Moment equations for a piecewise deterministic PDE

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Abstract

We analyze a piecewise deterministic PDE consisting of the diffusion equation on a finite interval Ω with randomly switching boundary conditions and diffusion coefficient. We proceed by spatially discretizing the diffusion equation using finite differences and constructing the Chapman–Kolmogorov (CK) equation for the resulting finite-dimensional stochastic hybrid system. We show how the CK equation can be used to generate a hierarchy of equations for the r-th moments of the stochastic field, which take the form of r-dimensional parabolic PDEs on Ω^r that couple to lower order moments at the boundaries. We explicitly solve the first and second order moment equations ($r = 2$). We then describe how the r-th moment of the stochastic PDE can be interpreted in terms of the splitting probability that r non-interacting Brownian particles all exit at the same boundary; although the particles are non-interacting, statistical correlations arise due to the fact that they all move in the same randomly switching environment. Hence the stochastic diffusion equation describes two levels of randomness: Brownian motion at the individual particle level and a randomly switching environment. Finally, in the limit of fast switching, we use a quasi-steady state approximation to reduce the piecewise deterministic PDE to an SPDE with multiplicative Gaussian noise in the bulk and a stochastically-driven boundary.

(Some figures may appear in colour only in the online journal)

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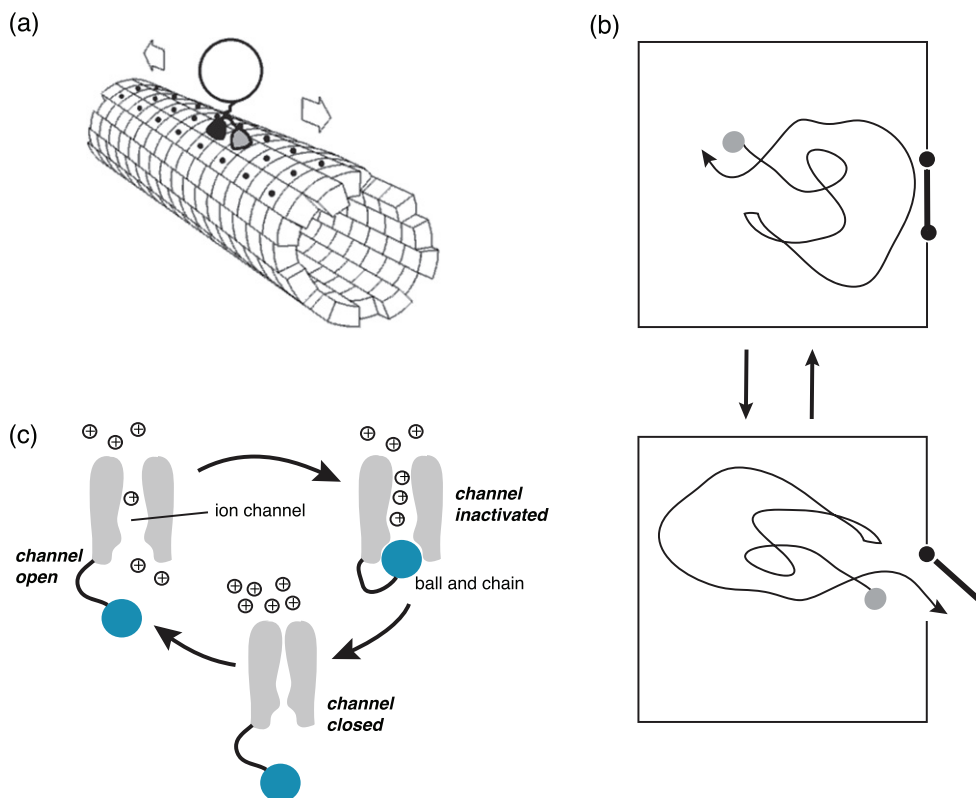
Figure 1. Examples of stochastic hybrid systems for ODEs. (a) Intermittent motion of a molecular motor. (b) Stochastically-gated Brownian motion. (c) Neuron with voltage-gated ion channels.

1. Introduction

There are a growing number of problems in biology that involve the coupling between a piecewise deterministic dynamical system in $\mathbb{R}^d$ and a time-homogeneous Markov chain on some discrete space Γ, resulting in a stochastic hybrid system [1], also known as a piecewise deterministic Markov process [2]. One simple example concerns the intermittent dynamics of a molecular motor moving along a cytoskeletal filament, with the continuous variable representing spatial position along the filament and the discrete variable denoting the motile state of the motor [3–9]; the latter could determine whether the motor is moving to the left or to the right, see figure 1(a). Another example is a macromolecule diffusing in some bounded intracellular domain, which contains a narrow channel within the boundary of the domain. One obtains a hybrid system if the channel is controlled by a stochastic gate that switches between an open and closed state (see figure 1(b)) or if the molecule switches between different conformational states, only some of which allow the molecule to pass through the channel [10]. In contrast to the previous example, the continuous dynamics now evolve according to a stochastic differential equation (SDE). A third important example is the membrane voltage fluctuations of a single neuron due to the stochastic opening and closing of ion channels [11–19], see figure 1(c). Here the discrete states of the ion channels evolve according to a continuous-time Markov process with voltage-dependent transition rates and,

in-between discrete jumps in the ion channel states, the membrane voltage evolves according to a deterministic equation that depends on the current state of the ion channels. In the limit that the number of ion channels goes to infinity, one can apply the law of large numbers and recover classical Hodgkin–Huxley type equations. However, finite-size effects can result in the noise-induced spontaneous firing of a neuron due to channel fluctuations. Stochastic hybrid systems also arise in neural networks [21] and gene networks [22, 23].

In all of the above examples, one can describe the evolution of the system in terms of a forward differential Chapman–Kolmogorov (CK) equation, which takes the form of a deterministic partial differential equation for the indexed set of probability densities $p_n(x, t)$ with $x \in \Omega \subset \mathbb{R}^d$ and $n \in \Gamma$. The CK equation is the starting point for various approximation schemes. For example, in the case of sufficiently fast switching between the discrete states, one can use a quasi-steady-state (QSS) approximation to reduce the CK equation to a Fokker–Planck (FP) equation [3, 8, 24]. Furthermore, when considering escape problems that are dominated by rare events (for which the diffusion approximation breaks down), one can use WKB methods and matched asymptotics [13, 18, 19] or large deviation theory [20, 25, 26].

In this paper, we consider a higher level of stochastic hybrid system, in which the piecewise deterministic dynamics itself evolves according to a partial differential equation. For concreteness, we focus on the diffusion equation on a finite interval with randomly switching boundary conditions. One can view it as a macroscopic model of many Brownian particles that all diffuse in the same randomly switching environment, which is a one-dimensional version of example (b) in figure 1. This type of piecewise deterministic PDE has recently been analyzed by Lawley *et al* [27] using the theory of random iterative systems. These authors assumed that the left-hand boundary is Dirichlet, and the right-hand boundary switches randomly between inhomogeneous Dirichlet and either Neumann or Dirichlet. In both cases they showed that the solution of the stochastic PDE converges in distribution to a random variable whose expectation satisfies a deterministic system of PDEs whose solution is a linear function of x. They also found that the gradient of the solution is a much more complicated function of parameters in the case of the Dirichlet–Neumann switching problem. Note that the switching boundary problem is distinct from stochastic PDEs driven by additive space–time Gaussian noise [28–31], since the former tends to induce stronger correlations at fine spatial scales.

We will address two important issues raised by the study of Lawley *et al* [27]. First, can one derive deterministic PDEs for higher moments of the random field and how do they couple to lower moments? Second, does the resulting hierarchy of deterministic PDEs (assuming it exists) have an interpretation in terms of the dynamics of individual Brownian particles? We will tackle both issues by developing an alternative approach to analyzing piecewise deterministic PDEs, based on discretizing space and constructing the CK equation for the resulting finite-dimensional stochastic hybrid system. We show how the CK equation can be used to determine the dynamics of the expectation of the stochastic field, thus recovering the results of Lawley *et al* [27] in a simpler fashion. This construction is then extended to generate a hierarchy of equations for the r-th moments, which take the form of r-dimensional parabolic PDEs on Ω^r that couple to lower order moments at the boundaries. We explicitly solve the second order moment equations ($r = 2$). Finally, we describe how the r-th moment of the stochastic PDE can be interpreted in terms of the splitting probability that r non-interacting Brownian particles all exit at the same boundary; although the particles are non-interacting, statistical correlations arise due to the fact that they all move in the same randomly switching environment. Hence the stochastic diffusion equation describes two

levels of randomness: Brownian motion at the individual particle level and a randomly switching environment.

The paper is organized as follows. In section 2, we briefly summarize some aspects of piecewise deterministic ODEs. We then introduce our piecewise deterministic PDE in section 3, and determine the CK equation for the corresponding ODE obtained using finite differences. The moment equations for Dirichlet–Dirichlet and Dirichlet–Neumann switching boundaries are constructed and analyzed in sections 4 and 5, respectively. The relationship between the moment equations and single Brownian particle dynamics is established in section 6. Finally, in section 7 we use formal perturbation methods to approximate the piecewise deterministic PDE in the limit of fast switching by an SPDE with multiplicative Gaussian noise in the bulk of the domain and a stochastically-driven boundary.

2. Piecewise deterministic ODE

Before proceeding to analyze a piecewise deterministic PDE, it is useful to recall some basic features of piecewise deterministic ODEs. The reasons are twofold: first, we will analyze the stochastic PDE by discretizing space, which yields a finite-dimensional stochastic hybrid system evolving according to a piecewise deterministic ODE. Second, we wish to relate the deterministic PDEs obtained by taking moments of the full stochastic PDE to the CK equations for system of Brownian particles. For the sake of illustration, consider a one-dimensional stochastic hybrid system whose states are described by a pair $(x, n) \in \Omega \times \{0, \cdots, K - 1\}$, where x is a continuous variable in an interval $\Omega = [0, L]$ and n a discrete internal state variable taking values in $\Gamma \equiv \{0, \cdots, K - 1\}$. (Note that one could easily extend the model to higher-dimensions, $x \in \mathbb{R}^d$. In this case Ω is taken to be a connected, bounded domain with a regular boundary $\partial\Omega$.) When the internal state is n, the system evolves according to the ODE

$$\dot{x} = F_n(x)/\tau, \tag{2.1}$$

where the vector field $F_n: \mathbb{R} \to \mathbb{R}$ is a continuous function, locally Lipschitz. That is, given a compact subset $\mathcal{K}$ of Ω, there exists a positive constant K_n such that

$$\left| F_n(x) - F_n(y) \right| \leqslant A_n \left| x - y \right|, \quad \forall\, x, y \in \Omega \tag{2.2}$$

for some constant A_n. Here τ is a fixed positive time constant that characterizes the relaxation rate of the x-dynamics. For the moment we do not specify what happens to the particle on the boundary $\partial\Omega$, see below.

In order to specify how the system jumps from one internal state to the other for each $n \in \Gamma$, we consider the positive time constant τ_n and the function $W_{nn'}(x)$ defined on $\Gamma \times \Gamma \times \mathbb{R}$ with $W_{nn}(x) = 0$ and $\sum_{m \in \Gamma} W_{mn}(x) = 1$ for all x, n. The hybrid evolution of the system can be described as follows. Suppose the system starts at time zero in the state (x_0, n_0). Call $x_0(t)$ the solution of (2.1) with $n = n_0$ such that $x_0(0) = x_0$. Let θ_1 be the random variable such that

$$\mathbb{P}\left(\theta_1 > t\right) = \exp\left(-\frac{t}{\tau_{n_0}}\right).$$

Then in the random time interval $[0, \theta_1)$ the state of the system is $(x_0(s), n_0)$. We draw a value of θ_1 from the corresponding probability density

$$p(t) = \frac{1}{\tau_{n_0}} \exp\left(-\frac{t}{\tau_{n_0}}\right).$$

If $\theta_1 = \infty$ then we are done, otherwise we choose an internal state $n_1 \in \Gamma$ with probability $W_{n_1 n_0}(x_0(\theta_1))$ and call $x_1(t)$ the solution of the following Cauchy problem on $[\theta_1, \infty)$:

$$\begin{cases} \dot{x}_1(t) &= F_{n_1}\big(x_1(t)\big)/\tau, \quad t \geqslant \theta_1, \\ x_1(\theta_1) &= x_0(\theta_1). \end{cases}$$

Iterating this procedure, we construct a sequence of increasing jumping times $(\theta_k)_{k \geqslant 0}$ (setting $\theta_0 = 0$) and a corresponding sequence of internal states $(n_k)_{k \geqslant 0}$. The evolution $(x(t), n(t))$ is then defined as

$$(x(t), n(t)) = \big(x_k(t), n_k\big), \quad \text{if } \theta_k \leqslant t < \theta_{k+1}. \tag{2.3}$$

Note that the path $x(t)$ is continuous and piecewise C^1. Moreover, although the evolution of the continuous variable $X(t)$ or the discrete variable $N(t)$ is non-Markovian, it can be proven that the joint evolution $(X(t), N(t))$ is a strong Markov process [2].

Given the iterative definition of the stochastic hybrid process, let $X(t)$ and $N(t)$ denote the stochastic continuous and discrete variables, respectively, at time t, $t > 0$, given the initial conditions $X(0) = x_0$, $N(0) = n_0$. Introduce the probability density $p_n(x, t) = p(x, n, t | x_0, n_0, 0)$ with

$$\mathbb{P}\big\{X(t) \in (x, x + \mathrm{d}x), N(t) = n \big| x_0, n_0\big\} = p\big(x, n, t \big| x_0, n_0, 0\big)\mathrm{d}x.$$

We also fix the units of time by setting $\tau = 1$ and introducing the scaling $W_{mn} \to W_{mn}/\tau_n$. It follows that p_n evolves according to the forward differential CK equation [1, 32]

$$\frac{\partial p_n}{\partial t} = -\frac{\partial}{\partial x}\Big[F_n(x)p_n(x, t)\Big] + \sum_{m \in \Gamma} A_{nm}(x)p_m(x, t), \tag{2.4}$$

with

$$A_{nm} = W_{nm} - \delta_{n,m} \sum_{k \in \Gamma} W_{km}. \tag{2.5}$$

Note that $\sum_{n=0}^{K-1} A_{nm} = 0 \quad \forall m \in \Gamma$. It remains to specify boundary conditions for the CK equation (2.4). A natural choice is an absorbing or reflecting boundary at each end. Thus, at $x = 0$ we would have either

$$p_n(0, t) = 0 \quad \forall n \quad \text{such that} \quad F_n(0) < 0 \quad \text{(absorbing)}$$

or

$$\sum_{n=0}^{K-1} F_n(0)p_n(0, t) = 0 \quad \text{(reflecting)},$$

and similarly at $x = L$. Hence, a particle that hits the first boundary condition is trapped (absorbed) there for all future time, while a particle that hits the second boundary condition is reflected back into the interior of the domain.

A simple example of a stochastic hybrid system is a molecular motor moving along a filament track of length L. Suppose that the motor exists in two states: moving to the right with speed v ($n = 0$) or moving to the left with velocity $-v$ ($n = 1$). Assume that transitions between the two states are given by the two-state Markov process, $n = 0, 1$

$$0 \underset{\alpha}{\overset{\beta}{\rightleftharpoons}} 1. \tag{2.6}$$

Given the fixed transition rates α, β, the CK equation takes the simple form

$$\frac{\partial p_0}{\partial t} = -v \frac{\partial p_0}{\partial x} - \beta p_0 + \alpha p_1, \tag{2.7a}$$

$$\frac{\partial p_1}{\partial t} = v \frac{\partial p_1}{\partial x} + \beta p_0 - \alpha p_1. \tag{2.7b}$$

At $x = 0$ the absorbing and reflecting boundary conditions are $p_1(0, t) = 0$ and $p_0(0, t) = p_1(0, t)$, respectively.

So far we have assumed that the continuous process is piecewise deterministic. However, it is straightforward to extend to the case where the continuous process is a piecewise SDE. That is, consider the piecewise Ito SDE

$$dX(t) = F_n(X) + \sqrt{2D_n(X)}\, dW(t), \tag{2.8}$$

where $n \in \Gamma$ and $W(t)$ is a Wiener process. The drift term $F_n(X)$ and diffusion term $D_n(X)$ are both taken to be Lipschitz. When the SDE is coupled to the discrete process on Γ, the stochastic dynamics can again be described by a differential CK equation, except now there is an additional diffusion term:

$$\frac{\partial p_n(x, t)}{\partial t} = -\frac{\partial}{\partial x}\Big[F_n(x)p_n(x, t)\Big] + \frac{\partial^2}{\partial x^2}\Big[D_n(x)p_n(x, t)\Big] + \sum_m A_{nm}(x)p_m(x, t). \tag{2.9}$$

Equation needs to be supplemented by boundary conditions at $x = 0, L$. For example, for each discrete state n one could impose an absorbing or reflecting boundary condition at each end. Hence for each n we would impose

$$p_n(0, t) = 0 \text{ (absorbing)} \quad \text{or} \quad F_n(0)p_n(0, t) - \frac{\partial D_n(x)p_n(x, t)}{\partial x}\bigg|_{x=0} = 0 \text{ (reflecting)}.$$

In the special case of a pure Brownian particle existing in two states ($n = 0, 1$) with spatially uniform diffusion coefficients D_0, D_1 and transition rates α, β, we have

$$\frac{\partial p_0}{\partial t} = D_0 \frac{\partial^2 p_0}{\partial x^2} - \beta p_0 + \alpha p_1, \tag{2.10a}$$

$$\frac{\partial p_1}{\partial t} = D_1 \frac{\partial^2 p_1}{\partial x^2} + \beta p_0 - \alpha p_1, \tag{2.10b}$$

with $p_n(x, t) = 0$ or $\partial_x p_n(x, t) = 0$ at $x = 0, L$.

3. Piecewise deterministic PDE

We now turn to a piecewise deterministic PDE with switching boundaries. Consider the indexed diffusion equation

$$\frac{\partial u}{\partial t} = D_n \frac{\partial^2 u}{\partial x^2}, \quad x \in [0, L], t > 0 \tag{3.1a}$$

with u satisfying the boundary conditions

$$B_n(u(0, t), u'(0, t)) = 0, \quad C_n(u(L, t), u'(L, t)) = 0 \tag{3.1b}$$

and $n \in I \subseteq \mathbb{Z}$ is a discrete internal state variable. We assume that the latter evolves according to a jump Markov process $m \to n$ with u-independent transition rates W_{nm}. The jump propagator $W_{nm} dt$ is the probability that the system switches from the discrete internal state m at time t to the discrete state n at time $t + dt$. The resulting stochastic process is an example of a piecewise deterministic PDE, in which $u(x, t)$ evolves deterministically between jumps in the discrete variable n. When n switches, both the diffusion coefficient and the boundary conditions change. In order to develop the basic theory, we will focus on the two-state Markov process (2.6) and consider two cases for the possible boundary conditions. We take the boundary conditions to be

$$u(0, t) = 0, \quad u(L, t) = \eta > 0 \text{ for } n = 0, \quad u(L, t) = 0 \text{ for } n = 1 \tag{3.2}$$

or

$$u(0, t) = 0, \quad u(L, t) = \eta > 0 \text{ for } n = 0, \quad \partial_x u(L, t) = 0 \text{ for } n = 1. \tag{3.3}$$

Thus, the left-hand boundary condition is Dirichlet and in the case of equation (3.2) the right-hand boundary randomly switches between inhomogeneous Dirichlet and homogeneous Dirichlet. In equation (3.3) the right-hand boundary randomly switches between inhomogeneous Dirichlet and homogeneous Neumann. Both of these particular cases with $D_0 = D_1$ were previously analyzed by Lawley *et al* [27] using the theory of random iterative systems. In particular, these authors showed that in either case $u(x, t)$ converges in distribution to a random variable whose expectation is a linear function of x.

In this paper, we develop an alternative approach to analyzing piecewise deterministic PDEs of the form (3.1a) by discretizing space and constructing the CK equation for the resulting finite-dimensional stochastic hybrid system. The first step is to spatially discretize the piecewise deterministic PDE (3.1a) using a finite-difference scheme. One of the nice features of this discretization is that we can incorporate the boundary conditions into the resulting discrete Laplacian. Introduce the lattice spacing a such that $(N + 1)a = L$ for integer N, and let $u_j = u(aj)$, $j = 0, \ldots, N + 1$. Then

$$\frac{du_i}{dt} = \sum_{j=1}^{N} \Delta_{ij}^n u_j + \eta_a \delta_{i,N} \delta_{n,0}, \quad i = 1, \ldots, N, \quad \eta_a = \frac{\eta D_0}{a^2} \tag{3.4}$$

for $n = 0, 1$. Away from the boundaries ($i \neq 1, N$), Δ_{ij}^n is given by the discrete Laplacian

$$\Delta_{ij}^n = \frac{D_n}{a^2} \Big[\delta_{i,j+1} + \delta_{i,j-1} - 2\delta_{i,j} \Big]. \tag{3.5a}$$

On the left-hand absorbing boundary we have $u_0 = 0$, whereas on the right-hand boundary we have in the case of Dirichlet–Dirichlet switching described in equation (3.2) that

$$u_{N+1} = \eta \text{ for } n = 0, \quad u_{N+1} = 0 \text{ for } n = 1,$$

and we have in the case of Dirichlet–Neumann switching described in equation (3.3)

$$u_{N+1} = \eta \text{ for } n = 0, \quad u_{N+1} - u_{N-1} = 0 \text{ for } n = 1.$$

These can be implemented by taking

$$\Delta_{1j}^0 = \frac{D_0}{a^2} \Big[\delta_{j,2} - 2\delta_{j,1} \Big], \quad \Delta_{Nj}^0 = \frac{D_0}{a^2} \Big[\delta_{N-1,j} - 2\delta_{N,j} \Big], \quad \Delta_{1j}^1 = \frac{D_1}{a^2} \Big[\delta_{j,2} - 2\delta_{j,1} \Big] \tag{3.5b}$$

and

$$\Delta_{Nj}^1 = \frac{D_1}{a^2}\Big[\delta_{N-1,j} - 2\delta_{N,j}\Big] \quad \text{or} \quad \Delta_{Nj}^1 = \frac{2D_1}{a^2}\Big[\delta_{N-1,j} - \delta_{N,j}\Big], \qquad (3.5c)$$

depending on if we are considering Dirichlet–Dirichlet or Dirichlet–Neumann switching.

Let $\mathbf{u}(t) = (u_1(t), \ldots, u_N(t))$ and introduce the probability density

$$\text{Prob}\{\mathbf{u}(t) \in (\mathbf{u}, \mathbf{u} + d\mathbf{u}), n(t) = n\} = p_n(\mathbf{u}, t)d\mathbf{u}, \qquad (3.6)$$

where we have dropped the explicit dependence on initial conditions. Following our analysis of piecewise deterministic ODEs in section 2, see equation (2.4), the CK equation for the stochastic hybrid system (3.4) is

$$\frac{\partial p_n}{\partial t} = -\sum_{i=1}^{N}\frac{\partial}{\partial u_i}\left[\left(\sum_{j=1}^{N}\Delta_{ij}^n u_j + \eta_a\delta_{i,N}\delta_{n,0}\right)p_n(\mathbf{u}, t)\right] + \sum_{m=0,1}A_{nm}p_m(\mathbf{u}, t), \quad (3.7)$$

where A is the matrix

$$A = \begin{bmatrix} -\beta & \alpha \\ \beta & -\alpha \end{bmatrix}. \qquad (3.8)$$

The left nullspace of the matrix A is spanned by the vector

$$\psi = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad (3.9)$$

and the right nullspace is spanned by

$$\rho \equiv \begin{pmatrix} \rho_0 \\ \rho_1 \end{pmatrix} = \frac{1}{\alpha + \beta}\begin{pmatrix} \alpha \\ \beta \end{pmatrix}. \qquad (3.10)$$

A simple application of the Perron–Frobenius theorem shows that the two state Markov process with master equation

$$\frac{dP_n(t)}{\partial t} = \sum_{m=0,1}A_{nm}P_m(t) \qquad (3.11)$$

is ergodic with $\lim_{t\to\infty} P_n(t) = \rho_n$.

4. Moment equations: Dirichlet–Dirichlet case

In this section, we consider the Dirichlet–Dirichlet switching of equation (3.2). Since the drift terms in the CK equation are linear in the u_j, it follows that we can obtain a closed set of equations for the moment hierarchy. Since the process switches between boundary conditions of the same type, the analysis of these moments equations is much simpler than the Dirichlet–Neumann switching of equation (3.3) that we consider in section 5. We will proceed by determining equations for the first and second moments.

4.1. First-order moments

Let

$$v_{n,k}(t) = \mathbb{E}\Big[u_k(t)1_{n(t)=n}\Big] = \int p_n(\mathbf{u}, t)u_k(t)d\mathbf{u}. \qquad (4.1)$$

Multiplying both sides of the CK equation (3.7) by $u_k(t)$ and integrating with respect to $\mathbf{u}$ gives (after integrating by parts and using that $p_n(\mathbf{u}, t) \to 0$ as $\mathbf{u} \to \infty$ by the maximum principle)

$$\frac{\mathrm{d}v_{n,k}}{\mathrm{d}t} = \sum_{j=1}^{N} \Delta_{kj}^{n} v_{n,j} + \eta_a \rho_0 \delta_{k,N} \delta_{n,0} + \sum_{m=0,1} A_{nm} v_{m,k}. \tag{4.2}$$

We have assumed that the initial discrete state is distributed according to the stationary distribution ρ_n so that

$$\int p_n(\mathbf{u}, t)\mathrm{d}\mathbf{u} = \rho_n.$$

If we now retake the continuum limit $a \to 0$, we obtain parabolic equations for

$$V_n(x, t) = \mathbb{E}\left[u(x, t) 1_{n(t)=n} \right]. \tag{4.3}$$

That is

$$\frac{\partial V_0}{\partial t} = D_0 \frac{\partial^2 V_0}{\partial x^2} - \beta V_0 + \alpha V_1, \tag{4.4a}$$

$$\frac{\partial V_1}{\partial t} = D_1 \frac{\partial^2 V_1}{\partial x^2} + \beta V_0 - \alpha V_1, \tag{4.4b}$$

with

$$V_0(0, t) = V_1(0, t) = 0, \quad V_0(L, t) = \rho_0 \eta > 0, \quad V_1(L, t) = 0. \tag{4.5}$$

It is now straightforward to recover the result of Lawley *et al* [27] by determining the steady-state solution of equations (4.4a) and (4.4b) for $D_0 = D_1 = 1$. First, note that

$$\mathbb{E}[u(x, t)] = V_0(x, t) + V_1(x, t). \tag{4.6}$$

Since equations (4.4a) and (4.4b) have a globally attracting steady-state, it follows that

$$\lim_{t \to \infty} \mathbb{E}[u(x, t)] = V(x) \equiv \sum_{n=0,1} V_n(x), \tag{4.7}$$

where $V_n(x) \equiv \lim_{t \to \infty} V_n(x, t)$. Setting $D_0 = D_1 = 1$ and adding equations (4.4a) and (4.4b) gives

$$\frac{\mathrm{d}^2 V}{\mathrm{d}x^2} = 0, \quad V(0) = 0, \quad V(L) = \rho_0 \eta. \tag{4.8}$$

Hence

$$V(x) = \frac{x}{L}\rho_0 \eta.$$

Setting $\xi = \sqrt{\alpha + \beta}$, it is also straightforward to obtain that

$$V_0(x) = \rho_0 \eta \left(\rho_1 \frac{\sinh (\xi x)}{\sinh (\xi L)} + \frac{\rho_0}{L}x \right) \quad \text{and} \quad V_1(x) = \rho_0 \rho_1 \eta \left(\frac{x}{L} - \frac{\sinh (\xi x)}{\sinh (\xi L)} \right).$$

4.2. Second-order moments

Let

$$v_{n,kl}(t) = \mathbb{E}\Big[u_k(t)u_l(t)1_{n(t)=n} \Big] = \int p_n(\mathbf{u},\, t)u_k(t)u_l(t)\mathrm{d}\mathbf{u}. \tag{4.9}$$

Multiplying both sides of the CK equation (3.7) by $u_k(t)u_l(t)$ and integrating with respect to $\mathbf{u}$ gives (after integration by parts)

$$\frac{\mathrm{d}v_{n,kl}}{\mathrm{d}t} = \sum_{j=1}^{N}\Big[\Delta_{kj}^n v_{n,jl} + \Delta_{lj}^n v_{n,jk} \Big] + \eta_a \delta_{n,0}\Big[v_{n,k}\delta_{l,N} + v_{n,l}\delta_{k,N} \Big] + \sum_{m=0,1} A_{nm} v_{m,kl}. \tag{4.10}$$

If we now retake the continuum limit $a \to 0$, we obtain a system of parabolic equations for the equal-time two-point correlations

$$C_n(x,\, y,\, t) = \mathbb{E}\Big[u(x,\, t)u(y,\, t)1_{n(t)=n} \Big], \tag{4.11}$$

given by

$$\frac{\partial C_0}{\partial t} = D_0 \frac{\partial^2 C_0}{\partial x^2} + D_0 \frac{\partial^2 C_0}{\partial y^2} - \beta C_0 + \alpha C_1, \tag{4.12a}$$

$$\frac{\partial C_1}{\partial t} = D_1 \frac{\partial^2 C_1}{\partial x^2} + D_1 \frac{\partial^2 C_1}{\partial y^2} + \beta C_0 - \alpha C_1. \tag{4.12b}$$

The two-point correlations couple to the first-order moments via the boundary conditions:

$$C_0(0,\, y,\, t) = C_0(x,\, 0,\, t) = C_1(x,\, 0,\, t) = C_1(0,\, y,\, t) = 0 \tag{4.13a}$$

and

$$\begin{aligned} C_0(L,\, y,\, t) &= \eta V_0(y,\, t), \quad C_0(x,\, L,\, t) = \eta V_0(x,\, t), \\ C_1(L,\, y,\, t) &= C_1(x,\, L,\, t) = 0. \end{aligned} \tag{4.13b}$$

To see why these are the correct boundary conditions, note that if $n(t) = 0$ and $x = L$, then $u(x,\, t) = \eta$ with probability one, and thus

$$C_0(L,\, y,\, t) = \mathbb{E}\Big[u(L,\, t)u(y,\, t)1_{n(t)=0} \Big] = \eta \mathbb{E}\Big[u(y,\, t)1_{n(t)=0} \Big] = \eta V_0(y,\, t).$$

Deriving the other boundary conditions is similar.

As in the case of the first-moment equations, we can solve for the steady-state correlations explicitly. Again, for simplicity, set $D_0 = D_1 = 1$ and define

$$\lim_{t \to \infty} \mathbb{E}[u(x,\, t)u(y,\, t)] = C(x,\, y) \equiv \sum_{n=0,1} C_n(x,\, y),$$

where $C_n(x,\, y) \equiv \lim_{t \to \infty} C_n(x,\, y,\, t)$. Adding the pair of equations (4.12a) and (4.12b) gives

$$\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} = 0, \tag{4.14}$$

with boundary conditions

$$C(0,\, y) = C(x,\, 0) = 0, \quad C(L,\, y) = \eta V_0(y) \quad C(x,\, L) = \eta V_0(x). \tag{4.15}$$

Using separation of variables, we find that

$$C(x, y) = \sum_{n>0} A_n [\sinh(n\pi x/L) \sin(n\pi y/L) + \sin(n\pi x/L) \sinh(n\pi y/L)], \qquad (4.16)$$

where

$$A_n = \frac{2\eta}{\sinh(n\pi)L} \int_0^L V_0(z) \sin(n\pi z/L) dz$$

$$= \frac{2\eta^2 \rho_0}{\sinh(n\pi)L} \frac{(-1)^{n+1}\left(n\pi/L + \rho_0 L\xi^2/(n\pi)\right)}{(n\pi/L)^2 + \xi^2}.$$

In figure 2 we plot the truncated Fourier series of C.

4.3. Higher-order moments

Equations for r-th order moments $r > 2$ can be obtained in a similar fashion. Let

$$v_{n,k_1\ldots k_r}^{(r)}(t) = \mathbb{E}\left[u_{k_1}(t)\ldots u_{k_r}(t)1_{n(t)=n}\right] = \int p_n(\mathbf{u}, t)u_{k_1}(t)\ldots u_{k_r}(t)d\mathbf{u}. \quad (4.17)$$

Multiplying both sides of the CK equation (3.7) by $u_{k_1}(t)\ldots u_{k_r}(t)$ and integrating with respect to $\mathbf{u}$ gives (after integration by parts)

$$\frac{dv_{n,k_1\ldots k_r}^{(r)}}{dt} = \sum_{l=1}^{r}\sum_{j=1}^{N} \Delta_{k_{l}j}^{n} v_{n,k_1\ldots k_{l-1}jk_{l+1}\ldots k_r}^{(r)} + \eta_a \delta_{n,0} \sum_{l=1}^{r} v_{n,k_1\ldots k_{l-1}k_l+1\ldots k_r}^{(r-1)}\delta_{k_l,N} + \sum_{m=0,1} A_{nm} v_{m,k_1\ldots k_r}^{(r)}.$$

If we now retake the continuum limit $a \to 0$, we obtain a system of parabolic equations for the equal-time r-point correlations

$$C_n^{(r)}(x, y) = \mathbb{E}\left[u(x_1, t)u(x_2, t)\ldots u(x_r, t)1_{n(t)=n}\right], \qquad (4.18)$$

given by

$$\frac{\partial C_0^{(r)}}{\partial t} = D_0 \sum_{l=1}^{r} \frac{\partial^2 C_0^{(r)}}{\partial x_l^2} - \beta C_0^{(r)} + \alpha C_1^{(r)}, \qquad (4.19a)$$

$$\frac{\partial C_1^{(r)}}{\partial t} = D_1 \sum_{l=1}^{r} \frac{\partial^2 C_0^{(r)}}{\partial x_l^2} + \beta C_0^{(r)} - \alpha C_1^{(r)}. \qquad (4.19b)$$

The r-point correlations couple to the $(r-1)$-order moments via the boundary conditions:

$$C_0^{(r)}(x_1, \ldots, x_r, t)\Big|_{x_l=0} = C_1^{(r)}(x_1, \ldots, x_r, t)\Big|_{x_l=0} = C_1^{(r)}(x_1, \ldots, x_r, t)\Big|_{x_l=L} = 0, \quad (4.20a)$$
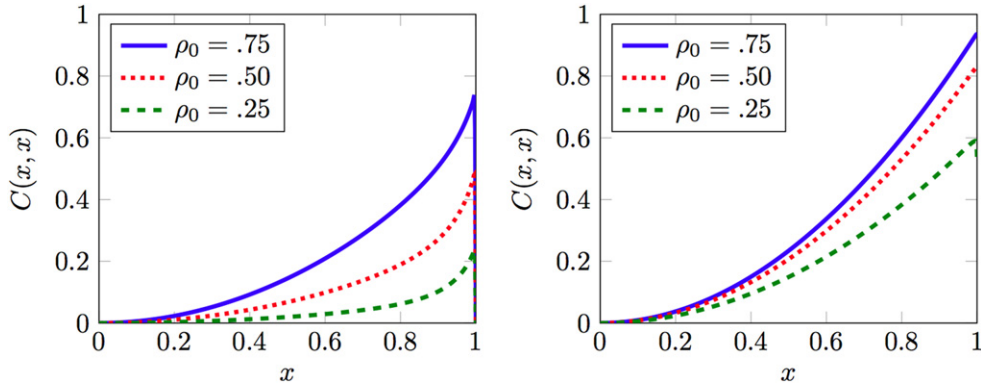
and

$$C_0^{(r)}(x_1, \ldots, x_r, t)\Big|_{x_l=L} = \eta C_0^{(r-1)}(x_1, \ldots, x_{l-1}, x_{l+1}\ldots, x_r, t), \qquad (4.20b)$$

for $l = 1,\ldots,r$.

5. Moment equations: Dirichlet–Neumann case

In this section, we consider the Dirichlet–Neumann switching of equation (3.3). As before, we will obtain a closed set of equations for the moment hierarchy. Since the process now

Figure 2. Plots of $C(x, x)$ for Dirichlet–Dirichlet switching on the left and Dirichlet–Neumann switching on the right. The parameters are $L = \eta = 1$, $\xi = 10$, and either $\rho_0 = 0.75$, 0.5, or 0.25. In each figure, the Fourier series is truncated after 200 terms. For the Dirichlet–Neumann switching, a 50 000-dimensional version of the infinite-dimensional system found in equation (5.25) is solved to estimate the Fourier coefficients.

switches between boundary conditions of different types, the analysis of these moments equations is much more complicated than the Dirichlet–Dirichlet switching of equation (3.3) that we considered above in section 4. Nevertheless, we will be able to solve for the first and second moments.

5.1. First-order moments

As in section 4, we define

$$V_n(x, t) = \mathbb{E}\Big[u(x, t) 1_{n(t)=n} \Big], \tag{5.1}$$

and obtain the parabolic equations

$$\frac{\partial V_0}{\partial t} = D_0 \frac{\partial^2 V_0}{\partial x^2} - \beta V_0 + \alpha V_1, \tag{5.2a}$$

$$\frac{\partial V_1}{\partial t} = D_1 \frac{\partial^2 V_1}{\partial x^2} + \beta V_0 - \alpha V_1, \tag{5.2b}$$

with

$$V_0(0, t) = V_1(0, t) = 0, \quad V_0(L, t) = \rho_0 \eta > 0, \quad \partial_x V_1(L, t) = 0. \tag{5.3}$$

To see why these are the correct boundary conditions, note that if $n(t) = 0$ and $x = L$, then $u(x, t) = \eta$ with probability one, and thus

$$V_0(L, t) = \mathbb{E}\Big[u(L, t) 1_{n(t)=0} \Big] = \eta \mathbb{P}(n(t) = 0) = \eta \rho_0.$$

Deriving the other boundary conditions is similar.

It is now straightforward to recover the result of Lawley *et al* [27] by determining the steady-state solution of equations (5.2a) and (5.2b) for $D_0 = D_1 = 1$. First, note that

$$\mathbb{E}[u(x, t)] = V_0(x, t) + V_1(x, t). \tag{5.4}$$

Since equations equations (5.2a) and (5.2b) have a globally attracting steady-state, it follows that

$$\lim_{t \to \infty} \mathbb{E}[u(x, t)] = V(x) \equiv \sum_{n=0,1} V_n(x), \tag{5.5}$$

where $V_n(x) \equiv \lim_{t \to \infty} V_n(x, t)$. Adding equations (5.2a) and (5.2b) and using the boundary conditions in equation (5.3) gives

$$\frac{d^2 V}{dx^2} = 0, \quad V(0) = 0, \quad V(L) = \rho_0 \eta + \kappa, \tag{5.6}$$

and $\kappa = V_1(L)$. Hence

$$V(x) = \frac{x}{L} \Big[\rho_0 \eta + \kappa \Big],$$

with

$$\frac{d^2 V_1}{dx^2} - (\alpha + \beta) V_1 = -\frac{\beta}{L} x \big(\rho_0 \eta + \kappa \big) \tag{5.7}$$

and $V_1(0) = 0, \partial_x V_1(L) = 0$. It follows that

$$V_1(x) = a e^{-\xi x} + b e^{\xi x} + \frac{\rho_1}{L} \big(\rho_0 \eta + \kappa \big) x,$$

with $\xi = \sqrt{\alpha + \beta}$. The boundary conditions imply that

$$a = -b, \quad 2\xi a \cosh(\xi L) = \frac{\rho_1}{L} \big(\rho_0 \eta + \kappa \big),$$

which yields the solution

$$V_1(x) = \rho_1 \big(\rho_0 \eta + \kappa \big) \left[-\frac{1}{\xi L} \frac{\sinh(\xi x)}{\cosh(\xi L)} + \frac{x}{L} \right]. \tag{5.8}$$

Finally, we obtain κ by setting $x = L$:

$$\kappa = \rho_1 \big(\rho_0 \eta + \kappa \big) \Big[1 - (\xi L)^{-1} \tanh(\xi L) \Big],$$

which can be rearranged to yield

$$\kappa = \rho_1 \rho_0 \eta \frac{1 - (\xi L)^{-1} \tanh(\xi L)}{\rho_0 + \rho_1 (\xi L)^{-1} \tanh(\xi L)}$$

and thus [27]

$$V(x) = \frac{x}{L} \frac{\eta}{1 + \big(\rho_1 / \rho_0 \big) (\xi L)^{-1} \tanh(\xi L)}. \tag{5.9}$$

In the limit $\xi \to \infty$ (fast switching)

$$V(x) = \frac{x}{L} \eta.$$

In section 6 we relate these first moments to a certain hitting probability for a particle diffusing in a random environment.

5.2. Second-order moments

As in section 4, we define

$$C_n(x, y, t) = \mathbb{E}\Big[u(x, t)u(y, t)1_{n(t)=n} \Big], \tag{5.10}$$

and obtain the parabolic equations

$$\frac{\partial C_0}{\partial t} = D_0\frac{\partial^2 C_0}{\partial x^2} + D_0\frac{\partial^2 C_0}{\partial y^2} - \beta C_0 + \alpha C_1, \tag{5.11a}$$

$$\frac{\partial C_1}{\partial t} = D_1\frac{\partial^2 C_1}{\partial x^2} + D_1\frac{\partial^2 C_1}{\partial y^2} + \beta C_0 - \alpha C_1. \tag{5.11b}$$

The two-point correlations couple to the first-order moments via the boundary conditions:

$$C_0(0, y, t) = C_0(x, 0, t) = C_1(x, 0, t) = C_1(0, y, t) = 0 \tag{5.12a}$$

and

$$C_0(L, y, t) = \eta V_0(y, t), \; C_0(x, L, t) = \eta V_0(x, t), \; \partial_x C_1(L, y, t)$$
$$= \partial_y C_1(x, L, t) = 0. \tag{5.12b}$$

As in the case of the first-moment equations, we can solve for the steady-state correlations explicitly. Again, for simplicity, set $D_0 = D_1 = 1$ and add the pair of equations (5.11a) and (5.11b). Define

$$\lim_{t \to \infty} \mathbb{E}[u(x, t)u(y, t)] = C(x, y) \equiv \sum_{n=0,1} C_n(x, y),$$

where $C_n(x, y) = \lim_{t \to \infty} C_n(x, y, t)$. Then we have

$$\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} = 0, \tag{5.13}$$

with boundary conditions

$$C(0, y) = C(x, 0) = 0 \tag{5.14a}$$

and

$$C(L, y) = \eta V_0(y) + C_1(L, y), \quad C(x, L) = \eta V_0(x) + C_1(x, L). \tag{5.14b}$$

Using separation of variables, we have $C(x, y) = f(x)g(y)$ with

$$\frac{f''(x)}{f(x)} = -\frac{g''(y)}{g(y)} = \pm \mu^2$$

for a constant μ. The general solution is

$$C(x, y) = \frac{A_0}{L^2}xy + \sum_{n>0}A_n[\sinh(n\pi x/L)\sin(n\pi y/L) + \sin(n\pi x/L)\sinh(n\pi y/L)]. \tag{5.15}$$

Note that

$$C(L, y) = A_0\frac{y}{L} + \sum_n A_n \sinh(n\pi)\sin(n\pi y/L) \tag{5.16a}$$

and

$$\partial_x C(L, y) = \frac{A_0}{L^2} y + \sum_n \frac{n\pi}{L} A_n \left[\cosh(n\pi) \sin(n\pi y/L) + (-1)^n \sinh(n\pi y/L) \right]. \qquad (5.16b)$$

It follows from equations (5.8) and (5.9) that

$$V_0(y) = \left(\rho_0 \eta + \kappa \right) \left[\frac{\rho_1}{\xi L} \frac{\sinh(\xi y)}{\cosh(\xi L)} + \rho_0 \frac{y}{L} \right].$$

Moreover, C_1 satisfies the equation

$$\frac{\partial^2 C_1}{\partial x^2} + \frac{\partial^2 C_1}{\partial y^2} - (\alpha + \beta) C_1(x, y) = -\beta C(x, y) \qquad (5.17)$$

with

$$C_1(x, 0) = C_1(0, y) = 0, \quad \partial_x C_1(L, y) = \partial_y C_1(x, L) = 0.$$

The general solution of C_1 is

$$C_1(x, y) = \rho_1 C(x, y) + B_0 [y \sinh(\xi x) + x \sinh(\xi y)]$$

$$+ \sum_{n>0} B_n \sinh \left(\sqrt{(n\pi/L)^2 + \xi^2} \, x \right) \sin(n\pi y/L)$$

$$+ \sum_{n>0} B_n \sin(n\pi x/L) \sinh \left(\sqrt{(n\pi/L)^2 + \xi^2} \, y \right). \qquad (5.18)$$

From the boundary conditions (5.14b)

$$\rho_0 C(L, y) = \eta V_0(y) + B_0 [y \sinh(\xi L) + L \sinh(\xi y)]$$

$$+ \sum_{n>0} B_n \sinh \left(\sqrt{(n\pi/L)^2 + \xi^2} \, L \right) \sin(n\pi y/L).$$

Equating terms on the two sides of this equation shows that

$$\rho_0 A_0 = \eta \rho_0 \left(\rho_0 \eta + \kappa \right) + B_0 L \sinh(\xi L), \qquad (5.19a)$$

$$\eta \left(\rho_0 \eta + \kappa \right) \frac{\rho_1}{\xi L \cosh(\xi L)} + B_0 L = 0, \qquad (5.19b)$$

and

$$\rho_0 A_n \sinh(n\pi) = B_n \sinh \left(\sqrt{(n\pi/L)^2 + \xi^2} \, L \right), \quad n > 0. \qquad (5.19c)$$

The first two equations determine A_0, B_0 and the remaining equations determine B_n in terms of A_n.

The final step is to determine the coefficients A_n, $n > 0$ using the other boundary condition $\partial_x C_1(L, y) = 0$. (By symmetry the boundary conditions at $y = L$ are automatically satisfied.) We thus require

$$-\rho_1 \partial_x C (L, y) = B_0 [(\xi y) \cosh (\xi L) + \sinh (\xi y)]$$
$$+ \sum_{n>0} \sqrt{(n\pi/L)^2 + \xi^2} B_n \cosh \left(\sqrt{(n\pi/L)^2 + \xi^2} L \right) \sin (n\pi y/L)$$
$$+ \sum_{n>0} (n\pi/L)(-1)^n B_n \sinh \left(\sqrt{(n\pi/L)^2 + \xi^2} y \right).$$

Using equation (5.16*b*) and rearranging gives

$$-\sum_{n>0} \gamma_n A_n \sin (n\pi y/L) = \left(B_0 \xi \cosh (\xi L) + \rho_1 A_0 /L^2 \right) y + B_0 \sinh (\xi y)$$
$$+ \sum_{n>0} \frac{n\pi}{L} (-1)^n$$
$$\times \left[\rho_1 A_n \sinh (n\pi y/L) + B_n \sinh \left(\sqrt{(n\pi/L)^2 + \xi^2} y \right) \right]$$
$$= \left(B_0 \xi \cosh (\xi L) + \rho_1 A_0 /L^2 \right) y + B_0 \sinh (\xi y)$$
$$+ \sum_{n>0} \frac{n\pi}{L} (-1)^n \left[\rho_1 \sinh (n\pi y/L) \right.$$
$$\left. + \rho_0 \sinh (n\pi) \frac{\sinh \left(\sqrt{(n\pi/L)^2 + \xi^2} y \right)}{\sinh \left(\sqrt{(n\pi/L)^2 + \xi^2} L \right)} \right] A_n, \tag{5.20}$$

where

$$\gamma_n A_n = \rho_1 \frac{n\pi}{L} \cosh (n\pi) A_n + \sqrt{(n\pi/L)^2 + \xi^2} B_n \cosh \left(\sqrt{(n\pi/L)^2 + \xi^2} L \right)$$
$$= \left[\rho_1 \frac{n\pi}{L} \cosh (n\pi) + \rho_0 \sqrt{(n\pi/L)^2 + \xi^2} \sinh (n\pi) \right.$$
$$\left. \times \operatorname{cotanh} \left(\sqrt{(n\pi/L)^2 + \xi^2} L \right) \right] A_n. \tag{5.21}$$

Multiplying both sides of equation (5.20) by $\sin (m\pi y/L)$ and integrating with respect to y yields

$$\frac{L}{2} \gamma_m A_m + \sum_{n>0} \Gamma_{mn} A_n = -\Lambda_m, \quad m > 0, \tag{5.22}$$

where

$$\Lambda_m = \int_0^L \sin (m\pi y/L) \left[\left(B_0 \xi \cosh (\xi L) + \rho_1 A_0 / L^2 \right) y + B_0 \sinh (\xi y) \right] dy \tag{5.23}$$

and

$$\Gamma_{mn} = \frac{n\pi}{L}(-1)^n \int_0^L \left[\rho_1 \sinh(n\pi y/L) + \rho_0 \sinh(n\pi)\frac{\sinh\left(\sqrt{(n\pi/L)^2 + \xi^2}\, y\right)}{\sinh\left(\sqrt{(n\pi/L)^2 + \xi^2}\, L\right)} \right]$$
$$\times \sin(m\pi y/L)\mathrm{d}y. \tag{5.24}$$

Using the integral formula

$$\int_0^L \sinh(\xi y)\sin(m\pi y/L)\mathrm{d}y = \frac{1}{4\mathrm{i}}\int_0^L \left[\mathrm{e}^{(\xi + \mathrm{i}m\pi/L)y} - \mathrm{e}^{(\xi - \mathrm{i}m\pi/L)y}\right]\mathrm{d}y - (\xi \to -\xi)$$

$$= \frac{1}{4\mathrm{i}}\frac{\mathrm{e}^{(\xi + \mathrm{i}m\pi/L)L} - 1}{\xi + \mathrm{i}m\pi/L} - \frac{1}{4\mathrm{i}}\frac{\mathrm{e}^{(\xi - \mathrm{i}m\pi/L)L} - 1}{\xi - \mathrm{i}m\pi/L} - (\xi \to -\xi)$$

$$= \frac{1}{2}\frac{1}{\xi^2 + (m\pi/L)^2}\left[\frac{m\pi}{L} - \frac{m\pi}{L}\cos(m\pi)\mathrm{e}^{\xi L}\right] - (\xi \to -\xi)$$

$$= (-1)^{m+1}\frac{m\pi/L}{\xi^2 + (m\pi/L)^2}\sinh(\xi L),$$

it follows that

$$\Gamma_{mn} = \frac{nm\pi^2}{L^2}(-1)^{n+m+1}\left[\rho_1\frac{\sinh(n\pi)}{(n\pi/L)^2 + (m\pi/L)^2} + \rho_0\frac{\sinh(n\pi)}{(n\pi/L)^2 + \xi^2 + (m\pi/L)^2}\right].$$

Similarly

$$\Lambda_m = \left(B_0\xi\cosh(\xi L) + \rho_1 A_0/L^2\right)\frac{L^2}{m\pi}(-1)^{m+1} + (-1)^{m+1}B_0\frac{m\pi/L}{\xi^2 + (m\pi/L)^2}\sinh(\xi L).$$

Introducing the change of coefficients (for $n > 0$)

$$\widehat{A}_n = \sinh(n\pi)A_n,$$

equation (5.22) can be rewritten as

$$\hat{\gamma}_m\widehat{A}_m + \sum_{n>0}(-1)^{n+m+1}\left[\frac{\rho_1 n}{n^2 + m^2} + \frac{\rho_0 n}{n^2 + (\xi L/\pi)^2 + m^2}\right]\widehat{A}_n = -\frac{\Lambda_m}{m}, \tag{5.25}$$

where

$$\hat{\gamma}_m = \frac{1}{2}\left[\rho_1\pi\coth(m\pi) + \rho_0\sqrt{\pi^2 + (\xi L/m)^2}\coth\left(\sqrt{(m\pi)^2 + (\xi L)^2}\right)\right].$$

If we assume that the infinite-dimensional matrix equation (5.25) has a unique solution, then taking the limit $m \to \infty$ shows that $\widehat{A}_m \sim 1/m^2$ for large m and thus $A_m \sim \mathrm{e}^{-m\pi}/m^2$ for large m. In figure 2 we plot estimates of $C(x, x)$ by truncating its Fourier series expansion in equation (5.15), where the coefficients are estimated by solving a truncated version of equation (5.25). We find that the numerical solution converges to a unique solution, except for a small boundary layer around $x = L$, which shrinks as more terms in our numerical approximation scheme are included. As a further consistency check, we note that the Dirichlet-Dirichelt and Dirichlet–Neumann numerical solutions match in the limit $\alpha \gg \beta$ ($\rho_0 \approx 1$), which is to be expected since both systems spend most of the time in the state corresponding to the inhomogeneous Dirichlet condition at $x = L$.

5.3. Higher-order moments

Analogous to section 4.3, one can show that the equal-time r-point correlations

$$C_n^{(r)}(x_1, x_2, ..., x_r) = \mathbb{E}\Big[u(x_1, t)u(x_2, t)...u(x_r, t)1_{n(t)=n}\Big], \qquad (5.26)$$

for the Dirichlet–Neumann problem satisfy the system of PDEs in equation (4.3) subject to the boundary conditions in equation (4.20b) and

$$C_0^{(r)}(x_1, ..., x_r, t)\Big|_{x_l=0} = C_1^{(r)}(x_1, ..., x_r, t)\Big|_{x_l=0} = \partial_{x_l}C_1^{(r)}(x_1, ..., x_r, t)\Big|_{x_l=L} = 0, (5.27)$$

for $l = 1,...,r$.

6. Particle perspective

The representation of solutions to certain second-order linear PDEs as statistics of solutions to associated SDEs is well established [32]. In this section, we relate the r-th moments of the random PDEs considered above to statistics of Brownian particles diffusing in a randomly switching environment. We find that after a simple rescaling, the r-th moment of the random PDE is the probability that r non-interacting Brownian particles all exit at the same boundary. Although the particles are non-interacting, statistical correlations arise due to the fact that they all move in the same randomly switching environment. Hence the stochastic diffusion equation describes two levels of randomness; Brownian motion at the individual particle level and a randomly switching environment. In section 6.1, we consider the Brownian particle situation corresponding to the Dirichlet–Neumann switching PDE of section 5. The particle situation corresponding to the Dirichlet–Dirichlet switching PDE of section 4 is similar and is explained briefly in section 6.2

6.1. Hitting probability: Dirichlet–Neumann case

The first-moment equations (5.2a) and (5.2b) are identical in form to the CK equation describing a single particle switching between two discrete internal states with distinct diffusion coefficients D_0, D_1 and boundary conditions. The one major difference is that within the single particle perspective, all boundary conditions are homogeneous. For example, suppose that there is an absorbing boundary at $x = 0$, whereas the boundary at $x = L$ is absorbing (reflecting) when the particle is in state $n = 0$ ($n = 1$)

$$\frac{\partial p_0}{\partial t} = D_0 \frac{\partial^2 p_0}{\partial x^2} - \beta p_0 + \alpha p_1, \qquad (6.1a)$$

$$\frac{\partial p_1}{\partial t} = D_1 \frac{\partial^2 p_1}{\partial x^2} + \beta p_0 - \alpha p_1, \qquad (6.1b)$$

with

$$p_0(0, t) = p_1(0, t) = 0, \quad p_0(L, t) = 0, \quad \partial_x p_1(L, t) = 0. \qquad (6.2)$$

Here $p_n(x, t) = p(x, n, t | y, m, 0)$ for y, m fixed is the probability density of finding the particle in discrete state n and position x at time t. For this example there is no non-trivial steady-state solution.

At the single particle level one is often interested in solving first passage problems. Quantities of particular interest are the splitting probability of exiting one end rather than the

other, and the associated conditional mean first-passage time. One way to determine these quantities is to consider the corresponding backward CK equation for $q_m(y, t) = p(x, n, t|y, m, 0)$ with x, n fixed:

$$\frac{\partial q_0}{\partial t} = D_0 \frac{\partial^2 q_0}{\partial y^2} - \beta[q_0 - q_1], \tag{6.3a}$$

$$\frac{\partial q_1}{\partial t} = D_1 \frac{\partial^2 q_1}{\partial y^2} + \alpha[q_0 - q_1]. \tag{6.3b}$$

Let $\gamma_m(y, t)$ be the total probability that the particle is absorbed at the end $x = L$, say, after time t given that it started at y in state m. That is,

$$\gamma_m(y, t) = -D_0 \int_t^\infty \frac{\partial p(L, 0, t'|y, m, 0)}{\partial x} dt'. \tag{6.4}$$

Differentiating equations (6.3a) and (6.3b) with respect to x and integrating with respect to t, we find that

$$\frac{\partial \gamma_0}{\partial t} = D_0 \frac{\partial^2 \gamma_0}{\partial y^2} - \beta[\gamma_0 - \gamma_1], \tag{6.5a}$$

$$\frac{\partial \gamma_1}{\partial t} = D_1 \frac{\partial^2 \gamma_1}{\partial y^2} + \alpha[\gamma_0 - \gamma_1]. \tag{6.5b}$$

The probability $\gamma_m(y, t)$ can be used to define two important quantities. The first is the hitting probability

$$\pi_m(y) = \gamma_m(y, 0) \tag{6.6}$$

and the second is the conditional mean first passage time $T_m(y)$

$$T_m(y) = -\int_0^\infty t \frac{\partial_t \gamma_m(y, t)}{\gamma_m(y, 0)} dt = \frac{\int_0^\infty \gamma_m(y, t) dt}{\gamma_m(y, 0)} \tag{6.7}$$

after integration by parts. Setting $t = 0$ in equations (6.5a) and (6.5b), and using $\partial_t \gamma_m(y, 0) = 0$ for all $y \neq L$ shows that

$$0 = D_0 \frac{\partial^2 \pi_0}{\partial y^2} - \beta[\pi_0 - \pi_1], \tag{6.8a}$$

$$0 = D_1 \frac{\partial^2 \pi_1}{\partial y^2} + \alpha[\pi_0 - \pi_1] \tag{6.8b}$$

with boundary conditions

$$\pi_0(0) = \pi_1(0) = 0, \quad \pi_0(L) = 1, \quad \partial_y \pi_1(L) = 0.$$

This hitting probability is closely related to the first moments of the piecewise deterministic PDE considered in section 5. Specifically, it is easy to check that

$$\pi_n(x) = \frac{1}{\rho_n \eta} V_n(x).$$

This equation can be thought of as a type of Feynman–Kac formula for relating diffusion in a random environment to a piecewise deterministic PDE. Furthermore, let $\pi_n^r(x_1, ..., x_r)$ be the

probability that r Brownian particles all exit at $x = L$ given that the initial positions of the Brownian particles are $x_1, ..., x_r$ and $n(0) = n$. Then

$$\pi_n^r(x_1, ..., x_r) = \frac{1}{\rho_n \eta^r} \lim_{t \to \infty} C_n^{(r)}(x_1, ..., x_r, t), \tag{6.9}$$

where $C_n^{(r)}$ is the r-th moment defined in equation (5.26). Though the particles are non-interacting, the probability that all r particles exit at $x = L$ is not the product of the probabilities of each particle exiting at $x = L$ because the particles are all diffusing in the same randomly switching environment. Equation (6.9) follows from writing down the backward equation for the joint probability density for r particles, and then constructing the multi-particle version of equation (6.4). The crucial step is determining the appropriate inhomogeneous boundary condition for the resulting r-dimensional time-independent PDE that determines the splitting probability. The boundary condition takes the form

$$\pi_0^{(r)}(x_1, \, ..., \, x_r)\Big|_{x_l = L} = \pi_0^{(r-1)}(x_1, \, ..., \, x_{l-1}, \, x_{l+1} ..., \, x_r), \tag{6.10}$$

for $l = 1, ..., r$. This ensures that if one of the particles starts on the right-hand boundary when the latter is in the state $n = 0$, then the particle is immediately removed and thus one just has to determine the splitting probability that the $r - 1$ remaining particles also exit at the right-hand boundary. Finally, performing a similar scaling to the first-moments yields the desired result.

Finally, we remark that the relationship found in this section between hitting probabilities of Brownian particles and moments for a related piecewise deterministic PDE can be generalized to systems with more than two boundary states. First, note that the forward equation, equation (6.1), was used to find moments of the piecewise deterministic PDE and the backward equation, equation (6.1), was used to find splitting probabilities for Brownian particles. Further, observe that when the forward equations and backward equations are viewed as matrix equations, then the matrix appearing in the backward equation is just the transpose of the matrix in the forward equation, and the matrix appearing in the backward equation is the generator for the Markov jump process controlling the boundary switching. This simple relation holds because the Markov jump process controlling the boundary switching has only two states and therefore must be reversible. If one considers more than two possible states for the boundary, one has to reverse the time of the Markov jump process controlling the switching to go between the particle perspective of this section (in which we study the backward equation) and the PDE perspective of the rest of this paper (in which we study the forward equation).

6.2. Hitting probability: Dirichlet–Dirichlet case

Consider r Brownian particles diffusing in the interval $[0, L]$ with absorbing boundary conditions at both endpoints. Let $n(t)$ be an independent Markov jump process and $\pi_n^r(x_1, ..., x_r)$ be the probability that all r particles exit at $x = L$ at times when $n(t) = 0$ given that the initial positions of the Brownian particles are $x_1, ..., x_r$ and $n(0) = n$. Then

$$\pi_n^r(x_1, ..., x_r) = \frac{1}{\rho_n \eta^r} \lim_{t \to \infty} C_n^{(r)}(x_1, ..., x_r, t), \tag{6.11}$$

where $C_n^{(r)}$ is the r-th moment of the Dirichlet–Dirichlet switching PDE defined in equation (4.18). This follows from an argument similar to the argument above in section 6.1.

7. QSS approximation

So far we have used finite differences and the continuum limit to derive exact equations for the moments of the piecewise deterministic PDE (3.1a). In this final section we use formal perturbation methods to derive an approximation of the PDE in the limit that the switching rates $\alpha, \beta \to \infty$, which takes the form of an SPDE with Gaussian spatiotemporal noise (when $D_0 \neq D_1$) and a randomly perturbed boundary condition. We will assume that the limit of the lattice spacing, $a \to 0$, and the limit of the switching rates, $\alpha, \beta \to 0$, commute, so that we can first carry out the QSS approximation of the spatially discrete process and then take the continuum limit.

First, introducing a small parameter, ϵ, and performing the rescalings $\alpha \to \alpha/\epsilon$ and $\beta \to \beta/\epsilon$, the CK equation (3.7) of the spatially discretized process can be written in the form

$$\frac{\partial p_n}{\partial t} = -\sum_{i=1}^{N} \frac{\partial}{\partial u_i} \Big[H_i^n(\mathbf{u}) p_n(\mathbf{u}, t) \Big] + \frac{1}{\epsilon} \sum_{m=0,1} A_{nm} p_m(\mathbf{u}, t), \tag{7.1}$$

with

$$H_i^n(\mathbf{u}) = \sum_{j=1}^{N} \Delta_{ij}^n u_j + \eta_a \delta_{i,N} \delta_{n,0}. \tag{7.2}$$

In the limit $\epsilon \to 0$, one can show that $p_n(\mathbf{u}, t) \to \rho_n \phi(\mathbf{u}, t)$ [26] with ϕ satisfying the Liouville equation

$$\frac{\partial \phi}{\partial t} = -\sum_{i=1}^{N} \frac{\partial}{\partial u_i} \overline{H}_i(\mathbf{u}) \phi(\mathbf{u}, t),$$

where

$$\overline{H}_i(\mathbf{u}) = \sum_{n=0,1} H_i^n(\mathbf{u}) \rho_n. \tag{7.3}$$

Assuming deterministic initial conditions, the Liouville equation is equivalent to the deterministic mean-field equation

$$\frac{\mathrm{d}u_i}{\mathrm{d}t} = \overline{H}_i(\mathbf{u}). \tag{7.4}$$

Taking the continuum limit of this equation using the discrete Laplacian given by equations (3.5a)–(3.5c) gives the deterministic diffusion equation

$$\frac{\partial u}{\partial t} = \overline{D} \frac{\partial^2 u}{\partial x^2} \tag{7.5a}$$

with $\overline{D} = \sum_{n=0,1} D_n \rho_n$ and the boundary conditions

$$u(0, t) = 0, \quad u(L, t) = \eta. \tag{7.5b}$$

This follows from the definition of $\overline{H}_i(\mathbf{u})$. Note that in the fast switching limit, the right-hand boundary condition reduces to inhomogeneous Dirichlet alone, that is, we do not obtain a Robin boundary condition that mixes Dirichlet and Neumann. First, this is consistent with the steady-state solution for the first moment, see equation (5.9). It is also consistent with the known relationship between random walks and diffusion equations in bounded domains. More specifically, in order to obtain a diffusion equation with a Robin boundary condition in the continuum limit of a random walk with a partially absorbing boundary, it is necessary to

take the probability of absorption for a random walker to be $O(a)$, where a is the lattice spacing [33]. This is clearly not the case here.

In the regime $0 < \epsilon \ll 1$, there are typically a large number of transitions between the discrete states $n = 0, 1$ while $\mathbf{u}$ hardly change at all. This suggests that the system rapidly converges to the above QSS solution, which will then be perturbed as $\mathbf{u}$ slowly evolves. The resulting perturbations can be analyzed using a QSS diffusion or adiabatic approximation, in which the CK equation (7.1) is approximated by a FP equation for the total density $\phi(\mathbf{u}, t) = \sum_n p_n(\mathbf{u}, t)$. The QSS approximation was first developed from a probabilistic perspective by Papanicolaou [34], see also [32]. It has subsequently been applied to a wide range of problems in biology, including bacterial chemotaxis [35], wave-like behavior in models of slow axonal transport [3, 4], and molecular motor-based models of random intermittent search [8, 9]. The first step in the QSS reduction is to introduce the decomposition

$$p_n(\mathbf{u}, t) = \phi(\mathbf{u}, t)\rho_n + \epsilon w_n(\mathbf{u}, t), \tag{7.6}$$

with

$$\phi(\mathbf{u}, t) = \sum_n p_n(\mathbf{u}, t), \quad \sum_n w_n(\mathbf{u}, t) = 0.$$

Substituting into equations (5.2a) and (5.2b) yields

$$\frac{\partial \phi(\mathbf{u}, t)}{\partial t}\rho_n + \epsilon \frac{\partial w_n(\mathbf{u}, t)}{\partial t} = -\sum_{i=1}^{N} \frac{\partial}{\partial u_i}\Big(H_i^n(\mathbf{u})\big[\phi(\mathbf{u}, t)\rho_n + \epsilon w_n(\mathbf{u}, t) \big]\Big)$$
$$+ \frac{1}{\epsilon} \sum_{m=0,1} A_{nm}\big[\phi(\mathbf{u}, t)\rho_m + \epsilon w_m(\mathbf{u}, t) \big]. \tag{7.7}$$

Summing both sides of equation (7.7) with respect to n then gives

$$\frac{\partial \phi(\mathbf{u}, t)}{\partial t} = -\sum_{i=1}^{N} \frac{\partial}{\partial u_i}\big(\overline{H}_i(\mathbf{u})\phi(\mathbf{u}, t)\big) - \epsilon \sum_{i=1}^{N} \frac{\partial}{\partial u_i}\Bigg(\sum_{n=0,1} H_i^n(\mathbf{u})w_n(\mathbf{u}, t)\Bigg). \tag{7.8}$$

Substituting equation (7.8) into (7.7) then gives

$$\epsilon \frac{\partial w_n(\mathbf{u}, t)}{\partial t} = -\rho_n \sum_{i=1}^{N} \frac{\partial}{\partial u_i}\Big(\big[H_i^n(\mathbf{u}) - \overline{H}_i(\mathbf{u})\big]\phi(\mathbf{u}, t)\Big) + \sum_{m=0,1} A_{nm} w_m(\mathbf{u}, t)$$
$$-\epsilon \sum_{i=1}^{N} \frac{\partial}{\partial u_i}\big(H_i^n(\mathbf{u})w_n(\mathbf{u}, t)\big) + \epsilon \rho_n \sum_{i=1}^{N} \frac{\partial}{\partial u_i}\Bigg(\sum_{m=0,1} H_i^m(\mathbf{u})w_m(\mathbf{u}, t)\Bigg).$$

Introduce the asymptotic expansion

$$w_n \sim w_n^0 + \epsilon w_n^1 + \epsilon^2 w_n^2 + \dots$$

and collect $O(1)$ terms:

$$\sum_{m=1}^{N} A_{nm} w_m(x, t) = \rho_n \sum_{i=1}^{N} \frac{\partial}{\partial u_i}\Big(\big[H_i^n(\mathbf{u}) - \overline{H}_i(\mathbf{u})\big]\phi(\mathbf{u}, t)\Big), \tag{7.9}$$

where we have dropped the superscript on w_n^0. The Fredholm alternative theorem shows that this has a solution, which is unique on imposing the condition $\sum_n w_n(x, t) = 0$. More explicitly, using the fact that $w_0 = -w_1$, we find that

$$w_0 = -\frac{\rho_0}{(\alpha + \beta)} \sum_{i=1}^{N} \frac{\partial}{\partial u_i} \left(\left[H_i^0(\mathbf{u}) - \overline{H}_i(\mathbf{u}) \right] \phi(\mathbf{u}, t) \right).$$

Finally, substituting this back into equation (7.8) and using $w_0 = -w_1$ yields the FP equation

$$\frac{\partial \phi(\mathbf{u}, t)}{\partial t} = -\sum_{i=1}^{N} \frac{\partial}{\partial u_i} \left(\overline{H}_i(\mathbf{u}) \phi(\mathbf{u}, t) \right)$$

$$+ \epsilon \frac{\rho_0 \rho_1}{(\alpha + \beta)} \sum_{i,j=1}^{N} \frac{\partial}{\partial u_i} \left[H_i^0(\mathbf{u}) - H_i^1(\mathbf{u}) \right] \frac{\partial}{\partial u_j} \left[H_j^0(\mathbf{u}) - H_j^1(\mathbf{u}) \right] \phi(\mathbf{u}, t), \quad (7.10)$$

which is of the Stratonovich form [32]. The corresponding SDE or Langevin equation is

$$dU_i = \overline{H}_i(\mathbf{u}) dt + \sqrt{2\epsilon \frac{\rho_0 \rho_1}{(\alpha + \beta)}} \left[H_i^0(\mathbf{u}) - H_i^1(\mathbf{u}) \right] dW(t), \quad (7.11)$$

where $W(t)$ is a Wiener process with

$$\langle dW(t) \rangle = 0, \quad \langle dW(t) dW(t) \rangle = \delta(t - t') dt \, dt'.$$

It remains to determine the resulting SPDE in the continuum limit $a \to 0$, where a is the lattice spacing of the discretization scheme, see section 3. This is straightforward to determine since, the Wiener process is space-independent, reflecting that switching between the discrete states $n = 0, 1$ applies globally. Thus, we obtain the SPDE (defined in the sense of Stratonovich)

$$dU(x, t) = \overline{D} \frac{\partial^2 U}{\partial x^2} dt + \sqrt{2\epsilon \frac{\rho_0 \rho_1}{(\alpha + \beta)}} \left[(D_0 - D_1) \frac{\partial^2 u}{\partial x^2} \right] dW(t) \quad (7.12a)$$

with the boundary conditions

$$u(0, t) = 0, \quad u(L, t) dt = \eta dt + \eta \sqrt{2\epsilon \frac{\beta}{\alpha(\alpha + \beta)}} \, dW(t). \quad (7.12b)$$

We have thus established that in the limit of fast switching, there is space-independent multiplicative noise in the bulk of the domain when switching in the diffusion coefficient occurs ($D_0 \neq D_1$) together with a randomly driven boundary condition at $x = L$.

8. Discussion

In this paper we have studied the one-dimensional diffusion equation with randomly switching boundary conditions and diffusion coefficient. To analyze this stochastic process, we discretized spaced and constructed the CK equation for the resulting finite-dimensional stochastic hybrid system. By retaking the continuum limit, we have derived boundary value problems that the moments of the process satisfy. In the case of the steady state first moment, the boundary value problem is a system of two ordinary differential equations which we solved to quickly recover results in [27]. Furthermore, we found Fourier series representations for the steady state second moment. We carry out these calculations in the case of switching between two Dirichlet boundary conditions and switching between a Dirichlet and a Neumann condition, noting that the analysis of the Dirichlet–Neumann case is significantly more complicated. Finally, we relate these piecewise deterministic PDEs to statistics for particles diffusing in a random environment, which can be interpreted as types of Feynman–Kac formulae.

For pedagogical reasons, we have focused on the specific example of the one-dimensional diffusion equation on a finite interval with two diffusion coefficients and two possible states for the boundary condition on one end of the interval. However, one can derive analogous moment equations for much more general piecewise deterministic PDE. One can consider general parabolic equations in higher-dimensions while allowing both the boundary conditions and the elliptic operator on the right-hand side of the PDE to randomly switch between arbitrarily many discrete states.

Of course, if the piecewise deterministic PDE under consideration is more complicated, then the resulting moment equations are more difficult to solve. Nevertheless, there are many examples for which the moment equations are explicitly solvable. For example, if we consider parabolic equations in one spatial dimension with N possible discrete states, then the resulting steady state first moment equations are simply a linear system of N ordinary differential equations.

Acknowledgments

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