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Feynman–Kac equation for Brownian non-Gaussian polymer diffusion

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Abstract

The motion of the polymer center of mass (CM) is driven by two stochastic terms that are Gaussian white noise generated by standard thermal stirring and chain polymerization processes, respectively. It can be described by the Langevin equation and is Brownian non-Gaussian by calculating the kurtosis. We derive the forward Fokker–Planck equation governing the joint distribution of the motion of CM and the chain polymerization process. The backward Fokker–Planck equation governing only the probability density function (PDF) of CM position for a given number of monomers is also derived. We derive the forward and backward Feynman–Kac equations for the functional distribution of the motion of the CM, respectively, and present some of their applications, which are validated by a deep learning method based on backward stochastic differential equations (BSDEs), i.e. the deep BSDE method.

Keywords: polymer, Brownian non-Gaussian, Fokker–Planck equation, Feynman–Kac equation, deep BSDE method

1. Introduction

A growing number of researchers are interested in Brownian non-Gaussian diffusion [1]. The mean squared displacement (MSD) of this type of diffusion shows a linear dependence on time t, but the PDF of the diffusion particle is strongly non-Gaussian [2]. Under the assumption of a large separation of timescales, the central limit theorem states that the distribution of the Fickian diffusion particle is Gaussian form for sufficient long time; however, it does

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not hold without this assumption [3]. The processes of Brownian non-Gaussian diffusion are ubiquitously observed in many complex systems. For example, in biology, it can be found in the process of lipid molecules or proteins embedded in into protein-dense lipid membranes [4, 5], biological cells [6–10], and anisotropic liquid crystals [11]. The authors have shown that the diffusion of passive tracers in thin films of swimming bacteria [12], in suspensions of flagellated eukaryotes [13] as well as in phospholipid tubes [3] is Brownian non-Gaussian by using numerical simulations. For more examples, one can see [14, 15]. In addition, [16–18] state that the motion of the center of mass (CM) of the polymer is Brownian non-Gaussian.

In this paper, we focus on the transport properties of the Brownian non-Gaussian diffusion process. There are two popular frameworks to describe diffusion from microscopic aspects, namely the random walk and the Langevin equation [19, 20]. Based on the random walk theory, the continuous time random walk (CTRW) [21-23] and the Lévy walk [24] are two representative models to describe anomalous diffusion. The Montroll-Weiss equation the CTRW model is derived by the traditional methods of Fourier and/or Laplace transforms. Combined with the concrete expressions of the waiting time and jump length distributions, the corresponding fractional Fokker–Planck equation [25-27] can be obtained, which is further used to analyze the transport properties of the stochastic dynamics. However, the fractional Fokker-Planck equation of the Lévy walk is not easy to solve due to its space-time coupled jump length by finite propagation velocity [24]. Hermite polynomial expansions [28] are introduced in [29] to solve this kind of problem. By this method, [30-32] respectively discuss the dynamics of Lévy walk in harmonic potential field, in mixed potential as well as in one dimensional uniform non-static media. The Langevin picture is usually used to describe diffusion under the action of external potential or noise induced by the fluctuating environment [33]. The ordinary Fokker–Planck equation and the spatial fractional Fokker–Planck equation [34–39] are respectively derived from the Langevin equation with Gaussian white noise and heavy-tailed stable noise, respectively. In addition, the effects of constant external force on the Lévy walk are also discussed under the Langevin picture in [40].

The functional of the diffusion particle trajectory x(t) is defined as $Y = \int_0^t U(x(\tau)) d\tau$, where U(x) is a prescribed function [41]. This type of functional is observed in many fields, ranging from physics [42–44] to finance [45, 46], hydrodynamics [47], etc. The equation governing the joint distribution of displacement and functional is called the forward Feynman-Kac equation, while the equation focusing only on the distribution of the functional Y is called the backward Feynman-Kac equation. The classical Feynman-Kac equation for Brownian motion was derived by Kac in 1949 in [48]. Later, the fractional Feynman–Kac equation for subdiffusion CTRW [49] is developed based on random walk theory. More and more Feynman-Kac equations are derived through this theoretical framework [50-54]. Furthermore, the forward Feynman-Kac equation under the Langevin picture with Gaussian white noise is derived using the Itô formula [55, 56]. For the more general overdamped Langevin equation with Lévy noise, [57] derives the corresponding Feynman–Kac equation. The Feynman–Kac equation has many applications, especially in calculating the distribution of statistical observables, since the statistical observables are closely related to the functionals. For example, the distribution of time spent in a given domain can be calculated by taking U(x) = 1 in the domain considered and U(x) = 0 otherwise [58, 59]. The above results can be further used to study the chemical reactions in kinetic as well as to obtain the first passage time [60]. Another representative application of functional distribution is presented in the study of NMR experiment [61].

In this paper, we aim to derive the Fokker–Planck equation and the Feynman–Kac equation of the polymer CM diffusion process described by the Langevin picture with Gaussian white noise. However, the diffusion coefficient is stochastic, determined by the chain polymerization process [62], which occurs as a birth-death process. This paper is organized as follows. In

section 2, we introduce the process of polymer CM diffusion. In section 3, we turn to the derivation of the Fokker–Planck equation of our considered model with the help of the Feynman– Kac equation of the chain polymerization process. The Feynman–Kac equation of the polymer CM position functional is discussed in section 4, and its applications are analyzed in sections 5 and 6 by deep BSDE method combined with Monte Carlo simulation. Finally, we conclude the paper with some discussions.

2. Introduction of the model

As stated in [18], the motion of polymer CM is Brownian non-Gaussian during the process of monomer polymerization/depolymerization. The microscopic equation corresponding to this model can be described by the following Langevin picture

$$dr(t) = \sqrt{2D(n(t))}dB(t), \qquad (1)$$

where r(t) represents the position of the polymer CM at time t, and n(t) represents the chain polymerization process and counts the number of monomers in the polymer. Notably, it is a stochastic process with a non-negative integer value. B(t) is a one-dimensional Brownian motion with mean 0 and variance t. The ordinary diffusion equation of the CM position is derived in [18] with the diffusion coefficient D(n), which is the chain polymerization process in the form of $\frac{D_0}{(n+n_{\min})^{\alpha}}$, where D_0 and α are given for the chosen polymer model [63, 64] and the minimum number of monomers in the polymer is recorded as n_{\min} [65].

The following is a brief introduction to the chain polymerization process n(t). Assume that the initial number of monomers in the polymer is n_0 , and $\lambda(n)$ is the association rate, which depends on the number of monomers n, while μ is the size independent dissociation rate. By changing the variable $n \mapsto n - n_{\min}$, [18, 66] derive the master equation governing the probability distribution of the chain polymerization process $P_N(n,t|n_0)$,

$$\begin{cases} \partial_t P_N(n,t|n_0) = \mu P_N(n+1,t|n_0) + \lambda(n-1)P_N(n-1,t|n_0) & n > 0, \\ -(\mu + \lambda(n))P_N(n,t|n_0), & n > 0, \\ \partial_t P_N(n,t|n_0) = \mu P_N(n+1,t|n_0) - \lambda(0)P_N(n,t|n_0), & n = 0. \end{cases}$$
(2)

The Monte Carlo simulations of $P_N(n,t|n_0)$ are shown on the left side of figure 1. In addition, [18] implies that a stationary distribution $P_N^*(n)$ can eventually be reached after sufficiently long time.

It is well known that the increment of Brownian motion is stationary and independent. Combined with its $\frac{1}{2}$ self-similarity, (1) can be rewritten in the following form

$$r(t) = B(s(t)), \qquad s(t) = \int_0^t 2D(n(\tau)) d\tau.$$
 (3)

Let G(r,s) be the PDF of the polymer CM position r the new 'time' scale s. According to the ordinary diffusion equation of Brownian motion, it has the form

$$\frac{\partial}{\partial s}G(r,s) = \frac{1}{2}\frac{\partial^2}{\partial r^2}G(r,s).$$
(4)



Figure 1. Numerical simulations of the distribution of the chain polymerization process $P_N(n,t|n_0)$ as well as the distribution of polymer CM position u(r,t). The above results are obtained by averaging over 10^4 realizations with $n_0 = 0$, $\alpha = 1$, $n_{\min} = 3$, $t = 10^3$ and $D_0 = \lambda = \mu = 1$.

Let u(r,t) be the PDF of the CM position r at real time t and S(s,t) the PDF of the stochastic process s(t). By the subordination theory [67] we get

$$u(r,t) = \int_0^\infty S(s,t) G(r,s) \,\mathrm{d}s. \tag{5}$$

Numerical simulations of the distribution of the polymer CM position u(r,t) are shown on the right side of figure 1. In addition, the asymptotic expression of the MSD in large time scale can be derived using (5). Starting with the definition of MSD and combining it with (5), we have

$$\langle r^{2}(t) \rangle = \left\langle \int_{0}^{t} \frac{2D_{0}}{(n(\tau) + n_{\min})^{\alpha}} d\tau \right\rangle$$

=
$$\sum_{n=0}^{\infty} \frac{2D_{0}}{(n + n_{\min})^{\alpha}} \int_{0}^{t} P_{N}(n, \tau | n_{0}) d\tau.$$
 (6)

For large time $t \gg t'$, a steady state can eventually be reached for the chain polymerization process; it holds that $P_N(n,t|n_0) \simeq P_N^*(n)$. By neglecting the lower order term of large time scale *t*, the MSD behaves as

$$\langle r^{2}(t) \rangle = \sum_{n=0}^{\infty} \frac{2D_{0}}{(n+n_{\min})^{\alpha}} \left(\int_{0}^{t'} P_{N}(n,\tau|n_{0}) \,\mathrm{d}\tau + \int_{t'}^{t} P_{N}(n,\tau|n_{0}) \,\mathrm{d}\tau \right)$$

$$\simeq \sum_{n=0}^{\infty} \frac{2D_{0}}{(n+n_{\min})^{\alpha}} \int_{t'}^{t} P_{N}^{*}(n) \,\mathrm{d}\tau$$

$$\simeq \sum_{n=0}^{\infty} \frac{2D_{0}}{(n+n_{\min})^{\alpha}} P_{N}^{*}(n) \,t = 2D_{\alpha}t,$$

$$(7)$$

where $D_{\alpha} = \sum_{n=0}^{\infty} \frac{D_0}{(n+n_{\min})^{\alpha}} P_N^*(n)$. This result is consistent with [18] and is verified numerically in figure 2. Furthermore, the non-Gaussian behavior of the motion of polymer CM is analyzed in [18] by calculating the kurtosis.



Figure 2. Numerical simulation of the MSD of polymer CM position. The result is obtained by averaging over 10^5 realizations. In addition, we take $\alpha = 0.5$, $n_{\min} = 3$, and $D_0 = \lambda = \mu = 1$. The squares and solid (red) line, respectively, represent the stochastic simulation result and theoretical result shown in (7).

In the next section, we will discuss the Fokker–Planck equation in light of the above research.

3. Derivation of the Fokker–Planck equation

Starting from (1), the ordinary diffusion equation governing only the distribution of the polymer CM position is derived in [18] with the form

$$\frac{\partial}{\partial t}u(r,t) = \frac{D_0}{\left(n(t) + n_{\min}\right)^{\alpha}} \frac{\partial^2}{\partial r^2}u(r,t).$$
(8)

It is closely related to the chain polymerization process n(t). The definition of a functional for the chain polymerization process n(t) satisfies

$$A(t) = \int_0^t U(n(\tau)) \,\mathrm{d}\tau,\tag{9}$$

where U(n) is a given function. In this section, we will derive the Fokker–Planck equation for the distribution of CM position and chain polymerization process using the Feynman–Kac equation for the chain polymerization process.

3.1. Forward Fokker-Planck equation

Starting with the definition of A(t), we first derive the forward Feynman–Kac equation of the chain polymerization process, which governs the joint distribution of the functional A(t) and the chain polymerization process n(t). The increment $\delta A(t)$ of A(t) during the small time interval τ satisfies $\delta A(t) = A(t + \tau) - A(t) = U(n(t))\tau$. Let Q(n,A,t) be the joint PDF of the functional A(t) and the monomer number n(t) in a polymer at time *t*. According to the theory of the chain polymerization process, we have

$$Q(n,A,t+\tau) = \mu\tau Q(n+1,A-U(n+1)\tau,t) +\lambda(n-1)\tau Q(n-1,A-U(n-1)\tau,t) +(1-\mu\tau-\lambda(n)\tau)Q(n,A-U(n)\tau,t),$$
(10)

where n > 0. The first term on the right hand side of the above equation states that the number of monomers in a polymer at time t is n + 1; during the time interval τ , the polymer dissociates with probability $\mu\tau$, resulting in the number of monomers in a polymer at time $t + \tau$ being n. Correspondingly, the functional at time t is $A - U(n+1)\tau$. The second term explains that there are n - 1 monomers in a polymer and the functional at time t is $A - U(n-1)\tau$, associated with the probability $\lambda(n-1)\tau$ during the time interval τ , which leads to the number of monomers increasing by 1 and the functional becoming A at time $t + \tau$. The third term means that during the time interval τ , the monomer neither dissociates nor associates with probability $1 - \mu\tau - \lambda(n)\tau$. The functional at time t is $A - U(n)\tau$. For the case n = 0 at time $t + \tau$, the number of monomers in a polymer at time t can only be 1 or 0. Combined with the chain polymerization process, we obtain

$$Q(0,A,t+\tau) = \mu \tau Q(1,A-U(1)\tau,t) + (1-\lambda(0)\tau)Q(0,A-U(0)\tau,t).$$
(11)

By taking the Fourier transform of $A \rightarrow p$ to (10), defined as

$$\widetilde{Q}(n,p,t) = \int_{-\infty}^{\infty} e^{-ipA} Q(n,A,t) \,\mathrm{d}A \tag{12}$$

and neglecting the higher order term of τ , we have

$$\widetilde{Q}(n,p,t+\tau) = \mu \tau \widetilde{Q}(n+1,p,t) + \lambda (n-1) \tau \widetilde{Q}(n-1,p,t) - (\mu \tau + \lambda (n) \tau - 1) \widetilde{Q}(n,p,t) - ipU(n) \tau \widetilde{Q}(n,p,t)$$
(13)

for n > 0. Rearranging the above equation and taking the limit $(\tau \rightarrow 0)$ results to

$$\frac{\partial}{\partial t}\widetilde{Q}(n,p,t) = \mu\widetilde{Q}(n+1,p,t) + \lambda(n-1)\widetilde{Q}(n-1,p,t) - (\mu+\lambda(n))\widetilde{Q}(n,p,t) - ipU(n)\widetilde{Q}(n,p,t).$$
(14)

Applying the same method to (11) yields

$$\frac{\partial}{\partial t}\widetilde{Q}(0,p,t) = \mu\widetilde{Q}(1,p,t) - \lambda(0)\widetilde{Q}(0,p,t) - ipU(0)\widetilde{Q}(0,p,t).$$
(15)

Define the operator

$$L_{ng}(n) = \begin{cases} \mu g(n+1) + \lambda (n-1) g(n-1) & n > 0, \\ -(\mu + \lambda (n)) g(n), & n = 0. \end{cases}$$
(16)

Then the forward Feynman-Kac equation of the chain polymerization process can be stated as

$$\frac{\partial}{\partial t}\widetilde{Q}(n,p,t) = L_n\widetilde{Q}(n,p,t) - ipU(n)\widetilde{Q}(n,p,t)$$
(17)

for $n \ge 0$. The probability distribution $P_N(n,t|n_0)$ of the chain polymerization process in (2) can be recovered by taking p = 0.

After taking the inverse Fourier transform $p \rightarrow A$, the forward Feynman–Kac equation in time-domain behaves as

$$\frac{\partial}{\partial t}Q(n,A,t) = L_nQ(n,A,t) - U(n)\frac{\partial}{\partial A}Q(n,A,t).$$
(18)

In particular, in the above equation, letting $U(n) = 2D(n) = \frac{2D_0}{(n+n_{\min})^{\alpha}}$ and A(t) = s(t), there exists

$$\frac{\partial}{\partial t}Q(n,s,t) = L_n Q(n,s,t) - \frac{2D_0}{(n+n_{\min})^{\alpha}} \frac{\partial}{\partial s}Q(n,s,t).$$
(19)

Next, we present the Fokker–Planck equation, which governs the distribution of the polymer CM position as well as chain polymerization process. Let u(n, r, t) be the joint PDF of CM position r(t) and chain polymerization process n(t). According to the property of the composite process r(t) = B(s(t)), we finally derive the Fokker–Planck equation (see appendix A for the derivation process)

$$\frac{\partial}{\partial t}u(n,r,t) = L_n u(n,r,t) + \frac{D_0}{\left(n+n_{\min}\right)^{\alpha}} \frac{\partial^2}{\partial r^2} u(n,r,t), \qquad (20)$$

which is called the forward Fokker–Planck equation. There are two reasons why the above equation is called the forward Fokker–Planck equation. On the one hand, it deals with the joint distribution of CM position and chain polymerization process. On the other hand, it is derived by using the forward Feynman–Kac equation of the chain polymerization process.

3.2. Backward Fokker-Planck equation

In this part, we derive the backward Fokker–Planck equation for CM diffusion, which focuses only on the distribution of the polymer CM position for a given initial number of monomers n_0 . The derivation is based on the backward Feynman–Kac equation of the chain polymerization process n(t). Let $Q_{n_0}(A, t)$ be the PDF of the functional A(t) at time t for a given n_0 . For a small time interval τ , we have

$$Q_{n_0}(A, t+\tau) = \mu \tau Q_{n_0-1} (A - U(n_0) \tau, t) + \lambda(n_0) \tau Q_{n_0+1} (A - U(n_0) \tau, t) + (1 - \mu \tau - \lambda(n_0) \tau) Q_{n_0} (A - U(n_0) \tau, t),$$
(21)

where $n_0 > 0$. That is, the number of monomers in the polymer is n_0 at the initial time; after the time interval τ , the monomer dissociates, associates, or remains unchanged with probability $\mu\tau$, $\lambda(n_0)\tau$, or $1 - \mu\tau - \lambda(n_0)\tau$, respectively, so that the number of monomers in the polymer is $n_0 - 1, n_0 + 1$, or n_0 . The functional in the time interval τ is $U(n_0)\tau$, so it should be $A - U(n_0)\tau$ in the remaining time. When $n_0 = 0$, it holds

$$Q_0(A, t+\tau) = \lambda(0)\tau Q_1(A - U(0)\tau, t) + (1 - \lambda(0)\tau)Q_0(A - U(0)\tau, t).$$
(22)

Taking the Fourier transform of (21) with $A \rightarrow p$ results in

$$Q_{n_0}(p,t+\tau) = \mu \tau Q_{n_0-1}(p,t) + \lambda(n_0) \tau Q_{n_0+1}(p,t) - (\mu \tau + \lambda(n_0) \tau - 1) \widetilde{Q}_{n_0}(p,t) - ip U(n_0) \tau \widetilde{Q}_{n_0}(p,t),$$
(23)

which can be rewritten as (for $\tau \rightarrow 0$)

$$\frac{\partial}{\partial t}\widetilde{Q}_{n_0}(p,t) = \mu \widetilde{Q}_{n_0-1}(p,t) + \lambda(n_0)\widetilde{Q}_{n_0+1}(p,t)
- (\mu + \lambda(n_0))\widetilde{Q}_{n_0}(p,t) - ipU(n_0)\widetilde{Q}_{n_0}(p,t).$$
(24)

Similarly, for (22), one can get

$$\frac{\partial}{\partial t}\widetilde{Q}_{0}(p,t) = \lambda(0)\widetilde{Q}_{1}(p,t) - \lambda(0)\widetilde{Q}_{0}(p,t) - ipU(0)\widetilde{Q}_{0}(p,t).$$
⁽²⁵⁾

Define the operator F_{n_0} as

$$F_{n_0}g(n_0) = \begin{cases} \mu g(n_0 - 1) + \lambda(n_0) g(n_0 + 1) & n_0 > 0, \\ -(\mu + \lambda(n_0)) g(n_0), & n_0 > 0, \\ \lambda(n_0) g(n_0 + 1) - \lambda(n_0) g(n_0), & n_0 = 0. \end{cases}$$
(26)

Then the backward Feynman–Kac equation corresponding to the chain polymerization process can be expressed as

$$\frac{\partial}{\partial t}\widetilde{Q}_{n_0}(p,t) = F_{n_0}\widetilde{Q}_{n_0}(p,t) - ipU(n_0)\widetilde{Q}_{n_0}(p,t).$$
(27)

Further, the inverse Fourier transform of (27) gives

$$\frac{\partial}{\partial t}Q_{n_0}(A,t) = F_{n_0}Q_{n_0}(A,t) - U(n_0)\frac{\partial}{\partial A}Q_{n_0}(A,t).$$
(28)

In particular, if we choose $U(n) = 2D(n) = \frac{2D_0}{(n+n_{\min})^{\alpha}}$ and A(t) = s(t), we have

$$\frac{\partial}{\partial t}Q_{n_0}(s,t) = F_{n_0}Q_{n_0}(s,t) - \frac{2D_0}{(n_0 + n_{\min})^{\alpha}}\frac{\partial}{\partial s}Q_{n_0}(s,t).$$
⁽²⁹⁾

Let $u_{n_0}(r,t)$ be the PDF of the CM position r(t) at time t when the initial number of monomers n_0 is given. Since r(t) = B(s(t)), we have

$$u_{n_0}(r,t) = \int_0^\infty G(r,s) Q_{n_0}(s,t) \,\mathrm{d}s.$$
(30)

Taking the derivative of time t and combining with (29) lead to the backward Fokker–Planck equation governing the position distribution of the polymer CM with a given n_0 , i.e.

$$\frac{\partial}{\partial t}u_{n_0}(r,t) = F_{n_0}u_{n_0}(r,t) + \frac{D_0}{(n_0 + n_{\min})^{\alpha}}\frac{\partial^2}{\partial r^2}u_{n_0}(r,t).$$
(31)

4. Derivation of the Feynman-Kac equation

In this section, we derive the Feynman–Kac equation of polymer CM diffusion. As in (9), we define the functional of the polymer CM position as

$$w(t) = \int_0^t U(r(\tau)) \,\mathrm{d}\tau. \tag{32}$$

4.1. Forward Feynman-Kac equation

From (1), the increment of the CM position $\delta r(t)$ during a small time interval $\tau (\tau \rightarrow 0)$ is

$$\delta r(t) = r(t+\tau) - r(t) = \sqrt{2D(n(t))}B(\tau)$$
(33)

in the Itô interpretation [68]. The distribution of the noise increment $\delta B(t)$ is the same as $B(\tau)$, satisfying [69]

$$\langle e^{-ikB(\tau)} \rangle = e^{-\frac{k^2}{2}\tau}.$$
(34)

According to the definition of the functional w(t) in (32), the increment during a small interval τ is

$$\delta w(t) = w(t+\tau) - w(t) = U(r(t))\tau.$$
(35)

Define u(n, r, w, t) as the joint PDF of CM position r(t), functional w(t), and chain polymerization process n(t) at time t. We will derive the forward Feynman–Kac equation of polymer CM diffusion, which governs the distribution of u(n, r, w, t). Taking the Fourier transform to u(n, r, w, t) with $n \rightarrow l, r \rightarrow k, w \rightarrow p$, we have

$$\widetilde{u}(l,k,p,t) = \sum_{n=0}^{\infty} e^{-iln} \int_{-\infty}^{\infty} e^{-ikr} dr \int_{-\infty}^{\infty} e^{-ipw} dw$$

$$\times \left\langle \delta_{n,n(t)} \delta\left(r - r(t)\right) \delta\left(w - w(t)\right) \right\rangle$$

$$= \left\langle e^{-iln(t)} e^{-ikr(t)} e^{-ipw(t)} \right\rangle,$$
(36)

where we have used the definition of discrete Fourier transform since n(t) is a discrete process. $\delta_{n,m}$ is the Kronecker delta function, defined as

$$\delta_{n,m} = \begin{cases} 1, & n = m, \\ 0, & n \neq m. \end{cases}$$

The increment of the joint PDF in Fourier space is defined as $\delta \tilde{u}(l,k,p,t) = \tilde{u}(l,k,p,t+\tau) - \tilde{u}(l,k,p,t)$, satisfying

$$\delta \widetilde{u}(l,k,p,t) = \left\langle e^{-iln(t+\tau)} e^{-ikr(t+\tau)} e^{-ipw(t+\tau)} \right\rangle - \left\langle e^{-iln(t)} e^{-ikr(t)} e^{-ipw(t)} \right\rangle.$$
(37)

Together with (33) and (35), it can be further written as

$$\delta \widetilde{u}(l,k,p,t) = \left\langle e^{-iln(t+\tau)} e^{-ik\left(r(t) + \sqrt{2D(n(t))}B(\tau)\right)} e^{-ip(w(t) + U(r(t))\tau)} \right\rangle$$

$$- \left\langle e^{-iln(t)} e^{-ikr(t)} e^{-ipw(t)} \right\rangle.$$
(38)

According to the theory of chain polymerization process, if $n(t + \tau) > 0$ we have

$$\begin{split} \delta \widetilde{u}\left(l,k,p,t\right) &= \tau \left\langle e^{-ikr(t)} e^{-ik\sqrt{2D(n(t))}B(\tau)} e^{-ipw(t)} e^{-ipU(r(t))\tau} e^{-iln(t)} e^{-il}\lambda\left(n\left(t\right)\right) \right\rangle \\ &+ \tau \left\langle e^{-ikr(t)} e^{-ik\sqrt{2D(n(t))}B(\tau)} e^{-ipw(t)} e^{-ipU(r(t))\tau} e^{-iln(t)} e^{il}\mu \right\rangle \\ &+ \left\langle e^{-ikr(t)} e^{-ik\sqrt{2D(n(t))}B(\tau)} e^{-ipw(t)} e^{-ipU(r(t))\tau} e^{-iln(t)} \right\rangle \\ &- \tau \left\langle e^{-ikr(t)} e^{-ik\sqrt{2D(n(t))}B(\tau)} e^{-ipw(t)} e^{-ipU(r(t))\tau} e^{-iln(t)} \left(\mu + \lambda(n(t))\right) \right\rangle \\ &- \left\langle e^{-ikr(t)} e^{-ipw(t)} e^{-iln(t)} \right\rangle. \end{split}$$

Since $B(\tau)$ is independent of the processes r(t) and n(t), combining with its characteristic function (34) and omitting the higher-order terms of the small time interval τ , we get

$$\begin{split} \delta \widetilde{u}\left(l,k,p,t\right) &\approx \tau \left\langle \lambda\left(n\left(t\right)\right) e^{-ikr\left(t\right)} e^{-ipw\left(t\right)} e^{-iln\left(t\right)} e^{-il} \right\rangle + \mu \tau \left\langle e^{-ikr\left(t\right)} e^{-ipw\left(t\right)} e^{-iln\left(t\right)} e^{il} \right\rangle \\ &- k^{2} \tau \left\langle D\left(n\left(t\right)\right) e^{-ikr\left(t\right)} e^{-ipw\left(t\right)} e^{-iln\left(t\right)} \right\rangle - ip \tau \left\langle U\left(r\left(t\right)\right) e^{-ikr\left(t\right)} e^{-ipw\left(t\right)} e^{-iln\left(t\right)} \right\rangle \\ &- \tau \left\langle \left(\mu + \lambda\left(n\left(t\right)\right)\right) e^{-ikr\left(t\right)} e^{-ipw\left(t\right)} e^{-iln\left(t\right)} \right\rangle. \end{split}$$

Dividing both sides by τ and taking the inverse Fourier transform with $l \to n, k \to r$, the forward Feynman–Kac equation of the CM functional is derived for the case $n(t+\tau) > 0$, which is

$$\frac{\partial}{\partial t}\widetilde{u}(n,r,p,t) = \lambda(n-1)\widetilde{u}(n-1,r,p,t) + \mu\widetilde{u}(n+1,r,p,t) - (\mu+\lambda(n))\widetilde{u}(n,r,p,t) + \frac{D_0}{(n+n_{\min})^{\alpha}}\frac{\partial^2}{\partial r^2}\widetilde{u}(n,r,p,t) - ipU(r)\widetilde{u}(n,r,p,t).$$
(39)

When $n(t + \tau) = 0$, the forward Feynman–Kac equation of the CM position functional can also be derived in a similar way. Taking the Fourier transform of the joint PDF $u(0, r, w, t + \tau)$ with $r \rightarrow k, w \rightarrow p$, we have

$$\begin{aligned} \widetilde{u}(0,k,p,t+\tau) &= \left\langle e^{-ikr(t)} e^{-ik\sqrt{2D(n(t))}B(\tau)} e^{-ipw(t)} e^{-ipU(r(t))\tau} \mu\tau \right\rangle \Big|_{n(t)=1} \\ &+ \left\langle e^{-ikr(t)} e^{-ik\sqrt{2D(n(t))}B(\tau)} e^{-ipw(t)} e^{-ipU(r(t))\tau} \left(1 - \lambda\left(n\left(t\right)\right)\tau\right) \right\rangle \Big|_{n(t)=0} \\ &= \mu\tau \left\langle e^{-ikr(t)} e^{-ipw(t)} \right\rangle \Big|_{n(t)=1} + \left\langle e^{-ikr(t)} e^{-ipw(t)} \right\rangle \Big|_{n(t)=0} \\ &- k^{2}\tau \left\langle e^{-ikr(t)}D(n(t))e^{-ipw(t)} \right\rangle \Big|_{n(t)=0} \\ &- ip\tau \left\langle U(r(t))e^{-ikr(t)} e^{-ipw(t)} \right\rangle \Big|_{n(t)=0} - \tau \left\langle e^{-ikr(t)} e^{-ipw(t)}\lambda(n(t)) \right\rangle \Big|_{n(t)=0} \\ &= \mu\tau\widetilde{u}(1,k,p,t) - \tau\lambda(0)\widetilde{u}(0,k,p,t) + \widetilde{u}(0,k,p,t) \\ &- k^{2}\frac{D_{0}}{n_{\min}^{\alpha}}\tau\widetilde{u}(0,k,p,t) - ip\tau\mathcal{F}_{r\to k}\left\{ U(r)\widetilde{u}(0,r,p,t) \right\}. \end{aligned}$$
(40)

$$\frac{\partial}{\partial t}\widetilde{u}(0,r,p,t) = \mu\widetilde{u}(1,r,p,t) - \lambda(0)\widetilde{u}(0,r,p,t) + \frac{D_0}{n_{\min}^{\alpha}}\frac{\partial^2}{\partial r^2}\widetilde{u}(0,r,p,t) - ipU(r)\widetilde{u}(0,r,p,t).$$
(41)

Together with the operator L_n defined in (16), we derive the forward Feynman–Kac equation for the CM position functional

$$\frac{\partial}{\partial t}\widetilde{u}(n,r,p,t) = L_n\widetilde{u}(n,r,p,t) + \frac{D_0}{(n+n_{\min})^{\alpha}}\frac{\partial^2}{\partial r^2}\widetilde{u}(n,r,p,t) - ipU(r)\widetilde{u}(n,r,p,t).$$
(42)

In particular, we recover the result of the forward Fokker–Planck equation (20) when taking p = 0. In this case, $\tilde{u}(n, r, p = 0, t) = \int_{-\infty}^{\infty} u(n, r, w, t) dw$ leads to the result of u(n, r, t), the joint PDF of CM position r(t) and the chain polymerization process n(t). Moreover, if the functional w is always non-negative, the Fourier transform of w can be replaced by the Laplace transform defined as $\hat{u}(n, r, p, t) = \int_{0}^{\infty} e^{-pw} f(n, r, w, t) dw$. Finally, the forward Feynman–Kac equation is obtained by replacing ip with p.

4.2. Backward Feynman-Kac equation

The forward Feynman–Kac equation emphasizes the joint distribution of CM position r(t), chain polymerization process n(t), and functional w(t). However, in some cases [49, 51], one pays attention only to the distribution of the functional w(t), which urges us to derive the backward Feynman–Kac equation for given n_0, r_0 . In this part we aim to derive the backward Feynman–Kac equation of the CM functional for specific n_0, r_0 .

Starting with (1), it can be noted that the diffusion coefficient depends on the timedependent chain polymerization process n(t), which causes the distribution of the CM position starting from the same position to be different during the same time interval. Therefore, the whole path r(t) has to be considered. The idea we adopt is to construct a new stochastic process to treat this problem. Define $\bar{r}(t) = (r(t), I(t))^{T}$ with the initial distribution $\bar{r}(0) = (r_0, I_0)^{T}$, where r(t) is the model under consideration and I(t) = t is a process with a deterministic variable. Taking the derivative with respect to time t, we obtain

$$d\bar{r}(t) = \begin{pmatrix} dr(t) \\ dt \end{pmatrix} = \begin{pmatrix} \sqrt{2D(N((0,1)\bar{r}))} dB(t) \\ dt \end{pmatrix},$$
(43)

which can be rewritten as

$$d\bar{r}(t) = \begin{pmatrix} \sqrt{2D\left(N((0,1)\bar{r})\right)} & 0\\ 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} dB(t)\\ dt \end{pmatrix}.$$
(44)

Now the diffusion coefficient in $\bar{r}(t)$ is independent of time *t*. We do not necessarily consider the whole path $\bar{r}(t)$ when deriving the backward Feynman–Kac equation of the stochastic process $\bar{r}(t)$.

Define the functional of $\bar{r}(t)$ as

$$\bar{w}(t) = \int_0^t U(\bar{r}(\tau)) \,\mathrm{d}\tau = \begin{pmatrix} \int_0^t U(r(\tau)) \,\mathrm{d}\tau \\ \int_0^t U(I(\tau)) \,\mathrm{d}\tau \end{pmatrix} = \begin{pmatrix} w(t) \\ m(t) \end{pmatrix},\tag{45}$$

where *U* is the same as the one in (32). Let $L_{n_0,\bar{r}_0}(\bar{w},t)$ be the PDF of the functional $\bar{w}(t)$ when the initial conditions n_0,\bar{r}_0 of the stochastic process $\bar{r}(t)$ are given. It can be written as $L_{n_0,\bar{r}_0}(w,m,t)$ since $\bar{w}(t) = (w(t),m(t))^{\mathrm{T}}$. Further it can be simplified as $L_{n_0,r_0}(w,m,t)$ since I(t) = t, which is a deterministic process. Let $u_{n_0,r_0}(w,t)$ be the PDF of the functional w(t) of the polymer CM diffusion process r(t) for given n_0, r_0 . There is no doubt,

$$u_{n_0,r_0}(w,t) = \int_{-\infty}^{\infty} L_{n_0,r_0}(w,m,t) dm$$

= $\mathcal{F}_{m \to p_0} \{ L_{n_0,r_0}(w,m,t) \} |_{p_0=0}.$ (46)

The increment of $L_{n_0,r_0}(w,m,t)$ during the small time interval τ is represented as $\delta L_{n_0,r_0}(w,m,t)$; respectively taking Fourier transform of $\delta L_{n_0,r_0}(w,m,t)$ with $w \to p, m \to p_0$, we have

$$\delta \widetilde{L}_{n_0,r_0}(p,p_0,t) = \left\langle e^{-ipw(t+\tau)|_{n_0,r_0} - ip_0m(t+\tau)|_{n_0,r_0}} \right\rangle - \left\langle e^{-ipw(t)|_{n_0,r_0} - ip_0m(t)|_{n_0,r_0}} \right\rangle,$$
(47)

where $w(t)|_{n_0,r_0}$ is the value of the functional w(t) at time *t* for given n_0, r_0 . Since $u_{n_0,r_0}(w,t) = \widetilde{L}_{n_0,r_0}(w,p_0,t)|_{p_0=0}$, the increment of $\delta u_{n_0,r_0}(w,t)$ in Fourier-space can be written as

$$\delta \widetilde{u}_{n_0,r_0}(p,t) = \left\langle e^{-ipw(t+\tau)|_{n_0,r_0}} \right\rangle - \left\langle e^{-ipw(t)|_{n_0,r_0}} \right\rangle.$$
(48)

We explore the relationship between the functional w(t) and the initial value of the stochastic process r(t). By the definition of the functional w(t) in (32), we have

$$w(t+\tau) = U(r_0)\tau + w(t)|_{n(\tau), r(\tau)}.$$
(49)

In addition, according to the Langevin equation (1), $r(\tau) = r_0 + \sqrt{2D(n_0)}B(\tau)$ holds under the Itô interpretation during a small time interval τ . Substituting the above results into (48), we have

$$\delta \widetilde{u}_{n_0,r_0}(p,t) = \left\langle \left\langle \left\langle e^{-ipU(r_0)\tau} e^{-ipw(t)|_{n(\tau),r_0} + \sqrt{2D(n_0)B(\tau)}} \right\rangle \right\rangle \right\rangle - \left\langle e^{-ipw(t)|_{n_0,r_0}} \right\rangle,$$
(50)

where the inner brackets of $\langle \langle \langle \cdot \rangle \rangle \rangle$ denote the average of w(t), while the outer two brackets denote the average of the Wiener process $B(\tau)$ and the chain polymerization process n(t),

respectively. According to the dynamics of monomer aggregation and disaggregation, one can get

$$\begin{split} \delta \widetilde{u}_{n_{0},r_{0}}\left(p,t\right) &= \left\langle \left\langle \mu \tau e^{-ipU(r_{0})\tau} e^{-ipw(t)|_{n_{0}-1,r_{0}} + \sqrt{2D(n_{0})}B(\tau)} \right\rangle \right\rangle \\ &+ \left\langle \left\langle \lambda(n_{0})\tau e^{-ipU(r_{0})\tau} e^{-ipw(t)|_{n_{0}+1,r_{0}} + \sqrt{2D(n_{0})}B(\tau)} \right\rangle \right\rangle \\ &+ \left\langle \left\langle \left(1 - \mu \tau - \lambda(n_{0})\tau\right) e^{-ipU(r_{0})\tau} e^{-ipw(t)|_{n_{0},r_{0}} + \sqrt{2D(n_{0})}B(\tau)} \right\rangle \right\rangle \end{split}$$
(51)
$$&- \left\langle e^{-ipw(t)|_{n_{0},r_{0}}} \right\rangle \end{split}$$

for $n_0 > 0$. Taking the Fourier transform of $\delta \tilde{u}_{n_0,r_0}(p,t)$ with $r_0 \to k_0$ and dropping the higherorder terms of τ , one can get

$$\begin{split} \delta \widetilde{u}_{n_{0},k_{0}}\left(p,t\right) &= \mu \tau \widetilde{u}_{n_{0}-1,k_{0}}\left(p,t\right) + \lambda\left(n_{0}\right) \tau \widetilde{u}_{n_{0}+1,k_{0}}\left(p,t\right) \\ &- \left(\mu + \lambda\left(n_{0}\right)\right) \tau \widetilde{u}_{n_{0},k_{0}}\left(p,t\right) - k_{0}^{2} D\left(n_{0}\right) \tau \widetilde{u}_{n_{0},k_{0}}\left(p,t\right) \\ &- i p \tau \mathcal{F}_{r_{0} \to k_{0}}\left\{U(r_{0}) \widetilde{u}_{n_{0},r_{0}}\left(p,t\right)\right\}. \end{split}$$
(52)

The details are given in appendix **B**. Taking the inverse Fourier transform of (52) with $k_0 \rightarrow r_0$, we finally obtain

$$\frac{\partial}{\partial t} \widetilde{u}_{n_0, r_0}(p, t) = \mu \widetilde{u}_{n_0 - 1, r_0}(p, t) + \lambda(n_0) \widetilde{u}_{n_0 + 1, r_0}(p, t)
- (\mu + \lambda(n_0)) \widetilde{u}_{n_0, r_0}(p, t) - ip U(r_0) \widetilde{u}_{n_0, r_0}(p, t)
+ \frac{D_0}{(n_0 + n_{\min})^{\alpha}} \frac{\partial^2}{\partial r_0^2} \widetilde{u}_{n_0, r_0}(p, t).$$
(53)

When $n_0 = 0$, according to the behavior of monomer aggregation and disaggregation, the increment of $\delta \widetilde{u}_{0,r_0}(p,t)$ can be expressed as

$$\begin{split} \delta \widetilde{u}_{0,r_{0}}(p,t) &= \left\langle \left\langle \lambda(0) \, \tau e^{-ipU(r_{0})\tau} e^{-ipw(t)|_{1,r_{0}} + \sqrt{2D(0)B(\tau)}} \right\rangle \right\rangle \\ &+ \left\langle \left\langle e^{-ipU(r_{0})\tau} e^{-ipw(t)|_{0,r_{0}} + \sqrt{2D(0)B(\tau)}} \right\rangle \right\rangle \\ &- \left\langle \left\langle \lambda(0) \, \tau e^{-ipU(r_{0})\tau} e^{-ipw(t)|_{0,r_{0}} + \sqrt{2D(0)B(\tau)}} \right\rangle \right\rangle \\ &- \left\langle e^{-ipw(t)|_{0,r_{0}}} \right\rangle. \end{split}$$
(54)

Following the above procedure, there exists

$$\frac{\partial}{\partial t} \widetilde{u}_{0,r_0}(p,t) = \lambda(0) \widetilde{u}_{1,r_0}(p,t) - \lambda(0) \widetilde{u}_{0,r_0}(p,t)
- ipU(r_0) \widetilde{u}_{0,r_0}(p,t) + \frac{D_0}{n_{\min}^{\alpha}} \frac{\partial^2}{\partial r_0^2} \widetilde{u}_{0,r_0}(p,t).$$
(55)

Together with the operator F_{n_0} defined in (26), the backward Feynman–Kac equation of the CM functional is derived as

$$\frac{\partial}{\partial t} \widetilde{u}_{n_0, r_0}(p, t) = F_{n_0} \widetilde{u}_{n_0, r_0}(p, t) - ip U(r_0) \widetilde{u}_{n_0, r_0}(p, t)
+ \frac{D_0}{(n_0 + n_{\min})^{\alpha}} \frac{\partial^2}{\partial r_0^2} \widetilde{u}_{n_0, r_0}(p, t).$$
(56)

In the following, we will solve the Feynman–Kac equation by the deep learning method [70] and use Monte Carlo simulation to simulate the corresponding stochastic process, the comparison of which verifies the effectiveness of the derived equation.

5. Deep BSDE method

Deep BSDE method is a deep learning method for solving high-dimensional partial differential equations (PDEs), which was proposed in [71]. In the work [70], we derive a discrete version of BSDE and generalize the deep BSDE method to solve equations with discrete operators. In this section, we briefly introduce the main ideas of the deep BSDE method.

5.1. PDEs and BSDEs

We consider a class of semilinear parabolic PDEs with infinite dimensional coupling. These PDEs can be represented as

$$\frac{\partial}{\partial t}u(n,r,p,t) + T_nu(n,r,p,t) + \frac{D_0}{(n+n_{\min})^{\alpha}}\frac{\partial^2}{\partial r^2}u(n,r,p,t) + f(n,r,p,u(n,r,p,t)) = 0$$
(57)

with the given terminal condition u(n,r,p,T) = g(n,r,p). Here the unknown is $u : \mathbb{N} \times \mathbb{R}^1 \times \mathbb{R}^1 \times [0,\infty) \to \mathbb{C}$,

$$T_n f(n) = \begin{cases} \alpha(n) \left(f(n+1) - f(n) \right) + \beta(n) \left(f(n-1) - f(n) \right), & n \ge 1, \\ \alpha(n) \left(f(1) - f(0) \right), & n = 0, \end{cases}$$
(58)

where $\alpha(n)$ and $\beta(n)$ are known functions that satisfy $\alpha(n), \beta(n) \ge 0$ for $n \in \mathbb{N}$, and $\beta(0) = 0$. It is easy to see that the equations (42) and (56) can both be transformed into the form of the equation (57).

Let n(t) be a birth-death process satisfying

$$\mathbb{P}(n(t+\tau) - n(t) = k | n(t) = n) = \begin{cases} \alpha(n)\tau + o(\tau), & k = 1, \\ \beta(n)\tau + o(\tau), & k = -1, \\ 1 - (\alpha(n) + \beta(n))\tau + o(\tau), & k = 0, \\ o(\tau), & \text{otherwise}, \end{cases}$$
(59)

and r(t) be a one-dimensional stochastic process satisfying

$$r(t) = r(0) + \int_0^t \sqrt{\frac{2D_0}{(n(\tau) + n_{\min})^{\alpha}}} dB(\tau).$$
(60)

$$u(n(t), r(t), p, t) - g(n(t), r(t), p)$$

$$= \int_{t}^{T} f(n(\tau), r(\tau), p, u(n(\tau), r(\tau), p, \tau)) d\tau$$

$$- \int_{t}^{T} \sqrt{\frac{2D_{0}}{(n(\tau) + n_{\min})^{\alpha}}} \frac{\partial}{\partial r} u(n(\tau), r(\tau), p, \tau) dB(\tau)$$

$$- \int_{t}^{T} \int_{\mathbb{Z} \setminus \{0\}} u(n(\tau-) + n, r(\tau), p, \tau) - u(n(\tau-), r(\tau), p, \tau) \widetilde{J}(d\tau, dn; n(\tau-)).$$
(61)

5.2. Deep BSDE method

Now, we can get the solution of the corresponding original equations by solving (60) and (61). We focus on the solution $u(n_0, r_0, p, 0)$, where $(n_0, r_0, p) \in \mathbb{N} \times \mathbb{R}^1 \times \mathbb{R}^1$ is already determined. We treat $u(n_0, r_0, p, 0) \approx \theta_{\phi}$ as a parameter in the model and consider BSDE (61) as the way to get the value of u at the terminal time T when $u(n(0) = n_0, r(0) = r_0, p, 0)$ and $\frac{\partial}{\partial r}u(n(t), r(t), p, t)$ and $u(n(t-) \pm 1, r(t), p, t)$ are known, where $\frac{\partial}{\partial r}u(n, r, p, t)$ is approximated by a neural network

$$\frac{\partial}{\partial r}u(n,r,p,t) \approx \psi_1(n,r,p,t|\theta_{\psi_1})$$
(62)

with parameters θ_{ψ_1} and $\delta_n^{\pm} u(n,r,t) = [u(n-1,r,t) - u(n,r,t), u(n+1,r,t) - u(n,r,t)]^T$ is approximated by a neural network

$$\delta_n^{\pm} u(n,r,p,t) \approx \psi_2(n,r,p,t|\theta_{\psi_2}) \tag{63}$$

with parameters θ_{ψ_2} .

On this basis, one can design the numerical schemes by discretizing time. Given a partition of the time interval $[0, t] : 0 = t_0 < t_1 < \cdots < t_{N-1} < t_N = T$, we consider the simple Euler scheme for $k = 0, 1, \dots, N-1$.

$$r(t_{k+1}) - r(t_k) = \sqrt{\frac{2D_0}{n(t_k) + n_{\min}}} \Delta B(t_k)$$
(64)

and

$$u(n(t_{k+1}), r(t_{k+1}), p, t_{k+1}) = u(n(t_k), r(t_k), p, t_k) - f(n(t_k), r(t_k), p, u(n(t_k), r(t_k), p, t_k)) \Delta t_k + \sqrt{\frac{2D_0}{(n(t_k) + n_{\min})^{\alpha}}} \frac{\partial}{\partial r} u(n(t_k), r(t_k), p, t_k) \Delta B(t_k) + u(n(t_{k+1}), r(t_k), p, t_k) - u(n(t_k), r(t_k), p, t_k) - F_n u(n(t_k), r(t_k), p, t_k),$$
(65)

where $\Delta t_k = t_{k+1} - t_k$, $\Delta B(t_k) = B(t_{k+1}) - B(t_k)$, and $n(t_{k+1}) - n(t_k)$ satisfies (59).

We take the discretized time $\{t_k\}_{0 \le k \le N}$, frequency p, the randomly generated paths $\{n(t_k)\}_{0 \le k \le N}$, $\{r(t_k)\}_{0 \le k \le N}$, and $\{B(t_k)\}_{0 \le k \le N}$ as the input data of the neural network. Let $\theta = \{\theta_{\phi}, \theta_{\psi_1}, \theta_{\psi_2}\}$, the final output $\hat{u}(\{n(t_k), r(t_k), p, B(t_k), t_k\}_{0 \le k \le N} | \theta)$ is obtained through the scheme (65) as an approximation of g(n(T), r(T), p). The difference from the given terminal conditions can be used to construct the loss function

$$\operatorname{Loss}\left(\theta\right) = \mathbb{E}\left[\left|g\left(n\left(T\right), r\left(T\right), p\right) - \hat{u}\left(\left\{r\left(t_{k}\right), p, n\left(t_{k}\right), B\left(t_{k}\right), t_{k}\right\}_{0 \leq k \leq N} |\theta\right)\right|^{2}\right].$$
(66)

6. Applications

In this section, we give some applications of the derived Feynman–Kac equations and solve them using the deep BSDE method and Monte Carlo simulation. To proceed, the original problem must first be transformed into a terminal problem by time transformation $t \rightarrow T - t$. All numerical examples are run on a desktop computer with a 3.40GHz Intel Core i7 processor and 32 GB memory.

6.1. Occupation time in the positive half-space

We first discuss the occupation time of the polymer CM position in r > 0 space. This application has been discussed for Brownian motion and non-Brownian case [51] from the backward Feynman–Kac equation. The functional corresponding to this application satisfies

$$w(t) = \int_0^t \Theta(r(\tau)) \,\mathrm{d}\tau,\tag{67}$$

where $\Theta(r) = 1$ for r > 0 and zero otherwise. To find the distribution of occupation times, we consider the backward Feynman–Kac equation

$$\frac{\partial}{\partial t}\tilde{u}_{n_{0},r_{0}}(p,t) + F_{n_{0}}\tilde{u}_{n_{0},r_{0}}(p,t) + \frac{D_{0}}{(n_{0}+n_{\min})^{\alpha}}\frac{\partial^{2}}{\partial r_{0}^{2}}\tilde{u}_{n_{0},r_{0}}(p,t) - ip\Theta(r_{0})\tilde{u}_{n_{0},r_{0}}(p,t) = 0$$
(68)

with terminal condition $\tilde{u}_{n_0,r_0}(p,T) = 1$. We calculate the occupation time distribution of the polymer CM on the positive half-space by solving the backward Feynman–Kac equation (68) using the deep BSDE method and Monte Carlo simulation, respectively.

Choosing $D_0 = 10$, $n_{\min} = 3$, $\alpha = 1$, $n_0 = 0$, $r_0 = 0$, T = 3, $\lambda(i) = 1$, and $\mu = 1$, we get the results of two methods (figure 3). In the simulation by the deep BSDE method, $p \in [-40, 40]$ is divided into 20 parts, and 20 models are trained in parallel, each model going through 40000 iterations of 256 batch size at 150 equidistant time steps (N = 150), with a learning rate of 0.001 for the first 20000 and 0.0001 for the last 20000 iterations. Then the solution in physical space is obtained by inverse Fourier transform. The 'exact solution' is obtained by simulating 1000000 particle trajectories using Monte Carlo simulation, and then numerically computing the probability density of the particle trajectory functional at [0,3]. The L_2 relative error between the solution obtained by the deep BSDE method and the solution obtained by the Monte Carlo simulation reaches 0.0002171. The results show that the solution obtained by solving equation (68) is consistent with the solution obtained by Monte Carlo simulation.



Figure 3. Plots of the probability density of occupation time of positive half-space of polymer CM at $n_0 = 0$, $r_0 = 0$, t = 0 (According to the time transformation $t \rightarrow T - t$, the physical time is 3), and $w \in [0,3]$, which are obtained by deep BSDE method and Monte Carlo simulation, respectively. The stars represent the 'exact solution' obtained by Monte Carlo simulation and the solid (blue) line is for the solution obtained by solving equation (68) using deep BSDE method and making inverse Fourier transform in three different frequency ranges [-4, 4], [-20, 20], and [-40, 40].

6.2. First passage time

In this subsection, we discuss the time that the polymer CM firstly passes through the boundary $\partial\Omega$. Assuming that the polymer CM moves freely in the domain $\Omega = [-L, L]$, the time at which the polymer CM firstly reaches the boundary $\pm L$ is called the first-passage time. The first-passage time is a direct application of the backward Feynman–Kac equation and the functional corresponding to this application is

$$w(t) = \int_0^t \Theta_{\Omega}(r(\tau)) \,\mathrm{d}\tau,\tag{69}$$

where $\Theta_{\Omega}(r) = 1$ for $r \in \Omega$ and zero otherwise.

To obtain the distribution of the first-passage time by solving the backward Feynman–Kac equation, we apply the absorption boundary condition $u_{n_0,r_0\in\partial\Omega}(w,t) = \delta(w)$ to the original equation, so consider the terminal boundary value problem

$$\frac{\partial}{\partial t} \widetilde{u}_{n_{0},r_{0}}(p,t) + F_{n_{0}} \widetilde{u}_{n_{0},r_{0}}(p,t) + \frac{D_{0}}{(n_{0}+n_{\min})^{\alpha}} \frac{\partial^{2}}{\partial r_{0}^{2}} \widetilde{u}_{n_{0},r_{0}}(p,t) - ip\Theta_{\Omega}(r_{0}) \widetilde{u}_{n_{0},r_{0}}(p,t) = 0$$
(70)

with terminal boundary conditions $\tilde{u}_{n_0,r_0}(p,T) = 1$ and $\tilde{u}_{n_0,r_0 \in \partial \Omega}(p,t) = 1$. It can be seen from the equation that we are actually calculating the distribution of survival time, so the distribution



Figure 4. Plots of the probability density of first passage time of polymer CM at $n_0 = 5$, $r_0 = 0$, t = 0 (According to the time transformation $t \rightarrow T - t$, the physical time is 10), and $w \in [0, 10]$, which are obtained by deep BSDE method and Monte Carlo simulation, respectively. The stars represent the 'exact solution' obtained by Monte Carlo simulation, and the solid (blue) line is for the solution obtained by solving equation (70) using deep BSDE method and making inverse Fourier transform.

of first passage time $\phi(w) = \lim_{t \to \infty} u_{n_0,r_0}(w,t)^3$ (Here $u_{n_0,r_0}(w,t)$ is the original one, i.e. no time transformation $t \to T - t$, where the same notation is used). By solving equation (70) with the deep BSDE method and Monte Carlo simulation, we obtain the distribution of the first passage time of polymer CM in one-dimensional case.

Choosing $D_0 = 10$, $n_{\min} = 3$, $\alpha = 1$, $n_0 = 5$, $r_0 = 0$, T = 10, $\lambda(i) = 1$, and $\mu = 1$, L = 2, we get the results of the two methods (figure 4). The BSDE solved by the deep BSDE method also has the boundary condition $\tilde{u}_{n(t),r(t)}(p,t) = 1$ for $r(t) \in \partial \Omega$. Stop the iteration when r(t) reaches the boundary, and calculate the boundary loss values. We divide $p \in [-10, 10]$ into five parts on average, and train five deep BSDE models in parallel, each model going through 40000 iterations of 256 batch size at 500 equidistant time steps (N = 500), with learning rate of 0.001 for the first 20000 and 0.0001 for the last 20000 iterations. Finally, the solution in physical space is obtained by inverse Fourier transform. The 'exact solution' is obtained by simulating 1000 000 particle trajectories using Monte Carlo simulation and then to numerically calculate the probability density of the particle trajectory functional at [0, 10]. The L_2 relative error between the solution obtained by the deep BSDE method and the solution obtained by the Monte Carlo simulation reaches 0.0001277. The results show that the solution obtained by solving equation (70) is consistent with the solution obtained by Monte Carlo simulation.

³ When $t \to +\infty$, the value of w defined by equation (69) is exactly the time spent of the particle firstly reaching the boundary. So, the solution of the equation is equal to the distribution of the first passage time when the physical time is large enough.

6.3. Joint distribution of position integral functional

In this subsection, we discuss the joint probability distribution of the size, position, and position integral functional for polymer CM. The functional corresponding to this application satisfies

$$w(t) = \int_0^t r(\tau) \,\mathrm{d}\tau. \tag{71}$$

Considering the forward Feynman-Kac equation

$$\frac{\partial}{\partial t}\widetilde{u}(n,r,p,t) + L_{n}\widetilde{u}(n,r,p,t) + \frac{D_{0}}{\left(n+n_{\min}\right)^{\alpha}}\frac{\partial^{2}}{\partial r^{2}}\widetilde{u}(n,r,p,t) - ipr\widetilde{u}(n,r,p,t) = 0,$$
(72)

with terminal condition $\tilde{u}(n,r,p,T) = g(n,r,p)$, we obtain the joint probability distribution by solving the forward Feynman–Kac equation (72) with the deep BSDE method and Monte Carlo simulation, respectively.

Choosing $D_0 = 1, n_{\min} = 3, \alpha = 1, n = 5, r = 0, T = 1, \lambda(i) = (50 - i)/10, \mu = 2$, and the terminal condition⁴

$$g(n,r,p) = \frac{\kappa_{\{0,\dots,9\}}(n)}{10(2\pi)^{\frac{1}{2}}} e^{-\frac{|r|^2}{2}},\tag{73}$$

we get the results of the two methods (figure 5). The results of the deep BSDE method go through 40000 iterations of 512 batch size at 50 equidistant time steps (N = 50), with learning rate of 0.0005 for the first 20000 and 0.0001 for the last 20000 iterations. The final results can then be obtained by the inverse Fourier transform. The L_2 relative error between the solution obtained by the deep BSDE method and the solution obtained by the Monte Carlo simulation reaches 0.00000024. The results show that the solution obtained by solving equation (72) is consistent with the solution obtained by Monte Carlo simulation.

7. Conclusion

We derive the Fokker–Planck equation and the Feynman–Kac equation for the dynamics of polymer CM diffusion which is described by the Langevin equation with Gaussian white noise. The diffusion coefficient corresponding to this model is a stochastic process called the chain polymerization process. The Fokker–Planck equation is derived with the help of the Feynman–Kac equation of chain polymerization process, termed as forward Fokker–Planck equation and backward Fokker–Planck equation, respectively. The forward Fokker–Planck equation governs the joint PDF of CM position and chain polymerization process while the backward Fokker–Planck equation of CM position for a given n_0 .

By defining a functional of the CM path, we derive the forward Feynman–Kac equation governing the joint PDF of the CM position, the functional, and the chain polymerization

⁴ The joint probability density $g(n,r,w) = \langle \delta_{n,n(0)} \delta(r-r(0)) \delta(w-w(0)) \rangle$ of n(0), r(0), and w(0) after the Fourier transform $w \to p$. We assume that r(0) satisfies the normal distribution and n(0) satisfies the uniform distribution of $\{0, 1, \dots, 9\}$, and that n(0) and r(0) are independent.



Figure 5. Plots of joint probability distribution of the size, position, and position integral functional for polymer CM at n = 5, r = 0, t = 0 (physical time is t = T = 1), and $w \in [-1, 1]$, which are obtained by deep BSDE method and Monte Carlo simulation respectively. Stars represent the 'exact solution' of Monte Carlo simulations while the solid (blue) line denotes the solution of (72) obtained by deep BSDE method.

process. The backward Feynman–Kac equation is also derived for given n_0, r_0 . Finally, we solve the Feynman–Kac equation using the deep BSDE method and Monte Carlo simulation through several classical application problems, respectively.

Data availability statement

The data cannot be made publicly available upon publication because they are not available in a format that is sufficiently accessible or reusable by other researchers. The data that support the findings of this study are available upon reasonable request from the authors.

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Appendix A. Derivation of (20)

Since r(t) = B(s(t)), it holds that [72]

$$u(n,r,t) = \int_0^\infty G(r,s) Q(n,s,t) \,\mathrm{d}s. \tag{A.1}$$

Taking the derivative of time t on both sides of the above equation and combining with (19) result in

$$\begin{split} \frac{\partial}{\partial t}u\left(n,r,t\right) &= \int_{0}^{\infty} G\left(r,s\right)\frac{\partial}{\partial t}Q\left(n,s,t\right) \mathrm{d}s\\ &= \int_{0}^{\infty} G\left(r,s\right)\left(L_{n}Q\left(n,s,t\right) - \frac{2D_{0}}{\left(n+n_{\min}\right)^{\alpha}}\frac{\partial}{\partial s}Q\left(n,s,t\right)\right)\mathrm{d}s\\ &= L_{n}u\left(n,r,t\right) - \frac{2D_{0}}{\left(n+n_{\min}\right)^{\alpha}}\int_{0}^{\infty} G\left(r,s\right)\frac{\partial}{\partial s}Q\left(n,s,t\right)\mathrm{d}s\\ &= L_{n}u\left(n,r,t\right) + \frac{2D_{0}}{\left(n+n_{\min}\right)^{\alpha}}\int_{0}^{\infty}Q\left(n,s,t\right)\frac{\partial}{\partial s}G\left(r,s\right)\mathrm{d}s\\ &= L_{n}u\left(n,r,t\right) + \frac{2D_{0}}{\left(n+n_{\min}\right)^{\alpha}}\int_{0}^{\infty}Q\left(n,s,t\right)\frac{1}{2}\frac{\partial^{2}}{\partial r^{2}}G\left(r,s\right)\mathrm{d}s\\ &= L_{n}u\left(n,r,t\right) + \frac{D_{0}}{\left(n+n_{\min}\right)^{\alpha}}\frac{\partial^{2}}{\partial r^{2}}u\left(n,r,t\right). \end{split}$$
(A.2)

Appendix B. Derivation process of (52)

Equation (51) can be further expanded as

$$\begin{split} \delta \widetilde{u}_{n_{0},r_{0}}\left(p,t\right) &= \left\langle \left\langle \mu \tau e^{-ipU(r_{0})\tau} e^{-ipw(t)|_{n_{0}-1,r_{0}} + \sqrt{2D(n_{0})}B(\tau)} \right\rangle \right\rangle \\ &+ \left\langle \left\langle \lambda(n_{0})\tau e^{-ipU(r_{0})\tau} e^{-ipw(t)|_{n_{0}+1,r_{0}} + \sqrt{2D(n_{0})}B(\tau)} \right\rangle \right\rangle \\ &+ \left\langle \left\langle e^{-ipU(r_{0})\tau} e^{-ipw(t)|_{n_{0},r_{0}} + \sqrt{2D(n_{0})}B(\tau)} \right\rangle \right\rangle \\ &- \left\langle \left\langle (\mu + \lambda(n_{0}))\tau e^{-ipU(r_{0})\tau} e^{-ipw(t)|_{n_{0},r_{0}} + \sqrt{2D(n_{0})}B(\tau)} \right\rangle \right\rangle \\ &- \left\langle e^{-ipw(t)|_{n_{0},r_{0}}} \right\rangle. \end{split}$$
(B.1)

According to the definition of Fourier transform with $r_0 \rightarrow k_0$, (B.1) becomes

$$\begin{split} \delta \widetilde{u}_{n_{0},k_{0}}\left(p,t\right) &= \mathcal{F}_{r_{0} \to k_{0}} \left\{ \left\langle \left\langle \mu \tau e^{-ipU(r_{0})\tau} e^{ik_{0}\sqrt{2D(n_{0})}B(\tau)} e^{-ipw(t)|_{n_{0}-1,r_{0}}} \right\rangle \right\rangle \right\} \\ &+ \mathcal{F}_{r_{0} \to k_{0}} \left\{ \left\langle \left\langle \lambda\left(n_{0}\right)\tau e^{-ipU(r_{0})\tau} e^{ik_{0}\sqrt{2D(n_{0})}B(\tau)} e^{-ipw(t)|_{n_{0}+1,r_{0}}} \right\rangle \right\rangle \right\} \\ &+ \mathcal{F}_{r_{0} \to k_{0}} \left\{ \left\langle \left\langle e^{-ipU(r_{0})\tau} e^{ik_{0}\sqrt{2D(n_{0})}B(\tau)} e^{-ipw(t)|_{n_{0},r_{0}}} \right\rangle \right\rangle \right\} \\ &- \mathcal{F}_{r_{0} \to k_{0}} \left\{ \left\langle \left\langle \left(\mu + \lambda\left(n_{0}\right)\right)\tau e^{-ipU(r_{0})\tau} e^{ik_{0}\sqrt{2D(n_{0})}B(\tau)} e^{-ipw(t)|_{n_{0},r_{0}}} \right\rangle \right\rangle \right\} \end{split}$$
(B.2)

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for $\tau \to 0$. Since the functional w(t) is independent with $B(\tau)$, it can be written as

$$\begin{split} \delta \widetilde{u}_{n_{0},k_{0}}\left(p,t\right) &= \mathcal{F}_{r_{0} \to k_{0}} \left\{ \left\langle \mu \tau e^{-ipU(r_{0})\tau} e^{-k_{0}^{2}D(n_{0})\tau} e^{-ipw(t)|_{n_{0}-1,r_{0}}} \right\rangle \right\} \\ &+ \mathcal{F}_{r_{0} \to k_{0}} \left\{ \left\langle \lambda\left(n_{0}\right)\tau e^{-ipU(r_{0})\tau} e^{-k_{0}^{2}D(n_{0})\tau} e^{-ipw(t)|_{n_{0}+1,r_{0}}} \right\rangle \right\} \\ &+ \mathcal{F}_{r_{0} \to k_{0}} \left\{ \left\langle e^{-ipU(r_{0})\tau} e^{-k_{0}^{2}D(n_{0})\tau} e^{-ipw(t)|_{n_{0},r_{0}}} \right\rangle \right\} \\ &- \mathcal{F}_{r_{0} \to k_{0}} \left\{ \left\langle \left(\mu + \lambda\left(n_{0}\right)\right)\tau e^{-ipU(r_{0})\tau} e^{-k_{0}^{2}D(n_{0})\tau} e^{-ipw(t)|_{n_{0},r_{0}}} \right\rangle \right\} \\ &- \left\langle e^{-ipw(t)|_{n_{0},k_{0}}} \right\rangle. \end{split}$$
(B.3)

By ignoring the higher-order terms of small time interval τ , it can be further simplified as

$$\begin{split} \delta \widetilde{u}_{n_{0},k_{0}}\left(p,t\right) &= \left\langle \mu \tau e^{-ipw(t)|_{n_{0}-1,k_{0}}} \right\rangle + \left\langle \lambda\left(n_{0}\right) \tau e^{-ipw(t)|_{n_{0}+1,k_{0}}} \right\rangle \\ &- \left\langle \left(\mu + \lambda\left(n_{0}\right)\right) \tau e^{-ipw(t)|_{n_{0},k_{0}}} \right\rangle - k_{0}^{2} \left\langle D\left(n_{0}\right) \tau e^{-ipw(t)|_{n_{0},k_{0}}} \right\rangle \\ &- ip\tau \mathcal{F}_{r_{0} \to k_{0}} \left\{ \left\langle U(r_{0}) e^{-ipw(t)|_{n_{0},r_{0}}} \right\rangle \right\}, \end{split}$$
(B.4)

which is equivalent to (52) in Fourier space.

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