A MULTISCALE APPROACH TO COMPUTATIONAL FLUID DYNAMICS

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ABSTRACT

We present a multiscale approach to computational fluid dynamics that contains Brownian configuration fields as a special case. The scheme is formulated in an Eulerian frame, and microstructural information is communicated to the macroscopic continuum via convection of slow modes of the microscopic configurational distribution function. The scheme can in principle be applied to any type of microstructural simulation. We present a simple test case of convected extensional flow of FENE dumbbells and compare to the exact solution.

KEYWORDS: MULTISCALE SIMULATION, BROWNIAN DYNAMICS, SUPG, FINITE ELEMENT, FENE, PROJECTION, DISTRIBUTION FUNCTION

INTRODUCTION

Recent developments in computational fluid dynamics and microstructural simulation techniques, as well as dramatic increases in computing power, have made conceivable the simulation of flows of microstructurally complex materials in complex geometries, directly from coarse-grained models of the microstructure, such as those outlined above. The basic idea of the approach is simple: at each time step the continuum equations of conservation of mass and momentum are solved via finite elements, self-consistently with microstructural (e.g. Brownian dynamics) simulations for the microstructure at each point in the flow. The promise of such *multiscale computational fluid dynamics* techniques is exciting, because the complexity and variety of fluids such as polymer solutions, fiber suspensions and colloids makes the construction of quantitatively accurate closed form constitutive models a daunting task. For example, the mere introduction of finitely extensible springs into the bead-spring theory of dilute polymer solutions – the FENE model -- precludes the construction of an exact evolution equation for the stress tensor [1]. However, the direct simulation, via Brownian dynamics, of the behaviour of such model polymers in a homogeneous flow is straightforward [2].

The first two-dimensional calculation to combine Brownian dynamics for the polymer microstructure with a finite element code for the solution of the continuum momentum and continuity equations was performed by Feigl, Laso and Öttinger [3], who computed the steady flow of a solution of Hookean dumbbells in an axisymmetric contraction. In their approach, the evaluation of an integral constitutive equation along streamlines was simply replaced by conventional Brownian dynamics simulations. Related calculations, but with microstructural models for which no closed form constitutive equation exists, have been performed by a number of groups [4–7]. Significant differences were found between the true microstructural behaviour and the behaviour predicted using approximate closed form constitutive models.

The natural reference frame for microstructural simulations (MS) of all types is Lagrangian, and in the above mentioned work, this reference frame was used. Nevertheless, there are drawbacks to using Lagrangian microstructural simulations in a computational fluid dynamics (CFD) calculation; all major CFD approaches except those developed for free-surface flows are Eulerian. An important development in multiscale CFD for complex fluids was the development of the Eulerian Brownian configuration fields (BCF) method [8]. As it stands, however, the BCF method is highly computationally demanding and suitable only in cases where the fluid microstructure is spatially very smooth. However, if the continuum hypothesis holds on the scale of the CFD calculation, we expect certain functions of the microstructural state, namely ensemble averages, to be smooth functions of spatial position. Furthermore, we expect that a finite number of such functions will describe the microstructure to the level of detail necessary to accurately compute the flow. These observations motivate our development of a new multiscale simulation method, which is purely Eulerian, encompasses BCF as a special case, and applies in principle to any type of microstructural simulation [9]. This approach and its performance on a model problem are detailed here. As will be seen, the results are extremely promising, thus providing strong motivation for further development of the approach.

METHOD

The central problem with constructing an Eulerian scheme for microstructural simulations in complex flows is how to "communicate" the microstructural information from point to point along pathlines in the flow. BCF solves this problem by solving a convection equation in physical space for each trajectory of the microstructural simulation. Since good statistics require large ensembles – 1000 trajectories are not unusual -- this is an expensive process. The fundamental idea underlying the present approach is that distribution functions can be accurately characterized by far fewer than 1000 pieces of information. Based on this idea we have developed the following scheme: at each (stationary) mesh point in the computational domain, the time-evolution of the microstructure $\mathbf{Q}$ from time n to $n+1$ consists of two parts, implemented as a straightforward splitting scheme:

1) a conventional Brownian dynamics (or other microstructural simulation) step. This updates the microstructure from its value $\mathbf{Q}^n$ at time step n to account for all effects except the convection of microstructure from

upstream; the result is an intermediate vector $\mathbf{Q}^*$;

2) a "convection step", where the microstructure is modified to account for the convection of microstructure from upstream. This is done by choosing a small number of properties of the microstructural distribution function, denoted by a vector $\mathbf{F}[\mathbf{Q}]$, project the microstructure onto these variables, and update them to reflect the effect of convection. Currently, the properties that are convected are chosen to be the lowest order moments of the microstructural distribution function [10]. First, we solve the convection equation

$$\mathbf{F}^{n+1} - \mathbf{F}^* = -\Delta t\, \mathbf{v} \cdot \nabla \mathbf{F}^{\mathbf{n+1}} \tag{1}$$

for $\mathbf{F}^{n+1} - \mathbf{F}^* = \Delta \mathbf{F}$. This gives the updated value of the projections – we now perform the (non-unique) step of updating the entire microstructure. Letting $\mathbf{Q}^{n+1} - \mathbf{Q}^* = \Delta \mathbf{Q}$ we note that to $\mathrm{O}(\Delta t)$

$$\Delta \mathbf{F} = \mathbf{L} \cdot \Delta \mathbf{Q} \tag{2}$$

where $\mathbf{L}$ is the Jacobian of $\mathbf{F}$. Because the dimension of $\mathbf{F}$ is much less than that of $\mathbf{Q}$, this problem is underdetermined. We solve it in the least squares sense, finding the smallest correction to the microstructure that conserves the vector $\mathbf{F}$. This solution scales linearly with the dimension of $\mathbf{Q}$. Note that if the properties to be conserved are chosen to be the microstructural state variables themselves, then the method reduces to BCF. Given the updated microstructure at the current time step, the corresponding stress is computed and the velocity field updated to satisfy conservation of mass and momentum. Because this method is in an Eulerian reference frame on a fixed mesh, it is relatively simple to implement, allowing well-developed finite- and spectral-element technology to be straightforwardly applied to the macroscopic flow simulation of very complex materials. For the purposes of the present work we call this scheme OSMM, for "Operator-Splitting Moment Matching", noting that moments are not the only, or even necessarily the best, projected variables to conserve.

We illustrate the promise of this approach with a simple example, a one-dimensional analogue of a finitely extensible bead-spring polymer model in flow. The flow domain is the region $0 < x < 1$ and all springs have equilibrium length upon entering the domain. The springs are convected through the domain with speed v while being acted upon by a stretching force modeling an extensional flow. The MS (in the Lagrangian frame) for this model is the Brownian dynamics simulation of the dimensionless stochastic differential equation

$$dq = \left[We\, q - \frac{1}{2} \frac{q}{1-q^2} \right] dt + \frac{1}{\sqrt{b}}\, dw \tag{3}$$

where w is a one-dimensional Wiener process with unit variance, b is the finite extensibility parameter, and We is the Weissenberg number. In this non-dimensionalization, $-1 < q < 1$. Note that because of the nonlinearity, the distribution of q is far from Gaussian. Furthermore, because the speed is constant, an "exact" solution can easily be obtained in the form of a time-dependent Lagrangian simulation, since time and spatial position are simply related: $x = vt$. This feature simplifies assessment of the performance of the Eulerian scheme. We implement the OSMM approach using a quadratic finite element discretization and SUPG weight functions to solve the convection step. Using $\mathbf{F} = \left\{ \langle q^2 \rangle, \langle q^4 \rangle, \langle q^6 \rangle, \langle q^8 \rangle, \langle q^{10} \rangle \right\}$ as the convected field variables yields the steady-state results shown in Figure 1, which are compared with "exact" results obtained by a Lagrangian simulation and the relation $x = vt$.

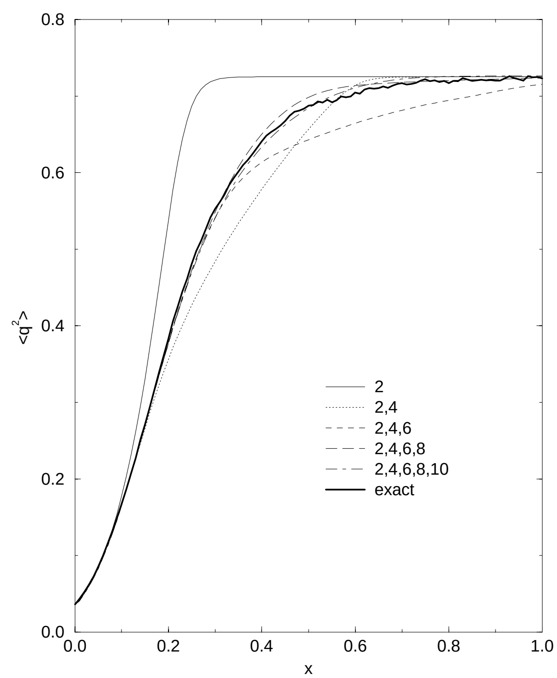

Figure 1. Steady-state profile for exact and OSMM with correction up to 10^{th} order. FENE dumbbells with b=25.0, We=4.0, De=0.1. The Deborah number De is defined such that a fluid element travels from $x = 0$ to $x = 1$ in time $t = De^{-1}$. Values of $\langle q^2 \rangle$ are in percent maximum extension. An ensemble size of 1000 dumbbells was used. The spatial domain was discretized with 50 quadratic elements.

We see that at $We = 2$ (4 times the critical Hookean extension rate) the dumbbell has a steady-state extension of approximately 85%. In this highly non-linear regime, moments up to 8^{th} order should be kept to adequately describe the spatial distribution. In general, the number of field variables that must be retained depends on the extent of the non-Gaussian behaviour of the distribution. Figure 2 shows the transient behaviour of the OSMM formulation and the "exact" solution using $\mathbf{F} = \left\{ \langle q^2 \rangle, \langle q^4 \rangle, \langle q^6 \rangle, \langle q^8 \rangle \right\}$. Again we see that the OSMM approach captures the transient behaviour well into the non-linear regime.

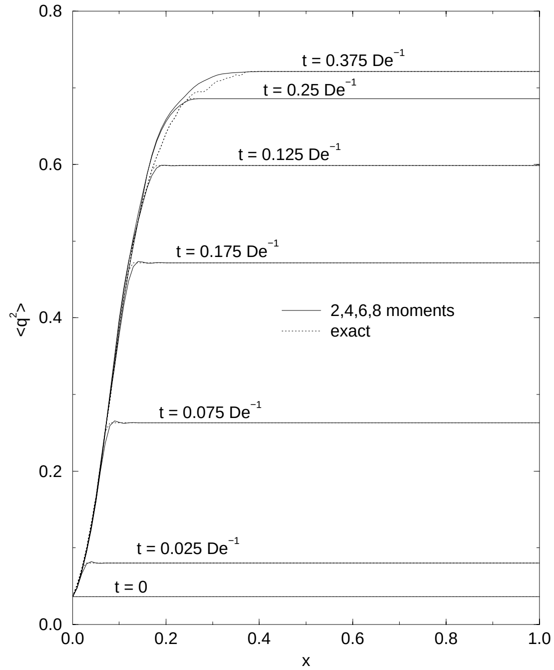

Figure 2. Transient comparison of exact and OSMM results. Parameters are the same as in Figure 1.

We feel that these results are highly promising – one way of rationalizing its success, at least on this simple model problem, is by noting that although an ensemble of 1000 (for example) may be necessary to obtain reasonable statistics for a Brownian dynamics simulations, far less information is actually necessary to capture the essential features of the distribution function. In this sense, OSMM is a model reduction approach to multiscale CFD. This methodology will now be integrated into a full two-dimensional transient flow solver and extended to Brownian dynamics of chain molecules, which incorporate charge effects and fluctuating hydrodynamic interactions [11].

Preliminary results projecting the microstructure onto Legendre polynomials rather than moments looks promising. Ultimately we expect the Legendre projection to be better as the series is rapidly converging. Also, since the Legendre polynomials are orthogonal with unity weighting function, the ensemble averages of the polynomials (the **F** 's) are the coefficients in the Legendre polynomial expansion of the configurational distribution function.

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