Spatially correlated noise and variance minimization in stochastic simulations

Raz Kupferman *, Yossi Shamai

Institute of Mathematics, The Hebrew University, Givat Ram Campus, Jerusalem 91904, Israel

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ABSTRACT

Brownian simulation methods have become a popular approach in computational rheology with the introduction of the CONNFFESSIT algorithm and the method of Brownian configuration fields in the 1990s. Jourdain et al. [B. Jourdain, C.L. Bris, T. Lelievre, On a variance reduction technique for micro–macro simulations of polymeric fluids, J. Non-Newton. Fluid Mech. 122 (2004) 91–106] pointed out that both methods can be viewed as variants that differ in the spatial correlation of the noise, which can be viewed as a computational parameter for statistical error minimization. We formulate an optimization problem of variance minimization with respect to the choice of noise correlation. Our analysis takes place in an infinite-dimensional function space. We solve the optimization problem analytically for the shear flow of a Hookean dumbbell model at steady state. Interestingly, we find that spatially uncorrelated noise, i.e., CONNFFESSIT minimizes the statistical error, although the precise meaning of this statement can only be interpreted as a limit of finite-dimensional approximations.

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1. Introduction

Brownian simulation methods were introduced in computational rheology in the early 1990s with the CONNFFESSIT method of Öttinger and co-workers [2], which is based on a mixed micro–macro formulation of the governing equations. The idea was to simulate an ensemble of particles (which represent the polymers in some coarse-grained sense), and to evaluate the stress tensor by averaging over contributions from particles in the vicinity of the point of interest. The use of Brownian simulations in computational rheology has been broadened later with the introduction of the method of Brownian configuration fields (BCF) [3], where instead of tracking individual "polymers", the local conformation of the polymers is represented by a finite collection of spatially continuous "conformation fields". These fields satisfy stochastic partial differential equations driven by mutually independent, spatially uniform Brownian noise. The stress is obtained by a suitable averaging over this finite collection of configuration fields. It has later been pointed out [1] that the CONNFFESSIT and the BCF methods can be viewed as variants of a larger family of stochastic approximation methods: they differ in that the first uses a Lagrangian formulation whereas the second uses a Eulerian formulation; more importantly, they differ in the spatial correlation of the Brownian noise. In fact, these two methods correspond to the extreme choices of spatially uniform noise (BCF) versus spatially uncorrelated noise (CONNFFESSIT). This observation has led to a more general formulation of stochastic simulations that are driven by Brownian noise with arbitrary spatial correlation. This correlation does not affect the "consistency" of the method, however it affects the variance of the solution, hence the statistical error.

A notable difference between CONNFFESSIT and BCF is that the latter yields solutions that are significantly smoother in space; this is not surprising, given the structure of the noise. This has at first led to a speculation that BCF is a "variance reduced" variant of CONNFFESSIT [4]. It was later realized, however, that smoothness does not necessarily imply a small variance. In fact, while in certain situations BCF yields velocity fields with a variance significantly lower than that obtained from CONNFFESSIT, the variance of the stress is much larger with BCF. Thus, the measure of variance reduction depends on how the statistical errors in the stress and in the velocity are weighted.

The question of how to use the freedom in the spatial correlation of the noise in order to minimize the statistical error was first addressed by Jourdain et al. in [1]. The optimization problem was formulated on a discrete level, for a specific finite element discretization. As an application, the optimal noise for a simple shear flow of a Hookean dumbbell fluid was computed. In [5] this question was addressed in a continuous framework, leading to an infinite-dimensional optimization problem, which was analyzed and solved in systems for which closed-form constitutive equations can be derived.

In this paper we first review the main results stated in [5]. Our presentation of the infinite-dimensional optimization problem is

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* Corresponding author.
E-mail addresses: raz@math.huji.ac.il (R. Kupferman),
yossish@math.huji.ac.il (Y. Shamai).

less technical than in [5]. In particular, we show how to apply it within the viscoelastic context. We calculate analytically the optimal noise correlation for the planar shear flow in the continuous setting. Interestingly, we find that the optimal choice is that of spatially uncorrelated noise, i.e., CONNFFESSIT. Ironically, we also show that BCF is the worst possible choice in terms of stress variance, thus totally rebutting the speculation in [4]. Even though the planar shear flow problem is simple, and somewhat degenerate compared to typical systems of interest, its solution is instructive, showing in particular the competition between variance minimization of velocity and stress.

The structure of this paper is as follows: In Section 2 we present the class of problems under consideration, namely, micro–macro models of incompressible polymeric fluids. In Sections 3 and 4 we formulate the variance minimization problem for Brownian simulation methods. In Section 5 we explain how the infinite-dimensional optimization problem can be approximated by sequences of finite-dimensional semi-definite programming problems. In Section 6 we study in detail the variance minimization problem for planar shear flow of a Hookean dumbbell fluid. A discussion follows in Section 7.

2. Coupled Stokes–Fokker-Planck systems

The equations that govern the flow of an incompressible fluid in the creeping flow regime are the Stokes system

$$-\nabla p + \nu_s \Delta \boldsymbol{u} + \operatorname{div} \boldsymbol{\tau} + \boldsymbol{f} = 0, \\ \operatorname{div} \boldsymbol{u} = 0, \tag{2.1}$$

where $\boldsymbol{u} = \boldsymbol{u}(\boldsymbol{x}, t)$ is the flow field, generally a three-dimensional vector field in a domain $\Omega \subseteq \mathbb{R}^3$, $p = p(\boldsymbol{x}, t)$ is the pressure, ν_s is the viscosity, and $\boldsymbol{f} = \boldsymbol{f}(\boldsymbol{x}, t)$ is an external force field. The tensor field $\boldsymbol{\tau} = \boldsymbol{\tau}(\boldsymbol{x}, t)$ is the polymeric extra-stress. In models that are derived from kinetic considerations, the stress field $\boldsymbol{\tau}$ is a local average over an ensemble of polymeric conformations. In a simple dumbbell model, for example, the conformation of a polymer is characterized by an end-to-end vector $\boldsymbol{q}$. If $\psi(\boldsymbol{q}, \boldsymbol{x}, t)$ denotes the probability density function (pdf) of finding a polymer in location $\boldsymbol{x}$ and time t in a conformation $\boldsymbol{q}$, then the stress is an ensemble average of the form

$$\boldsymbol{\tau}(\boldsymbol{x}, t) = \int_{\mathbb{R}^3} [\boldsymbol{q} \otimes \boldsymbol{F}(\boldsymbol{q})] \psi(\boldsymbol{q}, \boldsymbol{x}, t) \, d\boldsymbol{q}, \tag{2.2}$$

where $\boldsymbol{F}(\boldsymbol{q})$ is the force exerted by a polymer in conformation $\boldsymbol{q}$. The pdf ψ is governed by a Smoluchowski equation [6],

$$\frac{\partial \psi}{\partial t} + (\boldsymbol{u} \cdot \nabla)\psi = -\nabla_{\boldsymbol{q}} \cdot \{[(\nabla \boldsymbol{u})^T \boldsymbol{q} - \boldsymbol{F}(\boldsymbol{q})]\psi\} + \frac{1}{2}\Delta_{\boldsymbol{q}}\psi, \tag{2.3}$$

where ∇ denotes the gradient with respect to the spatial variable $\boldsymbol{x}$, and $\nabla_{\boldsymbol{q}}$, $\Delta_{\boldsymbol{q}}$ denote the gradient and the Laplacian with respect to the conformation variable $\boldsymbol{q}$. The coupled Stokes–Smoluchowski system (2.1)–(2.3) has to be supplemented by suitable initial and boundary conditions.

An observation that has been, to some extent, at the heart of the BCF method is that the *deterministic* Smoluchowski equation (2.3), which is derived from a random kinetic model, can be represented by a stochastic formulation. The somewhat non-trivial aspect of this alternative representation is that it involves stochastic partial differential equations (SPDEs) [7], which are much more technically involved than stochastic ordinary differential equations (SDEs).

Specifically, we introduce a function-valued stochastic process $\boldsymbol{q}(\boldsymbol{x}, t)$. For every time t, $\boldsymbol{q}(\boldsymbol{x}, t)$ is a random function of the spatial coordinates; we require this function to belong to the set of square integrable function L^2. The stochastic process $\boldsymbol{q}(\boldsymbol{x}, t)$ is governed by

the SPDE

$$\frac{d\boldsymbol{q}}{dt} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{q} = (\nabla \boldsymbol{u})^T \boldsymbol{q} - \boldsymbol{F}(\boldsymbol{q}) + \frac{d\boldsymbol{W}}{dt}, \tag{2.4}$$

where $\boldsymbol{W}(x, t)$ is a three-dimensional L^2-valued Brownian motion, standard in the sense that for every $\boldsymbol{x}$,

$$\mathbb{E}[d\boldsymbol{W}(\boldsymbol{x}, t) \otimes d\boldsymbol{W}(\boldsymbol{x}, t)] = \boldsymbol{I} \, dt, \tag{2.5}$$

where I is the identity matrix.

It can be shown (see [5] for details) that the Smoluchowski equation (2.3) governs the pdf that $\boldsymbol{q}(\boldsymbol{x}, t) = \boldsymbol{q}$. In this stochastic setting the stress is expressed as an expectation

$$\boldsymbol{\tau}(\boldsymbol{x}, t) = \mathbb{E}[\boldsymbol{q}(\boldsymbol{x}, t) \otimes \boldsymbol{F}(\boldsymbol{q}(\boldsymbol{x}, t))], \tag{2.6}$$

where the averaging is with respect to both the Brownian motion and the initial data, $\boldsymbol{q}_0(\boldsymbol{x}) = \boldsymbol{q}(\boldsymbol{x}, 0)$. Thus, the deterministic system (2.1)–(2.3) is replaced by the stochastic system (2.1), (2.4), (2.6).

Comments:

(1) A standard reference to the theory of function-valued stochastic processes and SPDEs is the book by Da Prato and Zabczyk [7].
(2) The transition between the deterministic and stochastic systems is relatively straightforward. In principle it requires the use of an infinite-dimensional version of Itô's formula, although in practice, one may use the standard Itô formula at any fixed value of space variable [5].
(3) The restriction (2.5) that the Brownian motion be standard is a point-wise condition, and does not uniquely determine the distribution of $\boldsymbol{W}(\boldsymbol{x}, t)$. A function-valued Brownian motion is characterized by a spatial auto-correlation function,

$$c(\boldsymbol{x}, \boldsymbol{y}) \, dt = \mathbb{E}[d\boldsymbol{W}(\boldsymbol{x}, t) \otimes d\boldsymbol{W}(\boldsymbol{y}, t)]. \tag{2.7}$$

The SPDE literature usually uses instead the notion of a correlation operator, but there is a simple equivalence between correlation operators and correlation functions. The remarkable fact is that the replacement of the deterministic system by the stochastic system holds for any choice of correlation function, provided that it satisfies (2.5), i.e., that $c(\boldsymbol{x}, \boldsymbol{x}) = \boldsymbol{I}$. That is, the constraints only involve the diagonal entries of the correlation function. This freedom in the choice of spatial correlation was first pointed out in [1].
(4) The non-uniqueness in the choice of spatial correlation can also be explained as follows: an SPDE of the form (2.4) induces an evolution on distributions in function space (e.g., it determines the probability that the function $\boldsymbol{q}(\cdot, t)$, at fixed time t, resides in any measurable set of functions). In contrast, the pdf $\psi(\boldsymbol{q}, \boldsymbol{x}, t)$ is, for every $\boldsymbol{x}$ and t, a distribution over a real-valued random variable. The distribution ψ is a marginal of the distribution in function space. The freedom in the choice of spatial correlation results from the fact that marginals do not uniquely determine multivariate distributions.

3. Brownian simulation methods

A practical approach for solving the stochastic system (2.1), (2.4), (2.6) is by Brownian simulations. The SPDE (2.4) for $\boldsymbol{q}(\boldsymbol{x}, t)$ is simulated by a collection of n realizations, $\boldsymbol{Q}_i(\boldsymbol{x}, t)$, $i = 1, \ldots, n$, which are driven by i.i.d Brownian motions $\boldsymbol{W}_i(\boldsymbol{x}, t)$. The processes $\boldsymbol{Q}_i(\boldsymbol{x}, t)$ approximate n independent realizations of $\boldsymbol{q}(\boldsymbol{x}, t)$. The stress, which is an expectation over all such trajectories, is approximated by an empirical mean over the random fields $\boldsymbol{Q}_i(\boldsymbol{x}, t)$. The solutions $\boldsymbol{u}(\boldsymbol{x}, t)$ and $\boldsymbol{\tau}(\boldsymbol{x}, t)$ are accordingly approximated by stochastic processes

$U(\boldsymbol{x}, t)$ and $\boldsymbol{T}(\boldsymbol{x}, t)$. The resulting stochastic scheme is

$$-\nabla P + \nu_s \Delta \boldsymbol{U} + \operatorname{div} \boldsymbol{T} + \boldsymbol{f} = 0,$$
$$\operatorname{div} \boldsymbol{U} = 0,$$
$$\boldsymbol{T} = \frac{1}{n} \sum_{i=1}^{n} \boldsymbol{Q}_i \otimes F(\boldsymbol{Q}_i), \tag{3.1}$$
$$\frac{\mathrm{d}\boldsymbol{Q}_i}{\mathrm{d}t} + (\boldsymbol{U} \cdot \nabla)\boldsymbol{Q}_i = (\nabla \boldsymbol{U})^T \boldsymbol{Q}_i - F(\boldsymbol{Q}_i) + \frac{\mathrm{d}\boldsymbol{W}_i}{\mathrm{d}t},$$

where $\boldsymbol{W}_i(\boldsymbol{x}, t)$, $i = 1, \ldots, n$ are i.i.d Brownian motions with spatial correlation function $c(\boldsymbol{x}, \boldsymbol{y})$, and $\boldsymbol{Q}_i(\cdot, 0)$ are i.i.d with the same distribution as $\boldsymbol{q}_0$.

As explained above, the consistency of the method is unaffected by the spatial correlation, $c(\boldsymbol{x}, \boldsymbol{y})$. An additional freedom is the distribution of the initial state $\boldsymbol{q}_0$, which should be consistent with the initial stress data,

$$\mathbb{E}[\boldsymbol{q}_0(\boldsymbol{x}) \otimes \boldsymbol{F}(\boldsymbol{q}_0(\boldsymbol{x}))] = \tau(\boldsymbol{x}, 0). \tag{3.2}$$

Here again, the restriction is on a marginal of the distribution of the initial state in the space of L^2-functions.

Different choices of correlation functions result in different Brownian simulation schemes. A spatially uniform Brownian motion, $c(\boldsymbol{x}, \boldsymbol{y}) \equiv \boldsymbol{I}$, corresponds to the BCF method. The CONNFFES-SIT method corresponds to a spatially uncorrelated (standard) Brownian motion. As pointed out in [5], such Brownian motion does not exist, in the sense that there does not exist an L^2 correlation function that corresponds to spatially uncorrelated noise. The CONNFFESSIT method can be defined as a limit of a sequence of correlation functions, $c_k(x, y)$, that converges to zero in L^2 as $k \to \infty$. Such sequence can be, for example, a sequence of piecewise-constant functions equal to zero everywhere except on a sequence of decreasing patches that include the diagonal, in which $c_k(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{I}$. It should be emphasized that spatially uncorrelated noise (δ-correlated) can be rigorously defined as an instance of so-called cylindrical Wiener processes [7]. Such a process is however non-standard.

We emphasize that we only address here the approximation of the probability space by a finite number of realizations. The PDE–SPDE system (3.1) also requires spatial and temporal discretizations. In particular, choices of Eulerian versus Lagrangian approximations lead to very different simulation methods.

The statistical error of the approximation scheme is defined as n times the sum of variances,

$$e(t) = n \mathbb{E}[\|\boldsymbol{\Delta}_u - \mathbb{E}(\boldsymbol{\Delta}_u)\|_2^2 + \|\boldsymbol{\Delta}_\tau - \mathbb{E}(\boldsymbol{\Delta}_\tau)\|_2^2], \tag{3.3}$$

where $\boldsymbol{\Delta}_u(\boldsymbol{x}, t) = \boldsymbol{U}(\boldsymbol{x}, t) - \boldsymbol{u}(\boldsymbol{x}, t)$ and $\boldsymbol{\Delta}_\tau(\boldsymbol{x}, t) = \boldsymbol{T}(\boldsymbol{x}, t) - \tau(\boldsymbol{x}, t)$, and $\| \cdot \|_2$ denotes the L^2-norm; for a matrix-valued function $\boldsymbol{M}(\boldsymbol{x})$,

$$\|\boldsymbol{M}\|_2^2 = \int_\Omega \operatorname{Tr}[\boldsymbol{M}(\boldsymbol{x})^T \boldsymbol{M}(\boldsymbol{x})] \, \mathrm{d}\boldsymbol{x}.$$

The reason we multiply the variance by n is to have a measure of the statistical error that converges to a constant as $n \to \infty$. The choice of statistical error is not unique. In particular, one may assign different weights to the stress and velocity variances. In particular, our presentation is made in dimensionless quantities. In a dimensional setting, the statistical errors associated with the velocity and the stress should be made comparable either by defining them as quantities of same dimensions, or, as dimensionless quantities, e.g., relative errors. The initial confusion about the reduction of variance by the BCF method is due precisely to the fact that BCF reduces the velocity variance on the account of an increase in the stress variance.

To rigorously define an optimization problem of statistical error minimization, one needs to identify the set of feasible correlation functions for which the Brownian simulations are defined, and obtain an explicit expression for the right-hand side of (3.3) in terms of the correlation function $c(\boldsymbol{x}, \boldsymbol{y})$, which is taken from the feasible set (more generally, one can also consider different choices of initial data distributions [5]). This is done in the next section.

4. The optimization problem

The main difficulties in expressing the statistical error (3.3) in terms of the spatial correlation function are: (i) the governing equations for the statistical error cannot be brought to closed-form; (ii) the n realizations $\boldsymbol{Q}_i$ are not independent, hence the variance of the difference $\boldsymbol{T} - \tau$ is not a summation over single-field contributions. To get more insight into the structure of the problem, we examine a particular example that is tractable, namely, the Hookean dumbbell model, where the force exerted by the polymers is linear in the end-to-end vector, $\boldsymbol{F}(\boldsymbol{q}) = k\boldsymbol{q}$. In this case, a closed-form PDE can be derived for the stress by multiplying the Smoluchowski equation (2.3) by $\boldsymbol{q} \otimes k\boldsymbol{q}$ and integrating over the configuration $\boldsymbol{q}$,

$$\frac{\partial \tau}{\partial t} + (\boldsymbol{u} \cdot \nabla)\tau = B(\boldsymbol{u}, \tau) - 2k\tau + k\boldsymbol{I}, \tag{4.1}$$

where $B(\boldsymbol{u}, \tau) = (\nabla \boldsymbol{u})^T \tau + \tau(\nabla \boldsymbol{u})$. The initial conditions for (4.1) are determined by the initial conditions for the Smoluchowski equation. Applying Itô's formula to the stochastic approximation of the stress, $\boldsymbol{T}$, and substituting the equations for $\boldsymbol{Q}_i$ results in an SPDE,

$$\frac{\mathrm{d}\boldsymbol{T}}{\mathrm{d}t} + (\boldsymbol{U} \cdot \nabla)\boldsymbol{T} = B(\boldsymbol{U}, \boldsymbol{T}) - 2k\boldsymbol{T} + k\boldsymbol{I} + \frac{2k}{n} \sum_{i=1}^{n} \boldsymbol{Q}_i \otimes \frac{\mathrm{d}\boldsymbol{W}_i}{\mathrm{d}t}, \tag{4.2}$$

with initial conditions determined by (2.4). Eq. (4.2) differs from (4.1) by a multiplicative noise term.

Since we expect the statistical error to be dominated by the variance, i.e., to scale like $1/\sqrt{n}$, we introduce the normalized errors,

$$\delta_u(\boldsymbol{x}, t) = \sqrt{n}(\boldsymbol{U}(\boldsymbol{x}, t) - \boldsymbol{u}(\boldsymbol{x}, t)),$$
$$\delta_\tau(\boldsymbol{x}, t) = \sqrt{n}(\boldsymbol{T}(\boldsymbol{x}, t) - \tau(\boldsymbol{x}, t)).$$

The evolution of δ_u is governed by the Stokes system,

$$-\nabla p + \nu_s \Delta \delta_u + \operatorname{div} \delta_\tau = 0,$$
$$\operatorname{div} \delta_u = 0. \tag{4.3}$$

Subtracting (4.1) from (4.2) and multiplying by $\sqrt{n}$ yields an evolution equation for δ_τ,

$$\frac{\mathrm{d}\delta_\tau}{\mathrm{d}t} + (\boldsymbol{u} \cdot \nabla)\delta_\tau + (\delta_u \cdot \nabla)\tau = B(\boldsymbol{u}, \delta_\tau) + B(\delta_u, \tau) - 2k\delta_\tau$$
$$+ \frac{2k}{\sqrt{n}} \sum_{i=1}^{n} \boldsymbol{Q}_i \otimes \frac{\mathrm{d}\boldsymbol{W}_i}{\mathrm{d}t} + \frac{1}{\sqrt{n}}(\delta_u \cdot \nabla)\delta_\tau + \frac{1}{\sqrt{n}}B(\delta_u, \delta_\tau). \tag{4.4}$$

The equations for $\boldsymbol{Q}_i$ take the form

$$\frac{\mathrm{d}\boldsymbol{Q}_i}{\mathrm{d}t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{Q}_i = (\nabla \boldsymbol{u})^T \boldsymbol{Q}_i - k\boldsymbol{Q}_i + \frac{\mathrm{d}\boldsymbol{W}_i}{\mathrm{d}t} + \frac{1}{\sqrt{n}}(\delta_u \cdot \nabla)\boldsymbol{Q}_i$$
$$+ \frac{1}{\sqrt{n}}(\nabla \delta_u)^T \boldsymbol{Q}_i. \tag{4.5}$$

For large n, the $O(1/\sqrt{n})$ terms can be neglected, so that to leading order,

$$\frac{\mathrm{d}\delta_\tau}{\mathrm{d}t} + (\boldsymbol{u} \cdot \nabla)\delta_\tau + (\delta_u \cdot \nabla)\tau$$
$$= B(\boldsymbol{u}, \delta_\tau) + B(\delta_u, \tau) - 2k\delta_\tau + \frac{2k}{\sqrt{n}} \sum_{i=1}^{n} \boldsymbol{Q}_i \otimes \frac{\mathrm{d}\boldsymbol{W}_i}{\mathrm{d}t}, \tag{4.6}$$

and

$$\frac{d\boldsymbol{Q}_i}{dt} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{Q}_i = ((\nabla \boldsymbol{u})^T - k)\boldsymbol{Q}_i + \frac{d\boldsymbol{W}_i}{dt}. \tag{4.7}$$

If the exact solutions $\boldsymbol{u}$ and $\boldsymbol{\tau}$ are given, then the coupled system (4.3), (4.6), (4.7), which governs the evolution of the normalized errors, is a closed system for $\boldsymbol{Q}_i$, δ_u and δ_τ.

Note that after the truncation of the $O(1/\sqrt{n})$ terms, the $\boldsymbol{Q}_i(\boldsymbol{x}, t)$ that are governed by (4.7) are independent; the weak coupling induced by the non-truncated dynamics (4.5) only affects higher order corrections. Furthermore, we observe that (4.6) is a non-homogenous linear equation for δ_τ, where the inhomogeneous term is a sum of independent noise terms. Since we are only interested in estimating the variance of δ_τ, we can replace the sum of independent noise terms by a single noise term that has the same first and second moments. Re-introducing $\boldsymbol{q}(\boldsymbol{x}, t)$ satisfying (2.4), we may therefore perform the substitution

$$\frac{2k}{\sqrt{n}} \sum_{i=1}^{n} \boldsymbol{Q}_i \otimes \frac{d\boldsymbol{W}_i}{dt} \rightarrow 2k\boldsymbol{q} \otimes \frac{d\boldsymbol{W}}{dt}. \tag{4.8}$$

The analysis of Eqs. (2.4), (4.3) and (4.6) with the substitution (4.8), is somewhat cumbersome due to the multi-component nature of the problem. To simplify the derivations, we focus in the remaining of this section on the stress variations, $\delta_\tau(\boldsymbol{x}, t)$, using the fact that the velocity variations, $\delta_u(\boldsymbol{x}, t)$, are expressible, through the Stokes system (4.3) as a linear function of the stress variations. We will revert to a separate analysis of velocity and stress variations in Section 6 where we solve the planar shear flow for a Hookean dumbbell model.

Thus, we rewrite the error dynamics in the more abstract (but compact) form,

$$\frac{d\delta_\tau}{dt} = A\delta_\tau + 2k\boldsymbol{q} \otimes \frac{d\boldsymbol{W}}{dt},$$
$$\frac{d\boldsymbol{q}}{dt} = B\boldsymbol{q} + \frac{d\boldsymbol{W}}{dt}, \tag{4.9}$$

where A and B are linear (differential) operators, and the initial conditions are $\delta_\tau(\boldsymbol{x}, 0)$ and $\boldsymbol{q}(\boldsymbol{x}, 0) = \boldsymbol{q}_0(\boldsymbol{x})$. The statistical error is

$$e(t) = \mathbb{E}\|\delta_\tau - \mathbb{E}(\delta_\tau)\|_2^2, \tag{4.10}$$

where the omission of the n-factor follows from the scaling of δ_τ.

System (4.9) is linear, hence the solution can be expressed in terms of the solution operators (or propagators) e^{At} and e^{Bt}. Specifically, $\boldsymbol{q}(\boldsymbol{x}, t)$ is given by

$$\boldsymbol{q}(\boldsymbol{x}, t) = e^{Bt}\boldsymbol{q}_0(\boldsymbol{x}) + \int_0^t e^{B(t-s)} d\boldsymbol{W}(\boldsymbol{x}, s),$$

whereas $\delta_\tau(\boldsymbol{x}, t)$ is given by

$$\delta_\tau(\boldsymbol{x}, t) = e^{At}\delta_\tau(\boldsymbol{x}, 0) + 2k \int_0^t e^{A(t-s)}(\boldsymbol{q}(\boldsymbol{x}, s) \otimes d\boldsymbol{W}(\boldsymbol{x}, s)).$$

It should be emphasized that the notation $e^{B(t-s)} d\boldsymbol{W}(\boldsymbol{x}, s)$, for example, means that the spatial operator $e^{B(t-s)}$ operates on the Brownian increment $d\boldsymbol{W}(\cdot, s)$, and then evaluated at the point $\boldsymbol{x}$.

In many situations of interest, the operators A and B are dissipative. Then the terms $e^{Bt}\boldsymbol{q}_0(\boldsymbol{x})$ and $e^{At}\delta_\tau(\boldsymbol{x}, 0)$ tend to zero as $t \rightarrow \infty$, and for large t the solution takes the form

$$\delta_\tau(\boldsymbol{x}, t) = 2k \int_0^t \int_0^s e^{A(t-s)}(e^{B(s-r)} d\boldsymbol{W}(\boldsymbol{x}, r) \otimes d\boldsymbol{W}(\boldsymbol{x}, s)).$$

Indeed, the long-time statistical error is independent of the initial data in dissipative systems.

At this point, it is useful to represent the propagators e^{At} and e^{Bt} by linear (possibly generalized) kernels, namely, for every matrix-valued function $\boldsymbol{M}(\boldsymbol{x})$ and vector-valued function $\boldsymbol{f}(\boldsymbol{x})$,

$$(e^{At}\boldsymbol{M})_{ij}(\boldsymbol{x}) = \int_\Omega a_{ijkl}(\boldsymbol{x}, \boldsymbol{y}, t)M_{kl}(\boldsymbol{y}) d\boldsymbol{y}, \quad i, j = 1, 2, 3,$$

$$(e^{Bt}\boldsymbol{f})_i(\boldsymbol{x}) = \int_\Omega b_{ik}(\boldsymbol{x}, \boldsymbol{y}, t)f_k(\boldsymbol{y}) d\boldsymbol{y}, \quad i = 1, 2, 3,$$

where we use the Einstein convention that repeated indices imply a summation. Then, the stress variation takes the form

$$[\delta_\tau(\boldsymbol{x}, t)]_{ij} = 2k \int_0^t \int_0^s \iint_\Omega a_{ijkl}(\boldsymbol{x}, \boldsymbol{y}, t-s)b_{km}(\boldsymbol{y}, \boldsymbol{z}, s-r)$$
$$\times d W_l(\boldsymbol{y}, s) d W_m(\boldsymbol{z}, r) d\boldsymbol{y} d\boldsymbol{z}.$$

Squaring, taking expectations using the fact that

$$\mathbb{E}[d W_i(\boldsymbol{x}, t_1) d W_j(\boldsymbol{y}, t_2)] = \delta(t_1 - t_2)c_{ij}(\boldsymbol{x}, \boldsymbol{y}) dt,$$

then integrating over $\boldsymbol{x}$ and summing over i, j, we obtain an expression for the mean statistical error, which is quadratic in the correlation function c,

$$e(t) = \iint \iint_\Omega m_{lqmn}(\boldsymbol{y}, \boldsymbol{y}', \boldsymbol{z}, \boldsymbol{z}', t)c_{lq}(\boldsymbol{y}, \boldsymbol{y}')$$
$$\times c_{mn}(\boldsymbol{z}, \boldsymbol{z}') d\boldsymbol{y} d\boldsymbol{y}' d\boldsymbol{z} d\boldsymbol{z}', \tag{4.11}$$

where

$$m_{lqmn}(\boldsymbol{y}, \boldsymbol{y}', \boldsymbol{z}, \boldsymbol{z}', t)$$
$$= 4k^2 \sum_{i,j} \int_0^t \int_0^s \int_\Omega a_{ijkl}(\boldsymbol{x}, \boldsymbol{y}, t-s)a_{ijpq}(\boldsymbol{x}, \boldsymbol{y}', t-s)b_{km}$$
$$\times (\boldsymbol{y}, \boldsymbol{z}, s-r)b_{pn}(\boldsymbol{y}', \boldsymbol{z}', s-r) d\boldsymbol{x} dr ds.$$

To rigorously define the optimization problem, we need to identify the set of admissible spatial correlation functions $c(\boldsymbol{x}, \boldsymbol{y})$. This is established by the following statement [5]:

An L^2 function $c(\boldsymbol{x}, \boldsymbol{y})$ is a spatial correlation function of a random L^2 function if and only if there exists an L^2 function $r(\boldsymbol{x}, \boldsymbol{y})$ such that

$$c(\boldsymbol{x}, \boldsymbol{y}) = \int r(\boldsymbol{x}, \boldsymbol{z})r(\boldsymbol{y}, \boldsymbol{z}) d\boldsymbol{z} \tag{4.12}$$

for almost every $\boldsymbol{x}, \boldsymbol{y}$.

In other words, the set of correlation functions $c(\boldsymbol{x}, \boldsymbol{y})$ can be indexed by the set of "square roots" $r(\boldsymbol{x}, \boldsymbol{y})$. Thus, the set of admissible correlation functions $c(\boldsymbol{x}, \boldsymbol{y})$ is

$$\mathcal{C} = \{c(\boldsymbol{x}, \boldsymbol{y}) = \int r(\boldsymbol{x}, \boldsymbol{z}) \otimes r(\boldsymbol{y}, \boldsymbol{z}) d\boldsymbol{z} : r \in L^2, \ c(\boldsymbol{x}, \boldsymbol{x}) = \boldsymbol{I}\}.$$

The optimization problem is

Find $c \in \mathcal{C}$ such that $e(t)$, given by (4.11), is minimal. \hfill (4.13)

Comments:

(1) An alternative description of the spatial correlation of the random function $\boldsymbol{W}(\boldsymbol{x}, t)$ is by the correlation operator $\boldsymbol{C}$, defined by its action on vector-valued functions,

$$[\boldsymbol{C}(\boldsymbol{f})(\boldsymbol{x})]_i = \int c_{ij}(\boldsymbol{x}, \boldsymbol{y})f_j(\boldsymbol{y}) d\boldsymbol{y}, \quad i = 1, 2, 3.$$

The statistical error then takes the more compact form

$$e(t) = \text{Tr}[\boldsymbol{M}(t)(\boldsymbol{C} \otimes \boldsymbol{C})], \tag{4.14}$$

where $\boldsymbol{M}(t)$ is an operators acting on $L^2 \otimes L^2$ defined by

$$[\boldsymbol{M}(t)(\boldsymbol{f} \otimes \boldsymbol{g})(\boldsymbol{x}, \boldsymbol{y})]_{ij} = \iint_{\Omega} m_{ijkl}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{x}', \boldsymbol{y}', t) \boldsymbol{f}_k(\boldsymbol{x}') \boldsymbol{g}_l(\boldsymbol{y}') \mathrm{d}\boldsymbol{x}' \mathrm{d}\boldsymbol{y}'.$$

(2) Condition (4.12) which defines the feasible set for which the Brownian simulations are defined, is equivalent to the requirement that the correlation operator $\boldsymbol{C}$ is symmetric positive semi-definite and has finite trace. This condition is necessary for the right-hand side of (4.14) to remain finite [7].

(3) The above optimization problem does not necessarily have a minimizer because the set of admissible correlation functions is neither closed nor bounded. In such case, we need to look for sequences $c_k(\boldsymbol{x}, \boldsymbol{y})$ of correlations functions such that the corresponding sequence of errors $e_k(t)$ converges to the infimum,

$$e_{\mathrm{inf}}(t) = \inf\{e(t) : c \in \mathcal{C}^W\}. \tag{4.15}$$

It is only in this context that CONNFFESSIT, for example, can be claimed to be optimal: the sequence of Brownian correlations, $c_k(\boldsymbol{x}, \boldsymbol{y})$, approaches a function that is zero everywhere, except for the diagonal where it must equal one. This function is equivalent (in L^2) to zero, which is not an admissible correlation function.

(4) The statistical error can be similarly developed in cases where A and B are not dissipative, resulting in a sum of two terms,

$$e(t) = e_1(t) + e_2(t),$$

where $e_2(t)$ is given by (4.11) and $e_1(t)$ depends on the distribution of $\boldsymbol{q}_0(\boldsymbol{x})$.

5. Finite-dimensional approximation

The optimization problem (4.13) cannot be solved analytically, except for very simple examples (see [5]). In general, it must be solved approximately. This can be done by discretizing the domain Ω and restricting the set of admissible correlation functions to functions that are piecewise constant with respect to the discretization. A general convergence theorem was proved in [5] asserting that as we refine the discretization, the sequence of optimizers yields a sequence of mean statistical errors that converges to the optimal statistical error e_{inf}.

We demonstrate the procedure for the case where Ω is a bounded one-dimensional interval $[a, b]$ and likewise, $\boldsymbol{q}$ and $\boldsymbol{W}$ are scalar fields. Using an N-point mesh,

$$x_k = a + (b-a)\frac{k - (1/2)}{N}, \quad k = 1, \ldots, N,$$

we approximate the integral (4.11)(without the indices, since we consider a one-dimensional system) by quadrature,

$$e(t) = \frac{1}{N^4} \sum_{l,q,m,n=1}^{N} m(x_l, x_q, x_m, x_n, t) c(x_l, x_q) c(x_m, x_n).$$

Defining the N-by-N and N^2-by-N^2 matrices, C and $M(t)$,

$$C_{lq} = \frac{1}{N} c(x_l, x_q), \quad \text{and} \quad M_{lN+m,qN+n}(t) = \frac{1}{N^2} m(t, x_l, x_q, x_m, x_n),$$

the statistical error takes the form,

$$e(t) = \mathrm{Tr}[M(t)(C \otimes C)], \tag{5.1}$$

where $\otimes$ denotes the Kronecker product for matrices. The matrix C is a symmetric positive semi-definite (spd) matrix, satisfying a constraint which follows from (2.5),

$$C_{ii} = \frac{1}{N}. \tag{5.2}$$

The infinite-dimensional optimization problem (4.13) is therefore approximated by the finite-dimensional minimization problem:

Find an spd matrix C satisfying (5.2) that minimizes (5.1). (5.3)

As stated above, the sequence of minimal errors converges to the lower bound of the error e_{inf} as $N \to \infty$. This does not imply, however, the convergence of the sequence of finite-dimensional optimizers.

The standard approach for solving finite-dimensional optimization problems of this form is by semi-definite programming algorithms [8]. These algorithms apply to convex optimization problems defined on the cone of symmetric positive semi-definite matrices, subject to affine constraints.

6. Planar shear flow of Hookean dumbbells

In this section we analyze the Hookean dumbbell model for the planar shear flow considered by Jourdain et al. in [1]. In this model, the momentum and mass conservation equations reduce to a scalar heat equation,

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial \tau}{\partial x}, \tag{6.1}$$

where $u(x, t)$ is the axial component of the velocity and $\tau(x, t)$ is the shear component of the conformation tensor, which is given by an expectation

$$\tau(x, t) = \mathbb{E}[q(x, t)r(t)], \tag{6.2}$$

where the function-valued and real-valued stochastic processes $q(x, t)$ and $r(t)$ satisfy a mixed SPDE–SDE system,

$$\frac{\mathrm{d}q}{\mathrm{d}t} = \frac{\partial u}{\partial x}r - \frac{q}{2} + \frac{\mathrm{d}W}{\mathrm{d}t},$$
$$\frac{\mathrm{d}r}{\mathrm{d}t} = -\frac{r}{2} + \frac{\mathrm{d}V}{\mathrm{d}t}. \tag{6.3}$$

Here $W(x, t)$ and $V(t)$ are independent function-valued and real-valued Brownian motions, and we denote by $c(x, y)$ the spatial correlation function of W. Note that $c(x, y)$ is now real-valued rather than matrix-valued. The domain is $x \in [0, 1]$. The boundary conditions are $u(0, t) = 1$ and $u(1, t) = 0$. There are no boundary conditions for $q(x, t)$; see Fig. 1 for a sketch of the geometry.

Introducing an auxiliary real-valued function $s(t) = \mathbb{E}[r^2(t)]$, which is a normal component of the conformation tensor, we obtain
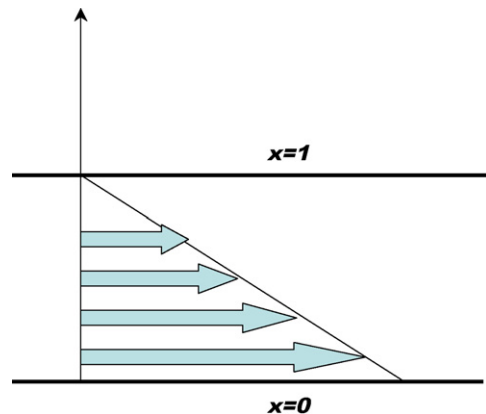

Fig. 1. Geometry of planar shear flow.

a closed-form system for $\tau(x, t)$, $s(t)$,

$$\frac{\partial \tau}{\partial t} = -\tau + \frac{\partial u}{\partial x} s,$$
$$\frac{ds}{dt} = -s + 1. \tag{6.4}$$

The "macroscopic" system (6.1), (6.4) governs the evolution of the shear flow. For long times, the solution tends to the steady-state

$$u(x) = 1 - x, \quad \tau(x) = -1, \quad s = 1.$$

The Brownian simulation scheme for the coupled system (6.1)–(6.3) is

$$\frac{dU}{dt} = \frac{\partial^2 U}{\partial x^2} + \frac{\partial T}{\partial x},$$
$$T(x, t) = \frac{1}{n} \sum_{i=1}^{n} Q_i(x, t) R_i(t), \tag{6.5}$$

where the sequences of stochastic processes $Q_i(x, t)$, $R_i(t)$ are approximations to independent realizations of the processes $q(x, t)$ and $r(t)$; they are governed by

$$\frac{dQ_i}{dt} = \frac{\partial U}{\partial x} R_i - \frac{Q_i}{2} + \frac{dW_i}{dt},$$
$$\frac{dR_i}{dt} = -\frac{R_i}{2} + \frac{dV_i}{dt}, \quad i = 1, \dots, n, \tag{6.6}$$

where $W_i(x, t)$ and $V_i(t)$ are sets of mutually independent function-valued and real-valued Brownian motions, such that the spatial correlation function of each $W_i(x, t)$ is $c(x, y)$. The boundary conditions are $U(0, t) = 1$, $U(1, t) = 0$. Since we are going to focus on long-time behavior, we may well assume that the deterministic system (6.1), (6.4) is initialized at steady state,

$$u(x, 0) = 1 - x, \quad \tau(x, 0) = -1, \quad s(0) = 1.$$

For the linearization to be a reasonable approximation for short time as well, we initialize the stochastic system (6.5), (6.6) such that

$$U(x, 0) = 1 - x, \quad \mathbb{E}[Q_i(x, 0) R_i] = -1, \quad \mathbb{E}[R_i^2(0)] = 1.$$

These choices are immaterial for the study of long-time behavior.

System (6.5)–(6.6) has a slightly different form than system (3.1). We therefore adapt the error analysis to the present case. We introduce the random function,

$$S(t) = \frac{1}{n} \sum_{i=1}^{n} R_i^2(t),$$

which is the stochastic approximation to $s(t)$. The pair $T(x, t)$, $S(t)$ is governed by the (non-closed) stochastic system

$$\frac{dT}{dt} = -T + \frac{\partial U}{\partial x} S + \frac{1}{n} \sum_{i=1}^{n} R_i \frac{dW_i}{dt} + \frac{1}{n} \sum_{i=1}^{n} Q_i \frac{dV_i}{dt},$$
$$\frac{dS}{dt} = -S + 1 + \frac{2}{n} \sum_{i=1}^{n} R_i \frac{dV_i}{dt}.$$

As in Section 4 we define normalized errors,

$$\delta_u(x, t) = \sqrt{n}(U(x, t) - u(x, t)),$$
$$\delta_\tau(x, t) = \sqrt{n}(T(x, t) - \tau(x, t)),$$
$$\delta_s(t) = \sqrt{n}(S(t) - s(t)).$$

The linearized equations for the normalized errors are

$$\frac{d\delta_u}{dt} = \frac{\partial^2 \delta_u}{\partial x^2} + \frac{\partial \delta_\tau}{\partial x},$$
$$\frac{d\delta_\tau}{dt} = s \frac{\partial \delta_u}{\partial x} - \delta_\tau + \frac{\partial u}{\partial x} \delta_s + \frac{1}{\sqrt{n}} \sum_{i=1}^{n} R_i \frac{dW_i}{dt} + \frac{1}{\sqrt{n}} \sum_{i=1}^{n} Q_i \frac{dV_i}{dt}, \tag{6.7}$$
$$\frac{d\delta_s}{dt} = -\delta_s + \frac{2}{\sqrt{n}} \sum_{i=1}^{n} R_i \frac{dV_i}{dt},$$

and the linearized equations for $Q_i(x, t)$ and $R_i(t)$ are

$$\frac{dQ_i}{dt} = \frac{\partial u}{\partial x} R_i - \frac{Q_i}{2} + \frac{dW_i}{dt},$$
$$\frac{dR_i}{dt} = -\frac{R_i}{2} + \frac{dV_i}{dt}, \quad i = 1, \dots, n. \tag{6.8}$$

As in Section 4 we observe that the $Q_i(x, t)$, $R_i(t)$ governed by (6.8) are independent, hence, applying the same considerations as in (4.8), the system (6.7) can be written in the form

$$\frac{d\delta_u}{dt} = \frac{\partial^2 \delta_u}{\partial x^2} + \frac{\partial \delta_\tau}{\partial x},$$
$$\frac{d\delta_\tau}{dt} = s \frac{\partial \delta_u}{\partial x} - \delta_\tau + \frac{\partial u}{\partial x} \delta_s + r \frac{dW}{dt} + q \frac{dV}{dt}, \tag{6.9}$$
$$\frac{d\delta_s}{dt} = -\delta_s + 2r \frac{dV}{dt},$$

where $q(x, t)$ and $r(t)$ are given by (6.3).

Often, one would like to evaluate the statistical errors in the velocity and in the shear-stress separately,

$$e_u(t) = \mathbb{E}\|\delta_u(\cdot, t)\|_2^2, \quad e_\tau(t) = \mathbb{E}\|\delta_\tau(\cdot, t)\|_2^2. \tag{6.10}$$

Since $s(t)$ was introduced as an auxiliary variable we do not account for the error associated with its approximation. The total statistical error is arbitrarily defined by setting equal weights for the two contributions,

$$e(t) = e_u(t) + e_\tau(t). \tag{6.11}$$

System (6.9) is an inhomogeneous linear system, whose solution is

$$\begin{pmatrix} \delta_u(x, t) \\ \delta_\tau(x, t) \\ \delta_s(t) \end{pmatrix} = e^{At} \begin{pmatrix} \delta_u(x, 0) \\ \delta_\tau(x, 0) \\ \delta_s(0) \end{pmatrix}$$
$$+ \int_0^t e^{A(t-t')} \begin{pmatrix} 0 \\ r(t') \, dW(x, t') + q(x, t') \, dV(t') \\ 2r(t') \, dV(t') \end{pmatrix}, \tag{6.12}$$

where

$$A = \begin{pmatrix} \dfrac{\partial^2}{\partial x^2} & \dfrac{\partial}{\partial x} & 0 \\ \dfrac{\partial}{\partial x} & -1 & -1 \\ 0 & 0 & -1 \end{pmatrix} \tag{6.13}$$

is an operator on the Hilbert space $L^2[0, 1] \times L^2[0, 1] \times \mathbb{R}$. The second derivative is endowed with vanishing Dirichlet boundary conditions. The operator A is dissipative hence the first term, which depends on the initial data can be neglected for long times. Furthermore, it is easy to verify that

$$e^{At} = \begin{pmatrix} B_{11}(t) & B_{12}(t) & 0 \\ B_{21}(t) & B_{22}(t) & -te^{-t} \\ 0 & 0 & e^{-t} \end{pmatrix},$$

where

$$\begin{pmatrix} B_{11}(t) & B_{12}(t) \\ B_{21}(t) & B_{22}(t) \end{pmatrix} = \exp\left\{ \begin{pmatrix} \dfrac{\partial^2}{\partial x^2} & \dfrac{\partial}{\partial x} \\ \dfrac{\partial}{\partial x} & -1 \end{pmatrix} t \right\}.$$

Denoting the (possibly singular) kernels of the $B_{ij}(t)$ by $b_{ij}(x, y, t)$, the long-time dependence of the normalized errors δ_u, δ_τ is

$$\delta_u(x, t) = \int_0^t \int_0^1 b_{12}(x, y, t - t') \, dn(y, t') \, dy,$$

$$\delta_\tau(x, t) = \int_0^t \int_0^1 b_{22}(x, y, t - t') \, dn(y, t') \, dy \qquad (6.14)$$

$$- \int_0^t (t - t') e^{-(t-t')} \, dm(t'),$$

where

$$dn(x, t) = r(t) \, dW(x, t) + q(x, t) \, dV(t), \quad dm(t) = 2r(t) \, dV(t).$$

Squaring the normalized errors and averaging we obtain

$$\mathbb{E}[\delta_u(x, t)]^2$$

$$= \int_0^t \iint_0^1 b_{12}(x, y, t - t') b_{12}(x, z, t - t') \mathbb{E}[dn(y, t') \, dn(z, t')] \, dy \, dz,$$

$$\mathbb{E}[\delta_\tau(x, t)]^2$$

$$= \int_0^t \iint_0^1 b_{22}(x, y, t - t') b_{22}(x, z, t - t') \mathbb{E}[dn(y, t') \, dn(z, t')] \, dy \, dz$$

$$- 2 \int_0^t \int_0^1 b_{22}(x, y, t - t')(t - t') e^{-(t-t')} \mathbb{E}[dn(y, t') \, dm(t')] \, dy$$

$$+ \int_0^t (t - t')^2 e^{-2(t-t')} \mathbb{E}[dm(t') \, dm(t')].$$

$$\qquad (6.15)$$

The independence of $W(x, t)$ and $V(t)$, and the spatial correlation function of $W(x, y)$ imply

$$\mathbb{E}[dW(y, t) \, dW(z, t)] = c(y, z) \, dt,$$

$$\mathbb{E}[dW(y, t) \, dV(t)] = 0, \qquad\qquad\qquad\qquad (6.16)$$

$$\mathbb{E}[dV(t) \, dV(t)] = dt,$$

from which we obtain

$$\mathbb{E}[dn(y, t) \, dn(z, t)] = (\mathbb{E}[r(t)^2] c(y, z) + \mathbb{E}[q(y, t) q(z, t)]) \, dt,$$

$$\mathbb{E}[dn(y, t) \, dm(t)] = 2\mathbb{E}[q(y, t) r(t)] \, dt,$$

$$\mathbb{E}[dm(t) \, dm(t)] = 4\mathbb{E}[r^2(t)] \, dt.$$

The correlation functions of $r(t)$ and $q(x, t)$ are obtained by integrating the stochastic system (6.3)

$$r(t) = r(0) e^{-t/2} + \int_0^t e^{-(t-t')/2} \, dV(t'),$$

$$q(x, t) = q(x, 0) e^{-t/2} + \int_0^t e^{-(t-t')/2} dW(x, t') - \int_0^t e^{-(t-t')/2} r(t') \, dt'.$$

At steady state

$$\mathbb{E}[r(t)^2] = 1, \quad \mathbb{E}[r(t) q(x, t)] = -1, \quad \mathbb{E}[q(x, t) q(y, t)] = c(x, y) + 2.$$

Substituting these correlations into (6.15) and integrating over x, we obtain as $t \to \infty$,

$$e_u = 2 \int_0^\infty \iiint_0^1 b_{12}(x, y, t) b_{12}(x, z, t)(1 + c(y, z)) \, dt \, dx \, dy \, dz,$$

$$e_\tau = 2 \int_0^\infty \iiint_0^1 b_{22}(x, y, t) b_{22}(x, z, t)(1 + c(y, z)) \, dt \, dx \, dy \, dz$$

$$\qquad (6.17)$$

$$+ 4 \int_0^\infty \iint_0^1 b_{22}(x, y, t) t e^{-t} \, dt \, dx \, dy$$

$$+ 4 \int_0^\infty \int_0^1 t^2 e^{-2t} \, dt \, dx.$$

Note that these mean statistical errors can be partitioned into terms that depend on the correlation $c(x, y)$ and terms that do not depend on the correlation. The latter, of course, do not affect the optimization problem. Also, the statistical error is an affine function of the correlation function rather than quadratic, as obtained in Section 4. Hence, an optimal correlation (if exists) is guaranteed to be on the boundary of the domain $\mathcal{C}$.

The three-dimensional linear space of constant functions is invariant under the operator A, and the restriction of e^{At} to constant functions can be calculated analytically. It is easy to see that in this case $B_{12}(t) = 0$ and $B_{22}(t) = e^{-t}$, from which we deduce that

$$\int_0^1 b_{12}(x, y, t) \, dy = 0 \quad \text{and} \quad \int_0^1 b_{22}(x, y, t) \, dy = e^{-t}.$$

Thus the terms in (6.17) that do not depend on the correlation function can be calculated, yielding

$$e_u = 2 \int_0^\infty \iiint_0^1 b_{12}(x, y, t) b_{12}(x, z, t) c(y, z) \, dt \, dx \, dy \, dz,$$

$$\qquad (6.18)$$

$$e_\tau = 3 + 2 \int_0^\infty \iiint_0^1 b_{22}(x, y, t) b_{22}(x, z, t) c(y, z) \, dt \, dx \, dy \, dz.$$

Eq. (6.18) can be further developed by formally expanding the kernel functions $b_{12}(x, y, t)$ and $b_{22}(x, y, t)$ in trigonometric series of the form

$$b_{12}(x, y, t) = \sum_{k=1}^\infty B_{12}(k, t) e_k(x) f_k(y),$$

$$\qquad (6.19)$$

$$b_{22}(x, y, t) = \sum_{k=0}^\infty B_{22}(k, t) e_k(x) e_k(y),$$

where

$$e_k(x) = \sqrt{2} \sin k\pi x, \quad k > 0,$$

$$f_k(x) = \sqrt{2} \cos k\pi x, \quad k > 0, \quad f_0(x) = 1.$$

The coefficients $B_{12}(k, t)$ and $B_{22}(k, t)$ are entries of the matrix-valued function

$$B(k, t) = \exp\left\{ \begin{pmatrix} -k^2 & -k \\ k & -1 \end{pmatrix} t \right\}. \qquad (6.20)$$

It can be verified that for large k,

$$B_{12}(k, t) \sim k^{-1} \quad \text{and} \quad B_{22}(k, t) \sim e^{-2t} + O(k^{-2}),$$

which implies that $\sum_{k=1}^\infty B_{12}(k, t) e_k(x) f_k(y)$ is convergent in L^2, while the series $\sum_{k=0}^\infty B_{22}(k, t) f_k(x) f_k(y)$ is convergent in the sense of distributions. Substituting (6.19) and (6.20) into (6.18), inverting

the order of the temporal and spatial integrations, and using the fact that

$$\int_0^\infty B_{12}^2(k,t)\,dt = \frac{1}{4\pi^2 k^2(1+\pi^2 k^2)},$$

$$\int_0^\infty B_{22}^2(k,t)\,dt = \frac{2+\pi^2 k^2}{4+4\pi^2 k^2},$$

we obtain the final expressions

$$e_u = 2\sum_{k=1}^\infty \frac{c_k}{4\pi^2 k^2(1+\pi^2 k^2)},$$

$$e_\tau = 3\frac{1}{2} + 2\sum_{k=0}^\infty \frac{c_k}{4+4\pi^2 k^2},$$
(6.21)

where

$$c_k = \iint_0^1 f_k(y)f_k(z)c(y,z)\,dy\,dz.$$

These expressions can now be used to derive the errors e_u and e_τ for a variety of correlation functions $c(x,y)$:

(1) The choice of spatially uniform correlation function, $c(x,y) = 1$, i.e., the BCF method, gives $c_0 = 1$ and $c_k = 0$ for $k > 0$, in which case we obtain

$$e_u = 0, \quad e_\tau = 4.$$

This result is in agreement with [1] where BCF was found to yield a vanishing statistical error in the velocity field.

(2) For any choice of correlation function of the form $c(x,y) = \cos \pi k(x-y)$, $k > 0$, the corresponding statistical errors are

$$e_u = \frac{2}{4\pi^2 k^2(1+\pi^2 k^2)}, \quad e_\tau = 3\frac{1}{2} + \frac{2}{4+4\pi^2 k^2}.$$

(3) CONNFFESSIT corresponds to a limit of correlation functions $c(x,y)$ that converge to zero in the off-diagonal entries while remaining equal to one on the diagonal, thus converge to zero in L^2. The corresponding statistical errors are therefore

$$e_u = 0, \quad e_\tau = 3\frac{1}{2}.$$

The fact that $e_u = 0$ is in agreement with [1], where it was shown that for uncorrelated noise the variance of the velocity is of the order of the mesh size.

Comments:

(1) The characterization (4.12) implies that for every choice of correlation function $c(x,y)$ and for every k

$$c_k = \int_0^1 \left(\int_0^1 f_k(y)r(x,y)\,dy \right)^2 dx,$$

where $r(x,y)$ is the "square root" of $c(x,y)$. Thus, $0 \le c_k \le 1$. Clearly, both sums in (6.21) are minimized when taking $c(x,y) \to 0$, hence the CONNFFESSIT method is optimal.
(2) Bessel's inequality implies that

$$\sum_{k=1}^\infty c_k \le \iint_0^1 r^2(x,y)\,dy = 1.$$

Thus, e_u is maximized by taking $c_1 = 1$ and $c_k = 0$ for every $k \ne 1$. The corresponding correlation function is $c(x,y) = \cos \pi(x-y)$. Similarly, e_τ is maximized by taking $c_0 = 1$ and $c_k = 0$ for every $k > 0$. Thus, the variance of the stress is maximized by the BCF method.

7. Discussion

We formulated an optimization problem in infinite-dimension for variance minimization in Brownian simulation methods. The optimization problem can be written in explicit form for micro–macro model for which closure into a macroscopic model is possible, although we believe that the resulting analysis provides insight into more general cases as well. Even for closable systems, the optimization problem can be solved analytically only in relatively simple cases. In practice, one has to approximate its solution by solving convex optimization problems in finite-dimension. We proved in [5] that the optimal variance can indeed be approached by the solution of finite-dimensional problems. Our analysis is based on a formal asymptotic expansion that uses an *a priori* estimate about the smallness of the statistical errors as $N \to \infty$.

We then solved analytically the optimization problem for the shear flow of a Hookean dumbbell model at steady state. Surprisingly perhaps, we find uncorrelated noise to be optimal. This result holds no matter how the variances in the velocity and the stress are weighted, as long as both have positive weights. The optimality of CONNFFESSIT is interesting, first because of the original speculation whereby BCF is a "noise-reduced" variant of CONNFFESSIT. Also, Jourdain et al. [1] found, in the context of a finite-dimensional discretization, that the optimal correlation has an oscillatory pattern. There is no contradiction between the two results, as the optimality of uncorrelated noise can only be interpreted as a limit. Had Jourdain et al. considered a sequence of mesh-refined solution, they would have seen that the off-diagonal terms of the optimal correlation function tend to zero. We emphasize that in practice, i.e., in a finite-dimensional setting, the optimal correlation may differ significantly from the optimal correlation in the continuum limit. For example, both BCF and CONNFFESSIT result in a vanishing statistical error for the velocity, whereas this is not the case in finite-dimensional settings.

A natural question is whether CONNFFESSIT remains optimal also in more general cases. We do not know the answer, and in particular, it may well be that the smoothness of the solutions of BCF becomes advantageous in strongly non-linear systems. Note that the linear shear flow problem leads to a variance that is an affine function of the noise correlation. In such case, the optimizer is guaranteed to reside on the boundary of the set of feasible correlations, $\mathcal{C}$. In non-linear cases, the variance is at least quadratic in the correlation function, so that the optimizer may well reside in the interior of $\mathcal{C}$.

Finally, we note that the differences between CONNFFESSIT and BCF for the shear flow problem are very mild; the variance changes by only 12%. It is unclear at this point whether differences may become much more pronounced in other models and geometries.

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