On a variance reduction technique for the micro-macro simulations of polymeric fluids.

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Abstract

The micro-macro simulations of polymeric fluids couple the mass and momentum conservation equations at the macroscopic level, with a stochastic differential equation which models the evolution of the polymer configurations at the microscopic level (Brownian dynamics simulation). Accordingly, the system is discretized by a finite element method coupled with a Monte Carlo method. All the discrete variables are random, and the accuracy of the result highly depends on the variance of these random variables. We give here some elements of numerical analysis on the crucial issue of variance reduction in order to get results of a better quality for a given computational cost. The present analytical study only deals with a one dimensional case, but nevertheless gives a track for computational strategies that may apply to the more physically relevant two and three dimensional cases.

Key words: CONNFFESSIT, Dumbbells, FENE, Variance reduction

1 Introduction and motivation

1.1 Micro-macro models of dilute solutions

In this paper, we focus on some micro-macro models of dilute solutions of polymers. Let us introduce briefly these models which now give rise to a lively and

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expanding field of computational simulation for non-Newtonian fluid dynamics (we refer the reader to [1,2,4,6,14] for some comprehensive surveys of the physical background). For the "macroscopic" part, the evolution of the velocity $\mathbf{u}$ and the pressure p is described by the momentum and mass conservation equations:

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u}\cdot\nabla\mathbf{u}\right)=\eta_s\Delta\mathbf{u}-\nabla p+\text{div }(\boldsymbol{\tau}_p)\ , \tag{1}$$

$$\text{div }(\mathbf{u})=0\ , \tag{2}$$

where $\boldsymbol{\tau}_p$ is an extra-stress tensor, due to the contribution of polymers. In order to derive the expression of this extra-stress tensor, one can use kinetic models of polymers. We deal here with the "dumbbell" model (a particular case of the Rouse model) in which a polymer is described by two beads linked by a spring (see Figure 1). The expression of the entropic force $\mathbf{F}$ in the spring, in term of the so-called end-to-end vector $\mathbf{X}$, can have more or less complicated expression, depending on the effects taken into account (excluded volume effects, finite extensibility of the polymer,...). We deal here with two types of forces (but our method is likely to apply to other cases of forces): a linear force: $\mathbf{F}(\mathbf{X})=\mathbf{F}_{HOOK}(\mathbf{X})=H\mathbf{X}$ (model of "Hookean dumbbells") or a non-linear force which takes into account the finite extensibility of the polymer (described by the non-dimensional parameter b): $\mathbf{F}(\mathbf{X})=\mathbf{F}_{FENE}(\mathbf{X})=H\frac{\mathbf{X}}{1-\frac{||\mathbf{X}||^2}{bk_BT/H}}$ (model of "FENE dumbbells"). The "microscopic" part of the model is the description of the evolution of the end-to-end vector $\mathbf{X}$ through a stochastic partial differential equation (Brownian dynamics simulation):

$$d\mathbf{X}+\mathbf{u}\cdot\nabla\mathbf{X}dt=\left(\nabla\mathbf{u}\mathbf{X}-\frac{2}{\zeta}\mathbf{F}(\mathbf{X})\right)dt+\frac{\sqrt{2}\sigma}{\zeta}d\mathbf{W}_t, \tag{3}$$

where ζ is a friction coefficient, $\sigma^2=2k_BT\zeta$ (T is the temperature) and $\mathbf{W}_t$ is a standard (multi-dimensional) Brownian motion. The expression of this extra-stress tensor $\boldsymbol{\tau}_p$ is then given by an expectation of a function of the configurations of the polymers (this is the Kramers expression):

$$\boldsymbol{\tau}_p=n\mathbb{E}(\mathbf{X}\otimes\mathbf{F}(\mathbf{X}))-nk_BT\text{Id}, \tag{4}$$

where n denotes the concentration of polymers.

It is to be noted that the "Hookean dumbbell" model described by equations (1), (2), (3) and (4), with $\mathbf{F}=\mathbf{F}_{HOOK}$ is equivalent to the famous Oldroyd-B model, which is usually written in a purely macroscopic differential or integral form (see [2] page 72). On the other hand, no closed differential or integral

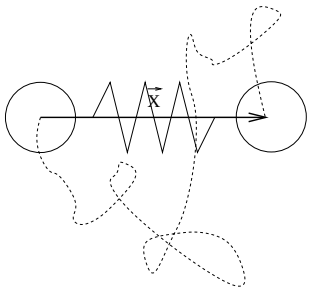


Fig. 1. The polymer (in dashed line) is modeled by a "dumbbell": two beads linked by a spring. The vector $\mathbf{X}$ which goes from one bead to the other is called the end-to-end vector.

equations on $\boldsymbol{\tau}_p$ have been found to be equivalent to the more realistic FENE model. Being more general than the purely macroscopic approach, the micro-macro approach seems all the more promising.

Once the system (1)-(4) is non-dimensionalised, it has the following form:

$$\mathrm{Re}\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = (1-\epsilon)\Delta\mathbf{u} - \nabla p + \mathrm{div}\,(\boldsymbol{\tau}_p)\ , \tag{5}$$

$$\mathrm{div}\,(\mathbf{u}) = 0\ , \tag{6}$$

$$\boldsymbol{\tau}_p = \frac{\epsilon}{\mathrm{We}}(\mu\mathbb{E}(\mathbf{X}\otimes\mathbf{F}(\mathbf{X})) - \mathrm{Id})\ , \tag{7}$$

$$d\mathbf{X} + \mathbf{u}\cdot\nabla\mathbf{X}dt = \left(\nabla\mathbf{u}\mathbf{X} - \frac{1}{2\mathrm{We}}\mathbf{F}(\mathbf{X})\right)dt + \frac{1}{\sqrt{\mathrm{We}\,\mu}}d\mathbf{W}_t, \tag{8}$$

with the following non-dimensional numbers:

$$\mathrm{Re} = \frac{\rho U L}{\eta}\ ,\ \mathrm{We} = \frac{\lambda U}{L}\ ,\ \epsilon = \frac{\eta_p}{\eta}\ ,\ \mu = \frac{L^2 H}{k_b T}\ , \tag{9}$$

and the following non-dimensional forces:

$$\mathbf{F}_{HOOK}(\mathbf{X}) = \mathbf{X}\ ,\ \mathbf{F}_{FENE}(\mathbf{X}) = \frac{\mathbf{X}}{1 - \frac{\mu||\mathbf{X}||^2}{b}}\ . \tag{10}$$

The numbers U and L denote the characteristic velocity and length, while λ (a relaxation time of the polymers) and η_p (the viscosity associated to the polymers) are defined by $\lambda = \frac{\zeta}{4H}$ and $\eta_p = nk_BT\lambda$.

This problem can be discretized by the so-called CONNFFESSIT method (see [10]), coupling a finite element method to discretize equations (5)-(6), standard Euler schemes in time for (5) and (8), and a Monte Carlo method to approximate the stress $\boldsymbol{\tau}_p$ in (7). Compared with a deterministic approach

which solves directly the Fokker-Planck equation associated to (8), the convergence of this stochastic approach scales efficiently with respect to the number of springs in the Rouse chain. However, the leading error in this kind of discretization is a statistical error due to the Monte Carlo method, and depends on the variance of the variables. Our aim here is to study the dependency of these variances in terms of the numerical parameters of the discretization.

More precisely, many authors (see Halin, Lielens, Keunings and Legat in [7] or Bonvin and Picasso in [3]) have observed that using a Brownian motion in (8) which does not depend on space, rather than a collection of Brownian motions uncorrelated from one Lagrangian trajectory to another, leads on the discretized problem to a reduction of the variance of the velocity $\mathbf{u}$ but also to an increase of the variance of the stress $\boldsymbol{\tau}_p$. After a discussion about the space-dependency of the Brownian motion in Section 2, we analyze in Section 3 this problem in the case of a pure shear flow. The momentum and mass conservation equations then reduce to a scalar heat equation (see Eq. (14) below). We then completely analyze the case of the long time behavior of the variances for Hookean dumbbells and recover by our analysis the observations mentioned above. We are also able to propose a strategy to reduce the variance on the stress in the shear flow case, at a given computational cost, by choosing an *ad hoc* correlation in space for the Brownian motion. In Section 4, we numerically test our strategy for Hookean and FENE springs in the one-dimensional case, leaving for the future numerical tests in dimensions 2 and 3. Other related issues are also addressed in this paper, such as the dependency of the variances in terms of the boundary conditions (see Remark 7) and the space step (see Section 5), or the dependency of the bias upon the number of realizations (see Section 5).

Remark 1 *Let us note that we do not consider in this paper other variance reduction methods like control variate methods or importance sampling methods, see [10,13,14] about these subjects.*

2 The dependency of the Brownian motion in space

As mentioned above, the main subject of the present work is the dependency upon the space variable of the Brownian motion $\mathbf{W}_t$. Let us look at this question from different viewpoints: the modeling viewpoint, that of the numerical simulations, and the mathematical viewpoint.

2.1 The modeling viewpoint

We recall that the derivation of (8) from kinetic theory requires that the Brownian motion on one bead of the dumbbell is independent of the Brownian motion which acts on the other bead (completely uncorrelated Brownian motion in space, see e.g. [14]). The modeling step therefore pushes forward the uncorrelated framework. Note however that this simple presentation is a little bit controversial in itself, as it may also seem quite natural that some kind of correlation in space between the Brownian motions appears (see [7] page 394). Indeed, the Brownian motion seen by a particle convected on one trajectory of the flow is somewhat correlated, at least at a sufficiently small scale, to another Brownian motion seen by a particle which follows a trajectory "close to the first one" (see Figure 2). The notion of "trajectory dependent" Brownian motion, that we will introduce and develop later in this section, is thus likely to be relevant. In the following, we will not discuss further the modeling and physical aspects of the correlation in space of the Brownian motions used. We rather focus on the numerical counterparts of these correlations.

2.2 The numerical viewpoint

Historically, the first of the two currently adopted approaches for the numerical simulation of (5)-(8) namely the CONNFFESSIT method, mimicked the modeling viewpoint. This method couples the macro-scale simulation with the Lagrangian approach for the micro-scale The first simulations (performed first on the start-up of a shear flow problem) accordingly made use of completely uncorrelated in space Brownian motions (see [10]). When the state of the art went to 2D simulations (see [11]), a Lagrangian computation of (8) was naturally adopted. In this framework, the authors used one Brownian motion per trajectory, all of them being independent from one another. Therefore, we may think of a collection of uncorrelated Brownian motions labelled by Lagrangian trajectories.

The second approach is the Eulerian one. It consisted in introducing the notion of configuration fields (see [8]): the end-to-end vector $\mathbf{X}_t$ is seen as an Eulerian variable that explicitly depends on the space variable $\mathbf{x}$. Equation (8) may then be solved in an Eulerian setting, which greatly simplifies the numerical implementation of the CONNFFESSIT method (no dumbbell tracking, no problem of dumbbell deletion or dumbbell relocation). In this approach, it is of course easier to take Brownian motions not depending on space. Nevertheless, one can imagine to keep the Brownian motions of the Lagrangian approach (a collection of uncorrelated Brownian motions labelled by the trajectories), for example by using a characteristic method to solve (8), but this road was

not followed. In fact, the use of configuration fields together with Brownian motions not depending on space has revealed to be a very efficient method to reduce variance of the velocity $\mathbf{u}$. In spite of the fact that the modeling issue is not settled, the use of a Brownian motion not depending on space on the discretized system can be seen as a pure numerical trick, that leads to a reduction of the variance of the velocity $\mathbf{u}$. Intuitively, this fact may be understood, since in (5), a derivative with respect to $\mathbf{x}$ of the stress is involved. But the situation is not so clear either. What is indeed counterintuitive (see Halin, Lielens, Keunings and Legat in [7] page 397 or Bonvin and Picasso in [3] page 197) is the fact that, contrary to what happens for the velocity field, the variance on the stress $\boldsymbol{\tau}_p$ increases when one goes from uncorrelated Brownian motions to a Brownian not depending on $\mathbf{x}$. Despite the lack of a theoretical understanding of this phenomenon, experts of the field seem to agree in the numerical simulations on the use of Brownian motions not depending on space, mainly because it leads to less noisy results in space, and because it greatly reduces the variance on the velocity. The state of the art of the numerical simulations seems to stay today on this point: use a Brownian motion not depending on space (see [8,15]).

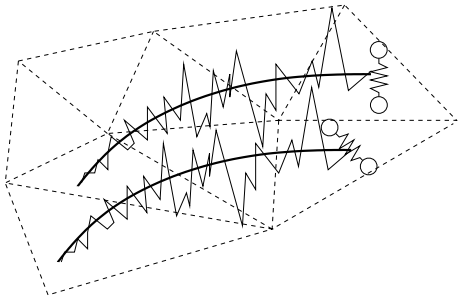


Fig. 2. Trajectories of two dumbbells, ending in two different cells: does each dumbbell "sees" the same noise, as is represented on this figure ?

2.3 The mathematical viewpoint

Let us now turn to mathematics. It is to be made precise at once that it is not straightforward to give a sense to the Eulerian system (5)-(8) at the continuous level with a Brownian motion depending on space. There are three ways to avoid the treatment of this delicate question. The first is to stay at the continuous level and turn to the Lagrangian form of (8) with Brownian motions depending on the trajectory. The second is to go at the discrete level: once being discretized in space, it is easy to give a proper meaning to (5)-(8), and to play with the dependence in space of the Brownian motion. A third way is to treat the shear flow case. Let us details these three approaches.

The continuous level

Let us introduce the Lagrangian form of (8), namely

$$d\tilde{\mathbf{X}}_t(\mathbf{x}) = \Big(\nabla \mathbf{u}(\mathbf{c}(0,\mathbf{x},t))\tilde{\mathbf{X}}_t(\mathbf{x}) - \frac{1}{2\mathrm{We}}\mathbf{F}(\tilde{\mathbf{X}}_t(\mathbf{x}))\Big)\,dt + \frac{1}{\sqrt{\mathrm{We}\,\mu}}d\tilde{\mathbf{W}}^{\mathbf{x}}_t, \quad (11)$$

where $\tilde{\mathbf{X}}_t(\mathbf{x}) = \mathbf{X}_t(\mathbf{c}(0,\mathbf{x},t))$ and

$$\begin{cases} \frac{d}{dt}\mathbf{c}(s,\mathbf{x},t) = \mathbf{u}(t,\mathbf{c}(s,\mathbf{x},t)), \\ \qquad\qquad \mathbf{c}(s,\mathbf{x},s) = \mathbf{x}. \end{cases} \quad (12)$$

We suppose here that the velocity field $\mathbf{u}(t,\mathbf{x})$ is smooth enough to define the characteristics. The stress $\tilde{\boldsymbol{\tau}_p}$ defined by (7), is then obtained by the following formula:

$$\tilde{\boldsymbol{\tau}_p}(t,\mathbf{x}) = \frac{\epsilon}{\mathrm{We}}\Big(\mu\mathbb{E}\Big(\tilde{\mathbf{X}}_t(\mathbf{c}(t,\mathbf{x},0)) \otimes \mathbf{F}(\tilde{\mathbf{X}}_t(\mathbf{c}(t,\mathbf{x},0)))\Big) - \mathrm{Id}\Big). \quad (13)$$

Notice that the stochastic differential equations (11) indexed by $\mathbf{x}$ are rigorously defined and are not coupled in space by (13).

Let us now consider a smooth solution $(\mathbf{u},\boldsymbol{\tau}_p)$ of (5)-(8) obtained with a Brownian motion which does not depend on the space variable, and asigns to each trajectory obtained by solving (12) a Brownian motion. Since the law of $\tilde{\mathbf{X}}$ (solution of (11)) is not influenced by the way the Brownian motions depend on the trajectory, we have $\tilde{\boldsymbol{\tau}_p} = \boldsymbol{\tau}_p$. Therefore, $(\mathbf{u},\boldsymbol{\tau}_p)$ will remain a solution to (5)-(8), whatever the dependency of the Brownian motions on the trajectory is. In other words, we have proved that the continuous solution $(\mathbf{u},\boldsymbol{\tau}_p)$ does not depend on the the way the Brownian motions depend on the trajectory, provided that the solution of the problem is unique and smooth enough.

The discrete level

Once the system (5)-(8) is discretized in space (say, by a finite element method, to fix the ideas), it is easy to give a proper meaning to (8) with a Brownian motion depending on space being understood that we in fact deal with a Brownian motion which depends polynomialy on the space variable (i.e. a discrete-in-space Brownian motion). Then, once one approaches the expectation (7) by an empirical mean, the results (and in particular their variances) may depend on the way the Brownian motion depends on trajectories.

If one considers that the scheme converges in the limit of the space step h and the time step δt go to zero, and the number of realizations goes to infinity, two questions then arise: May the limit depend on the dependency in space of the Brownian motions used ? What is the "best dependency" as far as the variance of the results is concerned ?

To the best of our knowledge, the first question is open: note for instance that contrary to the shear flow case, in a general geometry, the "discrete" streamlines themselves may be influenced by the dependency in space of the Brownian motion. As was pointed out in [15] (page 259), by using Brownian motions not depending on space, "completely unphysical correlations in the random forces at different positions are introduced". This crucial point would need further investigations.

Concerning the second question about the variance of the results, we have already pointed out that using a Brownian motion not depending on space leads to a reduction of the variance of the velocity $\mathbf{u}$, but an increasing of that on $\boldsymbol{\tau}_p$. Thus the natural question arises to find the best correlation in space, for the discrete-in-space Brownian, that will lead *in fine* to the least variance in the result for *both* $\mathbf{u}$ and $\boldsymbol{\tau}_p$.

The case of the shear flow

Let us now concentrate on the shear flow case, which will be the framework of the rest of this article. In this special geometry (see Figure 3 below), the transport term $\mathbf{u} \cdot \nabla \mathbf{X}$ vanishes on the left hand side of (8). Therefore, the streamlines are fixed, and one can then rigorously define, at the continuous level, the stochastic differential equation (8) for Brownian motions indexed by the space variable y. A given stochastic differential equation at macro point y does not interact with another one, at point $y' \neq y$, since (7) is a point-wise expectation. Therefore, the continuous solution $(\mathbf{u}, \boldsymbol{\tau}_p)$ does not depend on the way the Brownian motions depend on the space variable y (see Remark 8 in [9]).

Once the system is discretized, in the case of a shear flow and for Hookean dumbbells, we have shown in [9] that the convergence of the CONNFFESSIT scheme towards the unique continuous solution $(\mathbf{u}, \boldsymbol{\tau}_\mathbf{p})$ holds, whatever the correlation in space of the discrete-in-space Brownian motions is.

One aim in Section 3 is to contribute to the understanding of all the above observations and remarks. For this purpose, we consider a simple case, namely the start-up of shear flow problem which has been considered as a test case in many papers (see [10,15,3]). In this simple geometry, the Lagrangian and the Eulerian formulations are the same. The classical approaches adopted in the literature therefore amount in this case to the following alternative: the Brownian motions in each cells of the space discretization are either the same or completely uncorrelated. One could imagine to use other correlations in space of the Brownian motions, and this will be investigated in Section 3. It would even be possible to introduce correlations in space different from one time-step to another, but we have not considered this possibility in the following.

3 Explicit computations of variances in a simple case

3.1 A simple model: the pure shear flow

In order to simplify the problem and enable explicit computations, we consider in the following a simple geometry of the flow namely a pure shear flow (see Figure 3). Due to this special geometry, the velocity becomes a one-

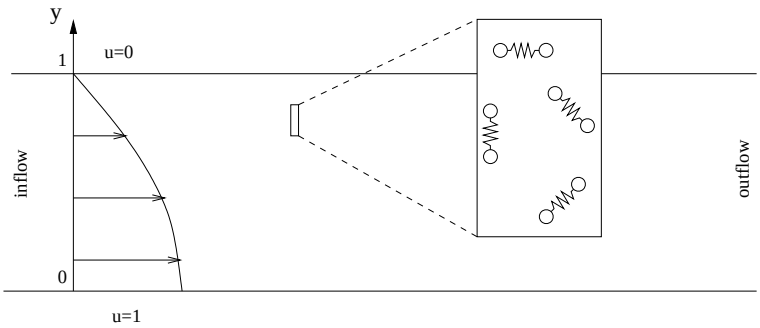


Fig. 3. Velocity profile in a shear flow of a dilute solution of polymers.

dimensional variable: $\mathbf{u}(t,\mathbf{x}) = (u(t,y),0)$, with the notation $\mathbf{x} = (x,y)$, and therefore the convective derivative $\mathbf{u}.\nabla$ is zero. One can thus show that the mass and momentum conservation equations reduce to a scalar heat equation. In addition to the above simplification of the geometry, we consider Hookean dumbbells. In the following, in order to simplify the notation, we choose the following values for the non-dimensional numbers: $\mathrm{Re} = 1/2$, $\mathrm{We} = 1$, $\epsilon = 1/2$, $\mu = 1$. Thus, the system (5)-(8) can be written in the following form:

$$\frac{\partial u}{\partial t}(t,y) = \frac{\partial^2 u}{\partial y^2}(t,y) + \frac{\partial\, \mathbb{E}(Y_t X_t(y))}{\partial y} \ , \tag{14}$$

$$dX_t(y) = \left(\frac{\partial u(t,y)}{\partial y} Y_t - \frac{X_t(y)}{2}\right) dt + dW_t(y) \ , \tag{15}$$

$$dY_t = -\frac{Y_t}{2} dt + dV_t \ , \tag{16}$$

where we have adopted the following notation for the components of $\mathbf{X}$ and $\mathbf{W}_t$: $\mathbf{X} = (X,Y)$ and $\mathbf{W}_t = (W_t, V_t)$. The system of equations is supplied with the following boundary and initial conditions:

$$u(0,y) = 0,\ X_0 \sim \mathcal{N}(0,1),\ Y_0 \sim \mathcal{N}(0,1),\ (X_0 \text{ and } Y_0 \text{ independent}),$$

$$u(t,0) = v(t) = v \min(1, 10\, t/T) \ ,\ u(t,1) = 0,$$

where T denotes the final time of the simulation and v is a constant denoting the velocity on the boundary, after a transition period in time of length $T/10$.

Note that, as explained in Section 2, we may let the Brownian motion W_t depend on space, and more precisely (see discussion above in Section 2) on trajectory. In the case that we consider, namely a shear flow, one can simply label the Brownian motions by the space variable y. The question is therefore how to define a process $(W_t(y))_{t\geq 0, y\in(0,1)}$. We impose the following constraints on the process $(W_t(y))_{t\geq 0, y\in(0,1)}$:

a) The process $(t, y) \to W_t(y)$ is a Gaussian process,
b) For a fixed $y \in (0, 1)$, $t \to W_t(y)$ is a Brownian motion,
c) The covariance in space $\mathbb{E}(W_t(x)W_t(y))$ does not depend on the time variable t.

Constraint b) is natural. We impose a) and c) in order to simplify and enable explicit computations. These assumptions clearly restrict the field of all possible $W_t(y)$ but we nevertheless believe they are general enough. Note that because of assumption a), the process $W_t(y)$ is completely determined by its covariance function.

We have chosen not to let the Brownian motion V_t depend on space since the process Y_t defined by (16) can be computed independently of the other unknowns u and X (see formula (24)). This point is of course specific to the Hookean case and will be modified in the FENE case (see Eq. (40) below).

3.2 The discretized problem

The CONNFFESSIT method applied to discretize system (14)-(16) can be written in the following way: assuming u_h^n, $X_{h,n}^j$ and Y_n^j are known, find $u_h^{n+1} \in V_h$ such that, for all $v \in V_h$,

$$\frac{1}{\delta t}\int_y (u_h^{n+1} - u_h^n)v = -\int_y \frac{\partial u_h^{n+1}}{\partial_y}\frac{\partial v}{\partial_y} - \int_y \tau_{h,n}\frac{\partial v}{\partial_y}, \tag{17}$$

$$\tau_{h,n} = \frac{1}{R}\sum_{j=1}^{R} X_{h,n}^j Y_n^j, \tag{18}$$

$$X_{h,n+1}^j - X_{h,n}^j = \left(\frac{\partial u_h^{n+1}}{\partial y}Y_n^j - \frac{1}{2}X_{h,n}^j\right)\delta t + \left(W_{h,t_{n+1}}^j - W_{h,t_n}^j\right), \tag{19}$$

$$Y_{n+1}^j - Y_n^j = -\frac{1}{2}Y_n^j\delta t + \left(V_{t_{n+1}}^j - V_{t_n}^j\right). \tag{20}$$

The indices n and j respectively denote the time index and the realization index: we indeed consider R trajectories of the random variables $X_{h,n}$ and Y_n ($1 \leq j \leq R$). The time interval $(0, T)$ is divided into N intervals, $\delta t = T/N$ and $t_n = n\,\delta t$. The subscript h indicates that we are considering space

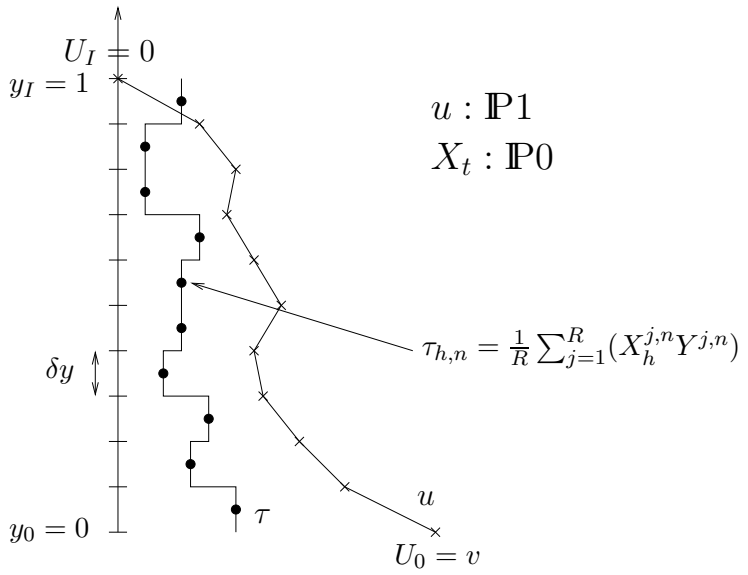


Fig. 4. Discretization of u and τ.

discretized variables. The random variables $\tau_{h,n}$ (or more precisely $\frac{1}{2}\tau_{h,n}$) are approximations of the off-diagonal component of the stress $\boldsymbol{\tau}_p$. The space of discretization V_h is a finite element space. In the following, we consider $V_h = \mathbb{P}1$, the space of continuous piecewise affine functions on a mesh of I cells of the interval $(0,1)$: $(y_0 = 0, y_1, ..., y_I = 1)$. The random variables $X^j_{h,n}$, $\tau_{h,n}$ and $\left(W^j_{h,t_{n+1}} - W^j_{h,t_n}\right)_{j,n}$ belong therefore naturally to the space $\partial_y V_h$ (in our case, $\partial_y \mathbb{P}1 = \mathbb{P}0$, see Figure 4). We can therefore associate to the piecewise constant in space functions $X^j_{h,n}$ and $\left(W^j_{h,t_{n+1}} - W^j_{h,t_n}\right)_{j,n}$ two vectors whose components are the values of these random variables on each cell (y_{i-1}, y_i) of the mesh: $\left(X^j_{i,n}\right)_{1\leq i\leq I}$ and $\left(W^j_{i,t_{n+1}} - W^j_{i,t_n}\right)_{1\leq i\leq I}$. Let us make precise that for $1 \leq j \leq R$, the processes $\left(W^j_{1,t}, ..., W^j_{I,t}, V^j_t\right)_{0\leq t\leq T}$ are independent and identically distributed Gaussian processes whose components are standard Brownian motions, the last one being independent from the first I ones. For a mathematical analysis of the system (14)-(16), and the convergence of the CONNFFESSIT method in this case, we refer to [9,12,5].

We now want to introduce some notation to make precise the dependency on space of the space-discretized Brownian motion $W^j_{h,t}$. Throughout this section, we will omit the superscript j which denotes the realization index, since the law of $W^j_{h,t}$ does not depend on j.

Since we choose a correlation in space which does not depend on time, the parameter we will consider in the following is the correlation matrix in space K defined by

$$K_{l,m} = \frac{1}{t}\mathbb{E}(W_{l,t}W_{m,t}), \tag{21}$$

where $1 \leq l \leq I$ and $1 \leq m \leq I$ denote two cell indices. With a slight abuse of

notation, we denote by W_t the I-dimensional process whose components are $W_{i,t}$: $W_t = (W_{1,t}, ..., W_{I,t})$, and thus, $K = \frac{1}{t}\mathrm{Cov}(W_t) = \frac{1}{t}\mathbb{E}(W_t \otimes W_t)$, where $\otimes$ denotes the tensorial product (for two vectors a and b in $\mathbb{R}^d$, $a \otimes b$ is the $d \times d$ matrix whose components are $(a_i\, b_j)_{1 \leq i \leq d,\, 1 \leq j \leq d}$).

If the components of W_t are independent, then $K = \mathrm{Id}$ and if the components of W_t are the same (W_t is not depending on space), then $K = J$, where J henceforth denotes the matrix with all components equal to 1.

In practice, in order to build the Brownian motion $W_t = (W_{1,t}, ..., W_{I,t})$, we consider a I-dimensional Brownian motion $\overline{W}_t$ (whose components are independent 1-dimensional Brownian motions) and compute W as an image by a linear application of $\overline{W}$: $W_t = N\overline{W}_t$ (N is a $I \times I$ matrix such that each line has an Euclidean norm equal to one). Therefore, $K = N({}^tN)$. To construct a Brownian motion not depending on space, one can take N such that $N_{i,j} = \delta_{1,j}$ and thus $K = J$ (δ denotes the Kronecker function). To build uncorrelated Brownian motions in space, one can consider $N = \mathrm{Id}$ and thus $K = \mathrm{Id}$.

In our simple case, one can consider that the correlation in space matrix K is just a numerical parameter. Indeed, we have shown (see Remark 8 in [9]) that whatever the correlation in space is, the scheme converges towards a unique solution $(u(t,y), \mathbb{E}(Y_t X_t(y))$. Therefore, the matrix K (or N) can be seen as another numerical parameter, that can be used to reduce the prefactor in the error $O(1/\sqrt{R})$ due to the Monte Carlo discretization (R denotes the number of realizations).

Note that in our numerical simulations (see Section 4), the spatial correlation of the initial variables is the same as the spatial correlation of the Brownian motions.

This simple problem presents the behavior already noticed in more complicated geometry: when one goes from $K = \mathrm{Id}$ (uncorrelated Brownian motions in space) to $K = J$ (a Brownian motion not depending on space), the variance on the velocity u_h^n decreases but the variance on the stress $\tau_{h,n}$ increases (see Section 4 and the curves labelled 'Wt(y)' and 'Wt' on Figure 6).

Remark 2 *One important remark is that the counterintuitive reduction of variance on the stress when one takes Brownian motions completely uncorrelated in space is intimately due to the coupling (in a probabilistic sense) between the variables u and X, or in other terms to the nonlinearity of the problem. If one performs the same simulation, but uses a pre-computed deterministic velocity u in (15), then the variance on τ is* not *reduced. Let us make precise this point. First observe that one can compute explicitly the expectations $\mathbb{E}(X_{h,n}Y_n)$ in the simple case of a shear flow, and use this deterministic computations to obtain a deterministic velocity u_h^n. One can then use this deterministic velocity*

in the computation of the stress with a Monte Carlo method in (18)-(20) and check that, whatever the correlation in space is, the variance obtained on τ for long time is about 0.058*, which is what we obtained in the worst case for the coupled system (see the curve labelled 'Wt' on Figure 6).*

Remark 3 *In [7], the authors have proposed the following explanation for the unexpected behavior of the variance on the stress: with Brownian motions not depending on space (and accordingly initial random variables not depending on space), the initial equilibrium distribution may not be correctly sampled. We have performed the computation with initial random variables uncorrelated in space and Brownian motions not depending on space and observed the same large variance on the stress, which seems to indicate, at least in the simple case considered here, that the major role is played by the space correlation of the Brownian motions and not by the initial value of the random variables.*

3.3 Dependency of the variance in term of the correlation in space

3.3.1 Computation of the variances

In the following, we want to explicitly compute the variances of the velocity and the stress solutions of the system (14)-(16). In order to enable explicit computations, we make the following simplifications:

- we focus on the long-time behavior of the system (14)-(16),
- accordingly to the previous assumption, we take $\dfrac{\partial u}{\partial t} = 0$ in (14),
- we consider only the space and Monte Carlo discretized system (no discretization in time),
- we consider only one dumbbell (i.e. one realization: $R = 1$).

We have checked all the conclusions we draw on this simplified case by numerical experiments on the long-time behavior of the time-dependent problem, for both Hookean and FENE dumbbells (see Section 4 below).

Taking into account these simplifications, we consider, instead of (14)-(16), the following system of equations:

$$-\frac{\partial^2 u(t,y)}{\partial y^2} = \frac{\partial\, \mathbb{E}(Y_t X_t(y))}{\partial y}, \tag{22}$$

$$dX_t(y) = \left(\frac{\partial u(t,y)}{\partial y} Y_t - \frac{X_t(y)}{2}\right) dt + dW_t(y), \tag{23}$$

$$Y_t = e^{-\frac{t}{2}} Y_0 + \int_0^t e^{\frac{s-t}{2}}\, dV_s. \tag{24}$$

Accordingly to Section 3.2, we consider a $\mathbb{P}1$ discretization in space on a uniform grid with I intervals (the space step is $\delta y = 1/I$). Since we consider only one dumbbell, we obtain the following discretization of (22)-(24), written in an algebraic form:

$$-MU(t) = Y_t B X_t + \mathrm{b}_1', \tag{25}$$

$$dX_t = \left(Y_t C U(t) + Y_t\, \mathrm{b}_2' - \frac{X_t}{2} \right) dt + dW_t, \tag{26}$$

where Y is a process with value in $\mathbb{R}$ defined by (24), U is a vector of size $(I-1)$ (because $u(y=0)$ and $u(y=1)$ are known) and X_t is now a $\mathbb{R}^I$-valued process (the $i-th$ components is the value of the discretization of X_t in cell (y_{i-1}, y_i)). Accordingly, W_t is now a process with value in $\mathbb{R}^I$. The matrices M, B and C are respectively of size $(I-1)\times(I-1)$, $(I-1)\times I$ and $I\times(I-1)$. One can easily check that, should the grid be uniform or not:

$$BC = M. \tag{27}$$

Here, we use a uniform grid in space and we obtain the finite differences matrices:

$$M = \frac{1}{\delta y^2} \begin{bmatrix} -2 & 1 & 0 & \dots & 0 \\ 1 & -2 & 1 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 1 & -2 & 1 \\ 0 & \dots & 0 & 1 & -2 \end{bmatrix}, \qquad B = \frac{1}{\delta y} \begin{bmatrix} -1 & 1 & 0 & \dots & 0 \\ 0 & -1 & 1 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & -1 & 1 \end{bmatrix},$$

$$C = -{}^t B = \frac{1}{\delta y} \begin{bmatrix} 1 & 0 & \dots & 0 \\ -1 & 1 & \dots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \dots & -1 & 1 \\ 0 & \dots & 0 & -1 \end{bmatrix}.$$

The vectors b_1' and b_2', of respective size $(I-1)$ and I, depend on the boundary conditions on u: $\mathrm{b}_1' = (v/\delta y^2, 0, \dots, 0)$, $\mathrm{b}_2' = (-v/\delta y, 0, \dots, 0)$.

We therefore have:

$$U(t) = -Y_t M^{-1} B X_t + \mathrm{b}_1, \tag{28}$$

$$dX_t = \left(-(Y_t)^2\, C M^{-1} B X_t + Y_t\, \mathrm{b}_2 - \frac{X_t}{2} \right) dt + dW_t, \tag{29}$$

where $\mathrm{b}_1 = -M^{-1}\mathrm{b}_1'$ and $\mathrm{b}_2 = -CM^{-1}\mathrm{b}_1' + \mathrm{b}_2'$ are two vectors depending on the boundary conditions on u. What can be easily checked is that $B\mathrm{b}_2 = 0$.

The aim of the remaining of this section is to analyze the covariance of the random variables U (the velocity) and Y_tX_t (the stress) in function of the covariance K in space of W_t (see Eq. 21). We first remark that the covariance of U can be expressed in function of the covariance of Y_tX_t:

$$\begin{aligned}\mathrm{Cov}(U(t)) &= \mathbb{E}(U(t)\otimes U(t)) - \mathbb{E}(U(t))\otimes\mathbb{E}(U(t)),\\ &= (M^{-1}B)\ \mathrm{Cov}(Y_tX_t)\ {}^t(M^{-1}B).\end{aligned} \tag{30}$$

Let us explain how we can compute $\mathrm{Cov}(Y_tX_t) = \mathbb{E}(Y_tX_t\otimes Y_tX_t) - \mathbb{E}(Y_tX_t)\otimes \mathbb{E}(Y_tX_t)$. First, from (29), one can compute the following expression of X:

$$\begin{aligned}X_t = &\exp\left(\int_0^t A(s)\,ds\right)X_0 + \int_0^t \exp\left(\int_s^t A(u)\,du\right)\mathrm{b}_2Y_s\,ds\\ &+\int_0^t \exp\left(\int_s^t A(u)\,du\right)dW_s,\end{aligned} \tag{31}$$

where

$$A(s) = -CM^{-1}B(Y_s)^2 - \frac{1}{2}\mathrm{Id}.$$

Note that $A(t)$ is a random matrix, which is $(Y_0, (V_s)_{s\le t})$-measurable. The last term in equation (31) makes sense since (Y_0, V) (and therefore Y) is independent from W.

The main Lemma that will be used in the sequel to compute the variances is the following:

Lemma 1 *The matrix $CM^{-1}B$ can be decomposed as follows:*

$$CM^{-1}B = Id - P,$$

where Id is the identity matrix of size $I\times I$ and P is the matrix of a projection on $\mathrm{Ker}(B)$.

Proof: The proof uses the fact that $BC = M$ (see (27)). A simple computation shows that:

$$(\mathrm{Id} - CM^{-1}B)(\mathrm{Id} - CM^{-1}B) = (\mathrm{Id} - CM^{-1}B),$$

and thus $P = \mathrm{Id} - CM^{-1}B$ is a projector. Besides, it is clear that $\mathrm{Ker}(B) \subset \{x,\, P(x) = x\}$. The converse inclusion is also easy to prove: if x is such that $P(x) = x$, then $CM^{-1}Bx = 0$ and therefore, by multiplying on the left by B,

one obtains $Bx = 0$. In a uniform in space mesh setting, one obtains $P = \delta y J$ where J is the $I \times I$ matrix with all components equal to 1. $\diamondsuit$

Using $A(s) = (Y_s)^2 P - \left(\frac{1}{2} + (Y_s)^2\right) \mathrm{Id}$ and the fact that, by Lemma 1, $P^n = P$, one obtains the following expression of $\exp\left(\int_s^t A(u)\, du\right)$:

$$\exp\left(\int_s^t A(u)\, du\right) = a(s,t)\mathrm{Id} + b(s,t)P, \tag{32}$$

where

$$a(s,t) = \exp\left(-\frac{t-s}{2}\right) \exp\left(-\int_s^t (Y_u)^2\, du\right),$$

and

$$b(s,t) = \exp\left(-\frac{t-s}{2}\right) \left(1 - \exp\left(-\int_s^t (Y_u)^2\, du\right)\right).$$

This leads to the following expression of $Y_t X_t$ (using the fact that $P\mathrm{b}_2 = \mathrm{b}_2$):

$$\begin{aligned} Y_t X_t = {} & Y_t\Big(a(0,t)\mathrm{Id} + b(0,t)P\Big)X_0 + Y_t \int_0^t \Big(a(s,t) + b(s,t)\Big) Y_s\, ds\, \mathrm{b}_2 \\ & + Y_t \int_0^t \Big(a(s,t)\mathrm{Id} + b(s,t)P\Big)\, dW_s. \end{aligned} \tag{33}$$

Remark 4 *These first computations allow us to explain the dependency of the variances upon the correlation in space of the Brownian motion as follows, at least in the particular case $K = Id$ or $K = J$. When the Brownian motions are completely uncorrelated in space ($K = Id$), one computes in the velocity equation (25) the difference between two independent random variables divided by the space step. It is therefore natural that this induces a variance much more important than in the case of a uniform in space Brownian motion ($K = J$). On the contrary, when we consider the equation (33) verified by X_t, we observe that the term $\int_0^t b(s,t)P\, dW_s$ (we recall that $P = \delta y J$) induces more variance in the case of a Brownian motion not depending on space for the same reason that, if G^i are i independent Gaussian random variables, $\mathrm{Var}\left(\sum_{i=1}^I G^i\right) < \mathrm{Var}\left(\sum_{i=1}^I G^1\right)$. Indeed, in the case of completely uncorrelated Brownian motions in space, the term $PdW_s = \delta y J dW_s$ leads to a sum of independent random variables, whose variance is less than a sum of one single random variable.*

We now turn to the computation of $\mathrm{Cov}(Y_t X_t)$. Using the independence of X_0, $(Y_s)_{s\le t}$, and $(W_s)_{s\le t}$, we check that the covariance between any two different terms of the right-hand-side of (33) is null. Therefore, we obtain the following expression of $\mathrm{Cov}(Y_t X_t)$:

$$\begin{aligned}\mathrm{Cov}(Y_tX_t) = &\mathbb{E}(a(0,t)^2Y_t^2)\,\mathbb{E}(X_0\otimes X_0) + \mathbb{E}(b(0,t)^2Y_t^2)P\,\mathbb{E}(X_0\otimes X_0)^tP\\ &+\mathbb{E}(a(0,t)b(0,t)Y_t^2)\,\left(P\mathbb{E}(X_0\otimes X_0) + \mathbb{E}(X_0\otimes X_0)^tP\right)\\ &+\mathbb{E}\left(\int_0^t \exp\left(-\frac{t-s}{2}\right)(Y_sY_t - \mathbb{E}\,(Y_sY_t))\,ds\right)^2 \mathrm{b}_2\otimes\mathrm{b}_2\\ &+\int_0^t \mathbb{E}(a(s,t)^2Y_t^2)\,ds\,K + \int_0^t \mathbb{E}(b(s,t)^2Y_t^2)\,ds\,PK^tP\\ &+\int_0^t \mathbb{E}(a(s,t)b(s,t)Y_t^2)\,ds\,(PK+K^tP). \qquad (34)\end{aligned}$$

We now want to take the limit $t\longrightarrow\infty$ in each of the terms of (34).

Using the fact that $a(0,t)\le\exp\left(-\frac{t}{2}\right)$ and $b(0,t)\le\exp\left(-\frac{t}{2}\right)$, one can see that the part of the covariance of Y_tX_t which depends on the initial condition X_0 goes to zero in the limit $t\to\infty$.

One can exactly compute (using the fact that $\mathbb{E}(Y_t^2)=1$ and $\mathbb{E}(Y_sY_t) = e^{-\frac{|s-t|}{2}}$) the part of the covariance of Y_tX_t which depends on b_2. We obtain:

$$\begin{aligned}&\mathbb{E}\left(\int_0^t \exp\left(-\frac{t-s}{2}\right)(Y_sY_t - \mathbb{E}\,(Y_sY_t))\,ds\right)^2\\ &= 4\exp(-2t)\,(-\exp(t)(1+t) + 4\exp(2t) - 4\exp(-3t/2) + 1) \qquad (35)\end{aligned}$$

which tends to 16 when t goes to ∞.

One can also show that the other terms in the expression (34) of the covariance of Y_tX_t have a limit when $t\to\infty$. Indeed, the sum of the three last terms of (34) writes :

$$I_t(K+PK^tP-PK-K^tP) + J_t(PK+K^tP-2PK^tP) + (1-\exp(-t))PK^tP$$

where

$$I_t = \int_0^t \exp(-t+s)\mathbb{E}\left(\exp\left(-2\int_s^t (Y_u)^2\,du\right)Y_t^2\right)\,ds$$

and

$$J_t = \int_0^t \exp(-t+s)\mathbb{E}\left(\exp\left(-\int_s^t (Y_u)^2\,du\right)Y_t^2\right)\,ds.$$

Clearly, I_t and J_t are smaller than $1-\exp(-t)$. Hence, it is enough to check that these terms are increasing to conclude that they have finite limits as $t\to\infty$, respectively denoted by α and β.

To prove that I_t is increasing, one can compute the following expression of I_t (by using the change of variable $r=t-s$ and the fact that, by stationarity, $(Y_u)_{t-r\le u\le t}$ and $(Y_u)_{0\le u\le r}$ have the same law):

$$
\begin{aligned}
I_t &= \int_0^t \exp(-t+s)\mathbb{E}\left(\exp\left(-2\int_s^t Y_u^2\,du\right)Y_t^2\right)\,ds \\
&= \int_0^t \exp(-r)\mathbb{E}\left(\exp\left(-2\int_{t-r}^t Y_u^2\,du\right)Y_t^2\right)\,dr \\
&= \int_0^t \exp(-r)\psi(r)\,dr
\end{aligned}
$$

where $\psi(r) = \mathbb{E}\left(\exp\left(-2\int_0^r (Y_u)^2\,du\right)Y_r^2\right)$ is a positive function. Using the same arguments, we obtain for J_t:

$$
J_t = \int_0^t \exp(-r)\mathbb{E}\left(\exp\left(-\int_0^r (Y_u)^2\,du\right)Y_r^2\right).
$$

These expressions clearly demonstrate that I and J are increasing.

This shows that, in the limit $t \to \infty$, $\mathrm{Cov}(Y_t X_t) = 16\,\mathrm{b}_2 \otimes \mathrm{b}_2 + \alpha_1 K + \alpha_2(K^t P + PK) + \alpha_3 PK^t P$, and thus (since $P =^t P$),

$$
\lim_{t\to\infty} \mathrm{Cov}(Y_t X_t) = 16\,\mathrm{b}_2 \otimes \mathrm{b}_2 + \alpha_1 K + \alpha_2(KP + PK) + \alpha_3 PKP, \tag{36}
$$

where $\alpha_1 = \alpha$, $\alpha_2 = \beta - \alpha$ and $\alpha_3 = 1 - 2\beta + \alpha$ are three positive constants.

Using (30) and the fact that $BP = 0$ et $B\mathrm{b}_2 = 0$, we obtain:

$$
\lim_{t\to\infty} \mathrm{Cov}(U(t)) = \alpha_1\, M^{-1} B\, K^{\,t}(M^{-1}B). \tag{37}
$$

Remark 5 *One can compute numerically the values of α_i, $i = 1, 2, 3$. We have found $\alpha \simeq 0.26$ and $\beta \simeq 0.39$. Therefore $\alpha_1 \simeq 0.26$, $\alpha_2 \simeq 0.13$ and $\alpha_3 \simeq 0.48$. Notice also that $\alpha_1 + 2\alpha_2 + \alpha_3 = 1$, which will be used later on.*

Remark 6 *All the computations we have made in this section can also be done with a mesh with non-constant space-steps. In particular, Lemma 1 holds with any mesh in space.*

Remark 7 *One can notice that the variance on the velocity is not influenced by the value of the boundary condition v on the velocity. This is not the case for the stress. In our simple case, since b_2 is a constant vector in space which is proportional to v, we observe that the variance on $Y_t X_t$ is* uniformly in space *influenced by v, and behaves like v^2 when $v \to \infty$. The boundary condition on the velocity therefore influences in the same manner the variance on the stress, at all points of the domain.*

3.3.2 Analysis of the cases $K = Id$ and $K = J$

On the basis of the main two results of the previous section (namely (36) and (37)), we can explain the way the variances on U and YX vary when ones

$t \longrightarrow \infty$	$\mathrm{Cov}(Y_t X_t)$ (stress)	$\mathrm{Cov}(U(t))$ (velocity)
W_t	$16\mathrm{b}_2 \otimes \mathrm{b}_2 + J$	0
$W_t(y)$	$16\mathrm{b}_2 \otimes \mathrm{b}_2 + \alpha_1 \mathrm{Id} + (1-\alpha_1)\delta y J$	$-\alpha_1 M^{-1}$

Fig. 5. Variances of u and τ (for long time) for a Brownian motion not depending on space (W_t) and for Brownian motions uncorrelated in space ($W_t(y)$). Notice that the covariance matrices of the stress (resp. of the velocity) are of size $I \times I$ (resp. $(I-1)\times(I-1)$) where $I = 1/\delta y$.

goes from completely uncorrelated Brownian motions in space ($K = \mathrm{Id}$) to a Brownian motion not depending on space ($K = J$).

In the case of a completely uncorrelated Brownian motion, we have $K = \mathrm{Id}$ and we obtain $\mathrm{Cov}(Y_t X_t) = 16\mathrm{b}_2 \otimes \mathrm{b}_2 + \alpha_1 \mathrm{Id} + (2\alpha_2 + \alpha_3)\delta y J = 16\mathrm{b}_2 \otimes \mathrm{b}_2 + \alpha_1 \mathrm{Id} + (1-\alpha_1)\delta y J$ and $\mathrm{Cov}(U(t)) = -\alpha_1 M^{-1}$.

In the case of a Brownian motion not depending on space, we have $K = J$ and we obtain $\mathrm{Cov}(Y_t X_t) = 16\mathrm{b}_2 \otimes \mathrm{b}_2 + (\alpha_1 + 2\alpha_2 + \alpha_3) J = 16\mathrm{b}_2 \otimes \mathrm{b}_2 + J$ and $\mathrm{Cov}(U(t)) = 0$ (since $BJ = 0$).

Table 5 summarizes the results we have obtained. These results corroborate the behavior of the numerical experiments and the observations of the authors in [3,7]. In particular, if one considers the variance of YX at a point in the middle of the flow, one obtains $C(b_2)+1$ with Wt and $C(b_2)+\alpha_1+(1-\alpha_1)\delta y \simeq C(b_2) + 0.26 + 0.74\delta y$ with Wt(y) (where $C(b_2)$ denotes a constant which depends on b_2): the variance reduces with a Brownian which depends on space (since $\delta y < 1$). Note also (see off-diagonal terms) the strong correlation which is introduced between the variables, at different point in space, when one uses a Brownian motion not depending on space.

3.3.3 Analysis of other correlation matrices K

We now want to further investigate the dependency of the variances in terms of K. What is of interest is the traces of these covariance matrices (renormalized by the number of cells), which measures the variance of the whole variable in space:

$$\begin{aligned}\delta y \,\mathrm{tr}\,(\mathrm{Cov}(Y_t X_t)) &= \alpha_1 + 16\delta y\, ||\mathrm{b}_2||^2 + (2\alpha_2 + \alpha_3)\delta y\, ||PN||^2, \\ &= \alpha_1 + 16\delta y\, ||\mathrm{b}_2||^2 + (1-\alpha_1)\delta y\, ||PN||^2,\end{aligned}$$

$$\delta y \,\mathrm{tr}\,(\mathrm{Cov}(U(t))) = \alpha_1 \delta y\, ||M^{-1}BN||^2,$$

where $||.||$ denotes the Frobenius or Euclidean norm and N is the matrix such that $K = N({}^tN)$ (see Section 3.2: N is a $I \times I$ matrix such that each line has a norm equal to one). We have obtained these expressions using some simple properties like $\mathrm{tr}\,(EF) = \mathrm{tr}\,(FE)$ for any matrices E and F, or $P^2 = P$. From these expressions of the variances, we can deduce the following:

- The minimum of the variance on U is zero and is obtained if and only if the Brownian motion does not depend on space. Indeed, $||M^{-1}BN|| = 0$ implies $BN = 0$, which implies that each line of N is the same.
- The minimum of the variance on Y_tX_t is $\alpha_1 + 16\delta y\,||\mathrm{b}_2||^2$. It is attained if and only if $PN = 0$ (and this is *not* the case with a Brownian motion not depending on space). This is equivalent to the fact that the sum of the components within each column of the matrix N is zero.

Let us now try to determine among all covariances matrices K such that the variance on Y_tX_t is minimum, the one that leads to a variance on $U(t)$ that is minimum.

Variance reduction using only one Brownian motion in space.

In a first step, we solve this question in the case when we use only one Brownian motion in space to construct K, in order to keep the same computational cost as in the case of a Brownian motion not depending on space. In other words, we can only choose $+W_t$ or $-W_t$ in each cell of the mesh. We can then state the following result: in case I is even, using only one Brownian in space, the covariance matrix K defined by $K_{i,j} = (-1)^{i+j}$ is such that, among all K possible such that the variance on X_t is minimum, the variance on $U(t)$ is minimum. To prove this result, one has to notice that we obtain all the admissible covariance matrices $K = N({}^tN)$ with the matrices N of the following form: the first column equal to $\epsilon = (\epsilon_1, ..., \epsilon_I)$ and zero elsewhere, with $\epsilon_i = \pm 1$, and $\sum_{i=1}^{I} \epsilon_i = 0$. The variance on U is then minimal if and only of the norm of $M^{-1}B\epsilon$ is minimal. But this vector $\nu = M^{-1}B\epsilon$ can also be interpreted as the solution in $\mathbb{P}1$ of the finite element discretization of the following problem: $\frac{\partial^2 r}{\partial y^2} = \frac{\partial \epsilon}{\partial y}$, where $y \in (0,1)$, with zero Dirichlet boundary conditions $r(0) = r(1) = 0$. Since the finite element solution is equal to the non-discretized solution, it is then obvious that the minimum of the norm of $\nu = M^{-1}B\epsilon$ is obtained, for example, with an oscillatory ϵ ($\epsilon = (1, -1, 1, -1, ...)$). We have plotted on Figure 6 the results obtained on the initial problem (14-16) in this case of an oscillatory-in-space Brownian motion (see the curves labelled '+/- Wt').

This result is interesting since it shows that, if the aim is to reduce the variance on Y_tX_t, one can further reduce the variances on *both* $U(t)$ and Y_tX_t, compared with the case of an uncorrelated Brownian motion (compare the curves labelled '+/- Wt' and 'Wt(y)' on Figure 6), and this using only *one* Brownian motion

in space.

Remark 8 *One could argue that the reduction of variance on the stress obtained by using Brownian motions uncorrelated in space is due to a kind of law of large numbers: we introduce more random numbers and therefore we reduce the variance, with of course more costly simulations. We have shown in this section that this argument does not hold, since the variance on YX can even be more reduced, using only one Brownian motion in space.*

Remark 9 *This reduction of variance using an oscillatory Brownian motion in space reminds us of the antithetic variables method, classically used in Monte Carlo simulations to reduce the variance.*

Variance reduction using arbitrarily many Brownian motions.

In a second step, we allow for the use of an arbitrary number of Brownian motions. We can reformulate the minimization problem we consider in the following:
Minimize $\mathrm{tr}\,(M^{-1}BK({}^tB)({}^tM^{-1}))$ among the matrices K such that:

- K is a symmetric matrix of size $I \times I$,
- K is positive,
- $\forall i,\ K_{i,i} = 1$,
- $\mathrm{tr}\,(KP) = 0$ (we recall that P is the orthogonal projector on the vector of size I: $(1, ..., 1)$).

This problem has a solution, since we minimize a linear function on a bounded convex closed set. We have solved this problem with the function 'lmisolver' of Scilab. We have used the covariance matrix obtained to construct a Brownian motion and perform a simulation on the initial time-dependent problem (14)-(16). The results plotted on Figure 6 show that we have indeed further reduced the variance on $U(t)$, with an optimal variance on Y_tX_t.

4 Numerical simulations

4.1 Hookean dumbbells

We here present some simple numerical experiments performed in the case of a pure shear flow with Hookean dumbbells on a uniform mesh (see Eq. (17)-(20)). The numerical parameters are: the number of cells I, the number of time step N, the number of realizations R, and the number of independent tests $NbTest$ we have performed in order to estimate the variances. The physical

parameters in all the simulations are: $v = 1$ (velocity on the boundary), $T = 5$ (final time of the simulation), $\epsilon = 0.9$, Re $= 0.1$, We $= 0.5$.

We can observe that, replacing a Brownian motion not depending on y (see the curves labelled 'Wt' on Figure 6) by Brownian motions completely uncorrelated in space (see the curves labelled 'Wt(y)' on Figure 6) results into:

- an increase of the variance of u (velocity) (the variance is multiplied by a factor of 250 for short times and 10^6 for long times: in fact, in case of a Brownian motion not depending on space, we have observed on our simple case that the variance on u seems to tend to zero as t goes to infinity),
- a decrease of the variance of τ (stress) (the variance is divided by about 5 for short times and 2 for long times).

We here observe, in our simple geometry, the same behaviour as other authors already noticed in more complex flows (see [3,7]) which legitimates a throughfull study of the 1D case.

We have also plotted on Figure 6 the results obtained with an oscillatory-in-space Brownian motion, and with the optimized covariance matrix.

4.2 FENE dumbbells

In the FENE case, the equations (14)-(16) become:

$$\frac{\partial u}{\partial t}(t,y) = \frac{\partial^2 u}{\partial y^2}(t,y) + \frac{\partial}{\partial y}\mathbb{E}\left(\frac{X_t(y)Y_t(y)}{1-(X_t(y)^2+Y_t(y)^2)/b}\right) , \tag{38}$$

$$dX_t(y) = \left(\frac{\partial u(t,y)}{\partial y}Y_t(y) - \frac{1}{2}\frac{X_t(y)}{1-(X_t(y)^2+Y_t(y)^2)/b}\right)dt + dW_t(y) , \tag{39}$$

$$dY_t(y) = -\frac{1}{2}\frac{Y_t(y)}{1-(X_t(y)^2+Y_t(y)^2)/b}dt + dV_t(y) , \tag{40}$$

One can notice that we may now let the Brownian motion V_t which acts on Y_t depends on space, since Y_t naturally depends on space.

Because of the nonlinear drift in the stochastic differential equations (39)-(40), we are not able to conduct the arguments of Section 3, even for this simple geometry. However, we have tested our three main correlations in space investigated in the Hookean dumbbell case, in the FENE framework (see Figure 7): Brownian motion not depending on space, uncorrelated Brownian motions in space, and oscillatory Brownian motion in space. In our simulations, the parameter b is equal to 20. Let us make precise the oscillatory Brownian motion

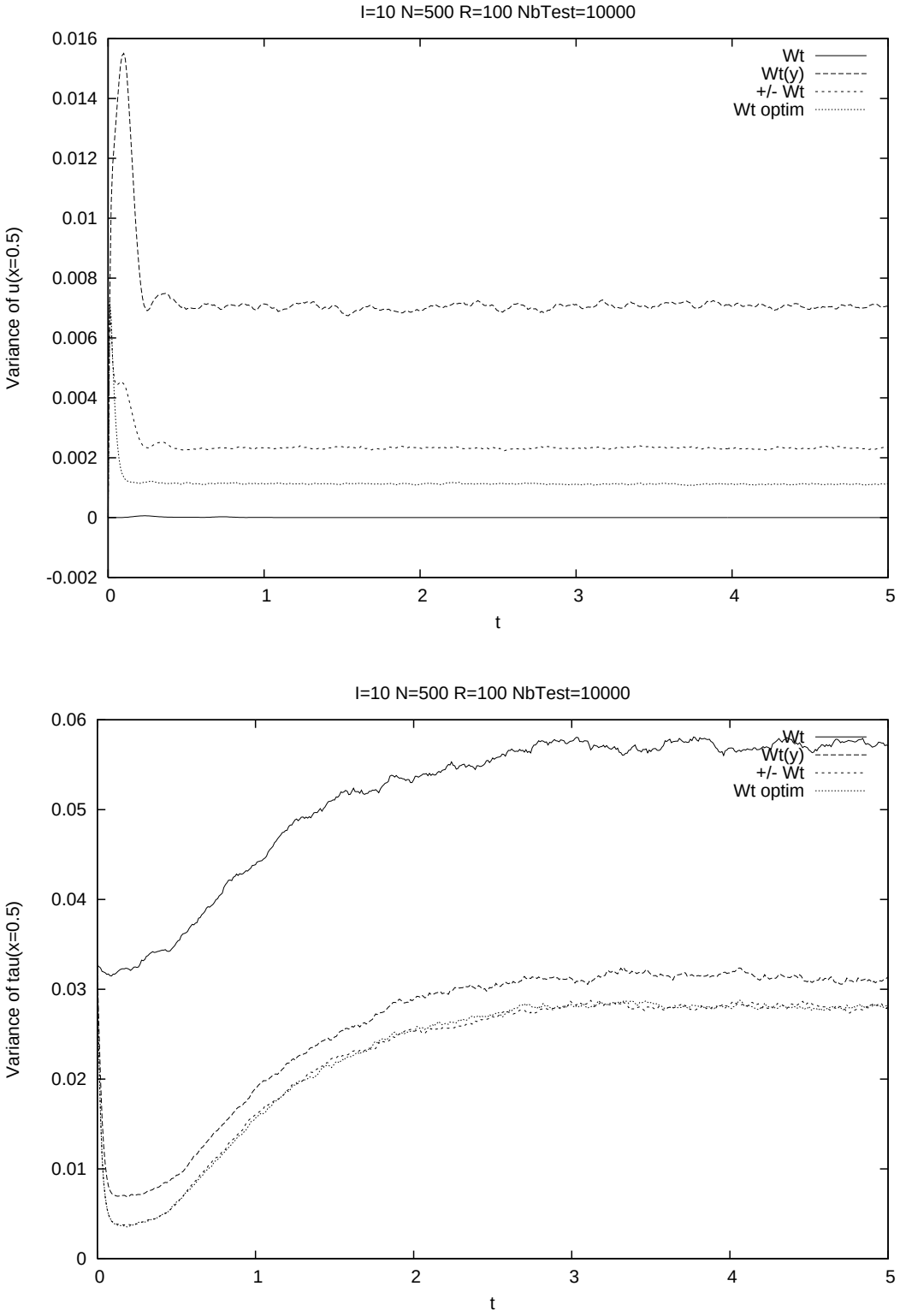


Fig. 6. Variances of u and τ (versus time) for different correlations in space: solid-line=Wt: a Brownian motion not depending on space ; long-dashed-line=Wt(y): completely uncorrelated Brownian motions in space ; short-dashed-line=+/-Wt: an oscillatory Brownian motion in space ; dotted-line=Wt optim: results obtained with an optimized correlation matrix.

we consider: from one cell to another, we have taken alternatively (W_t, V_t) or $(-W_t, V_t)$.

For example (see Figure 7), if one uses an oscillatory Brownian motion in space instead of a Brownian motion not depending on space, for short time ($t = 0.12$), the variance on the velocity is only multiplied by 3 but the variance on the stress is divided by 6, and is even better than for uncorrelated Brownian motions in space, which yet corresponds to a more costly simulation.

We can then draw the following conclusion: using only one Brownian motion in space (and therefore at a fixed computational cost), one can reduce the variance on τ compared to the case of a Brownian motion not depending on space, by using an oscillatory Brownian motion in space.

5 Related issues

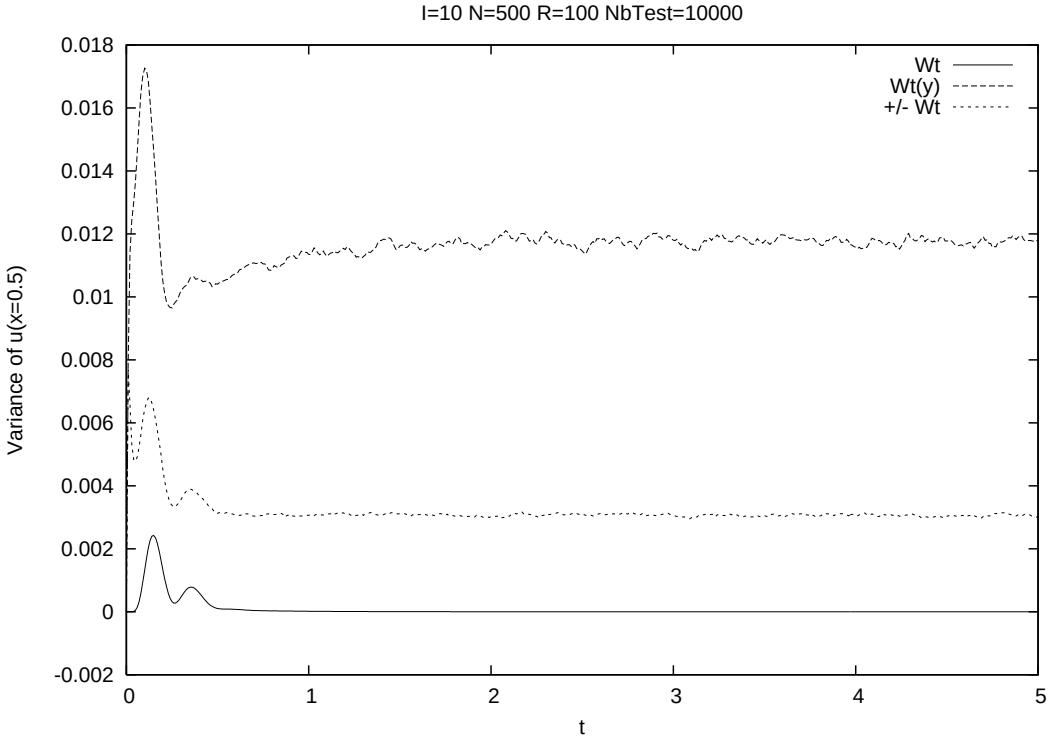
5.1 Dependency of the variances with respect to the space step δy

In Table 8, we give the dependency of the variances of $Y_t X_t$ and $U(t)$ for long time in our simple case. To derive this results, we have used the fact that $\mathrm{b}_2 = O(1)$ and $M^{-1} = O(\delta y)$. These last results can be numerically checked by observing that $\mathrm{b}_2 = (-1, -1, ..., -1)$ and $(M^{-1})_{i,i} = -\frac{i(I-i)}{I^3}$.

Remark 10 *In case of uncorrelated Brownian motions in space, we observe that the velocity becomes deterministic in the limit $\delta y \to 0$. This can be formally explained in our simple case by the fact that the velocity is an integral over the space of $Y_t X_t$: therefore, a kind of law of large numbers occurs when $\delta y \to 0$.*

5.2 Some remarks concerning the bias

The problem we consider is non-linear in the Mc Kean sense, since all the dumbbells are coupled through the velocity. Therefore, the law of each dumbbell depends on the total number of dumbbells R : to stress this dependency, we denote $(X_t^{j,R}, Y_t^{j,R})$ the end-to-end vector of the j-th dumbbell and $\overline{XY}_t^R = \frac{1}{R}\sum_{j=1}^R X_t^{j,R} Y_t^{j,R}$ the estimated stress. In general, this estimated stress is biased i.e. $\mathbb{E}(\overline{XY}_t^R) = \mathbb{E}(X_t^{j,R} Y_t^{j,R}) \neq \mathbb{E}(X_t Y_t)$, where (X_t, Y_t) is solution of (15)-(16). From a numerical point of view, one may compute the empirical mean of the estimated stress over NbTest independent experiments $\frac{1}{\mathrm{NbTest}}\sum_{k=1}^{\mathrm{NbTest}} \overline{XY}_t^{R,k}$, with the same number R of dumbbells.



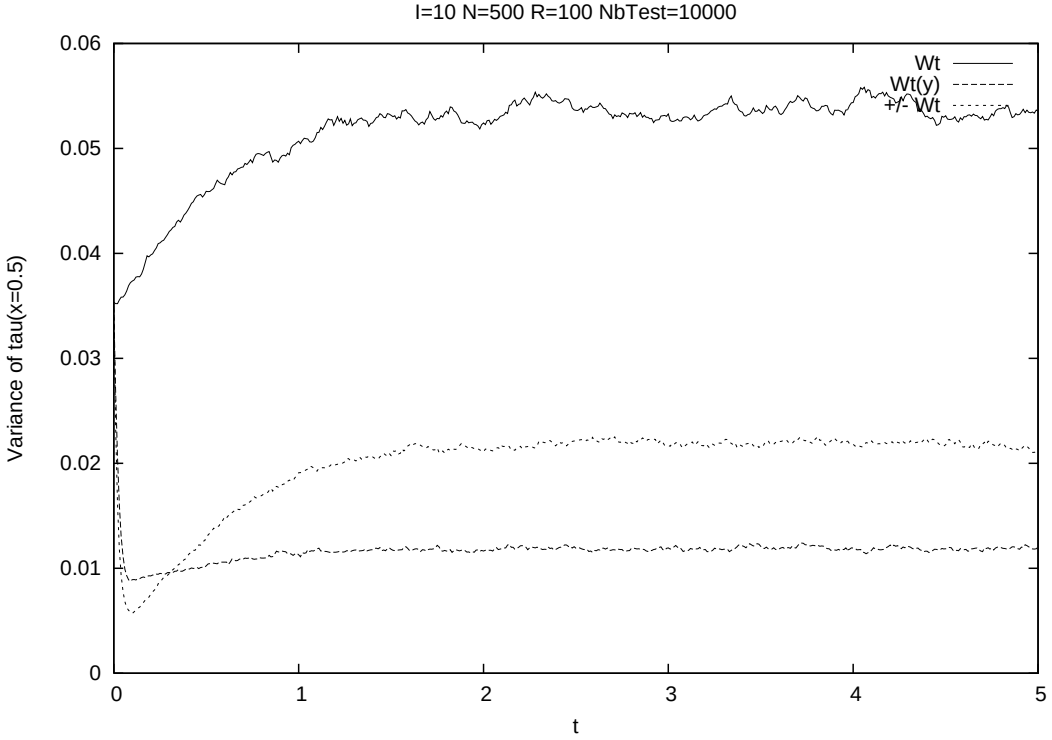


Fig. 7. In the case of FENE dumbbells: variances of u and τ versus time for different correlations in space: solid-line=Wt: a Brownian motion not depending on space ; long-dashed-line=Wt(y): completely uncorrelated Brownian motions in space ; short-dashed-line=+/-Wt: an oscillatory Brownian motion in space.

$t \longrightarrow \infty$	$\delta y \,\mathrm{tr}\,(\mathrm{Cov}(Y_t X_t))$ (stress)	$\delta y \,\mathrm{tr}\,(\mathrm{Cov}(U(t)))$ (velocity)
W_t	$O(1)$	0
$W_t(y)$	$O(1)$	$O(\delta y)$

Fig. 8. Dependency of the variances of u and τ (for long time) with respect to δy.

The error induced on the stress can be decomposed as follows:

$$\mathbb{E}(X_t Y_t) - \frac{1}{\mathrm{NbTest}} \sum_{k=1}^{\mathrm{NbTest}} \overline{XY}_t^{R,k} = \left(\mathbb{E}(X_t Y_t) - \mathbb{E}\left(\overline{XY}_t^{R}\right)\right) + \left(\mathbb{E}\left(\overline{XY}_t^{R}\right) - \frac{1}{\mathrm{NbTest}} \sum_{k=1}^{\mathrm{NbTest}} \overline{XY}_t^{R,k}\right).$$

The second term is the statistical error induced by the Monte Carlo method. The first term is a deterministic error, called the bias, which comes from the fact that the random variables $X_t^{j,R}$ et $Y_t^{j,R}$ are coupled (through the velocity). We have numerically observed a bias which is $O\left(\frac{1}{R}\right)$ (see the values obtained for $t = 0.1$ on Figure 9), which seems to be usual for this kind of coupling. In order to underline this dependency, we have performed a huge number of independent tests (NbTest = 10 000 000) to distinguish between the bias (which is typically $O\left(\frac{1}{R}\right)$) and the statistical error (which is typically $O\left(\frac{1}{\sqrt{R}}\right)$ for one single test). We also observe that for long time, the bias vanishes.

From this numerical observation, one can give an answer to the following classical question: in order to reduce the variance on the result, is it preferable to increase the number of dumbbells (R) or the number of tests (NbTest) ? Since the bias is $O\left(\frac{1}{R}\right)$ and the statistical error is $O\left(\frac{1}{\sqrt{R\,\mathrm{NbTest}}}\right)$, it does not make sense to choose NbTest such that NbTest $>> R$. Note that this conclusion also holds when one takes into account the computational cost for it is linear in both R and NbTest, since there are no complex interactions between the dumbbells.

The fact that the statistical error dominates the bias also shows the importance of understanding the variance of the results.

6 Conclusions

In this paper, we have explained what kind of dependency in space of the Brownian motion is natural to adopt in the micro-macro modeling of poly-

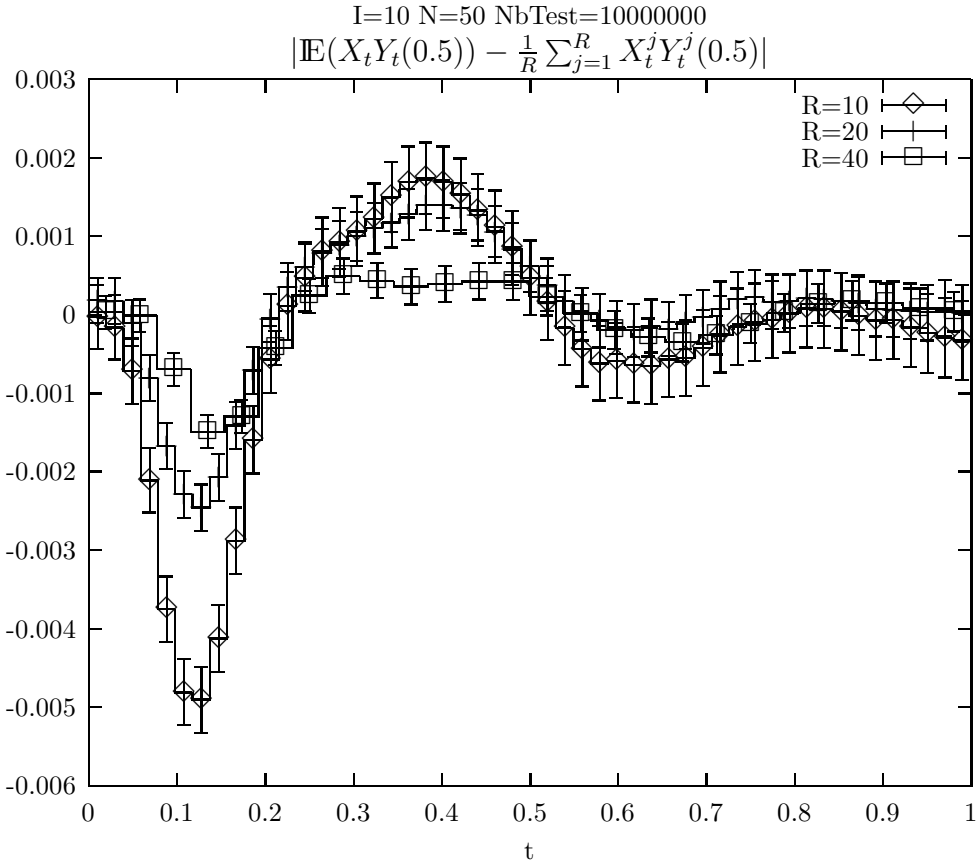


Fig. 9. Error between the estimator of τ and its exact value, at $y = 0.5$, in the Hookean dumbbell case.

meric fluids, namely some Brownian motions dependent in space through the Lagrangian trajectories of the flow.

We have then considered the pure shear flow for one single Hookean dumbbell in the long time limit and we have been able to prove on this simple case that:

a The variance on the velocity u is minimum when one considers a Brownian motion which is constant in space,
b The use of uncorrelated Brownian motions in space is not the best correlation in space to consider, if one wants to reduce the variance on the stress τ ; the use of an oscillatory-in-space Brownian motion is optimal as far as the variance on the stress is concerned,
c It is possible to reduce the variance on τ, compared to a Brownian motion which is constant in space, and this with the same computational cost.

On the simple case of a shear flow with Hookean dumbbells, we have checked by numerical experiments that point (c) above holds on the time-dependent problem, which validates our approach. We have also verified point (c) in the FENE case.

This analysis has shown the importance, for the variance of the results, of the interplay between the correlation matrix in space of the Brownian motions at the microscopic level and the matrices of the discretization of the differential operators at the macroscopic level.

As byproducts of our analysis, we have shown that:

- on our simple case and in the long time limit, the boundary condition does not influence the variance on the velocity but influences the variance on the stress, in the same manner at all points of the domain,
- on our simple case and in the long time limit, when one uses uncorrelated Brownian motions in space, the variance on the velocity goes to zero when the space-step δy goes to zero,
- since we have numerically observed that the bias is $O\left(\frac{1}{R}\right)$ and the statistical error is $O\left(\frac{1}{\sqrt{R\,\mathrm{NbTest}}}\right)$, where R denotes the number of dumbbells in each cell and NbTest the number of independent tests performed with R dumbbells, it does not make sense to choose NbTest such that NbTest $>> R$.

We have summarized these conclusions in Table 10.

Acknowledgments

This work has been inspired by a question asked by Roland Keunings, and initiated during the CEMRACS 2001 summer school with the contribution of Adrien Leygue. It is a pleasure to warmly thank these colleagues for their help as well as for their critical reading of a preliminary version of the manuscript.

References

[1] R.B. Bird, R.C. Armstrong, and O. Hassager. *Dynamics of polymeric liquids*, volume 1. Wiley Interscience, 1987.

[2] R.B. Bird, C.F. Curtiss, R.C. Armstrong, and O. Hassager. *Dynamics of polymeric liquids*, volume 2. Wiley Interscience, 1987.

[3] J. Bonvin and M. Picasso. Variance reduction methods for CONNFFESSIT-like simulations. *J. Non-Newtonian Fluid Mech.*, 84:191–215, 1999.

[4] M. Doi and S.F. Edwards. *The Theory of Polymer Dynamics*. International Series of Monographs on Physics. Oxford University Press, 1988.

[5] W. E, T.J. Li, and P.W. Zhang. Convergence of a stochastic method for the modeling of polymeric fluids. *Acta Mathematicae Applicatae Sinica, English Series*, 18(4):529–536, 2002.

	Rigorously proved	Numerically checked	Admitted in the literature
The dependency in space of the Brownian motion does not influence the continuous solution.	Shear flow with Hookean dumbbells or any flow with regular solutions and trajectorial dependency.		Any geometry, any spring, [8].
The CONNFFESSIT method converges to a unique continuous solution whatever the dependency in space.	Shear flow with Hookean dumbbells.	Shear flow or 4 to 1 contraction or journal bearing, [7,8,11].	Any flow, any spring, but a question in [15].
A Brownian motion not depending on space reduces the variance on u, but increases the variance on τ.	Shear flow for long time and Hookean dumbbell, $R = 1$.	Shear flow or 4 to 1 contraction with Hookean and FENE dumbbells, [7,3].	
One can reduce the variance on τ with *one single* Brownian motion.	Shear flow for long time and Hookean dumbbell, $R = 1$.	Shear flow with Hookean and FENE dumbbells.	
The boundary conditions influence the variance on τ but not on u.	Shear flow for long time and Hookean dumbbell, $R = 1$.	Shear flow with Hookean and FENE dumbbells.	
The variance on u is $O(\delta y)$ with uncorrelated Brownian motions.	Shear flow for long time and Hookean dumbbell, $R = 1$.	Shear flow with Hookean and FENE dumbbells.	
The bias is $O(1/R)$.		Shear flow with Hookean dumbbells.	

Fig. 10. Summary of the principle results.

[6] P.J. Flory. *Statistical Mechanics of Chain Molecules*. John Wiley and Sons, New York, 1969.

[7] P. Halin, G. Lielens, R. Keunings, and V. Legat. The Lagrangian particle method for macroscopic and micro-macro viscoelastic flow computations. *J. Non-Newtonian Fluid Mech.*, 79:387–403, 1998.

[8] M.A. Hulsen, A.P.G. van Heel, and B.H.A.A. van den Brule. Simulation of viscoelastic flows using Brownian configuration fields. *J. Non-Newtonian Fluid Mech.*, 70:79–101, 1997.

[9] B. Jourdain, T. Lelièvre, and C. Le Bris. Numerical analysis of micro-macro simulations of polymeric fluid flows: a simple case. *Math. Models and Methods in Applied Sciences*, 12(9):1205–1243, 2002.

[10] M. Laso and H.C. Öttinger. Calculation of viscoelastic flow using molecular models : The CONNFFESSIT approach. *J. Non-Newtonian Fluid Mech.*, 47:1–20, 1993.

[11] M. Laso, M. Picasso, and H.C. Öttinger. Two-dimensional, time-dependent viscoelastic flow calculations using CONNFFESSIT. *AIChE J.*, 43:877–892, 1997.

[12] T. Lelièvre. Optimal error estimate for the CONNFFESSIT approach in a simple case. *Computers and Fluids*, 2003. To appear.

[13] M. Melchior and H.C. Öttinger. Variance reduced simulations of polymer dynamics. *J. Chem. Phys.*, 105(8):3316–3331, 1996.

[14] H.C. Öttinger. *Stochastic Processes in Polymeric Fluids*. Springer, 1995.

[15] H.C. Öttinger, B.H.A.A. van den Brule, and M.A. Hulsen. Brownian configuration fields and variance reduced CONNFFESSIT. *J. Non-Newtonian Fluid Mech.*, 70:255–261, 1997.