# Continuous And Discrete Stochastic Models Related Through Finite Difference Forward Kolmogorov Equations

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*Abstract:* Discrete and continuous stochastic models that have approximate probability densities are identified through finite difference approximations of forward Kolmogorov equations (FKEs). Finite difference constructions of the FKE of an Itô stochastic differential equation (SDE) are shown to be identical to the FKEs of certain stochastic models that are discrete in time and state. This identification yields a family of discrete stochastic models with probability densities that approximate the probability density of the SDE model. Additionally, the FKE of a discrete stochastic model is shown to be equal to a finite difference equation of the FKE of a continuous stochastic model. This work gives greater understanding of how discrete and continuous stochastic models are related. Several examples in natural sciences illustrate joint application of realistic discrete and continuous stochastic models.

*Key-Words:* Stochastic model, forward Kolmogorov equation, SDE, FKE, finite difference, mathematical model

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## 1 Introduction

Forward Kolmogorov equations of a stochastic model, discrete in time and state, through Taylor series expansions in the time and state variables, leads to the forward Kolmogorov equation (FKE) of a certain Itô stochastic differential equation (SDE) model, [1], [2]. This result implies that the probability density of the continuous stochastic model approximates that of the discrete stochastic model. In applications, the relation between discrete and continuous stochastic models is useful in constructing physically or biologically realistic SDE models, [1], [2], [3], [4], [5], [6], [7].

The objective of the present investigation is to describe how discrete and continuous stochastic models are related through an interpretation of finite difference approximations of forward Kolmogorov equations. It is shown that finite difference constructions of the FKE of an Itô stochastic differential equation model are identical to the FKEs of certain discrete time and state stochastic models. This identification yields a family of discrete stochastic models with probability densities that approximate the probability density of the SDE model. Specifically, given a FKE associated with a SDE, a finite difference method for solving the FKE leads to a FKE of a discrete stochastic process and a collection of finite difference methods for solving the continuous FKE leads to a family of FKEs of corresponding discrete stochastic processes. Identification of a family of discrete stochastic models that have a similar dynamic behavior leads to a better understanding of the problem. Due to the many applications of discrete and continuous stochastic models, e.g., [1], [2], [3], [4], [5], [6], [7], this work raises awareness of how discrete and continuous models are related. One-dimensional problems are primarily considered in the present investigation. Several examples illustrate how finite differences are used to identify discrete and continuous stochastic models with approximate probability densities and how understanding of a problem is enhanced through joint application of these discrete and continuous stochastic models. Two of the examples are multidimensional.

Original contributions of this work include:

• Given a FKE of a continuous stochastic model, it is shown that a collection of finite difference methods leads to a family of discrete stochastic models.

• The FKE of a stochastic model, discrete in time and state, is shown to be equal to a finite difference equation of a FKE of a continuous model.

• For a problem modeled by a physically or biologically realistic discrete stochastic model, a corresponding approximate continuous stochastic model is identified through the finite difference methodology.

## 2 FKEs: Discrete And Continuous Stochastic Models

In this section, a stochastic differential equation, continuous in time and state, is given. The FKE of this SDE is approximated by a family of finite difference equations. It is shown how each of these finite difference equations generates a FKE of a stochastic model that is discrete in time and state. As all the discrete FKEs approximate the same continuous FKE, the probability densities of the different discrete stochastic models approximate each other. Also, when a discrete stochastic model, discrete in time and state is given, the FKE of this discrete stochastic model is shown to be equal to a finite difference equation of the FKE of a continuous stochastic model corresponding to a certain SDE.

### 2.1 Family Of Finite Difference Methods For A Continuous FKE

Consider the forward Kolmogorov equation for the continuous stochastic process $X(t)$

$$\begin{aligned}\frac{\partial p(t,x)}{\partial t} &= -\frac{\partial (f(t,x)p(t,x))}{\partial x} \\ &+ \frac{1}{2}\frac{\partial^2 (g(t,x)p(t,x))}{\partial x^2},\end{aligned} \tag{1}$$

with $p(0,x) = p_0(x)$ and $p(t,u_1) = p(t,u_2) = 0$, for $(t,x) \in U_T$ where $U_T = (0,T] \times U$ and $U = (u_1,u_2)$ for constants $u_2 > u_1$, [8], [9]. It is assumed that $g$ is positive on $\bar{U}_T$. The function $p$ in (1) is the approximate probability density, for $u_2 - u_1$ large, of solutions of the Itô SDE

$$dX(t) = f(t,X)dt + \sqrt{g(t,X)}dW(t), \tag{2}$$

with $X(0) \sim p_0(x)$, where $f$ and $\sqrt{g}$ are the drift and diffusion coefficients, [9], [10], [11]. A truncated domain $U \subset \mathbb{R}$ is considered here to facilitate the finite difference construction and the comparison with the discrete stochastic model. It is assumed that $u_2 - u_1$ is sufficiently large such that the probability density of FKE (1) on the truncated domain gives an accurate approximation to the probability density on $\mathbb{R}$ for time $0 \le t \le T$, such as when the density has Gaussian bounds, [12], [13], [14]. In particular, Gaussian upper and lower bounds exist to the fundamental solution of the forward Kolmogorov equation when the drift and diffusion coefficients are smooth, [13].

For existence and smoothness of the probability density $p$ of FKE (1), see, e.g., [8], [15], [16]. For example, probability density $p \in C^\infty(\bar{U}_T)$ exists if $p_0 \in C^\infty(\bar{U})$, $p_0(u_1) = p_0(u_2) = 0$, $g$ is positive on $\bar{U}_T$, and $f,g \in C^\infty(\bar{U}_T)$. In the present investigation, to estimate approximation errors, it is assumed that $g$ is positive on $\bar{U}_T$, probability density $p$ exists to (1), and $f,g,p \in C^3(\bar{U}_T)$.

A general explicit finite difference formulation of FKE (1) is defined, in a form to simplify comparison with discrete stochastic models, by the equation

$$\begin{aligned}p(t_{j+1},x_i) &= p(t_j,x_i) + \Delta t\, R(t_j,x_i) \\ &+ \varepsilon_{i,j}(\Delta t,\Delta x),\end{aligned} \tag{3}$$

for $i = 1,\ldots,M+1$ and $j = 1,2,\ldots,N$, where $x_i = u_1 + (i-1)\Delta x$ with $\Delta x = (u_2-u_1)/M$, and $t_j = (j-1)\Delta t$ with $T = N\Delta t$. In addition, $p(t_1,x_i) = p_0(x_i)$ and $p(t_j,x_1) = p(t_j,x_{M+1}) = 0$. The function $R(t_j,x_i)$ is given by

$$\begin{aligned}&R(t_j,x_i) = a_1(t_j,x_{i+2})p(t_j,x_{i+2}) + \\ &a_2(t_j,x_{i+1})p(t_j,x_{i+1}) - a_3(t_j,x_i)p(t_j,x_i) + \\ &a_4(t_j,x_{i-1})p(t_j,x_{i-1}) + a_5(t_j,x_{i-2})p(t_j,x_{i-2})\end{aligned} \tag{4}$$

where the functions $a_k(t,x)$ depend on $f(t,x)$ and $g(t,x)$ and are assumed to be nonnegative. In equation (3), $\varepsilon_{i,j}(\Delta t,\Delta x)$ is the truncation error in the finite difference approximation. (That is, $\varepsilon_{i,j}(\Delta t,\Delta x)$ is the error produced when the exact solution of the FKE is substituted into the approximate finite difference equations.)

The functions $a_k(t,x)$ for $k = 1,2,\ldots,5$ are selected so that the truncation error is small when $\Delta t$ and $\Delta x$ are small. By expanding all the terms in (3) and (4) in Taylor series about $t_j$ and $x_i$ and applying (1), then to obtain a truncation error of $O((\Delta t)^2) + O(\Delta t \Delta x)$, the functions $a_k$ satisfy

$$\begin{cases} a_1(t,x) + a_2(t,x) - a_3(t,x) \\ \quad + a_4(t,x) + a_5(t,x) = 0, \\ 2a_1(t,x) + a_2(t,x) - a_4(t,x) \\ \quad - 2a_5(t,x) = -f(t,x)/\Delta x, \\ 4a_1(t,x) + a_2(t,x) + a_4(t,x) \\ \quad + 4a_5(t,x) = g(t,x)/(\Delta x)^2. \end{cases} \tag{5}$$

For example, the terms in the Taylor expansions containing the partial derivatives $\partial(a_k(t,x)p(t,x))/\partial x\big|_{(t_j,x_i)}$ yield $2a_1 + a_2 - a_4 - 2a_5 = -f/\Delta x$. With values of $a_k$ that satisfy (5), the truncation error $\varepsilon_{i,j}$ in (3) satisfies $\max_{i,j}|\varepsilon_{i,j}(\Delta t,\Delta x)| \le \Delta t\,\varepsilon$ where

$$\begin{aligned}\varepsilon &= C_1 \Delta t \max_{(t,x)}\left(\left|\frac{\partial^2 p(t,x)}{\partial t^2}\right|\right) \\ &+ C_2(\Delta x)^3 \max_{k,(t,x)}\left(\left|\frac{\partial^3 (a_k(t,x)p(t,x))}{\partial x^3}\right|\right),\end{aligned} \tag{6}$$

for constants $C_1, C_2$. To readily construct families of difference methods using (5), the functions $a_k$ are assumed to satisfy the equations

$$a_k(t,x) = -\frac{b_k f(t,x)}{\Delta x} + \frac{c_k g(t,x)}{(\Delta x)^2}, \tag{7}$$

for $k = 1,2,\ldots,5$. By (5) and (7), the constants $b_k$ and $c_k$ satisfy the six equations

$$\begin{cases} b_1+b_2-b_3+b_4+b_5=0, \\ 2b_1+b_2-b_4-2b_5=1, \\ 4b_1+b_2+b_4+4b_5=0, \\ c_1+c_2-c_3+c_4+c_5=0, \\ 2c_1+c_2-c_4-2c_5=0, \\ 4c_1+c_2+c_4+4c_5=1, \end{cases} \tag{8}$$

under the condition that the resulting $a_k$, for $k = 1,2,\ldots,5$, are nonnegative. If the functions $R$ and $a_k$ of (4) and (7) are substituted into (3) and the equation is divided by $\Delta t$, the resulting equation is the standard, but general, finite difference formulation of FKE (1), [17]. In the present investigation, to facilitate comparison between the FKEs of discrete and continuous stochastic models, the finite difference methods are described by equations (3)-(8).

Based on the above formulation, the difference approximation $p_{j,i}$ to $p(t_j,x_i)$ is defined to exactly satisfy the finite difference equations

$$p_{j+1,i} = p_{j,i} + \Delta t\, R_{j,i}, \tag{9}$$

for $i = 1,\ldots,M+1$ and $j = 1,2,\ldots,N$ where

$$\begin{aligned} R_{j,i} \;=\; & a_1(t_j,x_{i+2})p_{j,i+2} + \\ & a_2(t_j,x_{i+1})p_{j,i+1} - a_3(t_j,x_i)p_{j,i} + \\ & a_4(t_j,x_{i-1})p_{j,i-1} + a_5(t_j,x_{i-2})p_{j,i-2}. \end{aligned} \tag{10}$$

In addition, $p_{1,i} = p_0(x_i)$ and $p_{j,1} = p_{j,M+1} = 0$ for $i = 1,\ldots,M+1$ and $j = 1,2,\ldots,N$. It is noted that (9) is identical in form to (3) but there is no truncation error term. The global error in the finite difference method, which takes into account the error accumulating with the time steps, is estimated using the truncation error.

To roughly estimate the global error in the finite difference method (9), a stability condition on the size of $\Delta t$ relative to $\Delta x$ is assumed of the form $\Delta t \max_{j,i} a_3(t_j,x_i) < 1$ (see, e.g., [17]). In addition, $L$ is defined as

$$\begin{aligned} L = \max_{j,i} \big| & a_1(t_j,x_{i+2}) + a_2(t_j,x_{i+1}) \\ & - a_3(t_j,x_i) + a_4(t_j,x_{i-1}) + a_5(t_j,x_{i-2}) \big|, \end{aligned} \tag{11}$$

where by (5)-(8), $L \le C_3 + O(\Delta x)$ with

$$C_3 = \max_{(t,x)} \Big( \Big| \frac{\partial f(t,x)}{\partial x} \Big| + \frac{1}{2} \Big| \frac{\partial^2 (g(t,x))}{\partial x^2} \Big| \Big). \tag{12}$$

Letting $e_j = \max_i |p_{j,i} - p(t_j,x_i)|$, then as $a_k(t_j,x_i) \ge 0$ for $k = 1,2,\ldots,5$,

$$e_j \le e_{j-1}(1 + L\Delta t) + \Delta t\, \varepsilon, \tag{13}$$

Table 1: Discrete stochastic model with indicated changes and probabilities in time interval $\Delta t$.

| Change in $X(t)$ | Probability of a change at time $t$ and state $x$ in time interval $\Delta t$ |
|---|---|
| $-2\Delta x$ | $a_1(t,x)\Delta t$ |
| $-\Delta x$ | $a_2(t,x)\Delta t$ |
| $0$ | $1 - a_3(t,x)\Delta t$ |
| $\Delta x$ | $a_4(t,x)\Delta t$ |
| $2\Delta x$ | $a_5(t,x)\Delta t$ |

*Source: created by the author.*

for $j = 1,\ldots,N$. From (13), the global error in the finite difference method satisfies

$$\max_j e_j \le \varepsilon \big( \exp(LT) - 1 \big)/L. \tag{14}$$

Thus, as $\varepsilon = O(\Delta t) + O(\Delta x)$, the global error between the continuous probability density and the finite difference solution is small when both $\Delta t$ and $\Delta x$ are small.

In the next subsection, a discrete stochastic model is defined based on the five functions $a_k \ge 0$ for $k = 1,2,\ldots,5$. If functions $f$ and $g$ of a continuous stochastic model are expressed in a certain way in terms of the $a_k$ for $k = 1,2,\ldots,5$, the FKE of the discrete stochastic model is equal to a finite difference approximation of the continuous FKE (1). This implies that the continuous probability density approximates the discrete probability density. On the other hand, based on the results of the present subsection, if the functions $f$ and $g$ of FKE (1) are given along with a collection of values $b_k$ and $c_k$ for $k = 1,2,\ldots,5$ that satisfy (8) and nonnegative functions $a_k$ for $k = 1,2,\ldots,5$ that satisfy (7), then a collection of discrete stochastic models are obtained whose FKEs are identical to finite difference approximations of the continuous stochastic model's FKE (1).

## 2.2 Continuous Stochastic Model Corresponding To A Discrete Model

The discrete stochastic model of Table 1 specifies five possible changes in time interval $\Delta t$ along with their respective probabilities. For clarity in the present investigation, five changes and exact probabilities are assumed in Table 1, but the model can be generalized to more than five changes and to probabilities with approximation errors of magnitude $O((\Delta t)^2)$. In Table 1, for the five indicated possible outcomes and probabilities in small time interval $\Delta t$, it is assumed that $a_k(t,x) \ge 0$ for $k = 1,2,\ldots,5$, $a_3(t,x) = a_1(t,x) + a_2(t,x) + a_4(t,x) + a_5(t,x)$, and $\max_{(t,x)} a_3(t,x)\Delta t < 1$. Random variable $X(t)$ takes discrete values $x_i = u_1 + (i-1)\Delta x$ for $i = 1,\ldots,M+1$ with $\Delta x = (u_2 -$

$u_1)/M$ and time $t$ is discrete with values $t_j = (j-1)\Delta t$ for $j = 1,2,\ldots,N+1$ and $T = N\Delta t$. The probability mass function for the discrete stochastic model is defined as $p_{j,i}\Delta x$, that is, $p_{j,i}\Delta x = P\big(X(t_j) = x_i\big)$. This definition is helpful so that the units of $p_{j,i}$ for the discrete stochastic model is consistent with the units of $p_{j,i}$ in equation (7) for the finite-difference approximation of the continuous stochastic model.

It is now shown, when the functions $a_k(t,x)$ in Table 1 are identical to those in equation (4), that the discrete model's FKE is equal to the finite difference equations (9)-(10) of the continuous stochastic model. The FKE of the discrete stochastic model follows directly from Table 1. When each term on both sides of the FKE is divided by $\Delta x$, the equation takes the simplified form

$$p_{j+1,i} = p_{j,i} + \Delta t\, R_{j,i}, \tag{15}$$

for $i = 1,\ldots,M+1$ and $j = 1,2,\ldots,N$ where

$$\begin{aligned} R_{j,i} \;=\; & a_1(t_j,x_{i+2})p_{j,i+2} + \\ & a_2(t_j,x_{i+1})p_{j,i+1} - a_3(t_j,x_i)p_{j,i} \\ & + a_4(t_j,x_{i-1})p_{j,i-1} + a_5(t_j,x_{i-2})p_{j,i-2}, \end{aligned} \tag{16}$$

with $p_{1,i} = p_0(x_i)$ and $p_{j,1} = p_{j,M+1} = 0$. As (15) and (16) are identical to (9) and (10), the FKE of the discrete stochastic model of Table 1 is identical to the finite difference equations (9)-(10) of the continuous FKE (1). To identify the functions $f$ and $g$ of the continuous stochastic model that corresponds with the finite difference equations, the terms in equations (3) and (4) are expanded in Taylor series about $t_j$ and $x_i$ as in the previous subsection. To obtain a low truncation error, the functions $f$ and $g$ in FKE (1) are identified as identical to those given in equation (5). Specifically,

$$\begin{cases} f(t,x) = \Delta x\big(-2a_1(t,x) - a_2(t,x) \\ \quad +a_4(t,x) + 2a_5(t,x)\big), \\ g(t,x) = (\Delta x)^2\big(4a_1(t,x) + a_2(t,x) \\ \quad +a_4(t,x) + 4a_5(t,x)\big). \end{cases} \tag{17}$$

Thus, given $a_k$, for $k = 1,2,\ldots,5$, of the discrete model of Table 1, the corresponding approximate continuous stochastic model has drift and diffusion coefficients $f$ and $g$ that satisfy (17). For $f$ and $g$ satisfying (17), by a similar argument to that in the previous subsection, the approximation error between the continuous and discrete probability densities decreases to zero as $\Delta t$ and $\Delta x$ decrease to zero.

The results and discussion of this section lead to the following theorem which summarizes and describes how the discrete and continuous stochastic models are related.

**Theorem 1**
**Part 1.** Assume that smooth nonnegative functions $a_k, k = 1,2,\ldots,5$ are given that define the discrete stochastic model described in Table 1. Let the drift and diffusion coefficients $f$ and $g$ be given by (17) with $g$ positive and assume that $p \in C^3(\bar{U}_T)$. Then, the probability density $p$ of the continuous stochastic model's FKE (1) approximates the probability density of the discrete stochastic model's FKE (15) for $(t,x) \in U_T$ with errors of $O(\Delta x) + O(\Delta t)$ for $\Delta t$ sufficiently small.
**Part 2.** On the other hand, assume that functions $f$ and $g$, with $g$ positive, are given which define a continuous stochastic model and $f,g,p \in C^3(\bar{U}_T)$. If the parameters $b_k$ and $c_k$ satisfy (8) and nonnegative functions $a_k$ satisfy (7) for $k = 1,2,\ldots,5$, then the resulting discrete stochastic models, described in Table 1, have FKEs (15) that are finite difference approximations of the continuous stochastic model's FKE (1) with global errors of $O(\Delta x) + O(\Delta t)$ for $\Delta t$ sufficiently small.

Several examples are presented to clarify this discussion. Suppose the discrete stochastic model in Table 1 has functions $a_1 = a_5 = 0$, $a_2$ and $a_4$ nonnegative, and $a_3 = a_1 + a_2 + a_4 + a_5$. Let $f$ and $g$ be given using (17) as

$$\begin{cases} f(t,x) = (a_4(t,x) - a_2(t,x))\Delta x, \\ g(t,x) = (a_2(t,x) + a_4(t,x))(\Delta x)^2. \end{cases} \tag{18}$$

Then, the discrete stochastic model's FKE is a finite difference approximation of the continuous stochastic model's FKE (1). Next, suppose instead that functions $f$ and $g$ are given for a continuous stochastic model and $b_1 = 0, b_2 = 1/2, b_3 = 0, b_4 = -1/2, b_5 = 0$, $c_1 = 0, c_2 = 1/2, c_3 = 1, c_4 = 1/2, c_5 = 0$. By (7), the functions $a_k$ are selected as

$$\begin{cases} a_1 = a_5 = 0, a_2 = \dfrac{-f}{2\Delta x} + \dfrac{g}{2(\Delta x)^2}, \\ a_3 = \dfrac{g}{(\Delta x)^2}, a_4 = \dfrac{f}{2\Delta x} + \dfrac{g}{2(\Delta x)^2}. \end{cases} \tag{19}$$

Then, if $a_2$ and $a_4$ are nonnegative, the resulting discrete stochastic model's FKE approximates the continuous stochastic model's FKE.

In the second example, suppose functions $f$ and $g$ are given in a continuous stochastic model and a common, important modeling situation is considered where the only changes in Table 1 for small time $\Delta t$ are 0 and $\pm\Delta x$ and so $a_1(t,x) = a_5(t,x) = 0$.

To find $a_2, a_3$, and $a_4$ in the corresponding discrete stochastic model, as $b_1 = b_5 = c_1 = c_5 = 0$, then by (8), $b_2 = c_2 = c_4 = 1/2$, $b_4 = -1/2$, $b_3 = 0$, and $c_3 = 1$. Thus, by (7), $a_2 = g/(2(\Delta x)^2) - f/(2\Delta x)$, $a_3 = g/(\Delta x)^2$, and $a_4 = g/(2(\Delta x)^2) + f/(2\Delta x)$. The discrete stochastic model's FKE in this case corresponds exactly with the central difference method for approximately solving the continuous model's FKE. This example indicates that, given a continuous stochastic model, a single discrete stochastic model is obtained that satisfies equations (7) and (8) and only allows nonzero changes $\pm\Delta x$ in a small time interval.

In the third example, suppose first that a discrete stochastic model is defined in Table 1 by the equations $a_5(t,x) = 0$, $a_1(t,x) = \phi_1(t,x)$, $a_2(t,x) = \phi_2(t,x)$, and $a_4(t,x) = \phi_2(t,x) + \phi_4(t,x)$ where $\phi_1(t,x)$, $\phi_2(t,x)$, and $\phi_4(t,x)$ are given nonnegative linearly independent functions. Using equations (17), the functions $f$ and $g$ for the corresponding continuous stochastic model satisfy $f(t,x)/\Delta x = (-2\phi_1(t,x) + \phi_4(t,x))$ and $g(t,x)/(\Delta x)^2 = (4\phi_1(t,x) + 2\phi_2(t,x) + \phi_4(t,x))$. Now suppose instead that a continuous stochastic model is defined by $f(t,x)/\Delta x = (-2\phi_1(t,x) + \phi_4(t,x))$ and $g(t,x)/(\Delta x)^2 = (4\phi_1(t,x) + 2\phi_2(t,x) + \phi_4(t,x))$ where $\phi_1(t,x)$, $\phi_2(t,x)$, and $\phi_4(t,x)$ are given nonnegative linearly independent functions. For this continuous model, the original discrete stochastic model is not in the family of models described by equations (7) and (8) as, for example, the function $a_1(t,x) = \phi_1(t,x)$ cannot be written as $-b_1 f(t,x)/\Delta x + c_1 g(t,x)/(\Delta x)^2$ for constants $b_1$ and $c_1$. The original discrete stochastic model's FKE is a special finite-difference approximation of the continuous model's FKE. Although the original discrete stochastic model is not a member of the family described by (7) and (8), many members of this family do exist such as the model with $a_1 = a_5 = 0$, $a_2 = 3\phi_1 + \phi_2$, $a_3 = 4\phi_1 + 2\phi_2 + \phi_4$, and $a_4 = \phi_1 + \phi_2 + \phi_4$, or the model with $a_2 = a_5 = 0$, $a_1 = \phi_1 + \phi_2/3$, $a_3 = \phi_1 + \phi_2 + \phi_4$, and $a_4 = 2\phi_2/3 + \phi_4$. Also, the probability densities of all these discrete stochastic models approximate each other as they approximate the same continuous probability density.

Finally, the family of discrete stochastic models that satisfy (5) may be empty. For example, if $\Delta x = 1$ and $f = 2g$ with $g$ positive, then there are no nonnegative functions $a_k, k = 1,2,\ldots,5$ that satisfy (5) as (5) gives $6a_1 + 2a_2 + 2a_5 = -g$. However, given $f$ and positive $g$, if $\Delta x$ can be made sufficiently small, nonnegative functions $a_k, k = 1,2,\ldots,5$ do exist that satisfy (5). For example, $a_1 = a_5 = 0$, $2a_2 = -f/\Delta x + g/(\Delta x)^2$, $2a_4 = f/\Delta x + g/(\Delta x)^2$, and $a_3 = g/(\Delta x)^2$.

# 3 Applications

Examples of several possible applications are described in this section. In the first example, how surface roughness changes with time during a smoothness process is studied through development of a physically reasonable discrete stochastic model. The discrete stochastic model leads to a corresponding SDE model which yields a formula for root mean square surface roughness as a function of time. In the second example, seed longevity is modeled by a discrete stochastic model. The corresponding continuous stochastic model yields insight, for example, into the coefficient of variation of sample batches. In addition, it is shown how corresponding discrete and continuous models may be identified for a multidimensional seed longevity problem. The third example illustrates how a hypothesized SDE model may be examined for realism by examining the corresponding discrete stochastic models. In the fourth example, the effects of demographic variability in the population dynamics of a two-dimensional biological control problem are studied. In the fifth example, the discrete stochastic model of a particular chemical reaction is studied. Another member of the same family of discrete stochastic models is described that has a similar probability density.

## 3.1 Progression of Surface Roughness Under Smoothing

In this example, the SDE corresponding to a discrete stochastic model is studied to find a relation for surface roughness as a function of time for a metal surface being smoothed through grinding. Root mean square surface roughness, $R_q(t)$, is defined as the standard deviation in the surface height at time $t$, [18]. It is desired to find a relation for $R_q(t)$ during surface smoothing. It is assumed that the initial roughness, $R_q(0)$, is known and that smoothing occurs through a grinding process where surface particles are removed during smoothing. To model the smoothing process, the surface height is assumed to be piecewise constant on a mesh with small mesh area $\Delta A$ and it is assumed that the heights on the mesh are independent. Let $X(t)$ be the height of the surface at a mesh position and notice that $R_q(t) = \sqrt{\mathrm{Var}(X(t))}$. Let $\gamma$ be the rate per unit surface area that particles separate from the surface during smoothing. It is assumed that a separating particle has volume $v$ and that the mesh area $\Delta A$ is greater than the particle cross-sectional area. A particle is removed with probability $\gamma \Delta A \Delta t$ in area $\Delta A$ in small time interval $\Delta t$. The term $E(X(0)) - v\gamma t$ is the average height of the surface at time $t$ and $X(t) - E(X(0)) + v\gamma t$ is the difference between the height at a mesh point and the average height of the surface. As particles more likely separate at high re-

Table 2: Surface height changes and probabilities in small time interval $\Delta t$.

| Change in mesh height $X(t)$ | Probability of change in $\Delta t$ |
|---|---|
| $-\nu/\Delta A$ | $\big(\gamma+\alpha Z(t)\big)\Delta t\Delta A$ |
| 0 | $1-\big(\gamma+\alpha Z(t)\big)\Delta t\Delta A$ |

*Source: created by the author.*

gions on the surface during grinding, the rate particles separate at a mesh position with height $X(t)$ is assumed to be equal to $\gamma+\alpha\big(X(t)-E(X(0))+\nu\gamma t\big)$ where the second term "corrects" the rate $\gamma$ for the height above or below the average surface height and where it is assumed that $\alpha E(X(0)) \leq \gamma$. Letting $Z(t) = X(t) - E(X(0)) + \nu\gamma t$, a discrete stochastic model for the height at each mesh point is described in Table 2 where $-\nu/\Delta A$ is the possible change in height for small time $\Delta t$ in mesh area $\Delta A$.

Using equation (17), the corresponding Itô SDE for this discrete stochastic model is given by

$$\begin{aligned} dX(t) &= -\nu\alpha\big(Z(t)+\gamma/\alpha\big)\,dt \\ &+ \sqrt{\nu^2\alpha\big(Z(t)+\gamma/\alpha\big)/\Delta A}\,dW(t), \end{aligned} \tag{20}$$

where $Z(t) = X(t) - E(X(0)) + \nu\gamma t$. Applying Itô's formula, [9], [10], [19], the variance of the mesh height is given by

$$\begin{aligned} \mathrm{Var}(X(t)) &= R_q^2(0)\exp(-bt) \\ &+ \nu\gamma\big(1-\exp(-bt)\big)/(2\alpha\Delta A), \end{aligned} \tag{21}$$

where $R_q(0)$ is the initial roughness and $b = 2\nu\alpha$. Equation (21) implies that an approximate formula for the roughness parameter $R_q(t)$ is given by

$$R_q(t) = \sqrt{R_q^2(0)\exp(-bt) + a(1-\exp(-bt))} \tag{22}$$

where $a$ and $b$ are constants. To test this result, the least squares fit is calculated for equation (22) to the roughness data reported in [20] for polishing a steel surface for different lengths of time. For this data, the least squares values of $a$ and $b$ are 0.00846 and 0.07950, respectively. The least squares curve of equation (22) to the data is presented in Figure 1. As can be seen from the figure, equation (22) fits well the roughness data.

## 3.2 Stochastic Modeling Of Seed Longevity

A problem in agriculture is the decline of seed fertility or viability with storage time, [21], [22]. Previously, seed germination data has generally been modeled by probit analysis where it is assumed that the

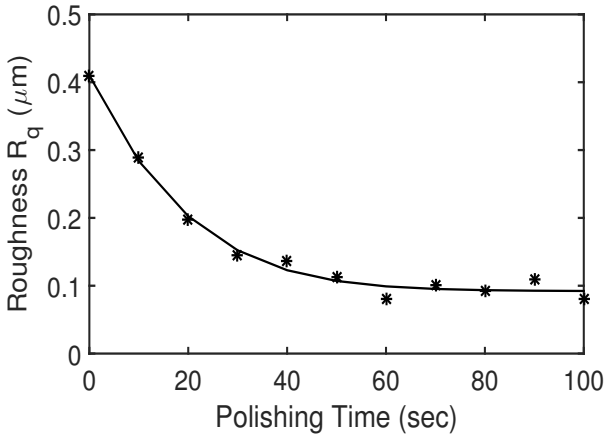



Figure 1: Comparison of equation (22) for roughness as a function of polishing time with data reported in [20] for steel. *Source: created by the author.*

Table 3: Changes in the number of viable seeds in small time interval $\Delta t$.

| Change $\Delta X$ | Probability of change |
|---|---|
| $-1$ | $kt^\gamma X(t)\Delta t$ |
| 0 | $1-kt^\gamma X(t)\Delta t$ |

*Source: created by the author.*

loss of the ability to germinate over time follows a normal distribution, [22]. In this example, a dynamic discrete stochastic model is derived from basic assumptions on loss of viability with time. The discrete stochastic model then leads to an approximate continuous SDE model which in turn provides approximations to the mean and variance of the number of fertile seeds with storage time. In addition, this example indicates how multidimensional problems can be treated in a manner similar to one-dimensional problems.

Viability of seeds in storage depends on storage time and on certain environmental conditions such as humidity and temperature. In this example, sample batches of seeds are considered each with total number $x_B$. Let $X(t)$ be the number of viable seeds in a sample batch at storage time $t$. It is assumed that the rate of change of the number of viable seeds is proportional to $X(t)$ and $t^\gamma$ where $\gamma$ is a constant. Let $k$ be a proportionality parameter which is assumed to depend on environmental conditions during storage. First, though, it is assumed that the environment is constant so $k$ is a constant. Based on these assumptions, a discrete model for the number of viable seeds with storage time $t$ is given in Table 3. From this ta-

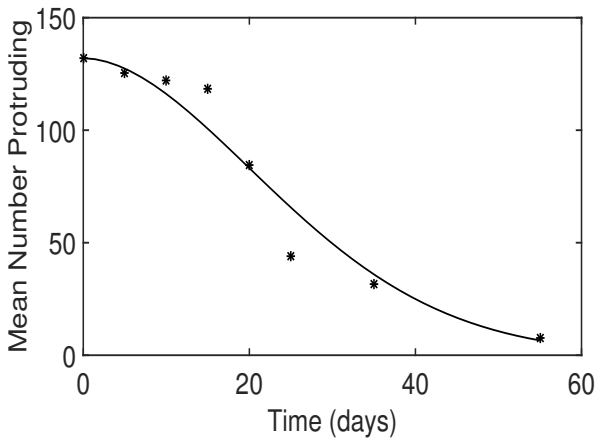



Figure 2: Data (from [21]) on mean number of tomato seeds sprouting in batches of 200 seeds compared with mean number $E(X(t)) = 135.5\exp(-t^{1.849}/550)$ using equation (24). *Source: created by the author.*

ble, the functions $f$ and $g$ for equation (1) are given from (17) as $f(t,x) = -kt^{\gamma}x(t)$ and $g(t,x) = kt^{\gamma}x(t)$ and the corresponding SDE has the form

$$dX(t) = -kt^{\gamma}X(t)dt + \sqrt{kt^{\gamma}X(t)}dW(t), \qquad (23)$$

with $X(0) \sim p_0(x)$, where $p_0$ is the probability density at $t = 0$ of the number of viable seeds for batches of size $x_B$. It is assumed that the mean and variance of density $p_0$ is $\bar{x}_0$ and $\sigma_0^2$, respectively. Using equation (23), the mean number of viable seeds in the batches, $E(X(t))$, satisfies for $t \geq 0$,

$$E(X(t)) = \bar{x}_0 \exp\big(-kt^{\gamma+1}/(\gamma+1)\big). \qquad (24)$$

To compare equation (24) with data, longevity data was considered for tomato seeds (of cultivar Gaucho) reported in reference [21] under a constant environment where $x_B = 200$ and $\bar{x}_0 = 135.5$. A least squares fit to the tomato seed data for the mean number of viable seeds with storage time gives $\gamma = 0.849$ and $k = 0.00336$ in equation (24). In Figure 2, the least squares fit is compared with the tomato seed data.

The SDE model (23) gives useful insight about the variability in number of viable seeds in the sample batches. For example, if $\bar{x}_0 \approx x_B$ and $\sigma_0^2 \approx 0$, the coefficient of variation for batches of seeds approximately satisfies

$$\frac{\sqrt{\mathrm{Var}(X(t))}}{E(X(t))} \approx \frac{\sqrt{z(t)}}{\sqrt{x_B}}, \qquad (25)$$

where $z(t) = \exp\big(kt^{\gamma+1}/(\gamma+1)\big) - 1$ indicating, for example, how the coefficient of variation in sample batches is improved by increasing the number of seeds, $x_B$, in batches.

Table 4: Changes and probabilities in $[X(t), K(t)]$ for small time interval $\Delta t$.

| Change | Probability of change |
|---|---|
| $[-1,0]$ | $K(t)t^{\gamma}X(t)\Delta t$ |
| $[0,\alpha]$ | $\beta_1 K(t)\Delta t + \beta_2(k_e - K(t))\Delta t$ |
| $[0,-\alpha]$ | $\beta_1 K(t)\Delta t - \beta_2(k_e - K(t))\Delta t$ |
| $[0,0]$ | $1 - K(t)t^{\gamma}X(t)\Delta t - 2\beta_1 K(t)\Delta t$ |

*Source: created by the author.*

In the remainder of this subsection, the stochastic model for seed viability is generalized to randomly varying storage conditions, for example, to randomly varying temperature and/or humidity. It is assumed, under the randomly varying environment, that the rate parameter $K(t)$ varies randomly with time about a mean value $k_e$. A discrete stochastic model for $X(t)$ and $K(t)$ is presented in Table 4 where $\alpha$, $\beta_1$ and $\beta_2$ are constants. Letting $x_i = x_{i-1} + 1$ and $k_m = k_{m-1} + \alpha$, the FKE for the discrete stochastic model of Table 4 has the form

$$\begin{aligned} p(t_{j+1},x_i,k_m) = {} & p(t_j,x_{i+1},k_m)u(t_j,x_{i+1},k_m)\Delta t \\ & + p(t_j,x_i,k_{m-1})v(t_j,k_{m-1})\Delta t \\ & + p(t_j,x_i,k_{m+1})w(t_j,k_{m+1})\Delta t \\ & + p(t_j,x_i,k_m)\big(1 - u(t_j,x_i,k_m)\Delta t \\ & - v(t_j,k_m)\Delta t - w(t_j,k_m)\Delta t\big), \end{aligned} \qquad (26)$$

where $u(t,x,k) = kt^{\gamma}x$, $v(t,k) = \beta_1 k + \beta_2(k_e - k)$, and $w(t,k) = \beta_1 k - \beta_2(k_e - k)$. Letting $f_1(t,x,k) = -u(t,x,k)$, $f_2(t,k) = \alpha(v(t,k) - w(t,k))$, $g_1(t,x,k) = u(t,x,k)$, and $g_2(t,k) = \alpha^2(v(t,k) + w(t,k))$, it is seen that the discrete stochastic model's FKE (26) are finite difference equations of the continuous model's FKE given by

$$\begin{aligned} \frac{\partial p}{\partial t} = {} & -\frac{\partial(f_1 p)}{\partial x} - \frac{\partial(f_2 p)}{\partial k} \\ & + \frac{1}{2}\frac{\partial^2(g_1 p)}{\partial x^2} + \frac{1}{2}\frac{\partial^2(g_2 p)}{\partial k^2} \end{aligned} \qquad (27)$$

where $p(t,x,k)$ is the probability density. Furthermore, the SDE system of the continuous model's FKE has the form

$$\begin{cases} dX(t) = -Kt^{\gamma}X dt + \sqrt{Kt^{\gamma}X}dW_1(t) \\ dK(t) = 2\alpha\beta_2(k_e - K)dt + \sqrt{2\alpha^2\beta_1 K}dW_2(t), \end{cases} \qquad (28)$$

with $X(0) \sim p_0(x)$ and $K(0) = k_0$ where $W_1(t)$ and $W_2(t)$ are independent Wiener processes. Computational solution of this SDE system may be helpful, for example, in studying the effects of randomly varying storage conditions on seed viability.

### 3.3 Checking the Realism of a SDE Model

Suppose a SDE model is hypothesized for a biological or physical phenomenon. Examining the discrete stochastic models that correspond with the SDE model can be helpful in determining whether the SDE model is reasonable biologically or physically. To illustrate this, a simple example is described.

Consider the pure birth process with demographic variability. It is hypothesized that the population size $X(t)$ at time $t$ satisfies the SDE

$$dX(t) = r_1 X(t)\,dt + (r_2 X(t))^{\alpha}\,dW(t), \qquad (29)$$

with $X(0) = 0$ where $r_1, r_2, \alpha > 0$ are constants. By inspection, $f(t,x) = r_1 x$ and $g(t,x) = (r_2 x)^{2\alpha}$. The discrete stochastic models that correspond with (29) are found by referring to Table 1 and equations (5) or (17). Assuming that the changes in the population size are either 0 or 1 for births in small time interval $\Delta t$, then $\Delta x = 1$ and $a_1 = a_2 = a_5 = 0$. In addition, equation (5) gives $a_4(x,t) = f(x,t) = r_1 x$, and $a_4(x,t) = g(x,t) = (r_2 x)^{2\alpha}$. Thus, for discrete stochastic models having population changes of 0 or 1 and corresponding with SDE (29), the results imply values of $\alpha = 1/2$ and $r_2 = r_1$ in (29). Thus, a reasonable SDE population model based on hypothesized model (29) is given by

$$dX(t) = r_1 X(t)\,dt + (r_1 X(t))^{1/2}\,dW(t). \qquad (30)$$

### 3.4 Plant Competition With Control

In this example, the effects of demographic variability in the population dynamics of a biological control problem are studied. A deterministic competition-control example described and studied in [23] is used as an illustration of transforming a deterministic problem into one involving discrete and continuous stochastic models. The problem involves competing native and invasive species and illustrates application to a multivariable problem.

Consider native and invasive species of competing plants with population levels $X(t)$ and $Y(t)$, respectively. A control is applied to limit the invasive species. How the randomness in the population levels affects the control is of interest in this example. Referring to [23], deterministic differential equations for $X(t)$ and $Y(t)$ for this example have the form

$$\begin{cases} \dfrac{dX(t)}{dt} = b_1(t,X(t)) - d_1(t,X(t),Y(t)), \\ \dfrac{dY(t)}{dt} = b_2(t,Y(t)) - d_2(t,X(t),Y(t)), \end{cases} \qquad (31)$$

with $X(0) = x_0, Y(0) = y_0$ where $b_1, d_1, b_2, d_2$ are birth and death rates of the native and invasive species, respectively, $t$ is time in years, and $0 \le u \le 1$ is a control parameter. In the present investigation, it is assumed that $u = 0.9$ and

$$\begin{cases} b_1(t,x) = 0.64x, \;\; b_2(t,y) = 0.8(1-\phi(t)u)y, \\ d_1(t,x,y) = (0.60 + 0.02x/x_0 + 0.05y/y_0)x, \\ d_2(t,x,y) = (0.70 + 0.05x/x_0 + 0.025y/y_0)y, \end{cases} \qquad (32)$$

where $\phi(t) = 1$ if $t - [t] < 1/10$ and $\phi(t) = 0$ if $t - [t] > 1/10$, where $[t]$ is the greatest integer in $t$. Thus, the control is applied for the first $1/10$ of each year. The control affects the reproduction rate of the invasive species. The discrete stochastic model derived from this discussion is described in Table 5 where unit changes may occur in $X(t)$ and $Y(t)$. The discrete stochastic model in Table 5 has the FKE

Table 5: Changes and probabilities in population sizes $[X(t), Y(t)]$ at time $t$ for small time interval $\Delta t$.

| Change in $[X(t), Y(t)]$ | Probability of change |
|---|---|
| $[1, 0]$ | $b_1(t, X(t))\Delta t$ |
| $[-1, 0]$ | $d_1(t, X(t), Y(t))\Delta t$ |
| $[0, 1]$ | $b_2(t, Y(t))\Delta t$ |
| $[0, -1]$ | $d_2(t, X(t), Y(t))\Delta t$ |

*Source: created by the author.*

$$\begin{aligned} p(t_{j+1},x_i,y_k) &= p(t_j,x_{i-1},y_k)b_1(t_j,x_{i-1})\Delta t \\ &+ p(t_j,x_i,y_{k-1})b_2(t_j,y_{k-1})\Delta t \\ &+ p(t_j,x_{i+1},y_k)d_1(t_j,x_{i+1},y_k)\Delta t \\ &+ p(t_j,x_i,y_{k+1})d_2(t_j,x_i,y_{k+1})\Delta t \\ &+ p(t_j,x_i,y_k)\big(1 - b_1(t_j,x_i)\Delta t - b_2(t_j,y_k)\Delta t\big) \\ &- p(t_j,x_i,y_k)\big(d_1(t_j,x_i,y_k)\Delta t + d_2(t_j,x_i,y_k)\Delta t\big). \end{aligned} \qquad (33)$$

Letting

$$\begin{cases} f_1(t,x,y) = b_1(t,x) - d_1(t,x,y), \\ f_2(t,x,y) = b_2(t,y) - d_2(t,x,y), \\ g_1(t,x,y) = b_1(t,x) + d_1(t,x,y), \\ g_2(t,x,y) = b_2(t,y) + d_2(t,x,y), \end{cases} \qquad (34)$$

and $\Delta x = \Delta y = 1$, it is seen that the FKE (33) of the discrete model is a central finite difference approximation of the continuous model's FKE

$$\begin{aligned} \frac{\partial p}{\partial t} &= -\frac{\partial (f_1 p)}{\partial x} - \frac{\partial (f_2 p)}{\partial y} \\ &+ \frac{1}{2}\frac{\partial^2 (g_1 p)}{\partial x^2} + \frac{1}{2}\frac{\partial^2 (g_2 p)}{\partial y^2}, \end{aligned} \qquad (35)$$

where $p(t,x,y)$ is the probability density. In addition, the corresponding Itô SDE system is given by

$$\begin{cases} dX = f_1(t,X,Y)\,dt + \sqrt{g_1(t,X,Y)}\,dW_1(t), \\ dY = f_2(t,X,Y)\,dt + \sqrt{g_2(t,X,Y)}\,dW_2(t), \end{cases} \qquad (36)$$

Table 6: Means and Standard Deviations in Natives and Invasives for the Discrete and Continuous Stochastic Models at $t = 2.5, 5.0$ and 7.5.

| Time (years) | Mean(Stdev) in Natives Discrete \| Continuous |
|---|---|
| 2.5 | 93.9(17.0) \| 93.5(16.8) |
| 5.0 | 89.3(23.0) \| 89.3(23.2) |
| 7.5 | 85.7(27.5) \| 86.0(27.7) |
| Time (years) | Mean(Stdev) in Invasives Discrete \| Continuous |
| 2.5 | 43.2(12.0) \| 42.5(11.8) |
| 5.0 | 40.4(16.1) \| 39.7(15.8) |
| 7.5 | 35.6(17.7) \| 35.0(17.4) |

*Source: created by the author.*

where $W_1(t)$ and $W_2(t)$ are independent standard Wiener processes. Individual trajectories of the SDE system (36) are simulated, for example, using numerical methods such as the Euler-Maruyama method, [9], [10].

A test comparison is made between the probability densities of the discrete and continuous stochastic models. The means and standard deviations of natives and invasives are calculated for the two stochastic models at $t = 2.5, 5.0$, and 7.5 years. The calculated values given in Table 6 show that the means and standard deviations of the discrete and continuous stochastic models are within 2% for $t = 2.5, 5.0, 7.5$.

The deterministic control equation (31) is compared to the stochastic SDE system (36) up to time $t = 30$, with $u = 0.9$, $x_0 = 100$, and $y_0 = 50$. With this level of control in the deterministic model, the native species (always) outcompetes the invasive species. However, for 5000 trajectories of the stochastic model's SDE system, the invasive species outcompetes the native species in about 18% of the stochastic population trajectories by time $t = 30$. For the SDE system, the proportion of the 5000 trajectories where the invasive population is greater than the native population is displayed in Figure 3 for $0 \le t \le 30$. These results indicate, for the population sizes considered in this example, that evaluating the control's effectiveness based solely on a deterministic control model can be misleading.

## 3.5 A Chemical Reaction Example

Consider reactions of three chemicals with molecular quantities $X(t)$, $Y(t)$, and $Z(t)$. (See, for example, the discussion in [24].) For simplicity, it is assumed that the numbers of molecules of $Y(t)$ and $Z(t)$ are large with respect to $X(t)$ and approximately constant so $Y(t) \approx y_0$ and $Z(t) \approx z_0$. Three reactions are assumed: $2X + Z \to U$, $X \to V$, and $X + Y \to 2X + W$, where

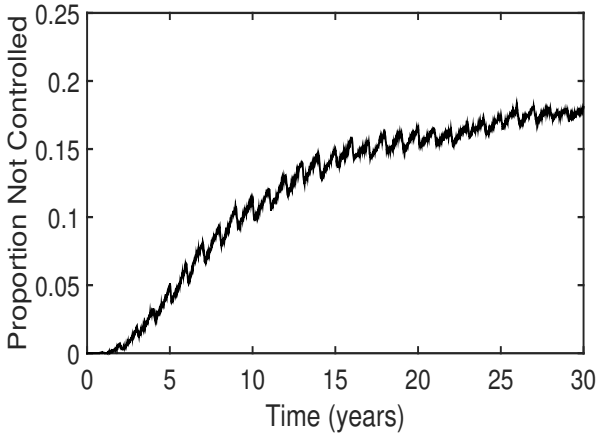



Figure 3: Proportion of 5000 trajectories where the invasive population is greater than native population at time $t$. *Source: created by the author.*

Table 7: Changes and probabilities of number of molecules of chemical reactant $X(t)$ for interval $\Delta t$.

| Change in $X(t)$ | Probability of change in time interval $\Delta t$ |
|---|---|
| $-2$ | $r_1 z_0 x(x-1)\Delta t$ |
| $-1$ | $r_2 x \Delta t$ |
| 0 | $1 - a_3(t,x)\Delta t$ |
| 1 | $r_4 y_0 x \Delta t$ |
| 2 | 0 |

*Source: created by the author.*

$U$, $V$, and $W$ are product chemicals. The probabilities of the three reactions for small $\Delta t$ are given in Table 7 where $r_1, r_2, r_4$ are rate constants, $Y(t) \approx y_0$, and $Z(t) \approx z_0$.

From Tables 1 and 7,

$$\begin{cases} a_1(t,x) = r_1 x(x-1) z_0, \\ a_2(t,x) = r_2 x, \\ a_3(t,x) = r_1 x(x-1) z_0 + r_2 x + r_4 x y_0, \\ a_4(t,x) = r_4 x y_0, \;\; a_5(t,x) = 0. \end{cases} \tag{37}$$

In addition, from (17) and (37) with $\Delta x = 1$,

$$\begin{cases} f(t,x) = r_4 y_0 x - 2 r_1 z_0 x(x-1) - r_2 x, \\ g(t,x) = r_4 y_0 x + 4 r_1 z_0 x(x-1) + r_2 x. \end{cases} \tag{38}$$

For this problem, the FKE of the corresponding continuous stochastic model has the form

$$\begin{aligned} \frac{\partial p(t,x)}{\partial t} &= -\frac{\partial \big(f(t,x)p(t,x)\big)}{\partial x} \\ &+ \frac{1}{2}\frac{\partial^2 \big(g(t,x)p(t,x)\big)}{\partial x^2}, \end{aligned} \tag{39}$$

Table 8: Changes and probabilities of number of molecules of reactant $\hat{X}(t)$ in small time interval $\Delta t$.

| Change in $\hat{X}(t)$ | Probability of change in $\Delta t$ |
|---|---|
| $-1$ | $(3r_1z_0x(x-1)+r_2x)\Delta t$ |
| 0 | $1-g(t,x)\Delta t$ |
| 1 | $(r_1z_0x(x-1)+r_4y_0x)\Delta t$ |

*Source: created by the author.*

where $p(t,x)$ in (39) is the probability density of the number of molecules $x$ at time $t$.

A central difference form of FKE (39) is now considered to give a second discrete stochastic model which will have approximately the same probability density as the stochastic model defined in Table 7. For this central finite difference method, $b_1 = 0, b_2 = 1/2, b_3 = 0, b_4 = -1/2, b_5 = 0$, $c_1 = 0, c_2 = 1/2, c_3 = 1, c_4 = 1/2, c_5 = 0$, and for these values $\hat{a}_1 = \hat{a}_5 = 0$, $\hat{a}_2 = -f/2 + g/2$, $\hat{a}_3 = g$, and $\hat{a}_4 = f/2 + g/2$. The discrete stochastic model for this central difference method is described in Table 8.

To computationally compare the probability densities of the two discrete models of Tables 7 and 8, the values of the parameters are selected as $r_1z_0 = 0.00002$, $r_2 = 0.002$, $r_4y_0 = 0.001$, with $x(0) = 100$, and $\Delta t = 0.25$. The probability densities are calculated at $t = 50$ using the FKEs of the discrete models of Tables 7 and 8. The calculated probability densities are displayed in Figure 4 which illustrates that the two densities closely approximate each other. This example indicates that a chemical reaction involving a single reactant changing with time can be approximated theoretically by a reaction that involves molecular changes of just $+1$ or $-1$ per time step. It is also noted for this example that if the reaction $X \to V$ is replaced by a reaction of the form $X + Q \to V$ with reaction rate $r_5q_0x$ where $Q(t) \approx q_0$, then the probability density $p(t,x)$ for the second set of reactions is approximately the same as for the original set of reactions when $q_0 = r_2/r_5$.

As another example, consider two sets of elementary chemical reactions. The first set of reactions is $H_{2(g)} + ICl_{(g)} \longrightarrow HI_{(g)} + HCl_{(g)}$ and $HI_{(g)} + ICl_{(g)} \longrightarrow I_{2(g)} + HCl_{(g)}$ with rate constants $r_1$ and $r_2$, respectively. The second set is $2NO_{(g)} \rightleftharpoons N_2O_{2(g)}$ and $N_2O_{2(g)} + O_{2(g)} \longrightarrow 2NO_{2(g)}$ with rate constants $r_3$ (forward), $r_{-3}$ (reverse), and $r_4$, respectively. In these reactions, suppose that the numbers of molecules of $H_2$, ICl, NO, and $O_2$ are initially large and approximately constant for the time interval considered with values $[H_2]$, [ICl], [NO], and $[O_2]$. Let the numbers of molecules of HI and $N_2O_2$ be denoted by $X(t)$ and $Y(t)$, respectively, with $X(0) = Y(0) = 0$. By constructing discrete stochastic models for $X(t)$ and $Y(t)$, it is straightforward to see that the corresponding continuous stochastic models for $X(t)$ and for $Y(t)$ are identical if $[NO]^2 = r_1[H_2][ICl]/r_3$ and $[O_2] = (r_2[ICl] - r_{-3})/r_4$. This implies, under these conditions, that the probability densities of $X(t)$ and $Y(t)$ approximate each other for these two sets of reactions.

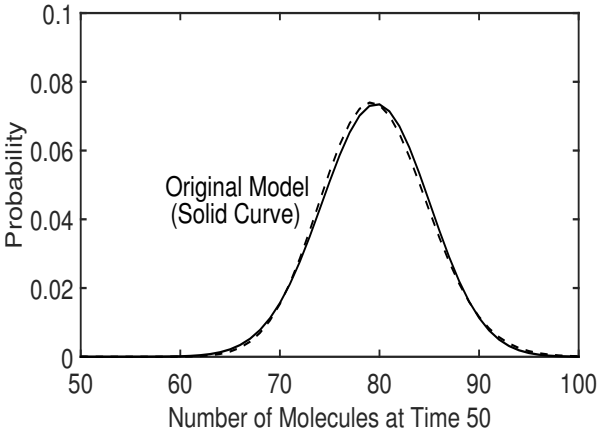



Figure 4: Probability densities of number of molecules at $t = 50$ for original and second models. *Source: created by the author.*

# 4 Summary And Future Work

In summary, discrete and continuous stochastic models are shown to be related through an interpretation of explicit finite difference methods of FKEs. A family of discrete stochastic models is identified with probability densities that approximate the density of a continuous stochastic model. The probability density of a continuous stochastic model is shown to approximate the probability density of a discrete stochastic model. For a given biologically or physically realistic discrete stochastic model, a corresponding approximate continuous stochastic model is identified through finite differences. The results are useful in the derivation, analysis, and joint application of realistic discrete and continuous stochastic models to applied problems in science and engineering.

There is potential for much future work. The discussion is generally limited to one dimension, only a basic one-dimensional error analysis is given, and solvability and smoothness results are described for one-dimensional parabolic PDEs. In future work, an increased explanation about multidimensional stochastic models is suggested with more-detailed error and convergence analyses of the numerical methods and with more numerical experiments. A detailed von Neumann stability analysis, a rigorous proof of

consistency and convergence in a suitable norm, and a precise discussion of the Courant-Friedrichs-Lewy condition is suggested for multiple dimensions. More general solvability and smoothness results applicable to the multidimensional parabolic PDEs could be considered and described. Furthermore, extending the results of the present investigation to a setting of implicit finite difference methodology is possible. That is, implicit finite difference equations of the continuous model's FKE could be related to implicit discrete models in a straightforward manner where the implicit discrete stochastic models are defined, for example, by generalizing the explicit discrete stochastic models described in Table 1. Finally, there are many more applications of the techniques described in this paper to derive and study various randomly varying problems in science, engineering, and agriculture. For example, future work may involve a more detailed study of seed longevity and plant competition with control.

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