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Convergence of a Stochastic Method for the Modeling of Polymeric Fluids

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Abstract We present a convergence analysis of a stochastic method for numerical modeling of complex fluids using Brownian configuration fields (BCF) for shear flows. The analysis takes into account the special structure of the stochastic partial differential equations for shear flows. We establish the optimal rate of convergence. We also analyze the nature of the error by providing its leading order asymptotics.

Keywords Brownian Configuration Fields (BCF), convergence analysis, dumbbell model
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1 Introduction

Stochastic methods have become an increasingly popular tool in modeling complex fluids, including polymeric fluids, liquid crystal flows, suspension and sedimentation. By modeling directly the dynamics and conformation of the macromolecules or particles in the solvent, they provide a direct link between the structure of the solute and the properties of the flows. Furthermore, this approach bypasses the need for empirical constitutive relations. However, stochastic methods also suffer from well-known difficulties, namely that the accuracy is often poor and the results are noisy. Therefore it is very important to understand the error in such methods in order to improve their accuracy. In this paper we analyze one of the most competitive stochastic method that uses Brownian configuration fields in the simplest flow geometry, the shear flow. We establish optimal rate of convergence and we analyze the nature of the error by providing its leading order asymptotics.

This paper is organized as follows. In the next section we give a short review of the stochastic dumbbell models for polymeric fluids. In Section 3 we prove the optimal error estimates and in Section 4 we analyze the leading order asymptotics of the error. Some conclusions are drawn in Section 5.

2 Stochastic Dumbbell Models

We consider the simplest situation where the polymers are modeled by dumbbells with two

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beads connected by a spring. Such models are discussed extensively in [1]. The configuration of the dumbbell is specified by the positional vector for the spring, denoted by $\boldsymbol{Q}$. The spring is convected and stretched by the flow and at the same time experiences the spring and Brownian forces. In the BCF approach, $\boldsymbol{Q}$ is viewed as a field. Its equation is then given by

$$\frac{\partial}{\partial t}\boldsymbol{Q}(\boldsymbol{x},t) + (\boldsymbol{u}\cdot\nabla)\boldsymbol{Q}(\boldsymbol{x},t) = (\nabla\boldsymbol{u})^T\boldsymbol{Q}(\boldsymbol{x},t) - \frac{2}{\zeta}\boldsymbol{F}\big(\boldsymbol{Q}(\boldsymbol{x},t)\big) + \sqrt{\frac{4k_BT}{\zeta}}\dot{\boldsymbol{W}}(t), \tag{1}$$

where $\boldsymbol{u}$ is the velocity field, $\boldsymbol{F(Q)}$ is the spring force, and $\dot{\boldsymbol{W}}(t)$ is temporal white noise, k_B is the Boltzmann constant, T is the temperature, ζ is the friction coefficient. The velocity field satisfies the momentum equation

$$\frac{\partial\boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} + \nabla p = \nu_s\Delta\boldsymbol{u} + \nabla\cdot\tau_p, \qquad \nabla\cdot\boldsymbol{u} = 0, \tag{2}$$

where ν_s is the solvent viscosity, τ_p is the extra stress due to the polymers. In the dilute limit, this polymeric stress is given by Kramers expression:

$$\tau_p = -nk_BT\boldsymbol{I} + n\big\langle\boldsymbol{F}(\boldsymbol{Q})\otimes\boldsymbol{Q}\big\rangle, \tag{3}$$

where n is the number density per unit volume of the polymers, $\otimes$ is tensor product, and $\langle\cdot\rangle$ denotes averaging with respect to the white noise.

Two special cases of the spring force law are of particular interest. The Hookean model for which $\boldsymbol{F}(\boldsymbol{Q}) = H\boldsymbol{Q}$ and the FENE model for which $\boldsymbol{F}(\boldsymbol{Q}) = \frac{H\boldsymbol{Q}}{1-Q^2/Q_0^2}$.

Introducing the non-dimensional parameters:

$$De = \frac{T_r}{T_c}, \qquad Re = \frac{\rho UL}{\nu}, \qquad \gamma = \frac{\eta_s}{\eta}, \tag{4}$$

where T_r is the typical relaxation time scale of spring, T_c is the typical convection time scale. We can rewrite (1)–(3) in non-dimensionalized form:

$$\begin{aligned}
&\frac{\partial\boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} + \nabla p = \frac{\gamma}{Re}\Delta\boldsymbol{u} + \frac{1-\gamma}{Re\,De}\nabla\cdot\tau_p \\
&\nabla\cdot\boldsymbol{u} = 0, \qquad \tau_p = \big\langle\boldsymbol{F}(\boldsymbol{Q})\otimes\boldsymbol{Q}\big\rangle \\
&\frac{\partial\boldsymbol{Q}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{Q} = (\nabla\boldsymbol{u})^T\boldsymbol{Q} - \frac{1}{2De}\boldsymbol{F}(\boldsymbol{Q}) + \frac{1}{\sqrt{De}}\dot{\boldsymbol{W}}(t).
\end{aligned} \tag{5}$$

Models of this type are drastically different from traditional models of polymeric fluids that invoke empirical constitutive relations in order to obtain a Navier-Stokes-like hydrodynamic equations. For a comparison between these two types of models, we refer to [3,11,15].

Laso and Öttinger seem to be the first to introduce simulation methods based on stochastic models of the type (5). They designed the so-called CONNFFESSIT (Calculation of Non-Newtonian Flow: Finite Elements and Stochastic Simulation Technique). A collection of N dumbbells at each grid point are evolved according to

$$\begin{cases}
\dfrac{d\boldsymbol{x}}{dt} = \boldsymbol{u}(x,t), \\
\dfrac{d\boldsymbol{Q}}{dt} = (\nabla\boldsymbol{u})^T\boldsymbol{Q}(\boldsymbol{x},t) - \dfrac{2}{\zeta}\boldsymbol{F}\big(\boldsymbol{Q}(x,t)\big) + \sqrt{\dfrac{4k_BT}{\zeta}}\dot{\boldsymbol{W}}(t).
\end{cases} \tag{6}$$

The polymeric stress is then calculated at each grid point by ensemble averaging over the N dumbbells. CONNFFESSIT is a Lagrangian method that follows the trajectories of the dumbbells. As such, it suffers from standard problems associated with Lagrangian methods, e.g. the distortion of the grid. This problem is amplified by the noise.

To overcome these difficulties, Hulsen et. al introduced a method that is based on the dynamics of configuration fields. The full model is then (5) and Hulsen et. al solve (5) using Eulerian methods. The configurations of the dumbbells are modeled by N fields $\boldsymbol{Q}_i(\boldsymbol{x}, t),\ i = 1, \cdots, N$. $\boldsymbol{Q}_i$ evolves independently according to (1), and the extra stress is again computed through ensemble averaging over the N fields at each grid point. This approach eliminates the problem with the distortion of the grids and also reduces the noise in the results.

As these methods become increasingly popular, interests in the numerical analysis of these methods grow[11,15]. However this does not seem to be an easy task because of the presence of the nonlinearity and the randomness. In this paper, we study a simple setup for the flow—the shear flow. In this case, the model has some special structure that can be exploited for the purpose of numerical analysis.

3 Convergence Analysis for Shear Flows

In the special case of pressure driven shear flows, we have

$$\boldsymbol{u} = \begin{pmatrix} u \\ 0 \end{pmatrix}, \qquad \nabla = \begin{pmatrix} 0 \\ \partial_y \end{pmatrix}, \qquad \nabla p = \begin{pmatrix} c \\ 0 \end{pmatrix},$$

the simplified form of equation (5) will be

$$\begin{cases} \partial_t u + c = \dfrac{\gamma}{Re}\partial_{yy} u + \dfrac{1-\gamma}{ReDe}\partial_y \langle Q_1 Q_2 \rangle, \\ \partial_t Q_1 = \Big(\partial_y u Q_2 - \dfrac{1}{2De} Q_1\Big) + \dfrac{1}{\sqrt{De}}\dot{W}_1, \\ \partial_t Q_2 = -\dfrac{1}{2De} Q_2 + \dfrac{1}{\sqrt{De}} \dot{W}_2. \end{cases} \tag{7}$$

Here c is the pressure gradient that drives the flow. For simplicity, we have restricted ourselves to the case of Hookean dumbbells.

After dropping the parameters in the equation above (for notational ease), we have

$$\begin{cases} \partial_t u + c = \partial_{yy} u + \partial_y \langle Q_1 Q_2 \rangle, \\ dQ_1 = (\partial_y u Q_2 - Q_1)\, dt + dW_1, \\ dQ_2 = (-Q_2)\, dt + dW_2 \end{cases} \tag{8}$$

with boundary condition $u|_{y=0} = u|_{y=1} = 0$ and initial condition $u|_{t=0} = 0,\ Q_{1i}, Q_{2i} \sim N(0,1)$.

Without loss of generality, we will consider a finite difference discretization of the field equations. At each grid point, we place N configuration fields $\boldsymbol{Q}_i$. For simplicity, we will not consider spatial discretization here since the modification to the analysis brought by the spatial discretization is quite standard. Therefore we will consider the following discretization

$$\begin{cases} \dfrac{u^{n+1} - u^n}{\Delta t} + c = \partial_{yy} u^{n+1} + \partial_y (\langle Q_1^n Q_2^n \rangle_N), \\ Q_{1i}^{n+1} = Q_{1i}^n + (\partial_y u^n Q_{2i}^n - Q_{1i}^n)\Delta t + dW_{1i}^n, \\ Q_{2i}^{n+1} = Q_{2i}^n + (-Q_{2i}^n)\Delta t + dW_{2i}^n, \end{cases} \tag{9}$$

where $dW_{1i}^n,\ dW_{2i}^n$ are i.i.d. (independent identically distributed) $N(0, \Delta t)$ random variables. Here and in the following we use $\langle \cdot \rangle_N$ to denote empirical averages, e.g.

$$\langle Q_1^n Q_2^n \rangle_N \triangleq \frac{1}{N} \sum_{i=1}^{N} Q_{1i}^n Q_{2i}^n.$$

Similarly we define

$$\langle f(Q_1^n, Q_2^n)\rangle_N = \frac{1}{N}\sum_{i=1}^{N} f(Q_{1i}^n, Q_{2i}^n).$$

We will use $\mathbb{E}$ to denote expectation with respect to the noises in (9).

Define $e^n = u^n - u(t_n),\ t_n = n\Delta t,\ \|e^n\|_0 = (\int_0^1 (e^n)^2\,dy)^{\frac{1}{2}}$, we then have

Theorem 3.1. *If the solution of equation (8) $u \in C^2\big([0,+\infty], C^2([0,1])\big)$, and Δt is sufficiently small, then except for a set of probability $\frac{1}{\Delta t}e^{-\delta N}$, for some fixed $\delta > 0$, we have $\|e^n\|_0 \le C\big(\Delta t + \frac{\xi}{\sqrt{N}}\big)$, where C is a constant independent of N and Δt, and $E\xi^2 \le$ constant.*

In order to prove this result, we need the following lemma about the discretization of SDE.

Lemma 3.1[7,10]**.** *Consider the stochastic differential equation $dX_t = A(t, X_t)\,dt + B(t, X_t)\,dW_t$. The Euler scheme $X^{n+1} = X^n + A(t_n, X^n)\Delta t + B(t_n, X^n)(W^{n+1} - W^n)$ is of weak order one, i.e. for any continuous $g(t,x)$, $\big|\mathbb{E}\big(g(t_n, X_{t_n})\big) - \mathbb{E}\big(g(t_n, X^n)\big)\big| \le C_g\Delta t$.*

Proof of Theorem 3.1. Taylor expansion of equation (8) at $t = t_n$ gives

$$u(t_{n+1}) - u(t_n) + c\Delta t = \partial_{yy}u(t_{n+1})\Delta t + \big(\partial_y\langle Q_1Q_2\rangle(t_n)\big)\,\Delta t + O\,(\Delta t^2),$$

then we have

$$e^{n+1} = e^n + \Delta t\partial_{yy}e^{n+1} + \Delta t\partial_y\big(\langle Q_1^nQ_2^n\rangle_N - \langle Q_1Q_2\rangle(t_n)\big) + O\,(\Delta t^2)$$

and a simple energy estimate shows

$$\begin{aligned}\|e^{n+1}\|_0^2 \le & (1+L\Delta t)\,\|e^n\|_0^2 + L\Delta t\big\|\langle Q_1^nQ_2^n\rangle_N - \langle Q_1Q_2\rangle(t_n)\big\|_0^2 \\ & - L\Delta t\,\|\partial_y e^{n+1}\|_0^2 + O\,(\Delta t^3),\end{aligned} \tag{10}$$

where $L = \frac{1}{1-\Delta t}$ and we have assumed that Δt is sufficiently small. Here and in the following C represents generic positive constant independent of n and Δt.

Next we consider the error of stress term

$$\big\|\langle Q_1^nQ_2^n\rangle_N - \langle Q_1Q_2\rangle(t_n)\big\|_0^2. \tag{11}$$

The error term (11) comes from two sources: the discretization of time and the approximation of the expectation by ensemble averaging. These two errors should be handled separately. Consider first

$$\begin{cases} \widetilde{Q}_1^{n+1} = \widetilde{Q}_1^n + \Delta t(\partial_y u(t_n)\widetilde{Q}_2^n - \widetilde{Q}_1^n) + dW_1^n, \\ \widetilde{Q}_2^{n+1} = \widetilde{Q}_2^n + \Delta t(-\widetilde{Q}_2^n) + dW_2^n, \end{cases} \tag{12}$$

where $u(t_n)$ is the value of exact solution u at time t_n. By Lemma 3.1, we have

$$\big|\langle Q_1Q_2\rangle(t_n) - \langle\widetilde{Q}_1\widetilde{Q}_2\rangle(t_n)\big| \le C\Delta t,$$

where C is a constant independent of Δt. Hence we have

$$\big\|\langle Q_1Q_2\rangle(t_n) - \langle\widetilde{Q}_1\widetilde{Q}_2\rangle(t_n)\big\|_0^2 \le C\Delta t^2.$$

Next we consider the BCF discretization of equation (12)

$$\begin{cases} \widehat{Q}_{1i}^{n+1} = \widehat{Q}_{1i}^n + \Delta t(\partial_y u(t_n)\widehat{Q}_{2i}^n - \widehat{Q}_{1i}^n) + dW_{1i}^n, \\ \widehat{Q}_{2i}^{n+1} = \widehat{Q}_{2i}^n + \Delta t(-\widehat{Q}_{2i}^n) + dW_{2i}^n \end{cases} \tag{13}$$

for $i = 1, \cdots, N$, where dW_{1i}^n, dW_{2i}^n are the same as in equation (9).

Note that the $\{\widehat{Q}_i\}$'s are independent for different i, it follows that

$$\mathbb{E}\big|\langle\widetilde{Q}_1\widetilde{Q}_2\rangle(t_n) - \langle\widehat{Q}_1^n\widehat{Q}_2^n\rangle_N\big|^2 \le \frac{\mathrm{Var}\,(\widetilde{Q}_1\widetilde{Q}_2)}{N}.$$

Lemma 3.2. *Under the assumption of Theorem 3.1, we have*

$$\int Var(\widetilde{Q}_1\widetilde{Q}_2)\,dy \le C$$

for some constant C.

The proof of this lemma will be deferred to later.

Thus we get

$$\mathbb{E}\big\|\langle\widetilde{Q}_1\widetilde{Q}_2\rangle - \langle\widehat{Q}_1^n\widehat{Q}_2^n\rangle_N\big\|_0^2 \le \frac{C}{N}. \tag{14}$$

Define

$$R^n = \langle Q_1^nQ_2^n\rangle_N - \langle\widehat{Q}_1^n\widehat{Q}_2^n\rangle_N,$$

we can decompose the error of the stress term (11) into three parts

$$\begin{aligned}
&\big\|\langle Q_1Q_2\rangle(t_n) - \langle Q_1^nQ_2^n\rangle_N\|_0^2\\
\le&\|\langle Q_1Q_2\rangle(t_n) - \langle\widetilde{Q}_1^n\widetilde{Q}_2^n\rangle\big\|_0^2 + \big\|\langle\widetilde{Q}_1^n\widetilde{Q}_2^n\rangle - \langle\widehat{Q}_1^n\widehat{Q}_2^n\rangle_N\big\|_0^2 + \big\|\langle\widehat{Q}_1^n\widehat{Q}_2^n\rangle_N - \langle Q_1^nQ_2^n\rangle_N\big\|_0^2\\
\le&C(\Delta t)^2 + \|R^n\|_0^2 + \big\|\langle\widetilde{Q}_1^n\widetilde{Q}_2^n\rangle - \langle\widehat{Q}_1^n\widehat{Q}_2^n\rangle_N\big\|_0^2.
\end{aligned} \tag{15}$$

Define $R_{1i}^n = Q_{1i}^n - \widehat{Q}_{1i}^n$ and $(R_1^n)^2 = \frac{1}{N}\sum\limits_{i=1}^{N}(R_{1i}^n)^2$, and notice that Q_2 is independent of u and y, we have $Q_{2i}^n = \widehat{Q}_{2i}^n$, thus

$$\|R^n\|_0^2 = \big\|\langle(Q_1^n - \widehat{Q}_1^n)Q_2^n\rangle_N\big\|_0^2 \le \|R_1^n\|_0^2\left\langle(Q_2^n)^2\right\rangle_N.$$

In order to control $\left\langle(Q_2^n)^2\right\rangle_N$, we will use large deviation estimates. Let $K_k = \left\langle(\widetilde{Q}_2^k)^2\right\rangle = \mathbb{E}(Q_{2i}^k)^2$. It is not difficult to prove that $K_k \le C$ since Q_2^n is simply the discretized Ornstein-Uhlenbeck process. Then

$$\left\langle(Q_2^k)^2\right\rangle_N \to K_k$$

as $N \to +\infty$. Furthermore, from Cramer's theorem, we have

$$\mathrm{Prob}\left\{\left\langle(Q_2^k)^2\right\rangle_N > K_k + 1\right\} \le e^{-\delta N}$$

for some $\delta > 0$ (see [14]).

Let $\Omega_k = \left\{\omega \in \Omega, \left\langle(Q_2^k)^2\right\rangle_N > K_k + 1\right\}$. $\Omega^n = \bigcup\limits_{k=1}^{n}\Omega_k$. We will now assume $\omega\overline{\in}\Omega^n$. We have

$$\mathrm{Prob}\,(\Omega^n) \le ne^{-\delta N}.$$

Since

$$R_{1i}^{n+1} = R_{1i}^n + \Delta t(\partial_y e^n Q_{2i}^n - R_{1i}^n) = (1-\Delta t)R_{1i}^n + \Delta t\partial_y e^n Q_{2i}^n.$$

Time R_{1i}^{n+1} to both sides and apply Cauchy inequality we have

$$\left\langle(R_1^{n+1})^2\right\rangle_N \le (1 + C\Delta t)\left\langle(R_1^n)^2\right\rangle_N + \Delta t(1 + C\Delta t)\,|\partial_y e^n|^2. \tag{16}$$

Let

$$\|R_1^n\|_0^2 = \int_0^1 \left\langle(R_1^n)^2\right\rangle_N dy,$$

then

$$\|R_1^{n+1}\|_0^2 \le (1+C\Delta t)\,\|R_1^n\|_0^2 + \Delta t(1+C\Delta t)\,\|\partial_y e^n\|_0^2. \tag{17}$$

From (10), we have, on $(\Omega^n)^c$,

$$\begin{aligned}\|e^{n+1}\|_0^2 \le &(1+\Delta t L)\,\|e^n\|_0^2 + C\Delta t\big(\Delta t^2 + \big\|\langle \widetilde{Q}_1^n\widetilde{Q}_2^n\rangle - \langle \widehat{Q}_1^n\widehat{Q}_2^n\rangle_N\big\|_0^2 + \|R_1^n\|_0^2\big)\\ &- L\Delta t\|\partial_y e^{n+1}\|_0^2 + O\left(\Delta t^3\right).\end{aligned} \tag{18}$$

Combining the inequalities (8) and (7), and noticing that $1 < L \le C$, we have

$$\begin{aligned}&\big(\|R_1^{n+1}\|_0^2 + \|e^{n+1}\|_0^2 + \Delta t\|\partial_y e^{n+1}\|_0^2\big)\\ \le &(1+C\Delta t)\left(\|R_1^n\|_0^2 + \|e^n\|_0^2 + \Delta t\|\partial_y e^n\|_0^2\right) + C\Delta t^3 + \Delta t\big\|\langle \widetilde{Q}_1^n\widetilde{Q}_2^n\rangle - \langle \widehat{Q}_1^n\widehat{Q}_2^n\rangle_N\big\|_0^2.\end{aligned} \tag{19}$$

By using the discrete Gronwall inequality, we obtain

$$\big(\|R_1^n\|_0^2 + \|e^n\|_0^2 + \Delta t\|\partial_y e^n\|_0^2\big) \tag{20}$$

$$\le C(\Delta t)^2 + \Delta t\sum_{k\le n}(1+C\Delta t)^{n-k}\big\|\langle \widetilde{Q}_1^k\widetilde{Q}_2^k\rangle - \langle \widehat{Q}_1^k\widehat{Q}_2^k\rangle_N\big\|_0^2. \tag{21}$$

Let

$$\xi_n^2 = N\Delta t\sum_{k\le n}(1+C\Delta t)^{n-k}\big\|\langle \widetilde{Q}_1^k\widetilde{Q}_2^k\rangle - \langle \widehat{Q}_1^k\widehat{Q}_2^k\rangle_N\big\|_0^2,$$

then from inequality (14), we have $E\xi_n^2 \le \text{Const}$. Hence on $(\Omega^n)^c$, we have

$$\|e^n\|_0 \le C\Big(\Delta t + \frac{\xi_n}{\sqrt{N}}\Big)$$

with $E\xi_n^2 \le \text{Const}$.

This proves the Theorem 3.1.

Proof of Lemma 3.2. In order to prove

$$\int \mathrm{Var}\,(\widetilde{Q}_1\widetilde{Q}_2)\,dy \le C,$$

we only need to show

$$\int \mathrm{Var}\,(Q_1Q_2)\,dy \le C.$$

We get this by a simple application of Lemma 3.1.

Define

$$\begin{aligned}&b_{11} = \langle Q_1^2\rangle, && b_{12} = \langle Q_1Q_2\rangle, && b_{22} = \langle Q_2^2\rangle,\\ &b_{1122} = \langle Q_1^2Q_2^2\rangle, && b_{1222} = \langle Q_1Q_2^3\rangle, && b_{2222} = \langle Q_2^4\rangle,\end{aligned}$$

then $\mathrm{Var}\,(Q_1Q_2) = b_{1122} - b_{12}^2$, we have the differential equations from equation (7),

$$\begin{pmatrix} b_{1122}\\ b_{1222}\\ b_{2222}\end{pmatrix}_t = \begin{pmatrix} -4 & 2\partial_y u & 0\\ 0 & -4 & \partial_y u\\ 0 & 0 & -4\end{pmatrix}\begin{pmatrix} b_{1122}\\ b_{1222}\\ b_{2222}\end{pmatrix} + \begin{pmatrix} 1 & 0 & 1\\ 0 & 3 & 0\\ 0 & 0 & 6\end{pmatrix}\begin{pmatrix} b_{11}\\ b_{12}\\ b_{22}\end{pmatrix},$$

$$\begin{pmatrix} b_{11}\\ b_{12}\\ b_{22}\end{pmatrix}_t = \begin{pmatrix} -2 & 2\partial_y u & 0\\ 0 & -2 & \partial_y u\\ 0 & 0 & -2\end{pmatrix}\begin{pmatrix} b_{11}\\ b_{12}\\ b_{22}\end{pmatrix} + \begin{pmatrix} 1\\ 0\\ 1\end{pmatrix}.$$

The steady state is

$$b_{1122} = \frac{1}{4}\Big(b_{11} + \frac{3}{2}\partial_y u b_{12} + \Big(1 + \frac{3}{4}\partial_y u^2\Big) b_{22}\Big),$$
$$b_{11} = \frac{1}{2} + \frac{1}{4}\partial_y u^2, \qquad b_{12} = \frac{1}{4}\partial_y u, \qquad b_{22} = \frac{1}{2}.$$

Finally we have $b_{1122} - b_{12}^2 = \frac{1}{4} + \frac{3}{16}\partial_y u^2$ when t tends to $+\infty$, then

$$\int \mathrm{Var}\,(Q_1 Q_2)\,dy \le C$$

if $u \in H_0^1\big([0,1]\big)$.

4 Asymptotic Analysis of the Error

In this section, we analyze the leading order structure of the error. For simplicity we will only consider the discretization in probability space, i.e. the error due to replacing the expectation values by empirically averaged values.

Consider the following stochastic scheme

$$\frac{\partial \boldsymbol{u}^N}{\partial t} + (\boldsymbol{u}^N \cdot \nabla)\boldsymbol{u}^N + \nabla p = \Delta \boldsymbol{u}^N + \nabla \cdot \tau_p^N, \qquad \nabla \cdot \boldsymbol{u}^N = 0, \tag{22}$$

$$\tau_p^N = \frac{1}{N}\sum_{i=1}^{N} \boldsymbol{G}(\boldsymbol{Q}_i^N), \tag{23}$$

$$\frac{\partial \boldsymbol{Q}_i^N}{\partial t} + (\boldsymbol{u}^N \cdot \nabla)\boldsymbol{Q}_i^N = (\nabla \boldsymbol{u}^N)^T \boldsymbol{Q}_i^N - \boldsymbol{F}(\boldsymbol{Q}_i^N) + \dot{\boldsymbol{W}}_i(t), \tag{24}$$

where $\boldsymbol{G}(\boldsymbol{Q}_i^N) = \boldsymbol{F}(\boldsymbol{Q}_i^N) \otimes \boldsymbol{Q}_i^N$.

We will compare $\boldsymbol{u}^N$ with $\boldsymbol{u}$ and $\boldsymbol{Q}_i^N$ with $\boldsymbol{Q}_i$, where $\boldsymbol{Q}_i$ is the solution of

$$\frac{\partial \boldsymbol{Q}_i}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{Q}_i = (\nabla \boldsymbol{u})^T \boldsymbol{Q}_i + \boldsymbol{F}(\boldsymbol{Q}_i) + \dot{\boldsymbol{W}}_i(t). \tag{25}$$

The noise terms in (24) and (25) are assumed to be the same.

Write

$$\boldsymbol{u}^N(\boldsymbol{x},t) - \boldsymbol{u}(\boldsymbol{x},t) = \frac{1}{\sqrt{N}}\boldsymbol{v}(\boldsymbol{x},t) + \cdots, \tag{26}$$

$$\boldsymbol{Q}_i^N(\boldsymbol{x},t) - \boldsymbol{Q}_i(\boldsymbol{x},t) = \frac{1}{\sqrt{N}}\boldsymbol{q}_i(\boldsymbol{x},t) + \cdots, \tag{27}$$

where the omitted terms are smaller compared with $\frac{1}{\sqrt{N}}$. Substituting (26) and (27) into (22)–(24), we obtain equations for $\boldsymbol{q}_i$ and $\boldsymbol{v}$:

$$\frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{v} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{u} = \Delta \boldsymbol{v} + \nabla \cdot \langle \boldsymbol{G}'(\boldsymbol{Q})\boldsymbol{q}\rangle + \nabla \cdot \xi(\boldsymbol{x},t), \tag{28}$$

$$\frac{\partial \boldsymbol{q}_i}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{q}_i + (\boldsymbol{v} \cdot \nabla)\boldsymbol{Q}_i = (\nabla \boldsymbol{u})^T \boldsymbol{q}_i + (\nabla \boldsymbol{v})^T \boldsymbol{Q}_i - \boldsymbol{F}'(\boldsymbol{Q}_i)\boldsymbol{q}_i, \tag{29}$$

where ξ is the noise term arising from

$$\frac{1}{N}\sum_{i=1}^{N} \boldsymbol{G}(\boldsymbol{Q}_i) - \big\langle \boldsymbol{G}(\boldsymbol{Q})\big\rangle = \frac{1}{\sqrt{N}}\xi(\boldsymbol{x},t) + \cdots. \tag{30}$$

From central limit theorem, ξ is Gaussian.

Having obtained the leading order expression for the error, we can design numerical methods to further reduce the fluctuations. This will be the research topic in the future.

5 Conclusion

In this paper, we give a rigorous analysis of BCF applied to 1D pressure driven shear flow for Hookean dumbbell model under suitable assumption on the regularity of $\boldsymbol{u}$. The convergence analysis takes into account the special structure of the stochastic differential equations. We obtain optimal order of accuracy for the error: $O\,(\Delta t + N^{-\frac{1}{2}})$. The leading order asymptotics of the error is also analyzed.

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References

[1] Bird, R.B., Hassager, O., Armstrong, R.C., Curtiss, C.F. Dynamics of polymeric liquids, Vol.2: Kinetic theory. (2nd ed.), Wiley-Interscience, New York (1987)
[2] Doi, M., Edwards, S.F. The theory of polymer dynamics. Oxford University Press, New York (1986)
[3] Feng, J., Leal, L.G. Simulating complex flows of liquid crystalline polymers using the Doi theory. *J. Rheol.*, 41, 1317–1335 (1997)
[4] Fishman, G.S. Monte Carlo: concepts, algorithms, and applications. Springer-Verlag, Heidelberg, New York (1995)
[5] De Gennes, P.G. Scaling concepts in polymer physics. Cornell Univ. Press, Ithaca, London (1979)
[6] Hulsen, M.A., van Heel, A.P.G., van den Brule, B.H.A.A. Simulation of viscoelastic flows using Brownian configuration fields. *J. Non-Newtonian Fluid Mech.*, 70, 79–101 (1997)
[7] Kloeden, P.E., Platen, E. Numerical solution of stochastic differential equations. Springer-Verlag, Heidelberg, New York (1995)
[8] Laso, M., Öttinger, H.C. Calculation of viscoelastic flow using molecular models: the CONNFFESSIT approach. *J. Non-Newtonian Fluid Mech.*, 47, 1–20 (1993)
[9] Liu, T.W. Flexible polymer chain dynamics and rheological properties in the steady flows. *J. Chem. Phys.*, 90, 5826–5842 (1989)
[10] Milstein, G.N. Numerical integration of stochastic differential equations. Kluwer Academic Publishers, Dordrecht, London, Norwell, New York (1995) (Translated from Russian)
[11] Nayak, R. Molecular simulation of liquid crystal polymer flow: a wavelet-finite element analysis. Ph D Thesis, MIT (1998)
[12] Oksendal, B. Stochastic differential equations: an introduction with applications. (4th ed.), Springer-Verlag, Heidelberg, New York (1998)
[13] Öttinger, H.C. Stochastic processes in polymeric liquids. Springer-Verlag, Heidelberg, New York (1996)
[14] Varadhan, S.R.S. Large deviation and applications. SIAM Press, Philadelphia (1984)
[15] Suen, J.K.C., Joo, Y.L., Armstrong, R.C. Molecular orientation effects in viscoelasticity. *Annu. Rev. Fluid Mech.*, 34, 417–444 (2002)