Computers and Mathematics with Applications 71 (2016) 2497–2512

Contents lists available at ScienceDirect

Computers and Mathematics with Applications

journal homepage: www.elsevier.com/locate/camwa

Generalized local and nonlocal master equations for some stochastic processes☆

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ARTICLE INFO

Article history:
Available online 12 November 2015

Keywords:
Nonlocal flux
Stochastic coagulation
Smoluchowski equation
Conservation law
Nonlocal diffusion
Fractional diffusion

ABSTRACT

In this paper, we present a study on generalized local and nonlocal equations for some stochastic processes. By considering the net flux change in a region determined by the transition probability, we derive the master equation to describe the evolution of the probability density function. Some examples, such as classical Fokker–Planck equations, models for Lévy process, and stochastic coagulation equations, are provided as illustrations. A particular application is a consistent derivation of coupled dynamical systems for spatially inhomogeneous stochastic coagulation processes.

1. Introduction

Given a stochastic process X_t, which may represent various processes such as the diffusion process, stochastic coagulation process, or continuous time random walk (CTRW), there are many methods to derive the evolution equation of its probability density function (PDF) $f = f(\mathbf{x}, t)$, which represents the probability that the system of interest is in the state $\mathbf{x}$ at time t. A general master equation in *differential* form may be written as [1]

$$f_t(\mathbf{x}, t') = \int_0^t \int_{\mathbb{R}^n} \Big[K(\mathbf{x}', \mathbf{x}, t-\tau) f(\mathbf{x}', \tau) - K(\mathbf{x}, \mathbf{x}', t-\tau) f(\mathbf{x}, \tau) \Big] \, \mathrm{d}\mathbf{x}' \mathrm{d}\tau, \tag{1.1}$$

where K is a *memory*-dependent nonlocal transition kernel [2] for general, and possibly non-Markovian, processes. For Markov processes which have no memory effect, Eq. (1.1) reduces to

$$f_t(\mathbf{x}, t) = \int_{\mathbb{R}^n} \Big[\gamma(\mathbf{x}', \mathbf{x}, t) f(\mathbf{x}', t) - \gamma(\mathbf{x}, \mathbf{x}', t) f(\mathbf{x}, t) \Big] \, \mathrm{d}\mathbf{x}', \tag{1.2}$$

where $\gamma(\mathbf{x}', \mathbf{x}, t)$ denotes the transition rate from $\mathbf{x}'$ to $\mathbf{x}$ at time t. In the *discrete time* form, (1.2) is often reformulated as

$$f(\mathbf{x}, t) - f(\mathbf{x}, t') = \int_{\mathbb{R}^n} \Big[p(\mathbf{x}', t'; \mathbf{x}, t) f(\mathbf{x}', t') - p(\mathbf{x}, t'; \mathbf{x}', t) f(\mathbf{x}, t') \Big] \, \mathrm{d}\mathbf{x}', \tag{1.3}$$

☆ Y. Zhao's research is supported by a grant from the Simons Foundation through No. 357963 and a start-up grant from George Washington University. Y. Ma's research is supported by Loyola Marymount University CSE continuing Faculty Research grant and a start-up grant from Loyola Marymount University. Q. Du's research is partially supported by the NSF grants DMS-1318586.

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http://dx.doi.org/10.1016/j.camwa.2015.09.030
0898-1221/

where $p(\mathbf{x}', t'; \mathbf{x}, t)$ represents the transition probability (TP) of a particle moving from $\mathbf{x}'$ at time t' to $\mathbf{x}$ at time t; the first part of the right hand side represents the incoming flux and the second part is the outgoing flux. Notice that

$$\int p(\mathbf{x}, t'; \mathbf{x}', t)\mathrm{d}\mathbf{x}' = 1,$$

the master equation (1.3) can thus be equivalently interpreted as the Chapman–Kolmogorov equation (CKE). There have been many works on the study of the evolution of Markov processes using the CKE, see for instance [3,4]. In [5], a nonlinear Fokker–Planck equation (FPE) of Markov processes is derived from the master equation in the gain–loss form by characterizing the transition probability. Master equations can also be applied to study non-Markov processes. For example, an equivalence is established between generalized master equations and continuous time random walks in [1]. In general, for either Markov or non-Markov processes, the master equation is completely determined by the transition kernel. For example, Taylor expansion of transition probability on CKE can be applied to derive the evolution equation of some Markov processes, but such a technique does not apply when there is nonlocal or non-Markovian effect [3,4]. On the other hand, it is possible to derive the evolution equation from the master equation (1.3) through a Taylor expansion on the PDF instead of the transition kernel. In this paper, we will mainly focus on the Markov process though our method can be extended to non-Markov process by taking into account the time integral over memory kernel terms. We present the derivations of the evolution equations for some Markov stochastic processes from the master equation in gain–loss form (1.3). Our approach is to consider a nonlocal flux as that in [6–8]. A key ingredient is to obtain an expression of the transition probability (TP) either explicitly or implicitly that is valid for both the local and nonlocal settings associated with complex transport and diffusion processes. We verify the derivations in the later sections. A particular application is a consistent derivation of spatial inhomogeneous stochastic coagulation process. In what follows, we present the generalized master equation framework in Section 1.1; then we apply it to some classical stochastic processes in Section 2 and relating stochastic processes involving nonlocal effect with nonlocal master equations in Section 3; this generalized master equation framework can be unified under the recently developed nonlocal vector calculus, and the details are given in Section 4; furthermore in Section 5, we establish rigorously a result on joint stochastic processes and show how the generalized master equation can be applicable to certain type of coupled dynamical system.

1.1. Generalized master equation framework

To present our approach, let us review the concept of conservation law. Assume $f(\mathbf{x}, t)$ is the PDF of a physical quantity $X = X_t$ such as heat, energy and mass. The total amount of X in a region $\Omega \in \mathbb{R}^n$ at time t is

$$\int_{\mathbf{x}\in\Omega} f(\mathbf{x}, t)\, \mathrm{d}\mathbf{x}.$$

X is conserved if it is only gained or lost through the domain boundaries without external sources. Let the vector field $\mathbf{F}(\mathbf{x}, t)$ be the flux. The conservation law implies that the rate of change of the density plus the divergence of the flux is equal to 0,

$$\frac{\partial f}{\partial t} + \nabla_x \cdot \mathbf{F} = 0. \tag{1.4}$$

The transport equation, the diffusion equation and the wave equation, can be derived from the principle of conservation law given the explicit form of the flux. Nevertheless, as discussed in [7,8], the flux $\mathbf{F}$ adopted in (1.4) is a local notion which is not always suitable for a general process X_t. On the other hand, it is possible to determine the TP $p(\mathbf{x}', t'; \mathbf{x}, t)$ which represents the probability that a particle is transferred from $\mathbf{x}'$ at time t' to $\mathbf{x}$ at time t. In [8], a notion of nonlocal flux was introduced to account for more general, nonlocal spatial interactions. The discussion here is intended for time-dependent processes but the principle is similar. We begin by rewriting the conservation law in a gain–loss form. Given a stochastic process X_t with its PDF $f(\mathbf{x}, t)$ representing a conserved physical quantity which is only gained or lost through the domain boundaries, then the quantity change in this domain Ω from time t' to t ($t' < t$) equals the net flux. The generalized equation of conservation law is written as

$$\int_{\mathbf{x}\in\Omega} f(\mathbf{x}, t)\, \mathrm{d}\mathbf{x} - \int_{\mathbf{x}\in\Omega} f(\mathbf{x}, t')\, \mathrm{d}\mathbf{x} = \mathcal{F}(\Omega, t', t) = \mathcal{F}^+(\Omega, t', t) - \mathcal{F}^-(\Omega, t', t), \tag{1.5}$$

where $\mathcal{F}^+$ and $\mathcal{F}^-$ represent the incoming flux and outgoing flux in the region Ω from t' to t respectively, and $\mathcal{F}(\Omega, t', t)$ is the net (*nonlocal*) flux for the region Ω or between Ω and Ω^c (the complement of Ω). More specifically, we write the incoming flux $\mathcal{F}^+(\Omega, t', t)$ in the region Ω in terms of the TP

$$\mathcal{F}^+(\Omega, t', t) = \int_{\mathbf{x}\in\Omega} \int_{\mathbf{x}'\in\Omega^c} p(\mathbf{x}', t'; \mathbf{x}, t) f(\mathbf{x}', t')\, \mathrm{d}\mathbf{x}'\mathrm{d}\mathbf{x}, \tag{1.6}$$

and the outgoing flux $\mathcal{F}^-(\Omega, t', t)$ by

$$\mathcal{F}^-(\Omega, t', t) = \int_{\mathbf{x}\in\Omega} \int_{\mathbf{x}'\in\Omega^c} p(\mathbf{x}, t'; \mathbf{x}', t) f(\mathbf{x}, t')\, \mathrm{d}\mathbf{x}'\mathrm{d}\mathbf{x}. \tag{1.7}$$

Combining these two terms, we have an explicit form of the flux $\mathcal{F}(\Omega, t', t)$:

$$\mathcal{F}(\Omega, t', t) = \int_{\mathbf{x}\in\Omega}\int_{\mathbf{x}'\in\Omega^c}\Big[p(\mathbf{x}', t'; \mathbf{x}, t)f(\mathbf{x}', t') - p(\mathbf{x}, t'; \mathbf{x}', t)f(\mathbf{x}, t')\Big]\mathrm{d}\mathbf{x}'\mathrm{d}\mathbf{x} \tag{1.8}$$

$$= \int_{\mathbf{x}\in\Omega}\int_{\mathbf{x}'\in\mathbb{R}^n}\Big[p(\mathbf{x}', t'; \mathbf{x}, t)f(\mathbf{x}', t') - p(\mathbf{x}, t'; \mathbf{x}', t)f(\mathbf{x}, t')\Big]\mathrm{d}\mathbf{x}'\mathrm{d}\mathbf{x}. \tag{1.9}$$

Introduce the function $F(\mathbf{x}, t', t)$ as

$$F(\mathbf{x}, t', t) = \int_{\mathbf{x}'\in\mathbb{R}^n}\Big[p(\mathbf{x}', t'; \mathbf{x}, t)f(\mathbf{x}', t') - p(\mathbf{x}, t'; \mathbf{x}', t)f(\mathbf{x}, t')\Big]\,\mathrm{d}\mathbf{x}' \tag{1.10}$$

and notice that Eq. (1.5) holds for any region Ω, we have the *strong pointwise form* of the master equation

$$f(\mathbf{x}, t) - f(\mathbf{x}, t') = F(\mathbf{x}, t', t) \tag{1.11}$$

Note that $\int_{\mathbf{x}'\in\mathbb{R}^n} p(\mathbf{x}, t'; \mathbf{x}', t)\,\mathrm{d}\mathbf{x}' = 1$, the master equation (1.11) matches with the Chapman–Kolmogorov equation (CKE)

$$f(\mathbf{x}, t) = \int_{\mathbf{x}'\in\mathbb{R}^n} p(\mathbf{x}', t'; \mathbf{x}, t)f(\mathbf{x}', t')\,\mathrm{d}\mathbf{x}'. \tag{1.12}$$

Furthermore, we have the master equation in *differential form*

$$f_t(\mathbf{x}, t) = \lim_{t'\to t}\frac{F(\mathbf{x}, t', t)}{\Delta t} \tag{1.13}$$

provided the limit exists.

When a stochastic process is homogeneous and symmetric in space and time (take Brownian motion as an example), namely

$$p(\mathbf{x}', t'; \mathbf{x}, t) = f(\mathbf{x} - \mathbf{x}', t - t') = f(\mathbf{x}' - \mathbf{x}, t - t') = p(\mathbf{x}, t'; \mathbf{x}', t),$$

the master equation (1.11) is simplified as

$$\begin{aligned} f(\mathbf{x}, t) - f(\mathbf{x}, t') &= \int_{\mathbf{x}'\in\mathbb{R}^n} f(\mathbf{x} - \mathbf{x}', t - t')(f(\mathbf{x}', t') - f(\mathbf{x}, t'))\,\mathrm{d}\mathbf{x}' \\ &= \sum_{n=1}^{\infty}\frac{\partial^n f(\mathbf{x}, t')}{\partial\mathbf{x}^n}\frac{1}{n!}\int_{\mathbf{x}'\in\mathbb{R}^n} f(\mathbf{x}' - \mathbf{x}, t - t')(\mathbf{x}' - \mathbf{x})^n\,\mathrm{d}\mathbf{x}' \\ &= \sum_{n=1}^{\infty}\frac{\partial^n f(\mathbf{x}, t')}{\partial\mathbf{x}^n}\frac{1}{n!}\int_{\tilde{\mathbf{x}}\in\mathbb{R}^n} f(\tilde{\mathbf{x}}, \triangle t)\tilde{\mathbf{x}}^n\,\mathrm{d}\tilde{\mathbf{x}}, \end{aligned}$$

where $\triangle t = t - t'$. Then we have the master equation in the form

$$f_t(\mathbf{x}, t) = \lim_{\triangle t\to 0}\sum_{n=1}^{\infty}\frac{\partial^n f(\mathbf{x}, t')}{\partial\mathbf{x}^n}\frac{1}{n!}\frac{E(X_{\triangle t}^n)}{\triangle t}, \tag{1.14}$$

where $E(X_{\triangle t}^n)$ is the n-th order moment of stochastic process X_t at time $t = \triangle t$. If we can find the moments explicitly, the evolution equation can be defined accordingly.

In the next section, the formulation (1.5)–(1.13) will be validated by deriving the evolution equations of some stochastic processes.

2. Master equations for some classical stochastic processes

For a number of stochastic processes studied in the literature, we know that $p(\mathbf{x}', t'; \mathbf{x}, t)$ only depends on the local points $\mathbf{x}, \mathbf{x}'$ and time, and so does the corresponding evolution equation. The derivation of the master equations for these processes is standard results from textbooks [9,10]. However, to show how the new formulation process (1.5)–(1.13) can be performed, here we give a complete derivation of the master equation for the one-dimensional Fokker–Planck and Lévy dynamics as an example.

2.1. Fokker–Planck equations

Consider the following Fokker–Planck equations (for drifted Brownian dynamics)

$$\mathrm{d}X_t = v(X_t, t)\mathrm{d}t + \sqrt{2\sigma}\mathrm{d}W_t \tag{2.1}$$

tracking the position of a diffusing particle in $\mathbb{R}^1$ at time t, where σ is a constant and W_t is a standard Brownian motion. For a small time step $\Delta t = t - t'$, we approximate the current position by forward Euler method,

$$X_t = x' + v(x', t')\Delta t + \sqrt{2\sigma}\omega, \tag{2.2}$$

where $\omega = W_t - W_{t'} \sim N(0, \Delta t)$ is Gaussian. Applying Taylor expansion on (2.2), we can further write X_t as

$$X_t = x' + v(x, t')\Delta t + (x' - x)\partial_x v(x, t')\Delta t + \sqrt{2\sigma}\omega, \tag{2.3}$$

which can be treated as a normal distribution with mean $x' + v(x, t')\Delta t + (x' - x)\partial_x v(x, t')\Delta t$ and variance $2\sigma\Delta t$. Then the TP reads

$$p(x', t'; x, t) = \frac{1}{\sqrt{2\pi\sigma\Delta t}} \exp\left(-\frac{|x - x' - v(x, t')\Delta t - (x' - x)\partial_x v(x, t')\Delta t|^2}{2\sigma\Delta t}\right), \tag{2.4}$$

and the master equation is

$$f(x, t) = \int p(x', t'; x, t) f(x', t')\, \mathrm{d}x' = \mathrm{I} + \mathrm{II} + \mathrm{III} + O(\Delta t^2), \tag{2.5}$$

where

$$\mathrm{I} = \int p(x', t'; x, t) f(x, t')\, \mathrm{d}x' = f(x, t')\big[1 - \partial_x v(x, t')\Delta t\big] + O(\Delta t^2),$$

$$\mathrm{II} = \int p(x', t'; x, t)(x' - x)\partial_x f(x, t')\, \mathrm{d}x' = -v(x, t')\Delta t\partial_x f(x, t') + O(\Delta t^2),$$

$$\mathrm{III} = \int p(x', t'; x, t)\frac{(x' - x)^2}{2}\partial_{xx} f(x, t')\, \mathrm{d}x' = \sigma\Delta t\partial_{xx} f(x, t') + O(\Delta t^2).$$

by simple calculation. Moving $f(x, t')$ in I to the left hand side of (2.5), dividing two sides by Δt and taking the limit $\Delta t \to 0$, we obtain the Fokker–Planck equation

$$\partial_t f(x, t) = -\partial_x\Big(v(x, t)f(x, t)\Big) + \sigma\partial_{xx} f(x, t). \tag{2.6}$$

Similar derivation can be applied on many other processes such as Lévy process. The key ingredient in the new formulation is to find the TP $p(\mathbf{x}', t'; \mathbf{x}, t)$ and then derive the flux function F.

2.2. Lévy process

If X is a one-dimensional Lévy process, then by Lévy–Itô decomposition, it can be decomposed into three independent parts [11,12]

$$X(t) = (bt + \sqrt{2\sigma}W_t) + \int_{|x|<1} x\tilde{N}(t, \mathrm{d}x) + \int_{|x|\geq 1} xN(t, \mathrm{d}x) \tag{2.7}$$

where $N(\mathrm{d}t, \mathrm{d}x)$ is the Poisson random measure, $\tilde{N}(\mathrm{d}t, \mathrm{d}x) = N(\mathrm{d}t, \mathrm{d}x) - \nu(\mathrm{d}x)\mathrm{d}t$ is the compensated Poisson random measure, and ν is the Lévy intensity measure defined on R and concentrated on $R \setminus \{0\}$, satisfying

$$\int_{R\setminus\{0\}} (x^2 \wedge 1)\nu(\mathrm{d}x) < \infty.$$

To derive the master equation governing the dynamics of the PDF $f(x, t)$ for the Lévy process in (2.7), we can study the three independent parts separately. First of all, the drifted Brownian part $bt + \sqrt{2\sigma}W_t$ make a contribution similar as in (2.6):

$$-\partial_x(bf(x, t)) + \sigma\partial_{xx} f(x, t). \tag{2.8}$$

Secondly, the Poisson integration $\int_{|x|\geq 1} xN(t, \mathrm{d}x)$ is a compound Poisson process which can be rewritten as

$$\int_{|x|\geq 1} xN(t, \mathrm{d}x) = \sum_{0\leq u\leq t} \Delta X(u)\chi_{|x|\geq 1}(\Delta X(u)) \tag{2.9}$$

where χ is the characteristic function, $\Delta X(t) = X(t) - X(t-)$ is the jump process associated with the Lévy process and $X(t-)$ is the left limit at the point t. Then the transition rate for this compound Poisson process is

$$\lim_{\Delta t\to 0}\frac{1}{\Delta t}p(x', t'; x, t) = \lim_{\Delta t\to 0}\frac{1}{\Delta t}p(0, 0; \Delta x, \Delta t) = \lim_{\Delta t\to 0}\frac{1}{\Delta t}P(\tau < \Delta t)\mu(\Delta x)$$

where τ is the waiting time for the compound Poisson process which is exponentially distributed random variable, $\tau \sim \exp(-\lambda t)$, with $\lambda = \nu(\{|x| \geq 1\})$, and μ is the law for the jump size random variable $\Delta X(\tau)$ which is given by [11,12]

$$\mu(B) = \frac{\nu(\{|x| \geq 1\} \cap B)}{\nu(\{|x| \geq 1\})}. \tag{2.10}$$

Notice that

$$P(\tau < \Delta t) = 1 - P(\tau \geq \Delta t) = 1 - \exp(-\lambda \Delta t) = \lambda \Delta t + O(\Delta t^2),$$

the transition rate becomes

$$\lim_{\Delta t \to 0} \frac{1}{\Delta t} p(x', t'; x, t) = \nu(\Delta x).$$

Hence the right hand side of Eq. (1.13) reads

$$\lim_{\Delta t \to 0} \frac{1}{\Delta t} F(x, t', t) = \int_{|z| \geq 1} (f(x - z, t) - f(x, t)) \nu(\mathrm{d}z) \tag{2.11}$$

which is the contribution of the Poisson integral $\int_{|x| \geq 1} xN(t, \mathrm{d}x)$. Thirdly, since the compensated Poisson integral $\int_{|x|<1} x\tilde{N}(t, \mathrm{d}x)$ is of the form,

$$\int_{|x|<1} x\tilde{N}(t, \mathrm{d}x) = \int_{|x|<1} xN(t, \mathrm{d}x) - t \int_{|x|<1} x\nu(\mathrm{d}x) = \mathrm{I} + \mathrm{II},$$

hence I makes a contribution of the form

$$\int_{|z|<1} (f(x - z, t) - f(x, t)) \nu(\mathrm{d}z), \tag{2.12}$$

which is similar as (2.11). II is a drift term and makes a contribution of the form

$$\partial_x f(x, t) \int_{|z|<1} z\nu(\mathrm{d}z). \tag{2.13}$$

Finally the combination of (2.8), (2.11), (2.12) and (2.13) yields the master equation for the Lévy process (2.7),

$$\partial_t f(x, t) = -\partial_x (bf(x, t)) + \sigma \partial_{xx} f(x, t) + \int_{R \setminus \{0\}} \Big[f(x - z, t) - f(x, t) + \chi_{|z|<1} z \partial_x f(x, t) \Big] \nu(\mathrm{d}z) \tag{2.14}$$

which is consistent with the results in [13,14]. The above equation gives rise to space-fractional equation. We refer to [15,16] for further studies. In the case of $b = \sigma = 0$ and a symmetric measure ν, we may view the nonlocal master equation as a nonlocal diffusion equation, see related discussions in [17,18].

3. Nonlocal equations for stochastic processes

The TPs of stochastic processes involving nonlocal effects depend on the density distribution in part of the entire space $\mathbb{R}^n$. In this section, we present one example of such a stochastic process, the stochastic coagulation process, whose evolution equation can also be derived by the master equation (1.11).

3.1. Stochastic coagulation equation

Stochastic coagulation equations [19] are also called as Smoluchowski equations [20] or population balance equations [21,22], which are often used to describe the rate of change of the concentration in time in a dynamic coagulation process and have been applied to a wide range of topics, such as aerosol growth, polymerization problems, and the kinetics of platelet aggregate formation and disaggregation. For example, researchers used them to study the heterotypic aggregation kinetics of platelets and neutrophils, most notably in the uniform shear field [21,22]. In [23,24], we applied it to model the polymorphonuclear neutrophils (PMN) and tumor cell adhesion in nonuniform shear flow in the parallel-plate flow chamber.

To begin with, we consider the spatially homogeneous coagulation equation. Let $N = N(x, t)$, $x \in \mathbb{R}^1$ be the particle volume density function representing the concentration of the particle of volume x at time t. The continuous coagulation equation reads

$$N_t(x, t) = \frac{1}{2} \int_0^x \beta(y, x - y) N(y, t) N(x - y, t) \mathrm{d}y - \int_0^\infty \beta(x, y) N(x, t) N(y, t) \mathrm{d}y \tag{3.1}$$

with an initial condition

$$N(x, 0) = N_0(x) \geq 0, \tag{3.2}$$

where $\beta(x, y)$ is called a coagulation kernel which describes the intensity of aggregation between particles of volumes x and y. The first term on the right-hand side of Eq. (3.1) indicates the fact that a particle of volume x can only be generated if two particles of volumes $x - y$ and y ($y \leq x$) aggregate. The second term says that each particle of volume x disappears after aggregating with any other particle. The coagulation kernel $\beta(x, y)$ is assumed to be non-negative and symmetric, i.e. $\beta(x, y) \geq 0$ and $\beta(x, y) = \beta(y, x)$ for all (x, y). In this paper, we only focus on the coagulation process, and ignore the fragmentation assumption, namely, the particle volume, as a function of time t, keeps non-decreasing. The complexity of the system (3.1)–(3.2) is determined by the form of $\beta(x, y)$.

A discrete version of the coagulation equation describing the rate of change of the concentration $N(i, t)$ of the particles with i monomers is given by:

$$\frac{\partial N(i, t)}{\partial t} = \frac{1}{2}\sum_{j=1}^{i-1} \beta(j, i-j)N(j, t)N(i-j, t) - \sum_{j=1}^{\infty} \beta(i, j)N(i, t)N(j, t)$$

with an initial condition $N(i, 0) = N_0(i)$, $(i = 1, 2, 3, \ldots)$. Here $\beta(i, j)$ is the coagulation kernel in discrete version.

The coagulation equations have various stochastic and deterministic formulations such as Chapman–Kolmogorov formulation, Marcus–Lushnikov formulation [19,25–27], and conservation law formulation [28] for spatially homogeneous coagulation equation. Sabelfeld [29] derived the spatially inhomogeneous equation by Lagrange model. In this section, we will derive the coagulation equation (3.1) from two different approaches—CKE (1.12) and conservation law.

3.2. Chapman–Kolmogorov equation

Coagulation kernel $\beta(u, v)$ is the incoming flux of particles per unit time for unit concentration. For the spatially homogeneous case, we assume particles are uniformly distributed, therefore, $\beta(u, v)N(v, t)$ is the coagulation number per unit time between the target particle of volume u and other particles of volume v at time t. This leads to the probabilistic interpretation of the coagulation kernel $\beta(u, v)$ [25,30,31]. More specifically, for small time Δt,

- $\beta(u, v)\Delta t$ stands for the probability of occurrence of aggregation per unit volume between particles of volume u and those of volume v during a time interval of length Δt;
- For a target particle of volume u, $\beta(u, v)N(v, t)\Delta t$ gives the probability of the target particle of volume u adhering to a particle of volume v in the next infinitesimal time interval $(t, t + \Delta t)$ per unit volume, and $\beta(u, v)N(v, t)\mathrm{d}v\Delta t$ gives the probability of the target particle of volume u adhering to a particle of volume v to $v + \mathrm{d}v$ in the next infinitesimal time interval $(t, t + \Delta t)$ per unit volume;
- $\beta(u, v)N(u, t)N(v, t)\mathrm{d}u\mathrm{d}v\Delta t$ presents the average number of aggregations per unit volume between the particles of volume u to $u + \mathrm{d}u$ and those of volume v to $v + \mathrm{d}v$ during $(t, t + \Delta t)$.

The probability representation of the coagulation kernel reveals the particle interaction theory in the stochastic coagulation system. It helps us to set up the stochastic coagulation model, and may apply the Monte Carlo method to simulate the stochastic system.

In a stochastic coagulation system, we focus on one particular particle and track its growth on size. Let X_t be a stochastic process representing the volume of this particle at time t. This stochastic process is a Markov process since the growth of the particle volume at time $t + \triangle t$ only depends on the volume at time t. Let the PDF of this stochastic process be $f(x, t)$. Notice that $f(x, t)\Delta t$ is the probability that $X_t = x$ during the time interval $(t, t + \Delta t)$, and $1/x$ gives the number of particles per unit volume, so $f(x, t)\Delta t/x$ provides the average number of particles of volume x per unit volume during the time interval $(t, t + \Delta t)$, which is the same as $N(x, t)\Delta t$. Hence, $f(x, t)$ and $N(x, t)$ are connected via

$$N(x, t) = f(x, t)/x. \tag{3.3}$$

Assume the particle volume $X_t = x$, then as we discussed in the circular bullets of the preceding paragraph, the probability that this particle will adhere to a particle of volume y in the next infinitesimal time interval $(t, t + \Delta t)$ is $\beta(x, y)N(y, t)\Delta t$. Hence, the probability that it will be unattached to any particle is $1 - \int_0^\infty \beta(x, y)\triangle tN(y, t)\mathrm{d}y$. If it sticks to a particle of volume y, then its particle volume will increase to $x + y$ at time $t + \triangle t$, that is, $X_{t+\triangle t} = x + y$. Otherwise, if there is no coagulation event taking place, $X_{t+\triangle t}$ will remain being x.

In general, we assume that the particle volume at time t is x. Then the TP of the coagulation process, the probability that a particle of volume x at t becomes volume $x + y$ at $t + \Delta t$, is given as:

$$p(x, t; x + y, t + \Delta t) = \begin{cases} \beta(x, y)\Delta tN(y, t), & y > 0 \\ 1 - \displaystyle\int_0^\infty \beta(x, z)\Delta tN(z, t)\mathrm{d}z, & y = 0 \\ 0, & y < 0 \end{cases} \tag{3.4}$$

or in other words

$$p(x', t'; x, t) = \begin{cases} \beta(x', x - x')\Delta t N(x - x', t), & x > x' \\ 1 - \int_0^\infty \beta(x', \hat{x})\Delta t N(\hat{x}, t)\mathrm{d}\hat{x}, & x = x' \\ 0. & x < x' \end{cases} \tag{3.5}$$

where $t = t' + \Delta t$. Therefore, the density function $f(x, t + \Delta t)$ satisfies the CKE (1.12):

$$f(x, t) = \int_0^x \beta(x', x - x')\Delta t N(x - x', t) f(x', t')\mathrm{d}x' + \left(1 - \int_0^\infty \beta(x, \hat{x})\Delta t N(\hat{x}, t)\mathrm{d}\hat{x}\right) f(x, t'). \tag{3.6}$$

Rearranging terms yields

$$\frac{f(x, t) - f(x, t')}{\Delta t} = \int_0^x \beta(x', x - x')N(x - x', t) f(x', t')\mathrm{d}x' - \int_0^\infty \beta(x, x') f(x, t')N(x', t)\mathrm{d}x'. \tag{3.7}$$

Taking the limit on the left-hand side as $\Delta t \to 0$ and noting the relation (3.3) yields an equation of $f(x, t)$ as follows:

$$f_t(x, t) = \int_0^x \frac{\beta(x', x - x')}{x - x'} f(x - x', t) f(x', t)\mathrm{d}x' - \int_0^\infty \frac{\beta(x, x')}{x'} f(x, t) f(x', t)\mathrm{d}x' \tag{3.8}$$

For the first integral on the right hand side of (3.8), we have

$$\begin{aligned} &\int_0^x \frac{\beta(x', x - x')}{x - x'} f(x', t) f(x - x', t)\mathrm{d}x' \\ &= \frac{1}{2}\int_0^x \frac{\beta(x', x - x')}{x - x'} f(x', t) f(x - x', t)\mathrm{d}x' + \frac{1}{2}\int_0^x \frac{\beta(x', x - x')}{x - x'} f(x', t) f(x - x', t)\mathrm{d}x' \\ &= \frac{1}{2}\int_0^x \frac{\beta(x', x - x')}{x - x'} f(x', t) f(x - x', t)\mathrm{d}x' + \frac{1}{2}\int_0^x \frac{\beta(x', x - x')}{x'} f(x', t) f(x - x', t)\mathrm{d}x' \\ &= \frac{x}{2}\int_0^x \beta(x', x - x')\frac{f(x', t)}{x'}\frac{f(x - x', t)}{x - x'}\mathrm{d}x' \end{aligned}$$

therefore, Eq. (3.8) becomes

$$f_t(x, t) = \frac{x}{2}\int_0^x \beta(x', x - x')\frac{f(x', t)}{x'}\frac{f(x - x', t)}{x - x'}\mathrm{d}x' - \int_0^\infty \frac{\beta(x, x')}{x'} f(x, t) f(x', t)\mathrm{d}x' \tag{3.9}$$

Divide the two sides of (3.9) by x, and apply the relation (3.3), we have

$$N_t(x, t) = \frac{1}{2}\int_0^x \beta(x', x - x')N(x', t)N(x - x', t)\mathrm{d}x' - \int_0^\infty \beta(x, x')N(x, t)N(x', t)\mathrm{d}x' \tag{3.10}$$

which is exactly the continuous coagulation equation (3.1) except that y is replaced by x' here.

3.3. Formulations as conservation laws

It is pointed out in [28] that the coagulation equation can be written in terms of the conservation law:

$$\frac{\partial}{\partial t} f(x, t) + \frac{\partial}{\partial x} F(x, t) = 0, \tag{3.11}$$

where the flux $F(x, t)$ is given by

$$F(x, t) = \int_0^x \int_{x-y}^\infty \frac{\beta(y, y')}{y'} f(y, t) f(y', t)\mathrm{d}y'\mathrm{d}y. \tag{3.12}$$

We will re-derive the flux formulation and reveal its relationship with (1.12). Recall the original definition of the net flux in Eq. (1.5). For arbitrary $x \in \mathbb{R}$, select the region $\Omega_x = [x, \infty)$ and set $\mathcal{F}(\Omega_x, t', t)$ to be the net flux to this region Ω_x from t' to t. Notice that the particles monotonically grow on size in the coagulation process, therefore the outgoing flux is zero, namely $\mathcal{F}^-(\Omega, t', t) = 0$. Therefore we have

$$\begin{aligned} \mathcal{F}(\Omega_x, t', t) =& \mathcal{F}^+(\Omega_x, t', t) \\ =& \int_{\mathbb{R}\setminus\Omega}\int_\Omega p(y, t'; z, t) f(y, t')\,\mathrm{d}z\mathrm{d}y \\ =& \Delta t \int_0^x \int_x^\infty \beta(y, z - y)N(z - y, t) f(y, t')\,\mathrm{d}z\mathrm{d}y. \end{aligned} \tag{3.13}$$

Dividing Δt on both sides of Eq. (1.5) and sending $\Delta t \to 0$ yields

$$\int_x^\infty \frac{\partial}{\partial t} f(x,t)dx = \int_0^x \int_x^\infty \beta(y, z-y)N(z-y,t)f(y,t)\,\mathrm{d}z\mathrm{d}y \tag{3.14}$$

right hand side of which is exactly the flux $F(x,t)$ in (3.12) by the change of variable $y' = z - y$. Taking the first order spatial derivative on both sides of (3.14), we obtain the evolution equation formulated in conservation law (3.11),

$$f_t(x,t) = -\frac{\partial}{\partial x}\int_0^x \int_x^\infty \beta(y, z-y)N(z-y,t)f(y,t)\,\mathrm{d}z\mathrm{d}y. \tag{3.15}$$

Eq. (3.15) implies the coagulation equation (3.1). Indeed, set

$$M(x,y) = \int_x^\infty \beta(y, z-y)N(z-y,t)f(y,t)\mathrm{d}z,$$

and apply the differentiation rule under the integral sign

$$\frac{\partial}{\partial x}\int_0^x M(x,y)\mathrm{d}y = M(x,x) + \int_0^x \frac{\partial}{\partial x}M(x,y)\mathrm{d}y,$$

consequently

$$\begin{aligned}
&\frac{\partial}{\partial x}\int_0^x \int_x^\infty \beta(y, z-y)N(z-y,t)f(y,t)\,\mathrm{d}z\mathrm{d}y \\
&\quad = \int_x^\infty \beta(x, z-x)N(z-x,t)f(x,t)\,\mathrm{d}z - \int_0^x \beta(y, x-y)N(x-y,t)f(y,t)\,\mathrm{d}y \\
&\quad = \int_0^\infty \beta(x,y)N(y,t)f(x,t)\,\mathrm{d}y - \int_0^x \beta(x-y,y)N(y,t)f(x-y,t)\,\mathrm{d}y
\end{aligned}$$

where the last step is due to the change of variables. Accordingly the conservation law (3.15) becomes

$$f_t(x,t) = -\int_0^\infty \beta(x,y)N(y,t)f(x,t)\,\mathrm{d}y + \int_0^x \beta(x-y,y)N(y,t)f(x-y,t)\,\mathrm{d}y$$

which is identical with (3.8) by noticing $N(y,t) = f(y,t)/y$. Then the calculation in (3.8)–(3.10) leads us again to the spatially homogeneous coagulation equation:

$$N_t(x,t) = \frac{1}{2}\int_0^x \beta(x-y,y)N(y,t)N(x-y,t)\,\mathrm{d}y - \int_0^\infty \beta(x,y)N(x,t)N(y,t)\,\mathrm{d}y.$$

4. Nonlocal fluxes, a nonlocal vector calculus and nonlocal conservation laws

In this section, we will review some recently developed theories in nonlocal vector calculus and relate them with our generalized master equation framework (1.5)–(1.13).

Introducing nonlocal operators like nonlocal gradient, nonlocal divergence and nonlocal curl operators in some recent works [7,6,8], the standard (local) calculus is generalized into a nonlocal vector calculus, from which the nonlocal fluxes, nonlocal conservation laws and nonlocal advection–diffusion problems are well established. In what follows we will give a brief review on the nonlocal calculus and nonlocal conservation laws (see the details in [7,6,8] and the references therein) and show the connection with our generalized master equation framework (1.5)–(1.13). For the sake of brevity, in this section, we suppress explicit reference to the time dependence of variables.

4.1. Nonlocal fluxes

For any point $\mathbf{x} \in \mathbb{R}^n$ and an integrable $\psi(\mathbf{x},\mathbf{y})$, the *nonlocal flux density* at $\mathbf{x}$ into $\tilde{\Omega}$ is defined as

$$\int_{\tilde{\Omega}} \psi(\mathbf{x},\mathbf{y})\mathrm{d}\mathbf{y}, \quad \forall \tilde{\Omega} \subseteq \mathbb{R}^n. \tag{4.1}$$

With such a definition, one can easily verify the following equivalent statements:

- $\psi(\mathbf{x},\mathbf{y})$ is an antisymmetric function, i.e., $\psi(\mathbf{x},\mathbf{y}) = -\psi(\mathbf{y},\mathbf{x})$;
- there are no self-interactions, i.e., $\int_{\tilde{\Omega}}\int_{\tilde{\Omega}} \psi(\mathbf{x},\mathbf{y})\,\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{x} = 0,\ \forall \tilde{\Omega} \subseteq \mathbb{R}^n$;
- for regions $\Omega_1, \Omega_2 \subset \mathbb{R}^n$, both having nonzero volume, one has the *nonlocal action–reaction principle*: $\int_{\Omega_1}\int_{\Omega_2} \psi(\mathbf{x},\mathbf{y})\,\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{x} + \int_{\Omega_2}\int_{\Omega_1} \psi(\mathbf{x},\mathbf{y})\,\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{x} = 0$.

For any two open regions $\Omega_1 \subseteq \mathbb{R}^n$ and $\Omega_2 \subseteq \mathbb{R}^n$ both having nonzero volume, the (scalar) *interaction* or *nonlocal flux from* Ω_1 *into* Ω_2 is defined by

$$\int_{\Omega_1}\int_{\Omega_2} \psi(\mathbf{x},\mathbf{y})\,\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{x}. \tag{4.2}$$

The nonlocal action–reaction principle states that the flux from Ω_1 into Ω_2 is equal and opposite to the flux from Ω_2 into Ω_1. The flux is *nonlocal* because the interaction may be nonzero even when the closures of Ω_1 and Ω_2 have an empty intersection, unlike local flux which is possibly nonzero only when Ω_1 and Ω_2 have a nonempty common boundary $\partial\Omega_{12} = \bar{\Omega}_1 \cap \bar{\Omega}_2$. Special forms of nonlocal fluxes will be illustrated later in the derivation of master equations for joint stochastic processes. More properties of nonlocal fluxes and comparisons with local fluxes can be found in [8].

4.2. A nonlocal vector calculus

Given the mappings $\boldsymbol{\nu}(\mathbf{x},\mathbf{y}), \boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\colon \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^k$ with $\boldsymbol{\alpha}$ being antisymmetric, i.e., $\boldsymbol{\alpha}(\mathbf{x},\mathbf{y}) = -\boldsymbol{\alpha}(\mathbf{y},\mathbf{x})$, the action of the *nonlocal divergence operator* $\mathcal{D}$ on $\boldsymbol{\nu}$ is defined as

$$\mathcal{D}(\boldsymbol{\nu})(\mathbf{x}) := \int_{\mathbb{R}^n} (\boldsymbol{\nu}(\mathbf{x},\mathbf{y}) + \boldsymbol{\nu}(\mathbf{y},\mathbf{x}))\cdot\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\,\mathrm{d}\mathbf{y}, \quad \mathbf{x}\in\mathbb{R}^n \tag{4.3}$$

where $\mathcal{D}(\boldsymbol{\nu}) : \mathbb{R}^n \to \mathbb{R}$.

Given the mapping $u(\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}$, the *adjoint operator* $\mathcal{D}^*$ *corresponding to* $\mathcal{D}$ is the operator whose action on u is given by

$$\mathcal{D}^*(u)(\mathbf{x},\mathbf{y}) = -(u(\mathbf{y}) - u(\mathbf{x}))\boldsymbol{\alpha}(\mathbf{x},\mathbf{y}), \quad \mathbf{x},\mathbf{y}\in\mathbb{R}^n, \tag{4.4}$$

where $\mathcal{D}^*(u) : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^k$, and we view $-\mathcal{D}^*$ as a *nonlocal gradient*.

Let $\boldsymbol{\Theta}(\mathbf{x},\mathbf{y}) = \boldsymbol{\Theta}(\mathbf{y},\mathbf{x}) : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^{k\times k}$ denote a second-order tensor satisfying $\boldsymbol{\Theta} = \boldsymbol{\Theta}^T$, then

$$\mathcal{D}(\boldsymbol{\Theta}\cdot\mathcal{D}^*u)(\mathbf{x}) = -2\int_{\mathbb{R}^n} (u(\mathbf{y}) - u(\mathbf{x}))\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\cdot(\boldsymbol{\Theta}(\mathbf{x},\mathbf{y})\cdot\boldsymbol{\alpha}(\mathbf{x},\mathbf{y}))\,\mathrm{d}\mathbf{y}, \quad \mathbf{x}\in\mathbb{R}^n$$

where $\mathcal{D}(\boldsymbol{\Theta}\cdot\mathcal{D}^*u) : \mathbb{R}^n \to \mathbb{R}$. Let $\gamma = \boldsymbol{\alpha}\cdot(\boldsymbol{\Theta}\cdot\boldsymbol{\alpha})$, and $\mathcal{L}(u) = -\mathcal{D}(\boldsymbol{\Theta}\cdot\mathcal{D}^*u)$, then for $u(\mathbf{x}) : \Omega \to \mathbb{R}$, the action of the linear operator $\mathcal{L}$ on the function $u(\mathbf{x})$ is simply

$$\mathcal{L}u(\mathbf{x}) := 2\int (u(\mathbf{y}) - u(\mathbf{x}))\gamma(\mathbf{x},\mathbf{y})\,\mathrm{d}\mathbf{y} \tag{4.5}$$

which is a composition of nonlocal divergence and gradient operators so that if $\boldsymbol{\Theta}$ is the identity tensor, $\mathcal{L}$ can be interpreted as a nonlocal Laplacian operator.

4.3. Nonlocal conservation laws

Let Ω denote a bounded, open set in $\mathbb{R}^n$. Nonlocal conservation laws have the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\tilde{\Omega}} q(\mathbf{x},t)\mathrm{d}\mathbf{x} = \int_{\tilde{\Omega}} b(\mathbf{x},t)\mathrm{d}\mathbf{x} - \mathcal{F}(\tilde{\Omega},\tilde{\Omega}_{\mathit{I}};q), \quad \forall\tilde{\Omega}\subseteq\Omega, t>0 \tag{4.6}$$

where $q(\mathbf{x},t)$ is the intensive quantity in some subdomain $\Omega\subset\mathbb{R}^n$, $b(\mathbf{x},t)$ denotes the source density for q in Ω, $\tilde{\Omega}_{\mathit{I}}$ is the interaction region corresponding to $\tilde{\Omega}$, and most importantly $\mathcal{D}$ is the flux operator defined as

$$\mathcal{F}_{\mathrm{nonloc}}(\Omega_1,\Omega_2;q) := \int_{\Omega_1}\int_{\Omega_2} (\boldsymbol{\nu}(\mathbf{x},\mathbf{y}) + \boldsymbol{\nu}(\mathbf{y},\mathbf{x}))\cdot\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{x}, \quad \Omega_1,\Omega_2\subset\mathbb{R}^n \tag{4.7}$$

which gives the nonlocal flux from Ω_1 into Ω_2. Here the vector $\boldsymbol{\nu}(\mathbf{x},\mathbf{y})$ has to be related to q through a constitutive relation.

By taking $\Omega_1 = \tilde{\Omega}$ and $\Omega_2 = \tilde{\Omega}_{\mathit{I}}$, the nonlocal flux can be written as follows:

$$\begin{aligned}
\mathcal{F}_{\mathrm{nonloc}}(\tilde{\Omega},\tilde{\Omega}_{\mathit{I}};q) &= \int_{\tilde{\Omega}}\int_{\tilde{\Omega}_{\mathit{I}}} (\boldsymbol{\nu}(\mathbf{x},\mathbf{y}) + \boldsymbol{\nu}(\mathbf{y},\mathbf{x}))\cdot\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{x}\\
&= -\int_{\tilde{\Omega}_{\mathit{I}}}\int_{\tilde{\Omega}} (\boldsymbol{\nu}(\mathbf{x},\mathbf{y}) + \boldsymbol{\nu}(\mathbf{y},\mathbf{x}))\cdot\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{x}\\
&= -\int_{\tilde{\Omega}_{\mathit{I}}}\int_{\tilde{\Omega}\cup\tilde{\Omega}_{\mathit{I}}} (\boldsymbol{\nu}(\mathbf{x},\mathbf{y}) + \boldsymbol{\nu}(\mathbf{y},\mathbf{x}))\cdot\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{x}, \quad \forall\tilde{\Omega}\subset\Omega,
\end{aligned}$$

so that the conservation laws (4.6) become

$$\int_{\tilde{\Omega}} \frac{\partial q}{\partial t} \mathrm{d}\mathbf{x} + \int_{\tilde{\Omega}_I} \mathcal{N}(\boldsymbol{\nu}) \mathrm{d}\mathbf{x} = \int_{\tilde{\Omega}} \left(\frac{\partial q}{\partial t} + \mathcal{D}(\boldsymbol{\nu}) \right) \mathrm{d}\mathbf{x} = \int_{\tilde{\Omega}} b \, \mathrm{d}\mathbf{x}, \quad \forall \tilde{\Omega} \subseteq \Omega, \tag{4.8}$$

where a nonlocal Gauss theorem [8] has been used, and from which it follows that, because $\tilde{\Omega}$ is arbitrary in Ω,

$$\frac{\partial q}{\partial t} + \mathcal{D}(\boldsymbol{\nu}) = b, \quad \forall \mathbf{x} \in \Omega. \tag{4.9}$$

The interaction vector $\boldsymbol{\nu}$ is related to the intensive quantity q through a constitutive relation. If taking $\boldsymbol{\nu} = \kappa \mathcal{D}^*(q)$, one can obtain the *nonlocal diffusion equation* [17,6,7].

$$\frac{\partial q}{\partial t} + \kappa \mathcal{D} \mathcal{D}^*(q) = b, \quad \forall \mathbf{x} \in \Omega.$$

4.4. Generalized master equations as nonlocal conservation laws

Back to our generalized master equation framework (1.5)–(1.13). Comparing (1.5)–(1.13) and (4.6)–(4.9), our generalized master equation framework can actually be unified to the nonlocal conservation laws by taking the source term $b(\mathbf{x}, t) = 0$ and

$$\boldsymbol{\nu} = \boldsymbol{\Theta} \cdot (\mathcal{D}^* q) - \boldsymbol{\mu} q \tag{4.10}$$

where $\boldsymbol{\mu} : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^k$ describes the nonlocal convection which is symmetric and translational invariant. Indeed, after inserting (4.10) into (4.9) and applying the definition of $\mathcal{D}(\boldsymbol{\nu})$ in (4.3), the conservation law (4.9) reads

$$q_t(\mathbf{x}, t) + \int_{\mathbb{R}^n} \gamma(\mathbf{x}, \mathbf{y}) q(\mathbf{x}, t) - \gamma(\mathbf{y}, \mathbf{x}) q(\mathbf{y}, t) \, \mathrm{d}\mathbf{y} = 0 \tag{4.11}$$

where the kernel $\gamma : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is of the form [7]

$$\gamma = 2\boldsymbol{\alpha} \cdot \boldsymbol{\Theta} \boldsymbol{\alpha} - \boldsymbol{\mu} \cdot \boldsymbol{\alpha}. \tag{4.12}$$

Our generalized master equation in differential form (1.13) is identical to (4.11) when taking γ as the transition rate

$$\gamma(\mathbf{x}, \mathbf{x}') := \lim_{\Delta t \to 0} \frac{p(\mathbf{x}, t; \mathbf{x}', t')}{\Delta t}, \tag{4.13}$$

where the time variable in γ is suppressed as we mentioned before.

On the other hand, for the applications of generalized master equation framework, we rather adopt the pointwise form (1.11) instead of the differential form (1.13) and (4.9) in most of the examples in this paper because it is easier to find the transition probability p than the transition rate γ. However, when having the cases where the transition rate can be simply found, one can easily apply the differential form (1.13) to derive the master equations.

Let $X(t)$ be a finite-range nonsymmetric Markov jump process. More precisely, let $X(t)$ denote the position of a diffusing particle at time t and $u(\mathbf{x}, t)$ be the probability density function. It is a jump process confined in Ω, the jump size is at most ϵ, and the jumps are not symmetric, namely, the TP $p(\mathbf{x}', t'; \mathbf{x}, t)$ is not symmetric on $\mathbf{x}$ and $\mathbf{x}'$. Once the particle leaves Ω, it will not re-enter. Assume the transition rate exists and only depends on the spatial distance

$$\gamma(\mathbf{x}', \mathbf{x}) := \gamma^\epsilon(\mathbf{x} - \mathbf{x}') := \lim_{\Delta t \to 0} \frac{p(\mathbf{x}', t'; \mathbf{x}, t)}{\Delta t}. \tag{4.14}$$

According to (1.13), it is easy to verify that $u(\mathbf{x}, t)$ satisfies

$$u_t(\mathbf{x}, t) = \int_{\mathbf{x}' \in \Omega} \left[\gamma^\epsilon(\mathbf{x} - \mathbf{x}') u(\mathbf{x}', t) - \gamma^\epsilon(\mathbf{x}' - \mathbf{x}) u(\mathbf{x}, t) \right] \mathrm{d}\mathbf{x}' \tag{4.15}$$

which is exactly the nonlocal convection–diffusion equation in [7]. Here the $\gamma^\epsilon(\mathbf{x})$ is compactly supported when $|\mathbf{x}| \leq \epsilon$ so that the particle jumps on a size of no larger than ϵ.

Additionally, if we consider a Markov jump process $X(t)$ in R^n (without confinement in Ω), where $X(t)$ denotes the position of a diffusing particle at time t, and assume the transition rate is in the form of Lévy jump intensity

$$\gamma(\mathbf{x}', \mathbf{x}) := \phi(\mathbf{x} - \mathbf{x}') \propto |\mathbf{x} - \mathbf{x}'|^{-\alpha - n} \tag{4.16}$$

where $0 < \alpha < 1$. Then the PDF $u(\mathbf{x}, t)$ satisfies a nonlocal fractional diffusion equation [32]:

$$u_t(\mathbf{x}, t) = \int_{R^n} \Big[u(\mathbf{x}', t) - u(\mathbf{x}, t) \Big] \gamma(\mathbf{x}, \mathbf{x}') \, \mathrm{d}\mathbf{x}' \tag{4.17}$$

and α indicates the nonlocal fractional Laplacian in n dimensions. This is consistent to the derivations given in Section 2.2.

5. Coupled dynamical system

In this section, we will apply the formulations (1.8)–(1.13) to the system in which two stochastic processes are coupled together. Based on the results presented in this section, we derive the spatially inhomogeneous coagulation equation, and also study the gene regulation in a stochastically changing environment.

5.1. Formulation

Let us consider a coupled system $Z(t) = (X_1(t), X_2(t))$ where X_1, X_2 are two random processes, and X_2 depends on X_1 as follows:

$$\mathrm{d}X_2 = V(X_2, t)\mathrm{d}t + C\mathrm{d}X_1 \tag{5.1}$$

where V is a smooth function, and C is a constant independent of X_1 and X_2. For this coupled system, we can define $f_q^{(n)}$ the n-times joint probability density in q random processes ($q = 1, 2$) similar as the single random process case [9] by denoting

$$f_q^{(n)}\big(\mathbf{x}_1^{(1)}, \ldots, \mathbf{x}_q^{(1)}, t_1; \ldots; \mathbf{x}_1^{(n)}, \ldots, \mathbf{x}_q^{(n)}, t_n\big)\mathrm{d}\mathbf{x}_1^{(1)} \ldots \mathrm{d}\mathbf{x}_q^{(1)} \ldots \mathrm{d}\mathbf{x}_1^{(n)} \ldots \mathrm{d}\mathbf{x}_q^{(n)}$$

as the probability that $X_1(t_1) \in \big(\mathbf{x}_1^{(1)}, \mathbf{x}_1^{(1)} + \mathrm{d}\mathbf{x}_1^{(1)}\big), \ldots, X_q(t_1) \in \big(\mathbf{x}_q^{(1)}, \mathbf{x}_q^{(1)} + \mathrm{d}\mathbf{x}_q^{(1)}\big), \ldots, X_1(t_n) \in \big(\mathbf{x}_1^{(n)}, \mathbf{x}_1^{(n)} + \mathrm{d}\mathbf{x}_1^{(n)}\big), \ldots, X_q(t_n) \in \big(\mathbf{x}_q^{(n)}, \mathbf{x}_q^{(n)} + \mathrm{d}\mathbf{x}_q^{(n)}\big)$. For instance, if $f_2^{(2)}(\mathbf{x}_1', \mathbf{x}_2', t'; \mathbf{x}_1, \mathbf{x}_2, t)$ is the two-times joint PDF describing the random system (X_1, X_2), the two-times joint probability density of the random process X_2 alone reads

$$f_1^{(2)}(\mathbf{x}_2', t'; \mathbf{x}_2, t) = \iint f_2^{(2)}(\mathbf{x}_1', \mathbf{x}_2', t'; \mathbf{x}_1, \mathbf{x}_2, t)\mathrm{d}\mathbf{x}_1'\mathrm{d}\mathbf{x}_1,$$

where and hereafter the integration domain for each variable is $\mathbb{R}^n$ and is omitted for the sake of brevity. In other words, we can obtain the joint probability density of the assigned random processes by integrating over the other processes. Additionally, we may express the TP in the following way:

Definition 5.1. For a coupled system of random processes $(X_1(t), X_2(t))$, we denote by $p(\mathbf{x}_1', \mathbf{x}_2', t'; \mathbf{x}_1, \mathbf{x}_2, t)$ the TP of (X_1, X_2) from t' to t, which is defined by

$$p(\mathbf{x}_1', \mathbf{x}_2', t'; \mathbf{x}_1, \mathbf{x}_2, t) = \frac{f_2^{(2)}(\mathbf{x}_1', \mathbf{x}_2', t'; \mathbf{x}_1, \mathbf{x}_2, t)}{f_2^{(1)}(\mathbf{x}_1', \mathbf{x}_2', t')} = \frac{f_2^{(2)}(\mathbf{x}_1', \mathbf{x}_2', t'; \mathbf{x}_1, \mathbf{x}_2, t)}{\iint f_2^{(2)}(\mathbf{x}_1', \mathbf{x}_2', t'; \mathbf{x}_1, \mathbf{x}_2, t)\mathrm{d}\mathbf{x}_1\mathrm{d}\mathbf{x}_2}.$$

What is more, since we are considering the coupled system $(X_1(t), X_2(t))$ with *one-way dependence* (5.1) between X_1 and X_2, the joint (or transition) probability density in X_2 conditioned by X_1 is important in our discussion.

Definition 5.2. For a coupled system of random processes $(X_1(t), X_2(t))$, we denote by $f_{X_2|X_1}(x_2, t|x_1', t')$ the conditional PDF of X_2 at t given X_1 at t', which is defined by

$$f_{X_2|X_1}(\mathbf{x}_2, t|\mathbf{x}_1', t') = \frac{\iint f_2^{(2)}(\mathbf{x}_1', \mathbf{x}_2', t'; \mathbf{x}_1, \mathbf{x}_2, t)\mathrm{d}\mathbf{x}_2'\mathrm{d}\mathbf{x}_1}{f_1^{(1)}(\mathbf{x}_1', t')} \tag{5.2}$$

and when $t' = t$, we define $f_{X_2|X_1}(\mathbf{x}_2, t|\mathbf{x}_1, t)$ by

$$f_{X_2|X_1}(\mathbf{x}_2, t|\mathbf{x}_1, t) = \frac{f_2^{(1)}(\mathbf{x}_1, \mathbf{x}_2, t)}{f_1^{(1)}(\mathbf{x}_1, t)} = \frac{\iint f_2^{(2)}(\mathbf{x}_1', \mathbf{x}_2', t'; \mathbf{x}_1, \mathbf{x}_2, t)\mathrm{d}\mathbf{x}_2'\mathrm{d}\mathbf{x}_1'}{f_1^{(1)}(\mathbf{x}_1, t)}. \tag{5.3}$$

Definition 5.3. For a coupled system of random processes $(X_1(t), X_2(t))$, we denote by $p_{X_i}(\mathbf{x}_i', t'; \mathbf{x}_i, t)$ the TP of X_i from t' to t, which is defined as

$$p_{X_i}(\mathbf{x}_i', t'; \mathbf{x}_i, t) = \frac{f_1^{(2)}(\mathbf{x}_i', t'; \mathbf{x}_i, t)}{f_1^{(1)}(\mathbf{x}_i', t')}, \quad i = 1, 2. \tag{5.4}$$

Definition 5.4. For a coupled system of random processes $(X_1(t), X_2(t))$, we denote by $p_{X_2|X_1}(\mathbf{x}_2', t'; \mathbf{x}_2, t|\mathbf{x}_1', t')$ the conditional TP of X_2 from t' to t given X_1, which is defined by

$$p_{X_2|X_1}(\mathbf{x}_2', t'; \mathbf{x}_2, t|\mathbf{x}_1', t') = \int p(\mathbf{x}_1', \mathbf{x}_2', t'; \mathbf{x}_1, \mathbf{x}_2, t)\mathrm{d}\mathbf{x}_1. \tag{5.5}$$

With all the above notations, we have the following lemma, which is simply the conditional version of the CKE:

Lemma 5.5. *Given a coupled system of stochastic processes $(X(t), Y(t))$, and assume $Y(t)$ depends on $X(t)$ as*

$$\mathrm{d}Y = V(Y,t)\mathrm{d}t + \mathrm{d}X \tag{5.6}$$

where V is a smooth function in terms of both Y and t. Then the conditional PDF $f_{Y|X}(\mathbf{y},t|\mathbf{x}',t')$ and the conditional TP $p_{Y|X}(\mathbf{y}',t'\to\mathbf{y},t|\mathbf{x}',t')$ as defined in Definitions 5.2 and 5.4 satisfy

$$\int p_{Y|X}(\mathbf{y}',t';\mathbf{y},t|\mathbf{x}',t')f_{Y|X}(\mathbf{y}',t'|\mathbf{x}',t')\mathrm{d}\mathbf{y}' = f_{Y|X}(\mathbf{y},t|\mathbf{x}',t'). \tag{5.7}$$

Proof. By Definitions 5.1–5.4, we have,

$$\begin{aligned}\mathrm{LHS} &= \int \frac{\int f_2^{(2)}(\mathbf{x}',\mathbf{y}',t';\mathbf{x},\mathbf{y},t)\mathrm{d}\mathbf{x}}{f_2^{(1)}(\mathbf{x}',\mathbf{y}',t')}\cdot\frac{f_2^{(1)}(\mathbf{x}',\mathbf{y}',t')}{f_1^{(1)}(\mathbf{x}',t')}\,\mathrm{d}\mathbf{y}'\\ &= \frac{1}{f_1^{(1)}(\mathbf{x}',t')}\iint f_2^{(2)}(\mathbf{x}',\mathbf{y}',t';\mathbf{x},\mathbf{y},t)\mathrm{d}\mathbf{y}'\mathrm{d}\mathbf{x} = f_{Y|X}(\mathbf{y},t|\mathbf{x}',t') = \mathrm{RHS}\end{aligned}$$

which implies the conditional version of the CKE. □

To make our notation simple without inducing any ambiguity, from now on we will drop off the subscript and superscript from joint probability density $f_q^{(n)}$. For instance

- $f(\mathbf{x},\mathbf{y},t)$ represents the one-time joint probability density in two random processes X and Y;
- $f(\mathbf{x}',\mathbf{y}',t';\mathbf{x},\mathbf{y},t)$ represents the two-times joint PDF in two random processes X and Y;
- $f(\mathbf{x}',\mathbf{y}',t';\mathbf{y},t)$ is defined by $f(\mathbf{x}',t';\mathbf{y},t) = \iint f_2^{(2)}(\mathbf{x}',\mathbf{y}',t';\mathbf{x},\mathbf{y},t)\mathrm{d}\mathbf{y}'\mathrm{d}\mathbf{x}$.

For a coupled system of random processes $(X(t), Y(t))$ satisfying the *one-way dependence* (5.6), the conservation law reads

$$\int_{\Omega_X\times\Omega_Y}\Big[f(\mathbf{x},\mathbf{y},t) - f(\mathbf{x},\mathbf{y},t')\Big]\,\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y} = \mathcal{F}(\Omega_X\times\Omega_Y,t',t), \tag{5.8}$$

where the flux $\mathcal{F}(\Omega_X\times\Omega_Y,t',t)$ is defined as:

$$\mathcal{F}(\Omega_X\times\Omega_Y,t',t) = \int_{\Omega_X\times\Omega_Y}\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y}\int_{\mathbb{R}_X^m\times\mathbb{R}_Y^n}\mathrm{d}\mathbf{x}'\mathrm{d}\mathbf{y}'\Big[p(\mathbf{x}',\mathbf{y}',t';\mathbf{x},\mathbf{y},t)f(\mathbf{x}',\mathbf{y}',t') - p(\mathbf{x},\mathbf{y},t';\mathbf{x}',\mathbf{y}',t)f(\mathbf{x},\mathbf{y},t')\Big]. \tag{5.9}$$

Notice that we use subscripts X, Y in $\mathbb{R}^m$, $\mathbb{R}^n$ to associate the integral variable with the integral domain. For the same purpose, we sometimes put the differentials together with the integral signs in order to indicate the correspondence between the integral variable and integral domain.

Now let us introduce the main theorem which we will apply onto two examples in the next sections.

Theorem 5.6. *Given a coupled system of stochastic processes $(X(t), Y(t))$. Assume $Y(t)$ depends on $X(t)$ by (5.6), and the TP $p(\mathbf{x}',\mathbf{y}',t';\mathbf{x},\mathbf{y},t)$ satisfies*

$$p(\mathbf{x}',\mathbf{y}',t';\mathbf{x},\mathbf{y},t) = p_X(\mathbf{x}',t';\mathbf{x},t)\cdot p_{Y|X}(\mathbf{y}',t';\mathbf{y},t|\mathbf{x}',t') \tag{5.10}$$

then the net flux $\mathcal{F}(\Omega_X\times\Omega_Y,t',t)$ can be simplified as

$$\mathcal{F}(\Omega_X\times\Omega_Y,t',t) = \int_{\Omega_Y}\mathcal{F}_X(\Omega_X,\mathbf{y},t',t)\,\mathrm{d}\mathbf{y} + \int_{\Omega_X}\mathcal{F}_Y(\Omega_Y,\mathbf{x},t',t)\,\mathrm{d}\mathbf{x}. \tag{5.11}$$

Here the nonlocal fluxes $\mathcal{F}_X(\Omega_X,\mathbf{y},t',t)$ and $\mathcal{F}_Y(\Omega_Y,\mathbf{x},t',t)$ are constructed as follows

$$\begin{aligned}\mathcal{F}_X(\Omega_X,\mathbf{y},t',t) &= \int_{\Omega_X}\mathrm{d}\mathbf{x}\int_{\mathbb{R}_X^m}\mathrm{d}\mathbf{x}'\Big[p_X(\mathbf{x}',t';\mathbf{x},t)f(\mathbf{x}',t';\mathbf{y},t) - p_X(\mathbf{x},t';\mathbf{x}',t)f(\mathbf{x},t';\mathbf{y},t)\Big],\\ \mathcal{F}_Y(\Omega_Y,\mathbf{x},t',t) &= \int_{\Omega_Y}\mathrm{d}\mathbf{y}\int_{\mathbb{R}_Y^n}\mathrm{d}\mathbf{y}'\Big[p_{Y|X}(\mathbf{y}',t';\mathbf{y},t|\mathbf{x},t')f(\mathbf{x},\mathbf{y}',t') - p_{Y|X}(\mathbf{y},t';\mathbf{y}',t|\mathbf{x},t')f(\mathbf{x},\mathbf{y},t')\Big].\end{aligned}$$

One may check that the properties given in Section 4.1 are satisfied. Furthermore, we have the pointwise master equation for the coupled system as

$$\begin{aligned}f(\mathbf{x},\mathbf{y},t) - f(\mathbf{x},\mathbf{y},t') &= \int_{\mathbb{R}_X^m}\Big[p_X(\mathbf{x}',t';\mathbf{x},t)f(\mathbf{x}',t';\mathbf{y},t) - p_X(\mathbf{x},t';\mathbf{x}',t)f(\mathbf{x},t';\mathbf{y},t)\Big]\mathrm{d}\mathbf{x}'\\ &\quad + \int_{\mathbb{R}_Y^n}\Big[p_{Y|X}(\mathbf{y}',t';\mathbf{y},t|x,t')f(\mathbf{x},\mathbf{y}',t') - p_{Y|X}(\mathbf{y},t';\mathbf{y}',t|\mathbf{x},t')f(\mathbf{x},\mathbf{y},t')\Big]\mathrm{d}\mathbf{y}'\end{aligned} \tag{5.12}$$

or in the differential form

$$f_t(\mathbf{x},\mathbf{y},t) = \lim_{\Delta t\to 0}\frac{1}{\Delta t}\int_{\mathbb{R}_X^m}\Big[p_X(\mathbf{x}',t';\mathbf{x},t)f(\mathbf{x}',\mathbf{y},t') - p_X(\mathbf{x},t';\mathbf{x}',t)f(\mathbf{x},\mathbf{y},t')\Big]\mathrm{d}\mathbf{x}' + \lim_{\Delta t\to 0}\frac{1}{\Delta t}\int_{\mathbb{R}_Y^n}\Big[p_{Y|X}(\mathbf{y}',t';\mathbf{y},t|\mathbf{x},t')f(\mathbf{x},\mathbf{y}',t') - p_{Y|X}(\mathbf{y},t';\mathbf{y}',t|\mathbf{x},t')f(\mathbf{x},\mathbf{y},t')\Big]\mathrm{d}\mathbf{y}'.$$

Proof. By adding and subtracting one term to Eq. (5.9), we have

$$\begin{aligned}&\mathcal{F}(\Omega_X\times\Omega_Y,t',t)\\ &= \int_{\Omega_X\times\Omega_Y}\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y}\int_{\mathbb{R}_X^m\times\mathbb{R}_Y^n}\mathrm{d}\mathbf{x}'\mathrm{d}\mathbf{y}'\Big[p(\mathbf{x}',\mathbf{y}',t';\mathbf{x},\mathbf{y},t)f(\mathbf{x}',\mathbf{y}',t') - p(\mathbf{x},\mathbf{y}',t';\mathbf{x}',\mathbf{y},t)f(\mathbf{x},\mathbf{y}',t')\Big]\\ &\quad+\Big[p(\mathbf{x},\mathbf{y}',t';\mathbf{x}',\mathbf{y},t)f(\mathbf{x},\mathbf{y}',t') - p(\mathbf{x},\mathbf{y},t';\mathbf{x}',\mathbf{y}',t)f(\mathbf{x},\mathbf{y},t')\Big]\\ &= \mathrm{I}+\mathrm{II}.\end{aligned}$$

For the part I, we apply Eq. (5.10) and Lemma 5.5,

$$\begin{aligned}\mathrm{I} &= \int_{\Omega_Y}\mathrm{d}\mathbf{y}\iint_{\Omega_X\times\mathbb{R}_X^m}\mathrm{d}\mathbf{x}'\mathrm{d}\mathbf{x}\int_{\mathbb{R}_Y^n}\mathrm{d}\mathbf{y}'\Big[p_X(\mathbf{x}',t';\mathbf{x},t)p_{Y|X}(\mathbf{y}',t';\mathbf{y},t|\mathbf{x}',t')f_X(\mathbf{x}',t')f_{Y|X}(\mathbf{y}',t'|\mathbf{x}',t')\\ &\quad- p_X(\mathbf{x},t';\mathbf{x}',t)p_{Y|X}(\mathbf{y}',t';\mathbf{y},t|\mathbf{x},t')f_X(\mathbf{x},t')f_{Y|X}(\mathbf{y}',t'|\mathbf{x},t')\Big]\\ &= \int_{\Omega_Y}\mathrm{d}\mathbf{y}\iint_{\Omega_X\times\mathbb{R}_X^m}\mathrm{d}\mathbf{x}'\mathrm{d}\mathbf{x}\Big[p_X(\mathbf{x}',t';\mathbf{x},t)f_X(\mathbf{x}',t')\int_{\mathbb{R}_Y^n}p_{Y|X}(\mathbf{y}',t';\mathbf{y},t|\mathbf{x}',t')f_{Y|X}(\mathbf{y}',t'|\mathbf{x}',t')\mathrm{d}\mathbf{y}'\\ &\quad- p_X(\mathbf{x},t';\mathbf{x}',t)f_X(\mathbf{x},t')\int_{\mathbb{R}_Y^n}p_{Y|X}(\mathbf{y}',t',\mathbf{y},t|\mathbf{x},t')f_{Y|X}(\mathbf{y}',t'|\mathbf{x},t')\mathrm{d}\mathbf{y}'\Big]\\ &= \int_{\Omega_Y}\mathrm{d}\mathbf{y}\iint_{\Omega_X\times\mathbb{R}_X^m}\mathrm{d}\mathbf{x}'\mathrm{d}\mathbf{x}\Big[p_X(\mathbf{x}',t';\mathbf{x},t)f_X(\mathbf{x}',t')f_{Y|X}(\mathbf{y},t|\mathbf{x}',t')\\ &\quad- p_X(\mathbf{x},t';\mathbf{x}',t)f_X(\mathbf{x},t')f_{Y|X}(\mathbf{y},t|\mathbf{x},t')\Big]\\ &= \int_{\Omega_Y}\mathrm{d}\mathbf{y}\iint_{\Omega_X\times\mathbb{R}_X^m}\mathrm{d}\mathbf{x}'\mathrm{d}\mathbf{x}\Big[p_X(\mathbf{x}',t';\mathbf{x},t)f(\mathbf{x}',t';\mathbf{y},t) - p_X(\mathbf{x},t';\mathbf{x}',t)f(\mathbf{x},t';\mathbf{y},t)\Big]\\ &= \int_{\Omega_Y}\mathcal{F}_X(\Omega_X,\mathbf{y},t',t)\,\mathrm{d}\mathbf{y}.\end{aligned}$$

Part II is easier,

$$\begin{aligned}\mathrm{II} &= \int_{\Omega_X}\mathrm{d}\mathbf{x}\iint_{\Omega_Y\times\mathbb{R}_Y^n}\mathrm{d}\mathbf{y}'\mathrm{d}\mathbf{y}\int_{\mathbb{R}_X^m}\mathrm{d}\mathbf{x}'\Big[p(\mathbf{x},\mathbf{y}',t';\mathbf{x}',\mathbf{y},t)f(\mathbf{x},\mathbf{y}',t') - p(\mathbf{x},\mathbf{y},t';\mathbf{x}',\mathbf{y}',t)f(\mathbf{x},\mathbf{y},t')\Big]\\ &= \int_{\Omega_X}\mathrm{d}\mathbf{x}\iint_{\Omega_Y\times\mathbb{R}_Y^n}\mathrm{d}\mathbf{y}'\mathrm{d}\mathbf{y}\Big[f(\mathbf{x},\mathbf{y}',t')\int_{\mathbb{R}_X^m}p(\mathbf{x},\mathbf{y}',t';\mathbf{x}',\mathbf{y},t)\mathrm{d}\mathbf{x}' - f(\mathbf{x},\mathbf{y},t')\int_{\mathbb{R}_X^m}p(\mathbf{x},\mathbf{y},t';\mathbf{x}',\mathbf{y}',t)\mathrm{d}\mathbf{x}'\Big]\\ &= \int_{\Omega_X}\mathrm{d}\mathbf{x}\iint_{\Omega_Y\times\mathbb{R}_Y^n}\mathrm{d}\mathbf{y}'\mathrm{d}\mathbf{y}\Big[p_{Y|X}(\mathbf{y}',t';\mathbf{y},t|\mathbf{x},t')f(\mathbf{x},\mathbf{y}',t') - p_{Y|X}(\mathbf{y},t';\mathbf{y}',t|\mathbf{x},t')f(\mathbf{x},\mathbf{y},t')\Big]\\ &= \int_{\Omega_X}\mathcal{F}_Y(\Omega_Y,\mathbf{x},t',t)\,\mathrm{d}\mathbf{x}.\end{aligned}$$

The master equation (5.12) is a direct consequence from the form (5.11). Notice that when $\Delta t\to 0$, we have

$$f(\mathbf{x},t',\mathbf{y},t)\to f(\mathbf{x},\mathbf{y},t') = f(\mathbf{x},\mathbf{y},t),$$

hence the master equation in differential form holds as well. □

5.2. Spatially inhomogeneous coagulation equation

Consider an inhomogeneous coagulation process:

$$Z_t = \begin{pmatrix}X_t\\ S_t\end{pmatrix}, \tag{5.13}$$

where S_t represents a stochastic coagulation process, and X_t describes a stochastic particle motion in $\mathbb{R}^n$ satisfying the Fokker–Planck dynamics:

$$\mathrm{d}X_t = V(X,t)\mathrm{d}t + \sqrt{2\sigma}\mathrm{d}W_t,$$

and the PDF is $f(\mathbf{x},s,t)$. In this coupled system, the coagulation process S_t depends on the particle motion X_t through the coagulation kernel $\beta = \beta(s,s',\mathbf{x})$. The TP of the inhomogeneous coagulation process Z is given by:

$$p(\mathbf{x}',s',t';\mathbf{x},s,t) = p_X(\mathbf{x}',t';\mathbf{x},t)\cdot p_{S|X}(s',t';s,t|\mathbf{x}',t'), \tag{5.14}$$

where $p_X(\mathbf{x}',t';\mathbf{x},t)$ represents the transition probability of the particle motion in $\mathbb{R}^n$, and $p_{S|X}(s',t';s,t|\mathbf{x}',t')$ represents the coagulation probability from (s',t') to (s,t) at position $\mathbf{x}'$, and reads

$$p_{S|X}(s',t';s,t|\mathbf{x}',t') = \begin{cases} \dfrac{\Delta t}{s-s'}\beta(s',s-s',\mathbf{x}')f(\mathbf{x}',s-s',t'), & s'<s,\\ 1-\Delta t\displaystyle\int_0^\infty \frac{1}{\hat{s}}\beta(s',\hat{s};\mathbf{x}',t')f(\mathbf{x}',\hat{s},t')\mathrm{d}\hat{s}, & s'=s,\\ 0, & s'>s. \end{cases} \tag{5.15}$$

Now we can derive the spatially inhomogeneous coagulation equation. First of all, Eq. (2.6) implies

$$\begin{aligned}&\lim_{\Delta t\to 0}\frac{1}{\Delta t}\int_{\mathbb{R}_X^m}\Big[p_X(\mathbf{x}',t';\mathbf{x},t)f(\mathbf{x}',s,t') - p_X(\mathbf{x},t';\mathbf{x}',t)f(\mathbf{x},s,t')\Big]\,\mathrm{d}\mathbf{x}'\\ &\quad = -\nabla_{\mathbf{x}}\cdot\Big(v(\mathbf{x},t)f(\mathbf{x},s,t)\Big) + \sigma\,\Delta_{\mathbf{x}}f(\mathbf{x},s,t).\end{aligned}$$

Similar as the derivation for the homogeneous coagulation equation in Section 3.1, we have

$$\begin{aligned}&\lim_{\Delta t\to 0}\frac{1}{\Delta t}\int_{\mathbb{R}_S}\Big[p_{S|X}(s',t';s,t|\mathbf{x},t')f(\mathbf{x},s',t') - p_{S|X}(s,t';s',t)f(\mathbf{x},s,t')\Big]\,\mathrm{d}s'\\ &\quad = \frac{s}{2}\int_0^s \beta(s',s-s',\mathbf{x})\frac{f(\mathbf{x},s',t)}{s'}\frac{f(\mathbf{x},s-s',t)}{s-s'}\mathrm{d}s' - \int_0^\infty \frac{\beta(s,s',\mathbf{x})}{s'}f(\mathbf{x},s,t)f(\mathbf{x},s',t)\mathrm{d}s'.\end{aligned}$$

Apply Theorem 5.6 and the relation $N(\mathbf{x},s,t) = f(\mathbf{x},s,t)/s$, we finally have the spatially inhomogeneous coagulation equation,

$$\begin{aligned}N_t(\mathbf{x},s,t) =& \frac{1}{2}\int_0^s \beta(s',s-s',\mathbf{x})N(\mathbf{x},s',t)N(\mathbf{x},s-s',t)\mathrm{d}s' - \int_0^\infty \beta(s,s',\mathbf{x})N(\mathbf{x},s',t)N(\mathbf{x},s,t)\mathrm{d}s'\\ &- \nabla_{\mathbf{x}}\cdot(v(\mathbf{x},t)N(\mathbf{x},s,t)) + \sigma\,\Delta_{\mathbf{x}}N(\mathbf{x},s,t).\end{aligned} \tag{5.16}$$

5.3. Dynamics in randomly varying environments

The stochastic processes in the examples we study previously are all Lévy processes, which means $\mathrm{d}X_t$ is independent of increment and stationary. In this section, we will study some non-Lévy processes in $\mathbb{R}^n$. For instance, if $\mathrm{d}X_t/\mathrm{d}t = R_t$, where R_t is a Markov process, then X_t is not Lévy process because $\mathrm{d}X_t$ does depend on different time t. In this case, we need to introduce a new state variable for R_t so that we can derive its evolution equation more conveniently by studying the coupled dynamical system. For example, a stochastic model is proposed in [33] to study gene regulation in a stochastically changing environment. This model is formulated by a differential equation driven by a continuous time two-state Markov process. The system is written as

$$\frac{\mathrm{d}X_t}{\mathrm{d}t} + \mu X_t = R_t, \tag{5.17}$$

where X_t is the expression level, μ is the degradation rate and R_t is a Markov process with two states $\mathbf{r}_0, \mathbf{r}_1 \in \mathbb{R}^n$ which represents the environmental inputs. The authors write the density function as the sum of two marginal density functions which corresponds to two states $\mathbf{r}_0$ and $\mathbf{r}_1$ respectively.

Actually we can study for a more general system. Mathematically, we assume the system is governed by the equation

$$\mathrm{d}X_t = \mu_1(X_t,t)\mathrm{d}t + \mu_2(X_t,t)\mathrm{d}W_t + \mu_3(X_t,t)\mathrm{d}Z_t + \mu_4(X_t,t)R_t\mathrm{d}t, \tag{5.18}$$

where W_t is a Brownian motion and Z_t is a CTRW. R_t is a continuous time, continuous state, and time homogeneous Markov jump process with exponential waiting time between jumps. We assume R_t is independent of X_t. Furthermore, we also assume the transition rate $\varphi(\mathbf{r}';\mathbf{r})$ from state $\mathbf{r}'$ to $\mathbf{r}$ exists, i.e.:

$$\varphi(\mathbf{r}';\mathbf{r}) = \lim_{\Delta t\to 0}\frac{p_R(\mathbf{r}',t';\mathbf{r},t)}{\Delta t}. \tag{5.19}$$

In the present paper, we only consider the simple case that X_t follows

$$\frac{\mathrm{d}X_t}{\mathrm{d}t} = \mu(X_t, t) + R_t \tag{5.20}$$

and denote by $f(\mathbf{r}, \mathbf{x}, t)$ the PDF for this system. The joint TP for this coupled system (X_t, R_t) is

$$\begin{aligned} p(\mathbf{x}', \mathbf{r}', t'; \mathbf{x}, \mathbf{r}, t) &= p_R(\mathbf{r}', t'; \mathbf{r}, t) p_{X|R}(\mathbf{x}', t'; \mathbf{x}, t|\mathbf{r}', t') \\ &= p_R(\mathbf{r}', t'; \mathbf{r}, t)\delta\Big(\mathbf{x} - \mathbf{x}' - \boldsymbol{\mu}(\mathbf{x}', t')\triangle t - \mathbf{r}'\triangle t\Big) \\ &= p_R(\mathbf{r}', t'; \mathbf{r}, t)\frac{\delta(\mathbf{x}' - \mathbf{x}_0)}{1 + \nabla_{\mathbf{x}} \cdot \boldsymbol{\mu}(\mathbf{x}_0, t')\triangle t} \end{aligned} \tag{5.21}$$

where $\mathbf{x}_0$ is the root of $g(\mathbf{x}') = \mathbf{x} - \mathbf{x}' - \boldsymbol{\mu}(\mathbf{x}', t')\triangle t - \mathbf{r}\triangle t = 0$ for small time step $\triangle t = t - t'$. And $\mathbf{x}_0$ approaches $\mathbf{x}$ as $\triangle t$ converges to 0. Then we have

$$\begin{aligned} &\lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_{\mathbb{R}^m} \Big[p_R(\mathbf{r}', t'; \mathbf{r}, t) f(\mathbf{r}', \mathbf{x}, t') - p_R(\mathbf{r}, t'; \mathbf{r}', t) f(\mathbf{r}, \mathbf{x}, t')\Big]\, \mathrm{d}\mathbf{r}' \\ &= \int_{\mathbb{R}^m} \Big[\phi(\mathbf{r}'; \mathbf{r}) f(\mathbf{r}', \mathbf{x}, t') - \phi(\mathbf{r}'; \mathbf{r}) f(\mathbf{r}, \mathbf{x}, t')\Big]\, \mathrm{d}\mathbf{r}' \end{aligned} \tag{5.22}$$

due to the assumption (5.19). Furthermore,

$$\begin{aligned} &\lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_{\mathbb{R}^n} \Big[p_{X|R}(\mathbf{x}', t'; \mathbf{x}, t|\mathbf{r}, t') f(\mathbf{r}, \mathbf{x}', t') - p_{X|R}(\mathbf{x}, t'; \mathbf{x}', t|\mathbf{r}, t') f(\mathbf{r}, \mathbf{x}, t')\Big] \mathrm{d}\mathbf{x}' \\ &= \lim_{\Delta t \to 0} \frac{1}{\Delta t} \left(\frac{f(\mathbf{r}, \mathbf{x}_0, t')}{1 + \nabla_{\mathbf{x}} \cdot \boldsymbol{\mu}(\mathbf{x}_0, t')\Delta t} - f(\mathbf{r}, \mathbf{x}, t')\right) \\ &= -f(\mathbf{r}, \mathbf{x}, t)\nabla_{\mathbf{x}} \cdot \boldsymbol{\mu}(\mathbf{x}, t) - \nabla_{\mathbf{x}} f(\mathbf{r}, \mathbf{x}, t) \cdot \Big(\boldsymbol{\mu}(\mathbf{x}, t) + \mathbf{r}\Big) \\ &= -\nabla_{\mathbf{x}} \cdot \Big(\big[\mathbf{r} + \boldsymbol{\mu}(\mathbf{x}, t)\big] f(\mathbf{r}, \mathbf{x}, t)\Big) \end{aligned} \tag{5.23}$$

where the Taylor expansion for $f(\mathbf{r}, \mathbf{x}_0, t')$ around $\mathbf{x}$ is applied on the second equality.

According to Theorem 5.6, we can combine Eqs. (5.22) and (5.23) and obtain the density equation

$$f_t + \nabla_{\mathbf{x}} \cdot ((\mathbf{r} + \boldsymbol{\mu}) f) = \int_{\mathbf{r}' \in \mathbb{R}^m} \big(\varphi(\mathbf{r}|\mathbf{r}') f(\mathbf{r}', \mathbf{x}, t) - \varphi(\mathbf{r}'|\mathbf{r}) f(\mathbf{r}, \mathbf{x}, t)\big)\, \mathrm{d}\mathbf{r}'. \tag{5.24}$$

Now let us consider the discrete case. Assume R_t is a finite states Markov process with n states $\{\mathbf{r}_i\}_{i=1}^n$. Denote the Q-matrix, i.e., infinitesimal generator by Q and the transition probability matrix by $P(t)$. $P_{\mathbf{r}'\mathbf{r}}(t)$ represents the TP from state $\mathbf{r}'$ to $\mathbf{r}$ within transition time t. By the fundamental knowledge of continuous time Markov process, we know $P'(t) = P(t)Q$ and

$$q_{\mathbf{r}} = \lim_{t \to 0} \frac{1 - P_{\mathbf{r}\mathbf{r}}(t)}{t}, \qquad q_{\mathbf{r}'\mathbf{r}} = \lim_{t \to 0} \frac{P_{\mathbf{r}'\mathbf{r}}(t)}{t},$$

where $q_{\mathbf{r}} = -Q_{\mathbf{r}\mathbf{r}}$ represents the transition rate from state $\mathbf{r}$ to $\mathbf{r}$, and $q_{r'r} = Q_{r'r}$ represents the transition rate from state $\mathbf{r}'$ to $\mathbf{r}$. Similarly we have the evolution equation:

$$f_t(\mathbf{r}, \mathbf{x}, t) + \nabla_{\mathbf{x}} \cdot \Big(\big[\mathbf{r} + \boldsymbol{\mu}(\mathbf{x}, t)\big] f(\mathbf{r}, \mathbf{x}, t)\Big) = -q_{\mathbf{r}} f(\mathbf{r}, \mathbf{x}, t) + \sum_{\mathbf{r}' \neq \mathbf{r}} q_{\mathbf{r}'\mathbf{r}} f(\mathbf{r}', \mathbf{x}, t). \tag{5.25}$$

If the drift term $\boldsymbol{\mu}(x, t) = -\mu\mathbf{x}$ as in [33] and the Markov process only has two states $\mathbf{r}_0, \mathbf{r}_1$, and the infinitesimal generator is given by

$$\begin{pmatrix} -\lambda_0 & \lambda_0 \\ \lambda_1 & -\lambda_1 \end{pmatrix},$$

then we reproduce the PDEs as in [33]:

$$\begin{aligned} f_t(\mathbf{r}_0, \mathbf{x}, t) + \nabla_{\mathbf{x}} \cdot [(\mathbf{r}_0 - \mu\mathbf{x}) f(\mathbf{r}_0, \mathbf{x}, t)] &= -\lambda_0 f(\mathbf{r}_0, \mathbf{x}, t) + \lambda_1 f(\mathbf{r}_1, \mathbf{x}, t), \\ f_t(\mathbf{r}_1, \mathbf{x}, t) + \nabla_{\mathbf{x}} \cdot [(\mathbf{r}_1 - \mu\mathbf{x}) f(\mathbf{r}_1, \mathbf{x}, t)] &= -\lambda_1 f(\mathbf{r}_1, \mathbf{x}, t) + \lambda_0 f(\mathbf{r}_0, \mathbf{x}, t). \end{aligned}$$

6. Summary

In this paper, we presented some generalized local and nonlocal master equations for various stochastic processes. We illustrated the applications of this framework to both classical cases such as Fokker–Planck equations and Lévy process, as well as nonlocal models such as stochastic coagulation equation. The formalism can be viewed as one of the examples of the recently developed nonlocal vector calculus. Most importantly, Theorem 5.6 arising from our study for the coupled system of stochastic processes has been proved and applied to spatially inhomogeneous coagulation processes and some dynamics in randomly varying environments. Our work has been limited to processes defined in the entire space. It is natural to consider the effect of the bounded domain as in the case of [32,6]. Extensions to non-Markovian processes are also possible and these interesting topics will be studied in the future.

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