) or the recent Chen and Fukushima (2012).

To set up the analytical framework, let u be a solution to problem (2.1) and consider the following variational form of the evolution equation in $L^2(\mathbb{R})$:

$$\frac{\partial}{\partial t}\int_{\mathbb{R}} u(t,x)v(x)\,\mathrm{d}x = -\int_{\mathbb{R}} \frac{1}{2}D(x)\frac{\partial u}{\partial x}(t,x)\frac{\partial v}{\partial x}(x)\,\mathrm{d}x, \quad v \in C_c^\infty(\mathbb{R}). \tag{3.1}$$

The associated process is obtained by identifying a semigroup generated by the bilinear form

$$\mathcal{E}(u,v) = \int_{\mathbb{R}} \frac{1}{2}D(x)\frac{\partial u}{\partial x}(x)\frac{\partial v}{\partial x}(x)\,\mathrm{d}x, \quad u, v \in C_c^\infty(\mathbb{R}), \tag{3.2}$$

in some Hilbert space. For the case of D given by (2.1), standard considerations show that $\mathcal{E}$ is "closable" on $L^2(\mathbb{R})$, namely, it extends to a closed bilinear form (also denoted by $\mathcal{E}$) on $L^2(\mathbb{R})$ with domain $\mathrm{Dom}(\mathcal{E}) = H^1(\mathbb{R})$, the Sobolev space of L^2 functions whose generalized derivatives are also square integrable functions. Here, "closed" means that $\mathcal{E}(u,u) \geq 0$ for all $u \in \mathrm{Dom}(\mathcal{E})$ and that $\mathrm{Dom}(\mathcal{E}) = H^1(\mathbb{R})$ is a Hilbert space with the inner product $\mathcal{E}_1(u,v) := \mathcal{E}(u,v) + (u,v)_{L_2(\mathbb{R})}$. The bilinear form $(\mathcal{E}, \mathrm{Dom}(\mathcal{E}))$ is "coercive" since $\mathcal{E}(u,v)^2 \leq \mathcal{E}_1(u,u)\mathcal{E}_1(v,v)$ and a "Dirichlet form" since

$$\mathcal{E}(u,u) \leq \mathcal{E}(u^+ \wedge 1, u^+ \wedge 1) \quad \text{for all } u, v \in \mathrm{Dom}(\mathcal{E}). \tag{3.3}$$

Finally, $(\mathcal{E}, \mathrm{Dom}(\mathcal{E}))$ is "regular" since $\mathrm{Dom}(\mathcal{E}) \cap C_c(\mathbb{R})$ is dense in $\mathrm{Dom}(\mathcal{E})$ with respect to the norm $u \mapsto \mathcal{E}(u,u)^{1/2}$. For such a form, there exists a unique closed, negative definite, linear operator $(\boldsymbol{\mathcal{A}}, \mathrm{Dom}(\boldsymbol{\mathcal{A}}))$ that satisfies the resolvent conditions of the Hille–Yosida theorem for generating the appropriate semigroup; namely, $(\lambda - \boldsymbol{\mathcal{A}})(\mathrm{Dom}(\boldsymbol{\mathcal{A}})) = L^2(\mathbb{R})$, $\lambda > 0$. This operator is given by

$$\mathrm{Dom}(\boldsymbol{\mathcal{A}}) \subset \mathrm{Dom}(\mathcal{E}) \quad \text{and} \quad \mathcal{E}(u,v) = (-\boldsymbol{\mathcal{A}}u, v) \quad \text{for all } u \in \mathrm{Dom}(\boldsymbol{\mathcal{A}}),\ v \in \mathrm{Dom}(\mathcal{E}). \tag{3.4}$$

Integration by parts on (3.2) yields

$$\boldsymbol{\mathcal{A}}f = \frac{1}{2}D\frac{\partial^2 f}{\partial x^2}, \quad \mathrm{Dom}(\boldsymbol{\mathcal{A}}) = \left\{ f \in H^1(\mathbb{R}) \cap H^2(\mathbb{R}^+) \cap H^2(\mathbb{R}^-) : D^+\frac{\partial f}{\partial x}(0^+) = D^-\frac{\partial f}{\partial x}(0^-) \right\}, \tag{3.5}$$

where $H^2(\mathbb{R}^\pm)$ denote the respective Sobolev spaces for twice (generalized) differentiable functions on $\mathbb{R}^\pm$. The operator $(\boldsymbol{\mathcal{A}}, \mathrm{Dom}(\boldsymbol{\mathcal{A}}))$ is the infinitesimal generator of a strongly continuous contraction semigroup $\{T_t : t \geq 0\}$ on $L^2(\mathbb{R})$ which is also sub-Markovian since $(\mathcal{E}, \mathrm{Dom}(\mathcal{E}))$ satisfies the Dirichlet form property (3.3). Note also that the conservative interface condition is encoded in $\mathrm{Dom}(\boldsymbol{\mathcal{A}})$ and makes the operator $\boldsymbol{\mathcal{A}}$ self-adjoint. The family of transition probabilities $p^*(t,\cdot,\cdot)$, $t > 0$ are recovered from the semigroup via, for bounded $A \in \mathcal{B}(\mathbb{R})$,

$$p^*(t,x,A) = T_t\mathbb{1}_A(x). \tag{3.6}$$

Since for $f \in \mathrm{Dom}(\boldsymbol{\mathcal{A}})$, the unique solution in $C([0,\infty)) \cap \mathrm{Dom}(\boldsymbol{\mathcal{A}})$ to $\frac{\partial u}{\partial t} = \boldsymbol{\mathcal{A}}u$, $u(0,x) = f(x)$ is $u(t,x) = \int_{\mathbb{R}} p^*(t,x,\mathrm{d}y) f(y)$ with p^* given in (2.5), then $T_t f = \int_{\mathbb{R}} p^*(t,\cdot,y) f(y)\,\mathrm{d}y$ almost everywhere for any $f \in L^2(\mathbb{R}) \cap L^\infty(\mathbb{R})$. The process X^* therefore has transition probabilities given by (2.5).

Feller's Natural Scale and Lévy's Time Change of Brownian Motion

In this subsection we outline the procedure leading to the characterization of X^* via Feller's natural scale and Lévy's time change of Brownian motion, and refer the reader to the more general references Revuz and Yor (1999), Karatzas and Shreve (1988), Bhattacharya and Waymire (2009) and others.

Let $a < x < b$ be arbitrary. The scale measure s_* of X^* is the unique (up to a multiplicative constant) measure that satisfies

$$\mathbb{P}_x\big(\tau^*_{(a,b)} = H^*_b\big) = \frac{s_*((a,x))}{s_*((a,b))}, \tag{3.7}$$

where $H^*_b := \inf\{t \ge 0 : X^*(t) = b\}$ denotes the *hitting time* of b, and $\tau^*_{(a,b)} := \inf\{t \ge 0 : X^*(t) \in \{a,b\}\}$ is the *escape time* from the interval (a,b) for $X^*(0) \in (a,b)$. The speed measure m_* of X^* is the unique Radon measure on Borel subsets of $\mathbb{R}$ such that

$$\mathbb{E}_x \tau^*_{(a,b)} = \int_a^b G_{a,b}(x,y) m_*(\mathrm{d}y), \tag{3.8}$$

where the so-called Green's function G of X^* is given by

$$G_{a,b}(x,y) = \frac{s_*((x \wedge y, a)) s_*((b, x \vee y))}{s_*((a,b))}. \tag{3.9}$$

The process X^* has speed and scale measures with piecewise constant density. Let $m_*(\mathrm{d}x) = m'_*(x)\,\mathrm{d}x$, $s_*(\mathrm{d}x) = s'_*(x)\,\mathrm{d}x$ with

$$\begin{aligned} m'_*(x) &= m^-_* \mathbb{1}_{(-\infty,0)}(x) + m^+_* \mathbb{1}_{(0,\infty)}(x), \\ s'_*(x) &= s^-_* \mathbb{1}_{(-\infty,0)}(x) + s^+_* \mathbb{1}_{(0,\infty)}(x). \end{aligned} \tag{3.10}$$

To determine the constants, let $(\mathcal{A}, \mathrm{Dom}(\mathcal{A}))$ denote the restriction of the operator $(\boldsymbol{\mathcal{A}}, \mathrm{Dom}(\boldsymbol{\mathcal{A}}))$ in (3.5) to the space of bounded continuous functions:

$$\begin{aligned} &\mathcal{A}f = \frac{1}{2} D \frac{\partial^2 f}{\partial x^2}, \\ &\mathrm{Dom}(\mathcal{A}) \\ &\quad = \Big\{ f \in C_b(\mathbb{R}) \cap C^2(\mathbb{R}^+) \cap C^2(\mathbb{R}^-) : \\ &\qquad\qquad D^+ \frac{\partial f}{\partial x}(0^+) = D^- \frac{\partial f}{\partial x}(0^-) \Big\}. \end{aligned} \tag{3.11}$$

Then $(\mathcal{A}, \mathrm{Dom}(\mathcal{A}))$ is also given by

$$\begin{aligned} \mathcal{A}f &= \frac{\mathrm{d}}{\mathrm{d}m_*} \frac{\mathrm{d}}{\mathrm{d}s_*} f, \\ \mathrm{Dom}(\mathcal{A}) &= \Big\{ f \in C_b(\mathbb{R}) : \frac{\mathrm{d}f}{\mathrm{d}s_*} \text{ is continuous} \Big\}, \end{aligned} \tag{3.12}$$

where $\frac{\mathrm{d}f}{\mathrm{d}s_*} = \frac{\mathrm{d}f}{\mathrm{d}x}\frac{\mathrm{d}x}{\mathrm{d}s_*} = \frac{\mathrm{d}f}{\mathrm{d}x} / \frac{\mathrm{d}s_*}{\mathrm{d}x}$. Matching the expressions for $\mathcal{A}$ above, one arrives at

$$s^+_* = \frac{c}{D^+}, \quad s^-_* = \frac{c}{D^-}, \quad m^+_* = m^-_* = \frac{2}{c}, \tag{3.13}$$

where c is any positive constant which we set equal to one for convenience.

Within this framework (see Revuz and Yor, 1999, page 310) one has the following:

THEOREM 3.1. *Physical skew diffusion X^* with D given by (2.1) is the unique Feller process on $\mathbb{R}$ with speed and scale measures $m_*(\mathrm{d}x) = m'_*(x)\,\mathrm{d}x$, $s_*(\mathrm{d}x) = s'_*(x)\,\mathrm{d}x$ with densities given by*

$$\begin{aligned} m'_*(x) &= 2, \\ s'_*(x) &= \frac{1}{D^-} \mathbb{1}_{(-\infty,0)}(x) + \frac{1}{D^+} \mathbb{1}_{(0,\infty)}(x). \end{aligned} \tag{3.14}$$

To see the propagation of local interface effects on the global features within this framework, let $a > 0$ and $0 < \varepsilon < a$, and use (3.7), (3.8) to obtain

$$\begin{aligned} \mathbb{E}_a \tau^*_{(a-\varepsilon, a+\varepsilon)} &= \frac{\varepsilon^2}{D^+}, \\ \mathbb{P}_a\big(\tau^*_{(a-\varepsilon,a+\varepsilon)} = H^*_{a-\varepsilon}\big) &= \frac{1}{2} \end{aligned} \tag{3.15}$$

as expected, since starting at a, X^* must behave like a diffusion process with diffusion coefficient D^+ up to the hitting time $H_0 > \tau_{(a-\varepsilon,a+\varepsilon)}$. On the other hand, for the process starting at the interface at $x = 0$, the effects of the heterogeneity are depicted by

$$\begin{aligned} \mathbb{E}_0 \tau^*_{(-\varepsilon,\varepsilon)} &= \frac{2\varepsilon^2}{D^+ + D^-}, \\ \mathbb{P}_0\big(\tau^*_{(-\varepsilon,\varepsilon)} = H^*_{-\varepsilon}\big) &= \frac{D^-}{D^+ + D^-}. \end{aligned} \tag{3.16}$$

Namely, the interface $x = 0$ "skews" the process, making it more likely to exit the symmetric interval $(-\varepsilon, \varepsilon)$ through the endpoint with highest diffusion coefficient value.

For a path-wise representation of the process X^* one may proceed by Lévy's time change of Brownian motion as follows. Let $B = \{B(t) : t \ge 0\}$ denote canonical standard Brownian motion on $(\Omega, \mathcal{F}, \{\mathbb{P}_x\}_{x \in \mathbb{R}})$ and consider the following additive functional

$$\phi(r) = \int_0^r \frac{1}{2}\frac{m_*'(B(t))}{s_*'(B(t))}\,\mathrm{d}t, \quad r \ge 0. \tag{3.17}$$

Let T be the inverse of ϕ, $T(t) = \inf\{s \ge 0 : \phi(s) = t\}$, then the process X^* has the following representation:

$$X^*(t) = s_*^{-1}\big(B\big(T(t)\big)\big), \quad t \ge 0, \tag{3.18}$$

where s_*^{-1} denotes the inverse of the function $x \mapsto s_*((0,x))$, $s_*^{-1}(x) = D(x)x$.

The representation obtained in (3.18) can be simplified further in order to write X^* as a function of a continuous martingale. Consider the time-change $Y(t) = B(T(t))$, where

$$\begin{aligned} T(t) &= \int_0^{T(t)} 2\frac{s_*'(B(r))}{m_*'(B(r))}\,\mathrm{d}\phi(r) \\ &= \int_0^t 2\frac{s_*'(Y(\rho))}{m_*'(Y(\rho))}\,\mathrm{d}\rho \end{aligned} \tag{3.19}$$

and, therefore, the quadratic variation of Y is $\langle Y\rangle(t) = T(t)$. But since $\phi(r)$ is continuous, increasing and finite, then so is T. Therefore (see Karatzas and Shreve, 1988, Theorem 4.2), there exists a probability space $(\tilde{\Omega}, \tilde{\mathcal{F}}, \{\tilde{\mathbb{P}}_x\}_{x\in\mathbb{R}})$ extending $(\Omega, \mathcal{F}, \{\mathbb{P}_x\}_{x\in\mathbb{R}})$ and with a Brownian motion $\tilde{B}$ defined such that

$$\begin{aligned} Y(t) &= \int_0^t Z(r)\,\mathrm{d}\tilde{B}(r), \\ T(t) = \langle Y\rangle(t) &= \int_0^t Z^2(r)\,\mathrm{d}r, \quad \tilde{\mathbb{P}}\text{-a.s.} \end{aligned} \tag{3.20}$$

for some measurable adapted process Z. It follows from (3.20) that $Z(t) = [2s_*'(Y(t))/m_*'(Y(t))]^{1/2}$. So one arrives at the following representation in terms of the martingale Y:

$$\begin{aligned} X^*(t) &= D\big(Y(t)\big)Y(t), \\ Y(t) &= \int_0^t \frac{1}{\sqrt{D(Y(r))}}\,\mathrm{d}\tilde{B}(r). \end{aligned} \tag{3.21}$$

Stochastic Calculus and Local Time

The representation of X^* in (3.21) again makes it evident that whenever the process is away from the interface, the trajectories of X^* can be obtained by simply re-scaling those of Brownian motion by the square root of the appropriate diffusion coefficient. However, it does not reveal the behavior of X^* at $x = 0$ and, in particular, the skewness property (3.16). This property must be produced by the effect of the jump in the value of the diffusion coefficient over the trajectories, during the "time" a particle occupies the interface. In order to quantify this effect then, one is naturally led to consider the properties of the local time of X^*.

We now briefly give some necessary background on the theory of local time for continuous semimartingales. The reader is referred to Revuz and Yor (1999) for the general theory followed here. Given a continuous semimartingale $X(t) = M(t) + V(t)$, where M is a martingale and V is an increasing process, we define its local time process L^X via

$$\begin{aligned} \big|X(t) - a\big| &= \big|X(0) - a\big| \\ &\quad + \int_0^t \operatorname{sign}_-\big(X(s) - a\big)\,\mathrm{d}X(s) \\ &\quad + L^X(t,a) \end{aligned} \tag{3.22}$$

with the convention $\operatorname{sign}_- = \mathbb{1}_{(0,\infty)} - \mathbb{1}_{(-\infty,0]}$. What we are calling local time in this paper is sometimes referred to in the literature as *right local time* since it satisfies almost surely

$$L^X(t,a) = \lim_{\varepsilon\downarrow 0}\frac{1}{\varepsilon}\int_0^t \mathbb{1}_{[a,a+\varepsilon)}\big(X(r)\big)\,\mathrm{d}\langle X\rangle(r). \tag{3.23}$$

The function $(t,a) \mapsto L^X(t,a)$ can be taken continuous in t and cadlag in a and its jumps are given by

$$\begin{aligned} L^X(t,a) - L^X\big(t,a^-\big) &= 2\int_0^t \mathbb{1}_{\{a\}}\big(X(s)\big)\,\mathrm{d}X(s) \\ &= 2\int_0^t \mathbb{1}_{\{a\}}\big(X(s)\big)\,\mathrm{d}V(s). \end{aligned} \tag{3.24}$$

In particular, if $X = M$ is a local martingale, then $(t,a) \mapsto L^X(t,a)$ can be taken bi-continuous.

The following basic formulae encompass the most significant properties of local time:

Itô–Tanaka formula. If f is a difference of convex functions and f_-' denotes its left derivative, then

$$\begin{aligned} f\big(X(t)\big) &= f\big(X(0)\big) + \int_0^t f_-'\big(X(s)\big)\,\mathrm{d}X(s) \\ &\quad + \frac{1}{2}\int_{\mathbb{R}} L^X(t,x)f''(\mathrm{d}x). \end{aligned} \tag{3.25}$$

Occupation times formula. For any positive Borel—measurable function F,

$$\int_0^t F\big(X(s)\big)\,\mathrm{d}\langle X\rangle(s) = \int_{\mathbb{R}} F(x)L^X(t,x)\,\mathrm{d}x. \tag{3.26}$$

Left-side local time. If X is a continuous semimartingale, then almost surely

$$L^X\big(t,a^-\big) = \lim_{\varepsilon\downarrow 0}\frac{1}{\varepsilon}\int_0^t \mathbb{1}_{(a-\varepsilon,a)}\big(X(r)\big)\,\mathrm{d}\langle X\rangle(r). \tag{3.27}$$

As a first step consider the representation of X^* in (3.21) as a nonsmooth function of the martingale Y. Applying the Itô–Tanaka formula to the function $f(x) = s_*^{-1}(x) = xD(x)$ and using the representation (3.21) of Y in terms of a Brownian motion B, one gets

$$\begin{aligned} X^*(t) &= \int_0^t D(Y(r))\,\mathrm{d}Y(r) + \frac{1}{2}(D^+ - D^-)L^Y(t,0) \\ &= \int_0^t \sqrt{D(X^*(r))}\,\mathrm{d}B(r) \\ &\quad + \frac{1}{2}(D^+ - D^-)L^Y(t,0). \end{aligned}$$

The local time of Y can be related to the local time L^* of X^* using (3.23). Note first that $\langle X^*\rangle(r) = D^2(X(r))\langle Y\rangle(r)$ for $r \geq 0$, then write

$$\begin{aligned} &L^Y(t,a) \\ &\quad = \lim_{\varepsilon\downarrow 0} \frac{1}{\varepsilon}\int_0^t \mathbb{1}_{[0,\varepsilon)}(Y(r))\,\mathrm{d}\langle Y\rangle(r) \\ &\quad = \lim_{\varepsilon\downarrow 0} \frac{1}{(D^+)^2\varepsilon}\int_0^t \mathbb{1}_{[0,D^+\varepsilon)}(X(r))\,\mathrm{d}\langle X\rangle(r) \\ &\quad = \frac{1}{D^+}L^*(t,0). \end{aligned} \tag{3.28}$$

We have arrived at the following representation of X^*.

THEOREM 3.2. *For a given $X(0)$, and on any filtered probability space carrying a Brownian motion B, physical skew diffusion X^* is the unique strong solution to the following stochastic differential equation*:

$$\begin{aligned} X(t) = X(0) &+ \int_0^t \sqrt{D(X(r))}\,\mathrm{d}B(r) \\ &+ \frac{(D^+ - D^-)}{2D^+}L^X(t,0). \end{aligned} \tag{3.29}$$

Equation (3.29) is a stochastic differential equation in terms of the local time of the unknown process. Le Gall (1984) studied the problem of existence and uniqueness of solutions for equations of this type and proved Theorem 3.2. In fact, he considered a larger set of equations which we review here for its relevance with regard to more general solute transport problems. For the sake of consistency with other parts of the present paper, we summarize his analysis in terms of the right local time defined in (3.22), in place of the symmetric local time used in Le Gall (1984).

Consider a finite signed measure ν such that $\nu(\{x\}) < 1$ for all $x \in \mathbb{R}$, and let ν^c be its continuous part. Also, let φ be a right-continuous function of bounded variation that is also strictly positive and bounded away from zero. Le Gall (1984) considered the following equation:

$$\begin{aligned} X(t) = X(0) &+ \int_0^t \varphi(X(r))\,\mathrm{d}B(r) \\ &+ \frac{1}{2}\int_{\mathbb{R}} L^X(t,x)\nu(\mathrm{d}x). \end{aligned} \tag{3.30}$$

In the case of equation (3.29), $\varphi = \sqrt{D}$ and $\nu = \frac{D^+ - D^-}{D^+}\delta_0$, in particular, $\nu^c \equiv 0$. The key to the analysis is to relate equation (3.30) to a stochastic differential equation without a local time term. In fact, Le Gall (1984) shows that if f_ν is a right-continuous function satisfying

$$f_\nu(x^-)\nu(\mathrm{d}x) + f_\nu'(\mathrm{d}x) = 0, \qquad x \in \mathbb{R}, \tag{3.31}$$

and $F_\nu(x) = \int_{-\infty}^x f_\nu(y)\,\mathrm{d}y$, then a process X is a solution to (3.30) if and only

$$\begin{aligned} &Y(t) = F_\nu(X(t)) \quad \text{satisfies} \\ &Y(t) = \int_0^t f_\nu(X(r))\varphi(X(r))\,\mathrm{d}B(r). \end{aligned} \tag{3.32}$$

Moreover, it is easy to show that the function f_ν is given by

$$f_\nu(x) = \exp(-\nu^c((-\infty,x]))\prod_{y\leq x}(1 - \nu(\{y\})). \tag{3.33}$$

Not surprisingly, when this procedure is applied to equation (3.29), one gets $f_\nu = 1/D$ and recovers problem (3.21). The existence and uniqueness of strong solutions to (3.29) follows then from the corresponding result for (3.21) which was established in Nakao (1972), and recently generalized substantially in Prokaj (2011) and Fernholz, Ichiba and Karatzas (2013).

It is important to note that the representation (3.29) gives the decomposition of the continuous semimartingale X^* as the sum of a continuous local martingale and an increasing process. It follows that the local time of X^* is not continuous at $x = 0$. In fact, by (3.24), we can compute

$$\frac{L^*(t,0)}{L^*(t,0^-)} = \frac{D^+}{D^-}, \qquad t \geq 0. \tag{3.34}$$

This, however, cannot be interpreted as skew diffusion "spending more time" on either side of the interface. To see this, we can use the alternative definitions (3.23), (3.27) of right and left local time. For X^*, (3.29) gives the quadratic variation $\langle X^*\rangle(t) = \int_0^t D(X(r))\,\mathrm{d}r$. In particular, the ratio between the time a particle spends just above the interface $x = 0$ up to time t and the time it spends just below that interface is

$$\lim_{\varepsilon\downarrow 0}\frac{\int_0^t \mathbb{1}_{[0,\varepsilon)}(X^*(r))\,\mathrm{d}r}{\int_0^t \mathbb{1}_{(-\varepsilon,0]}(X^*(r))\,\mathrm{d}r}$$

$$(3.35)\quad = \lim_{\varepsilon\downarrow 0}\frac{(\int_0^t \mathbb{1}_{[0,\varepsilon)}(X^*(r))\,\mathrm{d}\langle X^*\rangle(r))/D^+}{(\int_0^t \mathbb{1}_{(-\varepsilon,0]}(X^*(r))\,\mathrm{d}\langle X^*\rangle(r))/D^-} = 1, \quad t \ge 0.$$

We will return to such matters in the context of applications.

Discrete and Numerical Approximations

Skew random walk is a natural discretization of skew Brownian motion defined as follows.

DEFINITION 3.1. The *α-skew random walk* is a discrete Markov chain $\{Y_n : n = 0, 1, 2, \dots\}$ on the integers $\mathbb{Z}$ having transition probabilities

$$p_{ij}^{(\alpha)} = \begin{cases} \frac{1}{2}, & \text{if } i \ne 0,\ j = i \pm 1, \\ \alpha, & \text{if } i = 0,\ j = 1, \\ 1-\alpha, & \text{if } i = 0,\ j = -1. \end{cases}$$

Convergence of the distribution at a fixed time point was first announced in Harrison and Shepp (1981), where they indicated a "fourth moment proof" along the lines of that given for a simple symmetric random walk (i.e., $\alpha = 1/2$) based on convergence of finite-dimensional distributions. However, proving tightness is quite laborious and tricky due to the lack of independence of the increments. A full proof was given in Brooks and Chacon (1983). The remainder of this section describes an approach based on the Skorokhod embedding method within this more specialized framework. A more general functional central limit theorem is given in Cherny, Shiryaev and Yor (2002).

LEMMA 3.1 (Discrete excursion representation). *Let $S = \{S_n : n = 0, 1, \dots\}$ be a simple symmetric random walk starting at* 0, *and let $\tilde J_{\pi_1}, \tilde J_{\pi_2}, \dots$ denote an enumeration of the excursions of S away from zero for a fixed but arbitrary permutation π of the natural numbers. In particular, $|S_n| > 0$ if $n \in \tilde J_{\pi_k}$. Define*

$$S_0^{(\alpha)} = 0, \quad S_n^{(\alpha)} = \sum_{k=1}^{\infty} \mathbb{1}_{\tilde J_{\pi_k}}(n)\tilde A_k |S_n|, \quad n \ge 1,$$

where $\tilde A_1, \tilde A_2, \dots$ is an i.i.d. sequence of Bernoulli ± 1-random variables, independent of S, with $\mathbb{P}(\tilde A_1 = 1) = \alpha$. Then $S^{(\alpha)}$ is distributed as an α-skew random walk.

Define the polygonal random function $S^{(\alpha,n)}$ on [0, 1] as follows:

$$(3.36)\quad S^{(\alpha,n)}(t) := \frac{S_{k-1}^{(\alpha)}}{\sqrt{n}} - \frac{S_k^{(\alpha)} - S_{k-1}^{(\alpha)}}{\sqrt{n}}\left(t - \frac{k-1}{n}\right), \quad t \in \left[\frac{k-1}{n}, \frac{k}{n}\right], 1 \le k \le n.$$

That is, $S^{(\alpha,n)}(t) = \frac{S_k^{(\alpha)}}{\sqrt{n}}$ at points $t = \frac{k}{n}$ $(0 \le k \le n)$, and $t \mapsto S^{(\alpha,n)}(t)$ is linearly interpolated between the endpoints of each interval $[\frac{k-1}{n}, \frac{k}{n}]$.

Let us recall that by an application of the Skorokhod embedding theorem (e.g., see Bhattacharya and Waymire, 2007), there is a sequence of times $T_1 < T_2 < \cdots$ and a Brownian motion $\{B(t) : t \ge 0\}$ such that $B(T_1)$ has a symmetric Bernoulli ± 1-distribution, and $B(T_{i+1}) - B(T_i)$ $(i \ge 0)$ are i.i.d. with a symmetric ± 1-distribution. Moreover, $T_{i+1} - T_i$ $(i \ge 0)$ are i.i.d. with mean one. With this one may check the following:

LEMMA 3.2. *The discrete parameter stochastic process $\tilde S_0^{(\alpha)} = 0$, $\tilde S_m^{(\alpha)} := B^{(\alpha)}(T_m)$, $m = 1, 2, \dots$, is distributed as an α-skew random walk.*

Now it is a rather straightforward exercise to prove the following theorem as an application of the Skorokhod embedding theorem, similar to that for weak convergence of the simple random walk to Brownian motion found in Bhattacharya and Waymire (2007) and many other references.

THEOREM 3.3. *$S^{(\alpha,n)}$ converges in distribution to the α-skew Brownian motion $B^{(\alpha)}$ as $n \to \infty$.*

Since the rescaling function is continuous, it follows that the rescaled skew random walks converge in distribution to the physical skew diffusion. That is, recalling the definition of $s_{\sqrt{D}}$ at (2.10), one has the following:

COROLLARY 3.1. *The* (*polygonal*) *random walks X_n^*, $n \ge 1$, defined by*

$$X_n^*(t) = s_{\sqrt{D}}(\tilde S^{(\alpha^*,n)}(t)), \quad t \ge 0, n = 1, 2, \dots,$$

converge weakly to the physical skew diffusion process X^* on $C[0,\infty)$.

The convergence of the discretized process opens the door to numerical simulation schemes. Two important alternatives to numerical methods are naturally suggested, namely, numerical solutions to the p.d.e. (2.1) and/or numerical solutions to the stochastic equation (3.29). The self-adjoint character of the conservative interface conditions singles out the numerical treatment of the equations in each of its formulations (2.1) or (3.29). For example, standard off-the-shelf finite difference methods provide numerical solutions to (2.1) for the conservative interface condition. Similarly, in spite of the presence of the local time term in (3.29), an Euler/Muruyama method was designed by Martinez and Talay (2012) that preserves the order of convergence of the Euler method when the coefficients of the s.d.e. are smooth. They exploit the fact that in the case of the conservative interface condition there is a one-to-one piecewise linear transformation of the process that, with the aid of the Itô–Tanaka lemma, eliminates the local time term. As will be emphasized in the next section and in subsequent examples to follow, the conservative interface condition is only one of infinitely many other possibilities of interest to applications that require new approaches to numerical simulations of both the p.d.e. and s.d.e. Recently, in Lejay and Pichot (2012), Étoré and Martinez (2013) and in Bokil et al. (2013), new numerical methods, including both stochastic and deterministic schemes, are developed that apply to these more general interface conditions and restore the order of convergence previously available for the more restrictive case of the conservative interface.

General Interface Conditions

The particular form of the interface condition (2.3) arises naturally in the case of solute transport as continuity of flux is imposed. However, as will be seen for applications outside solute transport, the following more general problem is also of interest:

$$\begin{aligned} &\frac{\partial u}{\partial t} = \frac{1}{2} D \frac{\partial^2 u}{\partial x^2}, \\ &\lambda \frac{\partial u}{\partial x}(t, 0^+) = (1-\lambda) \frac{\partial u}{\partial x}(t, 0^-), \\ &u(t, 0^+) = u(t, 0^-), t > 0, \end{aligned} \tag{3.37}$$

for some $0 < \lambda < 1$. The Markov process associated with problem (3.37) can be found using any of the techniques described in this section (see Appuhamillage et al., 2011a, 2011b). In fact, skew Brownian motion plays an important role here as provided by the following extension of Theorem 2.1

THEOREM 3.4. *The Markov process associated with problem* (3.37) *is*

$$\begin{aligned} &X(t) = s_{\sqrt{D}}\bigl(B^{(\alpha)}(t)\bigr), \\ &t \ge 0, \alpha = \alpha(\lambda) = \frac{\lambda\sqrt{D^-}}{\lambda\sqrt{D^-} + (1-\lambda)\sqrt{D^+}}, \end{aligned} \tag{3.38}$$

where $s_{\sqrt{D}}$ *is given in* (2.10).

DEFINITION 3.2. We refer to the Markov process associated to problem (3.37) as skew diffusion. In the special case of the conservative interface condition for (2.1), we refer to $X \equiv X^*$ as the physical skew diffusion.

Ouknine (1990) characterizes skew diffusion processes as solutions to a particular family of stochastic differential equations of the form (3.30). In particular, applying Tanaka's formula gives that the process $X = s_{\sqrt{D}}(B^{(\alpha)})$ is a strong solution to

$$\begin{aligned} X(t) = X(0) &+ \int_0^t \sqrt{D\bigl(X(r)\bigr)}\, \mathrm{d}B(r) \\ &+ \frac{\alpha\sqrt{D^+} - (1-\alpha)\sqrt{D^-}}{2\alpha\sqrt{D^+}} L^X(t, 0). \end{aligned} \tag{3.39}$$

The next theorem follows:

THEOREM 3.5. *Let* $\gamma < 1$, *then the strong solution to*

$$\begin{aligned} X(t) = X(0) &+ \int_0^t \sqrt{D\bigl(X(r)\bigr)}\, \mathrm{d}B(r) \\ &+ \frac{\gamma}{2} L^X(t, 0) \end{aligned} \tag{3.40}$$

is given by $X = s_{\sqrt{D}}(B^{(\alpha)})$ *with*

$$\alpha = \frac{\sqrt{D^-}}{\sqrt{D^-} + \sqrt{D^+}(1-\gamma)}. \tag{3.41}$$

Note that matching the formulae for α in (3.38) and (3.41) gives

$$\lambda = \frac{1}{(2-\gamma)} \in (0, 1), \tag{3.42}$$

which expresses the discontinuities at the interface of $\frac{\partial u}{\partial x}$ in relation to those of the local time of the process.

Finally, as one can easily check by matching the operators in (3.37) with the characterization of the infinitesimal operator in (3.12), the family of skew diffusion processes coincides with the class of Markov processes with scale and speed measures having piecewise constant densities.

THEOREM 3.6. *Let* X *be a regular diffusion process with speed measure* m *and scale measure* s *having densities*

$$\begin{aligned} m'(x) &= m^- \mathbb{1}_{(-\infty,0]}(x) + m^+ \mathbb{1}_{(0,\infty)}(x), \\ s'(x) &= s^- \mathbb{1}_{(-\infty,0]}(x) + s^+ \mathbb{1}_{(0,\infty)}(x) \end{aligned} \tag{3.43}$$

for some $m^+, m^-, s^+, s^- > 0$. *Then* X *is given by*

$$X = s_{\sqrt{D}}(B^{(\alpha)}) \quad \text{with } D = \frac{2}{m's'}, \alpha = \frac{\sqrt{m^+s^-}}{\sqrt{m^-s^+} + \sqrt{m^+s^-}}. \tag{3.44}$$

While there is no denying the importance of the conservative interface condition in many physical applications, a primary goal of the present article is to illustrate both the ubiquity and special effects of more general interface conditions. This is especially relevant to certain biological and ecological applications where awareness of such effects might help to guide the determination of an appropriate interface condition. For example, in the following section, we introduce notions of *natural occupation time* and *natural local time* for the processes arising in this more general class of models. These are modifications of the more standard mathematical definitions of occupation and local time to adapt to the physical units of the model, that is, so that occupation time is in the units of time, for example. An interesting consequence is that continuity and ordering properties of these quantities can be obtained that illustrate the effect of a particular interface condition in the context of modeling ecological and natural processes, for example, in relation to modeling advection–dispersion of insect populations as considered in Cantrell and Cosner (2003), Okubo and Levin (2001).

4. APPLICATIONS IN THE PHYSICAL AND BIOLOGICAL SCIENCES

In this section several different areas of application are described. It is in this section that the Mathematics of Planet Earth theme is most clearly illustrated. Each application area involves a distinct manifestation of an interface effect.

It is fitting to first note that the general interface conditions introduced in (3.37) from a mathematical perspective already arise naturally in a class of physical problems involving heat conduction in heterogeneous media as follows. As treated, for example, in the classical reference Carslaw and Jaeger (1988), the equation of conservation of thermal energy in a thin rod composed of two semi-infinite rods with heat capacity $\rho^{\pm}$ and heat conductivity $\kappa^{\pm}$, respectively, is given by

$$\rho^{\pm} \frac{\partial u}{\partial t} = \kappa^{\pm} \frac{\partial^2 u}{\partial x^2} \tag{4.1}$$

with interface condition at $x = 0$, given by

$$u(t, 0^+) = u(t, 0^-), \quad \kappa^+ \frac{\partial u}{\partial x}(t, 0^+) = \kappa^- \frac{\partial u}{\partial x}(t, 0^-). \tag{4.2}$$

In the notation used in this paper, $D^{\pm} = \frac{\kappa^{\pm}}{\rho^{\pm}}$. The fact that the interface condition only depends on the heat conductivity coefficient leads to the interface condition

$$\lambda \frac{\partial u}{\partial x}(t, 0^+) = (1 - \lambda) \frac{\partial u}{\partial x}(t, 0^-), \tag{4.3}$$

where $\lambda = \kappa^+/(\kappa^+ + \kappa^-)$.

The further collection of examples provided below indicate various other contexts from biological, environmental and physical sciences in which the general interface conditions may arise. We begin, however, with a return to an example of solute transport in porous media for the first two illustrations of the theory. In particular, the condition (2.3) applies at the interfaces.

Heterogeneous Taylor–Aris Dispersion and Averaging Effects

Taylor–Aris dispersion is well known throughout the physical and biological sciences for its role in providing the effective rate of spread of a solute immersed in a homogeneous fluid flow as given by (1.1) in the case of Poisseuille flow directed along the horizontal axis of a cylindrical tube $\mathbf{G} = [0, \infty) \times G$ in terms of the *tube radius* R of the cross section G, the *molecular diffusion coefficient* D and the *maximum flow* v_0 (or *cross-sectional average* $v_0/4$) of the parabolic flow profile.[4] In the case $v_0 = 0$ the dispersion coincides with molecular diffusion, and when $D = 0$ the dispersion of solute is aligned with the parabolic profile of the flow. The relative contributions of these combined effects ($D > 0, v_0 > 0$) are captured time asymptotically in Taylor's remarkable insights, leading to the celebrated formula for an *effective dispersion rate*

$$\bar{D} = 2D + \frac{R^2 v_0^2}{96D}. \tag{4.4}$$

[4]Motivated by considerations of the stability of a viscous liquid to two-dimensional disturbances in a porous medium, Wooding (1960) adapted their analysis to obtain the corresponding formula for dispersion of a solute in a unidirectional parabolic flow between two parallel planes separated by a distance R. The geometry will effect the constants appearing in the formulae for effective dispersion rates in ways that are made clear by the general theorem of Bhattacharya and Gupta (1984).

Although originally developed by Taylor (1953) and refined by Aris (1956) using perturbation methods of partial differential equations, this was subsequently shown to be a manifestation of the central limit theorem for a concentration of Brownian motion particles advected by the flow in Bhattacharya and Gupta (1984) for the case of Lipshitz continuous dispersion and drift coefficients. In this context, the effective dispersion coefficient is a time-asymptotic *variance* parameter for the distribution of the position of an immersed particle. In the presence of heterogeneity, as is currently known, it had been loosely anticipated that the effective dispersion would be modified by "averaging;" for example, see Gelhar and Axness (1983). In this section we will see that as a result of an interface effect, the effective rate involves both *arithmetic* and *harmonic* averaging.

Consider (1.1) in a cylindrical domain $\mathbf{G} = \mathbb{R} \times G$ with a cross-section $G \subset \mathbb{R}^d$, which is a closed interval in the case $d = 1$, or a bounded region with a smooth boundary if $d = 2$. Suppose the drift $\mathbf{v}$ is parallel to the x_1-axis and the diffusivity is a diagonal matrix depending only on the transverse variables. Namely, for $d = 2$, $\mathbf{v} = (v_1, 0, 0)$ and $D = \operatorname{diag}(D_1, D_2, D_3)$ with $v_1 = v_1(x_2, x_3)$ and $D_i = D_i(x_2, x_3)$ being positive and bounded away from zero, $i = 1, 2, 3$. Let $c(t, \mathbf{x})$ be a solution, and consider its cross-sectional average,

$$(4.5)\qquad C(t, x) := \iint_G c(t, x, x_2, x_3)\,\mathrm{d}x_2\,\mathrm{d}x_3.$$

If $X(t) = (X_1(t), X_2(t), X_3(t))$, $t > 0$ is the diffusion process associated with the p.d.e. solved by c, then $C(t, \cdot)$ represents the (nonnormalized) marginal distribution of the longitudinal coordinate $X_1(t)$ for an initial uniform distribution of the transverse coordinates $(X_2(t), X_3(t))$ on G. The Taylor–Aris problem involves *homogenized* parameters $\bar{v}, \bar{D}$ such that on large space–time scales λx, $\lambda^2 t$, the weak limit

$$(4.6)\qquad \tilde{C}(t, x)\,\mathrm{d}x := \lim_{\lambda\to\infty} C(\lambda^2 t, \lambda x + \bar{v}\lambda^2 t)\lambda\,\mathrm{d}x$$

provides a centered solution

$$\bar{C}(t, x) = \tilde{C}(t, x - \bar{v}t)$$

to the homogenized partial differential equation,

$$(4.7)\qquad \frac{\partial \bar{C}}{\partial t} = \frac{1}{2}\bar{D}\frac{\partial^2 \bar{C}}{\partial x^2} - \bar{v}\frac{\partial \bar{C}}{\partial x}, \qquad t \ge 0, x \in \mathbb{R}.$$

The homogenized parameters $\bar{v}$, $\bar{D}$ are in fact the result of an ergodic theorem for the transverse Markov process with reflecting boundary; see (4.10). The following extension of Bhattacharya and Gupta (1984) can be obtained for the case of a layered medium with piecewise continuous coefficients; see Ramirez et al. (2006) where the original idea of Bhattacharya and Gupta (1984) to view the problem in accordance with (4.6) as a functional central limit theorem for $\{X_1(\lambda^2 t) - \bar{v}\lambda^2 t\}/\lambda$ as $\lambda \to \infty$ is shown to carry over to piecewise continuous coefficients as well.

THEOREM 4.1 (A generalized Taylor–Aris formula for piecewise continuous coefficients). *Assume $d = 2$. Let $\pi(\mathrm{d}x_2\,\mathrm{d}x_3)$ be the uniform probability measure on G, and let h be a solution in $L^2(G, \pi)$ to the boundary value problem*

$$(4.8)\qquad \begin{cases} \nabla \cdot (D_{2,3}\nabla h) = v_1 - \bar{v}, & (x_2, x_3) \in G, \\ (D_{2,3}\nabla h) \cdot \mathbf{n}_0 = 0, & (x_2, x_3) \in \partial G, \end{cases}$$

where $\mathbf{n}_0$ denotes the outward normal vector of G and $D_{2,3} = \operatorname{diag}(D_2, D_3)$. Then, for any $t > 0$, $x \in \mathbb{R}$, and Borel measurable $A \subseteq \mathbb{R}$ with $|\partial A| = 0$,

$$(4.9)\qquad \begin{aligned} &\lim_{\lambda\to\infty} \int_A C(\lambda^2 t, \lambda x + \bar{v}\lambda^2 t)\lambda\,\mathrm{d}x \\ &\quad = \int_A \bar{C}(t, x + \bar{v}t)\,\mathrm{d}x \end{aligned}$$

with homogenized parameters

$$(4.10)\qquad \begin{aligned} \bar{v} &= \iint_G v\pi(\mathrm{d}x_2\,\mathrm{d}x_3), \\ \bar{D} &= \iint_G \{D_1 + (D_{2,3}\nabla h) \cdot \nabla h\}\pi(\mathrm{d}x_2\,\mathrm{d}x_3). \end{aligned}$$

In the case $d = 1$, $D_{2,3}$ is the scalar D_2 which is piecewise constant, and we obtain (see Figure 3) the following corollary.

COROLLARY 4.1 (A generalized Taylor–Aris formula with piecewise constant coefficients). *Assume $d = 1$, $G = [a, b]$, and D has the form*

$$D = D(x_2) = \sum_{k=-m}^{M} D^{(k)} \mathbb{1}_{[l_k, l_{k+1})}(x_2),$$

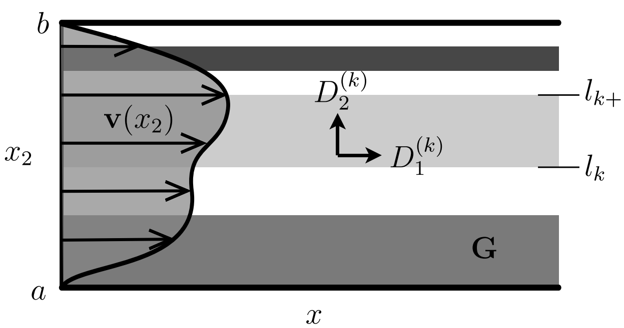

FIG. 3. *Two-dimensional advection dispersion through a layered medium. In the ongoing notation, $d = 1$, $G = [a, b]$, $\mathbf{G} = \mathbb{R} \times [a, b]$.*

$$D^{(k)} = \begin{bmatrix} D_1^{(k)} & 0 \\ 0 & D_2^{(k)} \end{bmatrix},$$

where $a = l_{-m} < l_{-m+1} < \cdots < l_M < l_{M+1} = b$ *is a collection of interfaces partitioning* $[a, b]$. *If* $D_1^{(k)} > 0$ *and* $D_2^{(k)} > 0$ *for all* k, *then the limit* (4.9) *of Theorem* 4.1 *holds with homogenized diffusion coefficient*

$$\bar{D} = \sum_{k=-m}^{M} \left\{ D_1^{(k)} \frac{l_{k+1} - l_k}{b - a} + \frac{1}{D_2^{(k)}} \int_{l_k}^{l_{k+1}} g(y)^2 \pi(\mathrm{d}y) \right\}, \tag{4.11}$$

where g *is given by*

$$g(y) = \int_a^y \big(v_1(x_2) - \bar{v}\big)\pi(\mathrm{d}x_2). \tag{4.12}$$

Thus, the first term of the effective dispersion rate (4.4) is replaced by a (weighted) arithmetic average, while the second term involves a (weighted) harmonic mean. In particular, for $G = [-R, R]$ with a single interface at 0 separating media with diffusion coefficient D^+ and D^-, respectively, and a parabolic velocity profile $v_1(x_2) = v_0(1 - (x_2/R)^2)$, the formula is

$$D = D_a + \frac{4v_0^2 R^2}{945 D_h}, \tag{4.13}$$

where

$$D_a = \frac{D^+ + D^-}{2}, \qquad D_h = \frac{1}{1/D^+ + 1/D^-}. \tag{4.14}$$

Physical Skew Diffusion and Stochastic Ordering of Breakthrough Curves

The topic addressed in this subsection was originally initiated as a result of observations resulting from laboratory experiments designed to empirically test and understand advection–dispersion in the presence of sharp interfaces, for example, experiments by Kuo et al. (1999), Hoteit et al. (2002) and Berkowitz et al. (2009). Such laboratory experiments have been rather sophisticated in the use of layers of sands and/or glass beads of different granularities and modern measurement technology. The specific interest is in the effect of the interface condition on so-called breakthrough curves, measuring the time required for an injected concentration at one location to appear at another. The basic phenomenon of interest to us here is captured by the following:

Question. Suppose that a dilute solute is injected at a point y units to the left of an interface at the origin and retrieved at a point y units to the right of the interface. Let D^- denote the (constant) dispersion coefficient to the left of the origin and D^+ that to the right, with, say, $D^- < D^+$ (see Figure 4). Conversely, suppose the solute is injected at a point y units to the right of the interface and retrieved at a point y units to the left. *In which of these two symmetric arrangements will the immersed solute most rapidly break through at the opposite end*?

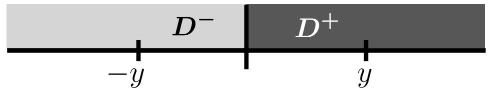

FIG. 4. *Interfacial schematic*.

The following results indicate that the question above can be answered by investigating the asymmetries in the hitting times of skew Brownian motion and skew diffusion.

LEMMA 4.1. *Fix* $y \geq 0$ *and let* $H_y^{(\alpha)} = \inf\{t \geq 0 : B^{(\alpha)}(t) = y\}$. *If* $0 < \alpha < 1/2$, *then*

$$\mathbb{P}_{-y}\big(H_y^{(\alpha)} > t\big) < \frac{\alpha}{1-\alpha}\mathbb{P}_y\big(H_{-y}^{(\alpha)} > t\big) < \mathbb{P}_y\big(H_{-y}^{(\alpha)} > t\big), \quad t > 0.$$

Recall that rescaling space by the respective diffusivities symmetrizes the transition probabilities when $\alpha = \alpha^*$, that is, for physical skew diffusion $X^*(t) = s_{\sqrt{D}}(B^{(\alpha^*)}(t))$. The following stochastic ordering of first passage times for physical skew diffusion provides a simple probabilistic basis for the symmetries and asymmetries predicted in experiments cited above. The proof is by a coupling and relies on an interesting balance between the specific conservative transmission parameter α^*, as well as the respective scalings on either side of the interface; see Appuhamillage et al. (2011a, 2011b) for details.

THEOREM 4.2. *Let* $H_y^* = \inf\{t \geq 0 : X^*(t) = y\}$. *Then, for* $y > 0$ *and* $D^- < D^+$,

$$\mathbb{P}_{-y}\big(H_y^* > t\big) \leq \frac{\sqrt{D^-}}{\sqrt{D^+}}\mathbb{P}_y\big(H_{-y}^* > t\big) < \mathbb{P}_y\big(H_{-y}^* > t\big), \quad t \geq 0.$$

To gain an alternative perspective on this phenomena, one may compute and compare the concentration curves as a function $t \to u(t, y)$ and $t \to u(t, -y)$ for a point injection at the interface; see Appuhamillage et al. (2011a, 2011b).

Interfacial Effects on Natural Residence and Local Times of Skew Diffusions

Within the ecology literature there is a recognition of the role of interfaces in "directing" movement from one habitat to another (e.g., see Fagan, Cantrell and Cosner, 1999; Cantrell and Cosner, 2003, page 112, and numerous references therein, as well as Okubo and Levin, 2001, page 265). The main point of the example described here is to highlight a natural role of nonconservative interfacial conditions in the models involving insect dispersal. Specifically, we will examine the effect of the interface on functionals such as residence times.

Fender's Blue butterfly provides a specific example that has been analyzed fairly extensively in both field experiments as well as mathematics. Fender's Blue is an endangered species of butterfly found in the Pacific Northwestern United States. The primary habitat patch is Kinkaid's Lupin flower.

Ecologists have focused substantial fieldwork efforts in examining the way in which organisms respond to habitat edges and the relationship to residence times in Lupin patches; see Schultz and Crone (2001). Sufficiently long residence (occupation) times are required for pollination, eggs, larvae and ultimate sustainability of the population. Empirical evidence points to a skewness in random walk models for butterfly movement at the path boundaries that have led to "biased random walk" and skew Brownian motion models in Schultz and Crone (2001), Cantrell and Cosner (2003), Okubo and Levin (2001), Fagan, Cantrell and Cosner (1999), Ovaskainen and Cornell (2003). The determination of proper interface conditions is primarily a statistical problem in such applications. However, as illustrated below, the role of local interfacial conditions is reflected in the behavior of residence times in ways that may be useful to the identification of interface conditions. In the framework of one-dimensional advection–dispersion one is therefore lead to consider the interface conditions (3.37) generalizing the conservative interface condition (2.3).

Note that $\lambda = 0$, $\lambda = 1$ correspond to reflection at the interface, while $\lambda = \frac{D^+}{D^+ + D^-}$ is the conservative interface condition (2.3) that gives rise to the process X^*. In particular, at the extremes the residence times of the positive half-line are obviously quite distinct. The following result interpolates between these extremes. The proof exploits the basic property of skew Brownian motion noted at the outset in (2.7), and essentially that

$$\mathbb{P}_0\big(B^{(\alpha)}(t) > 0\big) = \alpha, \quad t > 0. \tag{4.15}$$

This is easily checked from the definition and, intuitively, reflects the property that the excursion interval $J_{n(t)}$ of $|B|$ containing t results in a $[A_{n(t)} = +1]$ coin flip with probability α.

The following theorem involves a modification of the usual mathematical definition of *occupation time*, for example, as given in standard references such as Revuz and Yor (1999), in that integration is with respect to the Lebesgue measure in place of quadratic variation. We refer to this modification as *natural occupation time*.

DEFINITION 4.1. Let X be a continuous semimartingale. The *natural occupation time* of a Borel set A by X in time $[0, t]$ is defined by

$$\tilde{\Gamma}^X(A, t) = \int_0^t \mathbb{1}_A\big(X(s)\big)\,\mathrm{d}s.$$

One may note that this modification puts occupation time in the natural units of "time," while mathematical local time is in units of (area) "spatial length squared." As such, natural occupation time seems to be the more appropriate representation of *residence time* measurements, and we use it here for identifying regularities and properties of interest to the applications. Mathematical occupation time, on the other hand, has important roles to play in other theoretical contexts.

THEOREM 4.3. *Let $X^{(\alpha(\lambda))}$ denote skew diffusion defined in (3.38) for the dispersion coefficients D^+, D^- and interface parameter λ. Denote natural occupation time processes by*

$$\tilde{\Gamma}^+_\lambda(t) = \int_0^t \mathbb{1}_{(0,\infty)}\big(X^{(\alpha(\lambda))}(s)\big)\,\mathrm{d}s, \quad t \ge 0.$$

Similarly, let $\tilde{\Gamma}^-_\lambda(t) = t - \tilde{\Gamma}^+_\lambda(t)$, $t \ge 0$. Then,

$$\mathbb{E}\big(\tilde{\Gamma}^+_\lambda(t)\big) > \mathbb{E}\big(\tilde{\Gamma}^-_\lambda(t)\big), \quad t > 0,$$

if and only if

$$\lambda > \frac{\sqrt{D^+}}{\sqrt{D^+} + \sqrt{D^-}}$$

with equality when $\lambda = \frac{\sqrt{D^+}}{\sqrt{D^+}+\sqrt{D^-}}$.

It is noteworthy, therefore, that under the conservative interface condition more time is spent in the more volatile habitat, making such models questionable for many ecological contexts involving animal dispersion.

The conservative interface condition can also be characterized as the unique interface condition that gives the continuity of an analogous *natural local time* defined as follows.

DEFINITION 4.2. Let X be a continuous semimartingale. The *natural local time at a* $\tilde{L}^X(t,a) = \frac{1}{2}(\tilde{L}^{X,+}(t,a) + \tilde{L}^{X,-}(t,a))$ of X is defined by

$$\tilde{L}^{X,+}(t,a) = \lim_{\varepsilon \downarrow 0} \frac{1}{\varepsilon} \int_0^t \mathbb{1}_{[a,a+\varepsilon)}(X(s))\, \mathrm{d}s$$

and

$$\tilde{L}^{X,-}(t,a) = \lim_{\varepsilon \downarrow 0} \frac{1}{\varepsilon} \int_0^t \mathbb{1}_{(a-\varepsilon,a)}(X(s))\, \mathrm{d}s,$$

provided that the indicated limits exist almost surely.

With this definition, one has that

$$\tilde{\Gamma}^X(A,t) = \int_A \tilde{L}^X(t, \mathrm{d}a) \tag{4.16}$$

in complete analogy with the standard relation between local time and occupation time defined using the quadratic variation of the process X.

Recall that in the particular case of skew Brownian motion, the quadratic variation is simply $\langle B^{(\alpha)} \rangle(t) = t$. Therefore, the "symmetric local time" $\frac{1}{2}(L(^X(t,a) + L^X(t,a^-))$ [see Revuz and Yor, 1999 and equation (3.27)] agrees with the natural local time just defined. Moreover, the following relations among one-sided and symmetric local times at 0 are known; for example, see Ouknine (1990):

$$\begin{aligned} 2\alpha \tilde{L}^{B^{(\alpha)},+}(t,0) &= \tilde{L}^{B^{(\alpha)}}(t,0), \\ 2(1-\alpha)\tilde{L}^{B^{(\alpha)},-}(t,0) &= \tilde{L}^{B^{(\alpha)}}(t,0). \end{aligned} \tag{4.17}$$

In particular, the symmetric (natural) local time is continuous if and only if $\alpha = 1/2$.

The next theorem, a version of which was originally developed in Appuhamillage et al. (2012), extends the continuity of natural local time to the more general framework of the present paper. While the purpose here is not to explore the generality for which natural local time exists among all continuous semimartingales, according to the following theorem it does exist for skew diffusion. Moreover, continuity has a special significance for the determination of parameters.

THEOREM 4.4. *Let $X^{(\alpha(\lambda))}$ be the skew diffusion process with parameters $D^{\pm}, \lambda$. Then the natural local time of $X^{(\alpha(\lambda))}$ at* 0 *is continuous if and only if $\lambda = \frac{D^+}{D^+ + D^-}$, that is, if and only if $\alpha(\lambda) = \alpha^*$ and, thus, $X^{(\alpha^*)}$ is the physical skew diffusion.*

Thus, while at the macroscale of deterministic particle concentrations the determination of the transmission parameter α^* may be viewed as a consequence of the continuity of flux at the interface, at the scale of stochastic particle motions, it is determined by a condition of continuity of natural local time at the interface.

Dispersion of Organisms in River Networks

River networks are known to control the flux of water and sediment over most landscapes on the planet earth. Moreover, transport of water, organisms, sediment, nutrients and contaminants on river networks plays a central role in modern hydrology and ecology. River networks constitute, in particular, fundamental ecosystems whose populations are dependent upon the interconnectivity and heterogeneity of the different reaches that form the network (Fagan, 2002).

Mathematically, river networks are modeled as directed binary graphs. A long tradition of research in hydrology and geomorphology has narrowed the class of graphs observed in natural river basins, the relationships between physical variables involved in transport and the topological properties of such networks; for example, see Rodriguez-Iturbe and Rinaldo (2001), Peckham (1995), Barndorff-Nielsen (1998) and references therein. It is therefore natural to extend the linear advection–diffusion (2.1) to a binary graph in an effort to advance the understanding of the relationship between network topology, physical properties of rivers and dispersal of organisms.

The first steps toward an extension of skew Brownian motion to an infinite star-shaped graph was introduced by Walsh (1978) as a natural mathematical extension of skew Brownian motion on $\mathbb{R}$. A general theory of advection–diffusion processes on arbitrary graphs was subsequently initiated by Freidlin and Wentzell (1993).

To fix ideas in the context of river networks, consider a connected binary directed tree graph Γ as depicted in Figure 5. Each edge e models a stream reach of length l_e between two junctions and is assumed to be isomorphic to the interval $[0, l_e]$. Also, each edge e has associated strictly positive parameters v_e, A_e and D_e, denoting the mean water velocity, cross-sectional area and diffusion coefficient of the organisms in that reach. The endpoints $x = 0$ and $x = l_e$ correspond to the downstream and upstream nodes, respectively. The set of nodes in Γ can be divided into three subsets: the singleton root node ϕ, the set $I(\Gamma)$ of internal nodes connecting three edges, and the set $U(\Gamma)$ of upstream nodes n of "tributary edges" or "leaves" of Γ.

Considering the spatio-temporal evolution of the density of suspended organisms in Γ, and imposing conservation of mass throughout, one arrives at the following extension of (2.1) to the network:

$$\frac{\partial u_e}{\partial t} = \frac{1}{2} D_e \frac{\partial^2 u_e}{\partial x^2} - v_e \frac{\partial u_e}{\partial x}, \qquad x \in [0, l_e],\ e \in \Gamma, \tag{4.18}$$

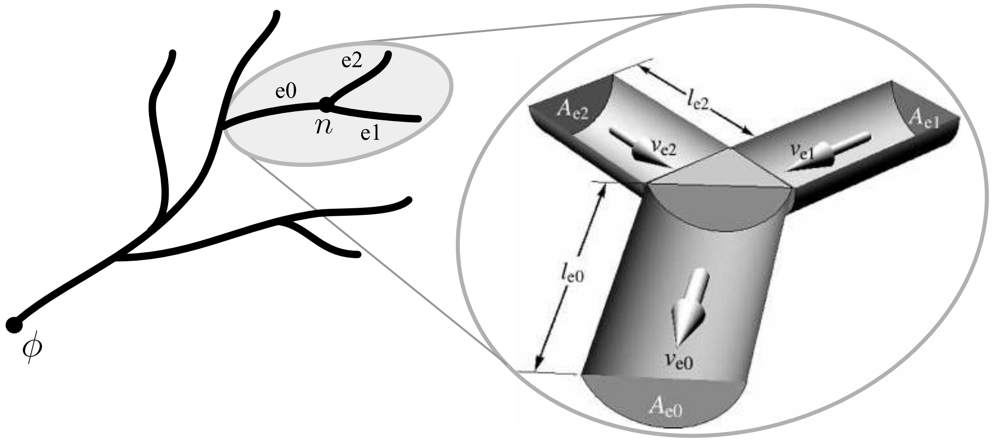

FIG. 5. *Schematic of a river network Γ with root node ϕ. The inset shows three edges connected at an internal node n representing the junction where two tributaries merge to form a new channel.*

where u_e denotes the restriction of the function u to edge e. Only functions that are continuous on each edge of Γ and twice continuously differentiable on the interior of each edge are considered. For an internal node where edges $e1$, $e2$ join to form edge $e0$, the appropriate extension of (2.3) reads

$$A_{e0}D_{e0}\frac{\partial u_{e0}}{\partial x}(t,l_{e0}) = A_{e1}D_{e1}\frac{\partial u_{e1}}{\partial x}(t,0)+A_{e2}D_{e2}\frac{\partial u_{e2}}{\partial x}(t,0). \tag{4.19}$$

Here, we also have assumed that water discharge is conserved at river junctions, namely, $A_{e1}v_{e1}+A_{e2}v_{e2}=A_{e0}v_{e0}$.

Several different behaviors can be prescribed at the boundary nodes of Γ. In particular, following Speirs and Gurney (2001), Lutscher, Pachepsky and Lewis (2005), Lutscher, Lewis and McCauley (2006), one may consider an ecological scenario where organisms do not leave the network through channel sources, and an abrupt change of flow conditions occur at ϕ that removes organisms from Γ, for example, a waterfall, a fast flowing river, a lake, the ocean or human disturbances. This can be coded mathematically by requiring

$$u(t,\phi)=0, \qquad \frac{\partial u}{\partial x}(t,n)=0, \quad n\in U(\Gamma), t\geq 0. \tag{4.20}$$

As shown in Freidlin and Sheu (2000), Freidlin and Wentzell (1993), the spatial operator on the left-hand side of (4.18) along with conditions (4.19, 4.20) is the infinitesimal generator of a Feller Markov process $X=\{X(t), t\geq 0\}$ on Γ with continuous sample paths that can be written as $X(t)=(x(t),e(t))$ with $e(t)$ being the edge the process occupies at time t, and $x(t)\in[0,l_{e(t)}]$, $t\geq 0$. Moreover, one has the analogous representation to (3.29): there exists a one-dimensional Brownian motion B and an increasing process L such that

$$\mathrm{d}x(t)=\sqrt{D_{e(t)}}\,\mathrm{d}B(t)-v_{e(t)}\,\mathrm{d}t+\mathrm{d}L(t), \tag{4.21}$$

where L only increases when $x(t)=0$. The three-way heterogeneity at internal nodes has a skewing effect on the sample paths analogous to property (3.16) of skew diffusion: let $H_\varepsilon^x=\inf\{t\geq 0: x(t)=\varepsilon\}$ and n denote the node connecting edges $e0, e1, e2$, then

$$\lim_{\varepsilon\to 0^+}\mathbb{P}\big(e(H_\varepsilon^x)=ei\,|\,X(0)=n\big) = \frac{A_{ei}D_{ei}}{A_{e0}D_{e0}+A_{e1}D_{e1}+A_{e2}D_{e2}}, \quad i=0,1,2. \tag{4.22}$$

An important contribution of advection–diffusion models in riverine ecology revolves about the classical “drift paradox,” whereby it was observed in Müller (1954) that although individual organisms in streams are subject to downstream drift, the average location of the population is not observed to move downstream over time, and thereby persists. In this regard, Speirs and Gurney (2001), Lutscher, Pachepsky and Lewis (2005), Lutscher, Lewis and McCauley (2006) obtain conditions on the channel length, drift velocity and population dynamics under which the population as a whole can persist along a single channel assuming that the movement of individuals is given by an advection–diffusion process of the form (1.2). Results of this type define resolutions of the drift paradox that can be useful to managers of ecological preserves.

Ecological persistence problems on river networks involve models in which individuals move within Γ via a jump process: an organism initially located at $y \in \Gamma$ jumps to the position $X(\tau_\sigma)$, where τ_σ is an exponentially distributed random variable that represents the time the individual spends dispersing within the water column. The resulting *dispersal kernel*, as it is known in the ecological literature, is therefore given by

$$k(y,x) = \mathbb{P}_y\bigl(X(\tau_\sigma) \in \mathrm{d}x\bigr) = \int_0^\infty \sigma e^{-\sigma t} p(t,y,x)\,\mathrm{d}t, \quad x, y \in \Gamma, \tag{4.23}$$

where $p(t,y,x)$ are the transition probability densities of X, the fundamental solution to problem (4.18), (4.19) and (4.20).

In the solutions noted above by Speirs and Gurney (2001), Lutscher, Pachepsky and Lewis (2005), Lutscher, Lewis and McCauley (2006), the evolution of the population u in the single channel $[0,l]$ is assumed to be given by[5]

$$\frac{\partial u}{\partial t}(t,x) = ru(t,x) - \lambda u(t,x) + \int_0^l \lambda k(y,x) u(t,y)\,\mathrm{d}y, \tag{4.24}$$

where $r > 0$ is the net population growth rate[6] and λ is the jump rate. Of course, in the case of a single channel there is not an interface and the model for $p(t,y,x)$ is simply Brownian motion with drift v and diffusion coefficient D.[7] Persistence is defined by instability of the solution $u = 0$ to (4.24).

An extension from the interval $[0,l]$ to tree networks Γ was developed in Ramirez (2012b), wherein the dispersal kernel (4.23) is explicitly solved. Moreover, Ramirez (2012b) permits nontrivial events of upstream migration, which are proposed in Speirs and Gurney (2001) to be the key to explaining the drift paradox. In particular, Ramirez (2012a) provides bounds on the minimum net growth rate r of individuals required for persistence of the population evolution in Γ via the dispersal kernel (4.23).

[5]Although Lutscher, Pachepsky and Lewis (2005) view (4.24) as "derived" from a regime-switching model, the argument is flawed. On the other hand, one may simply view (4.24) as a distinct population model. Felder and Waymire (2013) have recently shown, however, that the conditions on the parameters for persistence for the regime-switching model differ from those for (4.24).

[6]More general dynamics are considered, however, the results depend on the linear form in (4.24).

[7]Speirs and Gurney (2001), Lutscher, Lewis and McCauley (2006) permit more general models for $p(t,y,x)$, although the Brownian motion model is a primary example.

Coastal Upwelling, Fisheries and Continuity of Natural Local Time

Night satellite images of the earth show a striking concentration of fishing flotillas exploiting the ocean bounty off the coast of southern South America between approximately latitude 40 and 50 degrees south. This activity takes place in a narrow strip that follows the continental shelf break of South America where the cold nutrient rich waters of the Malvinas current reach the surface of the Atlantic Ocean in a process described as upwelling (see Figure 6). A mathematical model that approximately describes the location of the upwelling is given by the *arrested topographic wave* equation. Obtained under various simplifying assumptions, such as hydrostatic approximation and geostrophic balance, the equations determine the ocean-free surface elevation $\eta(x,y)$ as the solution of

$$\frac{\partial \eta}{\partial y} = -\frac{r}{f}\frac{1}{h(x)}\frac{\partial^2 \eta}{\partial x^2}. \tag{4.25}$$

Here x is the distance from the shore, y is the along-shore coordinate, $r > 0$ is the bottom friction, $f < 0$ is the Coriolis parameter and $h(x)$ is the derivative of the depth of the ocean at x. As part of the derivation of the equation, the orientation of the along-shore axis y is determined by the direction of motion of the current;

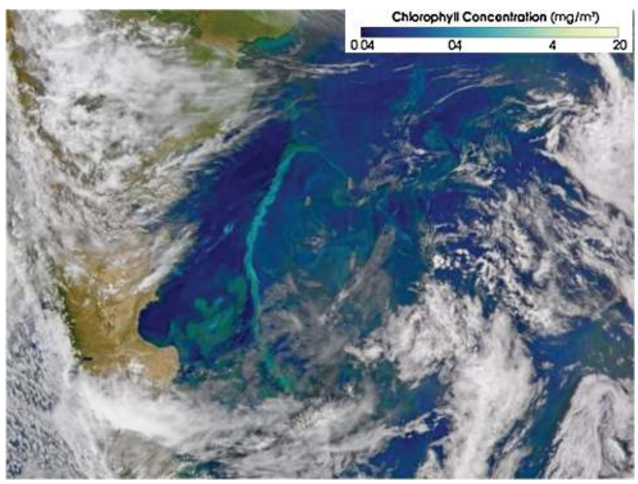

FIG. 6. *Phytoplankton bloom in Malvinas/Falklands current off the Atlantic coast of southern South America. Provided by the SeaWiFS Project, NASA/Goddard Space Flight Center and ORBIMAGE.*

see Matano and Palma (2008) and references within. As a consequence, (4.25) can be thought of as a diffusion equation where y plays the role of time.

The main features of the upwelling process are obtained by considering a bottom topography in which the slope $h(x)$ is piecewise constant, $h^{\pm}$ with a discontinuity at the continental shelf brake $x = l$. At the "interface" the conservation of mass transport by the current leads to the conditions

$$\begin{aligned} \eta(l^-, y) &= \eta(l^+, y), \\ \frac{\partial \eta}{\partial x}(l^-, y) &= \frac{\partial \eta}{\partial x}(l^+, y). \end{aligned} \tag{4.26}$$

This equation corresponds to (3.37) with

$$D^{\pm} = -\frac{r}{f h^{\pm}}, \quad \lambda = 1/2.$$

While the conservative interface conditions (2.3) are ubiquitous in the hydrological literature, the conditions (4.26) are mathematically natural. If one follows the general theory of time changes in the context of martingale problems as presented in Stroock and Varadhan (2006), the interface conditions of the arrested topographic wave are the ones that can obtained by a direct application of this theory. Indeed, with the time change $\tau(t) = \int_0^t \frac{1}{D(w(s))}\,ds$ one obtains that $X(t) = B(\tau(t)), t \geq 0$, is the Markov process corresponding to the problem (4.25) with interface condition (4.26). Alternatively, one can obtain $X(t) = s_{\sqrt{D}}(B^{\alpha^{\#}}(t)), t \geq 0$, where $\alpha^{\#} = \sqrt{D^-}/(\sqrt{D^+} + \sqrt{D^-})$.

5. COMPLEMENTARY RESULTS AND OPEN PROBLEMS

The main goal of this article has been to develop basic pathways to the frontiers of advection–dispersion research in the presence of interfacial effects from a probabilistic point of view. The example of one-dimensional processes with point interfaces is rich enough to provide realistic illustrations of the diverse effects on quantities arising in the applied sciences and engineering, however, it falls far short of a general mathematical framework. In addition, even in the one-dimensional context, the examples were selected to highlight various significant interfacial effects, but without an attempt to be comprehensive. However, the relative consequences of these effects do not seem to be widely recognized in the science literature in terms of the specification of the interfacial condition. As a result, the conservative interface condition is often adopted as the default consideration.

In this section we indicate some related results and open problems at the frontiers of research in this general area of advection–dispersion.

An alternative approach has also been partially developed by Portenko (1990), also see Aryasova and Portenko (2008), in the context of pdes whose coefficients may be generalized functions. Specifically, Aryasova and Portenko (2008) permits singular drift terms but requires smooth dispersion coefficients. A somewhat heuristic development of ideas along these lines in the context of dispersion in porous media was explored in LaBolle, Quastel and Fogg (1998) and LaBolle et al. (2000) that may also provide effective approaches to problems of this type. Certainly this provides an intriguing mathematical framework to explore, especially for problems in higher dimensions.

The definitions pertaining to breakthrough curves have various not necessarily equivalent formulations in the science and engineering literature. While first passage time is of obvious probabilistic interest, in the presence of advection the time profile of the *flux-averaged concentration* at a point is also sometimes adopted. The flux-averaged concentration is expressed in terms of the spatial derivatives of $u(t, x)$; see Appuhamillage et al. (2010). For the case of a discontinuous medium, this means that the concentration at the interface depends upon the derivatives on both the left and the right at the interface. However, these gradients evolve differently in the coarse and fine media. This means that, at the interface, the gradients of the concentration do depend upon the configuration (fine-to-coarse versus coarse-to-fine), and this dependency essentially breaks the symmetry that can be observed for the breakthrough curve of the resident concentration. This provides an alternative response to the fine-to-coarse vs. coarse-to-fine breakthrough curves, as this is explicitly computable in the presence of advection (see Appuhamillage et al., 2010, 2011b). The determination of the corresponding first passage times is unsolved in this generality. However, Appuhamillage and Sheldon (2012) recently computed an explicit expression for the density of the first passage time of skew Brownian motion.

The numerical methods by Martinez and Talay (2012) and Bokil et al. (2013) are more generally valid for piecewise continuous in place of piecewise constant diffusion coefficients. However, the methods are exclusively for the one-dimensional problems. The corresponding problems in a higher dimension are largely untreated. Similarly, as suggested by the examples, in many applications of biological interest in which the conservative interface condition is inappropriate, the determination of the proper interface condition involves statistical inference. The papers by Brillinger et al. (2002) and Brillinger (2003) provide some perspective on statistical inference for stochastic differential equations with smooth coefficients with ecological applications that might be expanded to this context. The upwelling example treated here is also a resource for possible explanation of migratory patterns being monitored by ocean ecologists in the context of oceanic flow properties; for example, see Acha et al. (2004).

The three theorems presented in Section 3 illustrate different approaches to deal with the effects of discontinuities of coefficients in the model equations. As problems in earth, physical and social sciences present situations in which abrupt changes in the parameters are more common, there is a need to develop an understanding from diverse points of view of the effect of these discontinuities in easily observable (macroscopic) quantities, as well as in refined, local properties of the processes involved. The results in Section 4 illustrate some of these effects in local time and occupation time as well as in the sustainability of ecosystems.

As remarked in previous sections, the tools that have been developed so far apply to one-dimensional problems, or problems on networks that preserve a one-dimensional structure along its branches. An outstanding open problem is to develop a more comprehensive approach to problems with discontinuities across hypersurfaces in several space dimensions. In this direction, Peskir (2007) obtains an extension of the Itô–Tanaka formula to the case where discontinuities occur across the graph of a function. This result, however, does not apply to the case when discontinuities occur, for example, across the surface of a sphere and severely limits its applicability since in many problems of interest, the discontinuities occur across the boundary of bounded sets. Two cases have been investigated in this regard: Decamps, Goovaerts and Schoutens (2006) constructs a skew Bessel process from its scale and speed measures and proves that such a process is the radial component of a "generalized diffusion process" (in the language of Portenko (1990)) with a drift term concentrated on the boundary of a sphere. Second, the family of planar diffusions with rank-dependent diffusion coefficients, thoroughly studied in Fernholz et al. (2013), Fernholz, Ichiba and Karatzas (2013), include the case of a diffusion process in $\mathbb{R}^2$ with discontinuous diffusion coefficient along the line $x = y$.

While full generalization of skew diffusion to problems in dimension greater than one is yet to be completed, some progress has been made for heterogeneous diffusion on graphs, as seen, for example, in Section 4 in the context of river networks. Additionally, for strong-swimming species whose movements are not dependent on the water velocity, Gutierrez et al. (2012) have used analysis on the operator in (4.18) with $v_e = 0$ for all edges to study the time required to eradicate invasive species in a river network.

At a more foundational level, Hairer and Manson (2010) obtain a one-dimensional skew diffusion as a limit in the diffusive scale of solutions of stochastic differential equations with a periodic drift coefficient outside an interval centered at the origin. In the limit the diffusion coefficients are determined in a classical manner, while the skewness is characterized in terms of a Zvonkin type transform of the drift. Moreover, in Hairer and Manson (2011) a similar limit is analyzed for a stochastic differential equation with periodic drift in all directions outside a finite region centered on a hyperplane in $\mathbb{R}^k$. The limiting diffusion has an infinitesimal generator with discontinuous coefficients for which the diffusion coefficient is classically determined. In turn, the domain of the generator determining the interface conditions is characterized through relations on the normal derivatives from both sides of the hyperplane and tangential derivatives. Such results illustrate the promise of a rich mathematical theory as research on interfacial effects goes forward.

A perhaps intermediate step between skew diffusion and diffusion on graphs is the case of problem (2.1) with a piecewise diffusion coefficient taking more than two or an infinite number of values. Namely, one might consider, as in Corollary 4.1, a one-dimensional medium with multiple interfaces. Define

$$D(x) = \sum_{k\in\mathbb{Z}} D^{(k)} \mathbb{1}_{(x_k, x_{k+1})}(x), \tag{5.1}$$

where $\{x_k : k \in \mathbb{Z}\}$ is a sequence of real numbers with no accumulation points and $\{D^{(k)} : k \in \mathbb{Z}\}$ are positive numbers uniformly bounded away from zero. The flux continuity condition (2.3) extends to the multiple interface case as $D^{(k-1)} f'(x_k^-) = D^{(k)} f'(x_k^+)$, $k \in \mathbb{Z}$. The associated process is denoted by X_M^* and is referred to as "multiple skew diffusion."

Using a framework very similar to that presented in Section 3, Ramirez (2011) characterizes X_M^* in terms of a process exhibiting skewness of paths at several points: "multiple skew Brownian motion." More precisely, let $\boldsymbol{\alpha} = \{\alpha_k : k \in \mathbb{Z}\}$ be a sequence with $\alpha_k \in (0, \frac{1}{2}) \cup (\frac{1}{2}, 1)$ and consider interfaces $\{y_k : k \in \mathbb{Z}\}$ with no accumulation points. The process $B^{\boldsymbol{\alpha}}$ is defined as the Feller process with generator $\mathcal{A}^{\boldsymbol{\alpha}} f = \frac{1}{2} f''$ acting on functions $f \in C_b(\mathbb{R})$ that are twice continuously differentiable inside each (y_k, y_{k+1}) and that satisfy $\alpha_k f'(y_k^+) = (1-\alpha_k) f'(y_k^-)$ for all $k \in \mathbb{Z}$. Not surprisingly, "multiple skew diffusion" is given by

$$X_M^*(t) = s_{\sqrt{D}}\big(B^{\boldsymbol{\alpha}^*}(t)\big), \tag{5.2}$$

where $s_{\sqrt{D}}$ denotes here the continuous piecewise linear function with $s_{\sqrt{D}}(0) = 0$ and $s'_{\sqrt{D}}(x) = D^{(k)}$ for $x \in (x_k, x_{k+1})$, and $B^{\boldsymbol{\alpha}^*}$ is multiple skew Brownian motion with interfaces $\{s_{\sqrt{D}}^{-1}(x_k) : k \in \mathbb{Z}\}$ and skewness sequence

$$\alpha_k = \frac{\sqrt{D_k}}{\sqrt{D_k} + \sqrt{D_{k-1}}}, \quad k \in \mathbb{Z}. \tag{5.3}$$

Processes of the form X_M^* can be used in the context of transport within layered media, as exemplified in Figure 3. In particular, Ramirez (2011) analyzes such a process to determine the asymptotic behavior of particles undergoing advection–diffusion on a periodic infinite layered medium composed of two phases: a matrix of slow diffusive transport with periodic cracks where fast diffusion dominates.

ACKNOWLEDGMENTS

The authors are especially grateful for the careful reading and comments by the reviewers that greatly improved the exposition. Professor Enrique Thomann acknowledges fellowship support of the NSF Institute for Mathematics and its Applications at the University of Minnesota during the academic year 2012–2013. The authors Thomann and Waymire were supported in part by NSF Grants DMS-11-22699 and DMS-10-31251.

REFERENCES

ACHA, E. M., MIANZAN, H. W., GUERRERO, R. A., FAVERO, M. and BAVA, J. (2004). Marine fronts at the continental shelves of austral South America: Physical and ecological processes. *Journal of Marine Systems* **44** 83–105.

APPUHAMILLAGE, T. and SHELDON, D. (2012). First passage time of skew Brownian motion. *J. Appl. Probab.* **49** 685–696. MR3012092

APPUHAMILLAGE, T. A., BOKIL, V. A., THOMANN, E. A., WAYMIRE, E. C. and WOOD, B. D. (2010). Solute transport across an interface: A Fickian theory for skewness in breakthrough curves. *Water Resour. Res.* **46** W07511.

APPUHAMILLAGE, T., BOKIL, V., THOMANN, E., WAYMIRE, E. and WOOD, B. (2011a). Corrections for "Occupation and local times for skew Brownian motion with applications to dispersion across an interface." *Ann. Appl. Probab.* **21** 2050–2051. MR2884059

APPUHAMILLAGE, T., BOKIL, V., THOMANN, E., WAYMIRE, E. and WOOD, B. (2011b). Occupation and local times for skew Brownian motion with applications to dispersion across an interface. *Ann. Appl. Probab.* **21** 183–214. MR2759199

APPUHAMILLAGE, T. A., BOKIL, V. A., THOMANN, E. A., WAYMIRE, E. C. and WOOD, B. D. (2012). Interfacial phenomena and natural local time. Unpublished manuscript. Available at arXiv:1204.0271.

ARIS, R. (1956). On the dispersion of a solute particle in a fluid moving through a tube. *Proc. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci.* **235** 67–77.

ARYASOVA, O. V. and PORTENKO, M. I. (2008). A uniqueness theorem for the martingale problem describing a diffusion in media with membranes. *Theory Stoch. Process.* **14** 1–9. MR2479727

BARNDORFF-NIELSEN, O. E. (1998). Stochastic Methods in Hydrology: Rain, Landforms and Floods, Volume 7. In *Advanced Series on Statistical Science and Applied Probability*. World Scientific, Singapore.

BERKOWITZ, B., CORTIS, A., DROR, I. and SCHER, H. (2009). Laboratory experiments on dispersive transport across interfaces: The role of flow direction. *Water Resour. Res.* **45** 2.

BHATTACHARYA, R. N. and GUPTA, V. K. (1984). On the Taylor–Aris theory of solute transport in a capillary. *SIAM J. Appl. Math.* **44** 33–39. MR0729999

BHATTACHARYA, R. N. and WAYMIRE, E. C. (2009). Stochastic processes with applications. *SIAM Classics in Applied Mathematics* **61**. Originally published: Wiley, New York. MR1054645

BHATTACHARYA, R. and WAYMIRE, E. C. (2007). *A Basic Course in Probability Theory*. Springer, New York. MR2331066

BOKIL, V. A., GIBSON, N. L., NGUYEN, S. T., THOMANN, E. A. and WAYMIRE, E. C. (2013). Numerical methods for linear diffusion equations in the presence of an interface. Preprint. Available at arXiv:1310.8248 [math.NA].

BRILLINGER, D. R. R. (2003). Sampling constrained animal motion using stochastic differential equations. In *Probability, Statistics and Their Applications: Papers in Honor of Rabi Bhattacharya*. *Institute of Mathematical Statistics Lecture Notes—Monograph Series* **41** 35–48. IMS, Beachwood, OH. MR1999410

BRILLINGER, D. R., PREISLER, H. K., AGER, A. A., KIE, J. G. and STEWART, B. S. (2002). Employing stochastic differential equations to model wildlife motion. *Bull. Braz. Math. Soc.* (*N.S.*) **33** 385–408. Fifth Brazilian School in Probability (Ubatuba, 2001). MR1978835

BROOKS, J. K. and CHACON, R. V. (1983). Diffusions as a limit of stretched Brownian motions. *Adv. Math.* **49** 109–122. MR0714586

CANTRELL, R. S. and COSNER, C. (2003). *Spatial Ecology via Reaction–Diffusion Equations*. Wiley, Chichester. MR2191264

CARSLAW, H. S. and JAEGER, J. C. (1988). *Conduction of Heat in Solids*, 2nd ed. Oxford Univ. Press, New York. MR0959730

CHEN, Z.-Q. and FUKUSHIMA, M. (2012). *Symmetric Markov Processes, Time Change, and Boundary Theory*. *London Mathematical Society Monographs Series* **35**. Princeton Univ. Press, Princeton, NJ. MR2849840

CHERNY, A. S., SHIRYAEV, A. N. and YOR, M. (2002). Limit behaviour of the "horizontal–vertical" random walk and some extensions of the Donsker–Prokhorov invariance principle. *Teor. Veroyatn. Primen.* **47** 498–517. MR1975425

DECAMPS, M., GOOVAERTS, M. and SCHOUTENS, W. (2006). Asymmetric skew Bessel processes and their applications to finance. *J. Comput. Appl. Math.* **186** 130–147. MR2190302

ÉTORÉ, P. and MARTINEZ, M. (2013). Exact simulation of one-dimensional stochastic differential equations involving the local time at zero of the unknown process. *Monte Carlo Methods Appl.* **19** 41–71. MR3039402

FAGAN, W. F. (2002). Connectivity, fragmentation, and extinction risk in dendritic metapopulations. *Ecology* **83** 3243–3249.

FAGAN, W. F., CANTRELL, R. S. and COSNER, C. (1999). How habitat edges change species interactions. *The American Naturalist* **153** 165–182.

FELDER, W. and WAYMIRE, E. C. (2013). On the drift paradox in a regime-switching mode. Preprint. Available at arXiv:1304.1208.

FERNHOLZ, E. R., ICHIBA, T. and KARATZAS, I. (2013). Two Brownian particles with rank-based characteristics and skew-elastic collisions. *Stochastic Process. Appl.* **123** 2999–3026. MR3062434

FERNHOLZ, E. R., ICHIBA, T., KARATZAS, I. and PROKAJ, V. (2013). Planar diffusions with rank-based characteristics and perturbed Tanaka equations. *Probab. Theory Related Fields* **156** 343–374. MR3055262

FREIDLIN, M. and SHEU, S.-J. (2000). Diffusion processes on graphs: Stochastic differential equations, large deviation principle. *Probab. Theory Related Fields* **116** 181–220. MR1743769

FREIDLIN, M. I. and WENTZELL, A. D. (1993). Diffusion processes on graphs and the averaging principle. *Ann. Probab.* **21** 2215–2245. MR1245308

FUKUSHIMA, M., OSHIMA, Y. and TAKEDA, M. (1994). *Dirichlet Forms and Symmetric Markov Processes. de Gruyter Studies in Mathematics* **19**. de Gruyter, Berlin. MR1303354

GELHAR, L. W. and AXNESS, C. L. (1983). Three-dimensional stochastic analysis of macrodispersion in aquifers. *Water Resour. Res.* **19** 161–180.

GUTIERREZ, J. B., HURDAL, M. K., PARSHAD, R. D. and TEEM, J. L. (2012). Analysis of the Trojan Y chromosome model for eradication of invasive species in a dendritic riverine system. *J. Math. Biol.* **64** 319–340. MR2864846

HAIRER, M. and MANSON, C. (2010). Periodic homogenization with an interface: The one-dimensional case. *Stochastic Process. Appl.* **120** 1589–1605. MR2653267

HAIRER, M. and MANSON, C. (2011). Periodic homogenization with an interface: The multi-dimensional case. *Ann. Probab.* **39** 648–682. MR2789509

HARRISON, J. M. and SHEPP, L. A. (1981). On skew Brownian motion. *Ann. Probab.* **9** 309–313. MR0606993

HOTEIT, H., MOSE, R., YOUNES, A., LEHMANN, F. and ACKERER, P. (2002). Three-dimensional modeling of mass transfer in porous media using the mixed hybrid finite elements and the random-walk methods. *Math. Geol.* **34** 435–456. MR1951790

ITÔ, K. and MCKEAN, H. P. JR. (1963). Brownian motions on a half line. *Illinois J. Math.* **7** 181–231. MR0154338

KARATZAS, I. and SHREVE, S. E. (1988). *Brownian Motion and Stochastic Calculus. Graduate Texts in Mathematics* **113**. Springer, New York. MR0917065

KUO, R. H., IRWIN, N. C., GREENKORN, R. A. and CUSHMAN, J. H. (1999). Experimental investigation of mixing in aperiodic heterogeneous porous media: Comparison with stochastic transport theory. *Transp. Porous Media* **37** 169–182.

LABOLLE, E. M., QUASTEL, J. and FOGG, G. E. (1998). Diffusion theory for transport in porous media: Transition-probability densities of diffusion processes corresponding to advection–dispersion equations. *Water Resour. Res.* **34** 1685–1693.

LABOLLE, E. M., QUASTEL, J., FOGG, G. E. and GRAVNER, J. (2000). Diffusion processes in composite porous media and their numerical integration by random walks: Generalized stochastic differential equations with discontinuous coefficients. *Water Resour. Res.* **36** 1685–1693.

LE GALL, J. F. (1984). One-dimensional stochastic differential equations involving the local times of the unknown process. In *Stochastic Analysis and Applications* (*Swansea*, 1983). *Lecture Notes in Math.* **1095** 51–82. Springer, Berlin. MR0777514

LEJAY, A. (2006). On the constructions of the skew Brownian motion. *Probab. Surv.* **3** 413–466. MR2280299

LEJAY, A. and PICHOT, G. (2012). Simulating diffusion processes in discontinuous media: A numerical scheme with constant time steps. *J. Comput. Phys.* **231** 7299–7314. MR2969713

LUTSCHER, F., LEWIS, M. A. and MCCAULEY, E. (2006). Effects of heterogeneity on spread and persistence in rivers. *Bull. Math. Biol.* **68** 2129–2160. MR2293837

LUTSCHER, F., PACHEPSKY, E. and LEWIS, M. A. (2005). The effect of dispersal patterns on stream populations. *SIAM Rev.* **47** 749–772 (electronic). MR2212398

MA, Z. M. and RÖCKNER, M. (1992). *Introduction to the Theory of* (*Nonsymmetric*) *Dirichlet Forms*. Springer, Berlin. MR1214375

MARTINEZ, M. and TALAY, D. (2012). One-dimensional parabolic diffraction equations: Pointwise estimates and discretization of related stochastic differential equations with weighted local times. *Electron. J. Probab.* **17** 1–32. MR2912504

MATANO, R. and PALMA, E. (2008). On the upwelling of downwelling currents. *Journal of Physical Oceanography* **38** 2482–2500.

MÜLLER, K. (1954). Investigations on the organic drift in north swedish streams. *Rep. Inst. Freshwat. Res. Drottningholm* **35** 133–148.

NAKAO, S. (1972). On the pathwise uniqueness of solutions of one-dimensional stochastic differential equations. *Osaka J. Math.* **9** 513–518. MR0326840

OKUBO, A. and LEVIN, S. A. (2001). *Diffusion and Ecological Problems*: *Modern Perspectives*, 2nd ed. *Interdisciplinary Applied Mathematics* **14**. Springer, New York. MR1895041

OUKNINE, Y. (1990). Le "Skew-Brownian motion" et les processus qui en dérivent. *Teor. Veroyatn. Primen.* **35** 173–179. MR1050069

OVASKAINEN, O. and CORNELL, S. J. (2003). Biased movement at a boundary and conditional occupancy times for diffusion processes. *J. Appl. Probab.* **40** 557–580. MR1993253

PECKHAM, S. D. (1995). New results for self-similar trees with applications to river networks. *Water Resources Research* **31** 1023–1029.

PERRIN, J. (1913). *Les Atomes/Par Jean Perrin*, *Avec* 13 *Figures*. F. Alcan, Paris.

PESKIR, G. (2007). A change-of-variable formula with local time on surfaces. In *Séminaire de Probabilités XL. Lecture Notes in Math.* **1899** 69–96. Springer, Berlin. MR2408999

PORTENKO, N. I. (1990). *Generalized Diffusion Processes. Translations of Mathematical Monographs* **83**. Amer. Math. Soc., Providence, RI. MR1104660

PROKAJ, V. (2011). The solution of the perturbed Tanaka—Equation is pathwise unique. Available at arXiv:1104.0740.

RAMIREZ, J. M. (2011). Multi-skewed Brownian motion and diffusion in layered media. *Proc. Amer. Math. Soc.* **139** 3739–3752. MR2813404

RAMIREZ, J. M. (2012a). Population persistence under advection–diffusion in river networks. *J. Math. Biol.* **65** 919–942. MR2984129

RAMIREZ, J. M. (2012b). Green's functions for Sturm–Liouville problems on directed tree graphs. *Rev. Colombiana Mat.* **46** 15–25. MR2945668

RAMIREZ, J. M., THOMANN, E. A., WAYMIRE, E. C., HAGGERTY, R. and WOOD, B. (2006). A generalized Taylor–Aris formula and skew diffusion. *Multiscale Model. Simul.* **5** 786–801. MR2257235

REVUZ, D. and YOR, M. (1999). *Continuous Martingales and Brownian Motion*, 3rd ed. *Grundlehren der Mathematischen Wissenschaften* [*Fundamental Principles of Mathematical Sciences*] **293**. Springer, Berlin. MR1725357

RODRIGUEZ-ITURBE, I. and RINALDO, A. (2001). *Fractal River Basins*: *Chance and Self-Organization*. Cambridge Univ. Press, Cambridge.

SCHULTZ, C. B. and CRONE, E. E. (2001). Edge-mediated dispersal behavior in a prairie butterfly. *Ecology* **82** 1879–1892.

SPEIRS, D. C. and GURNEY, W. S. C. (2001). Population persistence in rivers and estuaries. *Ecology* **82** 1219–1237.

STROOCK, D. W. and VARADHAN, S. R. S. (2006). *Multidimensional Diffusion Processes*. Springer, Berlin. Reprint of the 1997 edition. MR2190038

TAYLOR, G. I. (1953). Dispersion of a soluble matter in solvent flowing through a tube. *Proc. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci.* **219** 186–203.

WALSH, J. B. (1978). A diffusion with a discontinuous local time. *Astérisque* **52–53** 37–45.

WOODING, R. A. (1960). Rayleigh instability of a thermal boundary layer in flow through a porous medium. *J. Fluid Mech.* **9** 183–192. MR0120977