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ON THE NUMERICAL SIMULATION OF FLOWS OF POLYMER SOLUTIONS USING HIGH-ORDER METHODS BASED ON THE FOKKER-PLANCK EQUATION

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The present paper provides evidence of the affordability and competitiveness of Fokker-Planck-based methods when compared with stochastic simulation techniques. We apply an FP-based method to solve flow of a FENE fluid past a confined cylinder. We then solve uniaxial extensional flow for a reptation model due to Öttinger[1] at a high extensional rate. In both cases the FP method is seen, for comparable levels of accuracy, to cost only a small fraction of the equivalent stochastic approach.

1. Introduction

The equations of conservation of mass and of linear momentum for the inertialess flow of an incompressible polymer solution are

$$\boldsymbol{\nabla} \cdot \mathbf{v}^{j+1} = 0, \tag{1}$$

$$\boldsymbol{\nabla} p^{j+1} - \eta_s \boldsymbol{\nabla}^2 \mathbf{v}^{j+1} = \boldsymbol{\nabla} \cdot \boldsymbol{\tau}^j, \tag{2}$$

where p denotes the pressure, $\mathbf{v}$ the velocity field, $\boldsymbol{\tau}$ the elastic extra-stress tensor and η_s the solvent viscosity. The superscripts on the variables indicate a possible iterative or time-marching scheme where the elastic stress calculation is decoupled from that of the velocity-pressure pair. Traditionally, and in the interests of tractability, a closed-form constitutive equation for $\boldsymbol{\tau}$ of differential or integral type has been added to the conservation laws (1)-(2). However, in deriving such an equation - using a closure approximation, for example - unacceptably large steps

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away from the underlying physics may be taken. In the so-called "micro-macro" approach to computational rheology, kinetic theory models for the polymer configurations are coupled with the macroscopic conservation laws. The trend to date has been to solve stochastic differential equations for the polymer configurations.[2,3] Coolness - if not outright opposition - to the idea of solving an equivalent Fokker-Planck (FP) equation for the polymeric configuration probability density function (pdf) has been expressed in the literature, either on the grounds of ideology[3] or of fears of excessive computational cost.[4]

Indeed, very little has been done until recently to advocate FP-based methods as a convenient way of computing a macroscopic elastic stress. Exceptions are the papers of Warner[5] and Fan[6,7,8] on steady-state shearing flows and small amplitude oscillatory shear flows of dumbbell models. Fan[9] also computed the material functions for steady-state shear flow and uniaxial extensional flow of rigid rod-like molecular suspensions. In part II of the paper Fan[10] performed what, to our knowledge at least, were the first computations in the published literature of complex flows using the FP equation. In recent work by the MIT group[11,12,13] the discontinuous Galerkin method has been used for spatially discretizing the FP equation for dumbbell and Doi models and a Daubechies wavelet basis employed for representations in configurational space.

It is our purpose in the present paper to provide evidence of the affordability and competitiveness of FP-based methods when compared with stochastic simulation techniques. In Section 4 we apply an FP-based method to solve flow of a FENE fluid past a confined cylinder. We then solve uniaxial extensional flow for a reptation model due to Öttinger[1] at a high extensional rate. In both cases the FP method is seen, for comparable levels of accuracy, to cost only a small fraction of the equivalent stochastic approach.

2. A FENE Model for Dilute Polymer Solutions

In our modeling of dilute polymeric solutions we will represent the polymer chains by dumbbells which consist of two beads connected by a spring. A dumbbell whose centre of mass is at $\mathbf{x}$ at time t is fully described by a configuration end-to-end vector $\mathbf{q}(t, \mathbf{x})$.

Let $\psi(t, \mathbf{x}, \mathbf{q})$ be the pdf of the random process $\mathbf{q}(t, \mathbf{x})$. Then ψ for the FENE model satisfies the FP equation

$$\frac{D\psi}{Dt} + \mathrm{div}_{\mathbf{q}} \left((\boldsymbol{\kappa}\mathbf{q} - \frac{1}{2\lambda}\mathbf{F}(\mathbf{q}))\psi \right) = \frac{1}{2\lambda}\Delta_{\mathbf{q}}\psi, \tag{3}$$

where D/Dt is the material derivative, $\boldsymbol{\kappa}$ the transposed velocity gradient tensor ($\kappa_{ij} = \partial u_i/\partial x_j$), λ the relaxation time of the fluid and $\mathbf{F}(\mathbf{q})$ the inter-connecting spring force, which takes the following form for FENE dumbbells:

$$\mathbf{F}(\mathbf{q}) = \frac{\mathbf{q}}{1 - \dfrac{|\mathbf{q}|^2}{b}}. \tag{4}$$

In the relation above, $\sqrt{b}$ represents the maximum extensibility of the dumbbells and for two-dimensional configurational space we may write $\mathbf{q} = \mathbf{q}(r, \theta)$ where $r \in [0, \sqrt{b}]$ and $\theta \in [0, 2\pi]$ are polar coordinates. The computation of the velocity field with (1)-(2) is decoupled from that of the pdf, so that in equation (3), we can assume that the velocity gradient is known.

In our calculations the equilibrium pdf is supplied as the initial condition for ψ and the boundary conditions $\psi(t, \mathbf{x}, \sqrt{b}, \theta) = 0$ and $\frac{\partial \psi}{\partial r}(t, \mathbf{x}, 0, \theta) = 0$, are imposed.

2.1. *Numerical scheme*

We use a two-part time-splitting scheme to solve (3). Since two-dimensional configurational space for this problem is a disc of radius $\sqrt{b}$, a Fourier/Gauss-Legendre Galerkin spectral method is suitable for solving the first half time step in configurational space. The second half time step involves a convection problem and is solved in real space using an SUPG spectral element method. The details of the time-splitting scheme and discrete approximations used may be found in the recent paper of Chauvière and Lozinski.[14]

With $\psi^{j+1} = \psi((j+1)\Delta t, \mathbf{x}, r, \theta)$ thus computed at all quadrature points in both configurational and real space, the polymeric extra-stress $\boldsymbol{\tau}$ is found using the Kramers expression

$$\boldsymbol{\tau}^{j+1}(t, \mathbf{x}) = \frac{\eta_p}{\lambda} \left(\frac{b+2}{b} \right) \left(-\mathbf{I} + \int_{\theta=0}^{2\pi} \int_{r=0}^{\sqrt{b}} \mathbf{q} \otimes \mathbf{F}(\mathbf{q}) \psi^{j+1}(t, \mathbf{x}, r, \theta) r \, dr \, d\theta \right), \quad (5)$$

where η_p denotes the polymeric viscosity. The index j is now incremented by unity and the algorithm returns to (1)-(2).

3. The Uniform Öttinger (UÖ) Model for Concentrated Polymer Solutions and Melts

The UÖ model[1] features a maximum allowable extension ratio λ_{max}, and the evolution equation for the chain stretching ratio λ is

$$\dot{\lambda} = \frac{D\lambda}{Dt} = \lambda \boldsymbol{\kappa} : \mathbf{S} - \frac{1}{\tau_s} \frac{\left(\lambda^2 - 1\right) \lambda_{max}^2}{\lambda \left(\lambda_{max}^2 - \lambda^2\right)}. \quad (6)$$

The second term on the right-hand side of (6) is a dissipative contribution, denoted hereafter by $\dot{\lambda}_{dissip}$.

The FP equation for the configuration pdf $\psi(t, \mathbf{x}, \mathbf{u}, s)$ assumes the form

$$\frac{D\psi}{Dt} = -\frac{\partial}{\partial \mathbf{u}} \cdot [(\mathbf{I} - \mathbf{uu}) \cdot \boldsymbol{\kappa} \cdot \mathbf{u} \psi] - \frac{\partial}{\partial s} \left(\dot{s}_{tot} \psi \right) - \frac{\dot{\lambda}_{dissip}}{\lambda} \psi + \frac{1}{\pi^2 \tau_d} \frac{\partial^2 \psi}{\partial s^2} + D \frac{\partial^2 \psi}{\partial \mathbf{u}^2}, \quad (7)$$

where the drift velocity $\dot{s}_{tot} = -\frac{1}{\lambda} \left(s - \frac{1}{2} \right) \dot{\lambda}_{dissip}$ and D is an orientational diffusion coefficient. The vector $\mathbf{u}$ is a unit tangent vector for a polymer chain at the nor-

malized position $s \in [0,1]$. The physical significance of the terms in (7) is discussed by Öttinger[1] and by Fang et al.[15]

The boundary conditions for the FP equation (7) are

$$\psi(t,\mathbf{x},\mathbf{u},s) = \frac{1}{4\pi}\delta(|\mathbf{u}|-1), \quad s=0,1, \tag{8}$$

and the initial conditions ($j=0$) are chosen as $\lambda^0 = 1$ and $\psi^0 = 1/4\pi$.

3.1. *Numerical scheme*

Since the FP equation (7) contains derivatives in both configurational and physical space, it is too expensive to solve it in a completely implicit way. On the other hand, it is better to treat the convective terms in physical space implicitly for stability reasons. As a compromise, we split every time step into two half time steps, the first one (explicit) accounting for the dependencies in configurational space and the second one (implicit) for those in physical space.

We discretize the equations appearing in the first half time step in configurational space using a Galerkin spectral method, and the basis chosen consists of spherical harmonics and Lagrange interpolating polynomials based on the Gauss-Lobatto-Legendre points. An SUPG spectral element method is then used to treat the convection equations featuring in the second half time step. Full details of the time marching scheme and of the polynomial representation of the pdf ψ in real and configurational space may be found in the paper of Lozinski et al.[16]

Finally, the polymeric extra-stress tensor $\boldsymbol{\tau}$ is computed from a quadrature evaluation of

$$\boldsymbol{\tau}^{j+1}(t,\mathbf{x}) = 5G_0\left[1+\frac{\lambda^2-1}{1-(\lambda/\lambda_{max})^2}\right] \times \int_{s=0}^{1}\int_{\theta=0}^{\pi}\int_{\varphi=0}^{2\pi}\psi^{j+1}(t,\mathbf{x},\mathbf{u}(\theta,\varphi),s)\mathbf{u}(\theta,\varphi)\otimes\mathbf{u}(\theta,\varphi)\sin\theta\, d\varphi d\theta ds, \tag{9}$$

where G_0 is an elastic modulus. The algorithm increments the index j by unity and returns to the Stokes system (1)-(2).

4. Numerical Results

In this section we present some results of computations with the FENE and UÖ models using the FP equations (3) and (7), and compare these with those of stochastic simulations.

The results shown in Fig. 1 are for flow of a FENE fluid past a cylinder placed symmetrically in a planar channel. The same spectral element mesh (26 elements) is used in real space for all the computations and the results shown are the profiles of the elastic normal stress component τ_{xx} on the surface of the cylinder and along the downstream channel axis of symmetry. For the FP method described in Section 2 ψ was represented in configurational space by 6 Fourier modes in the

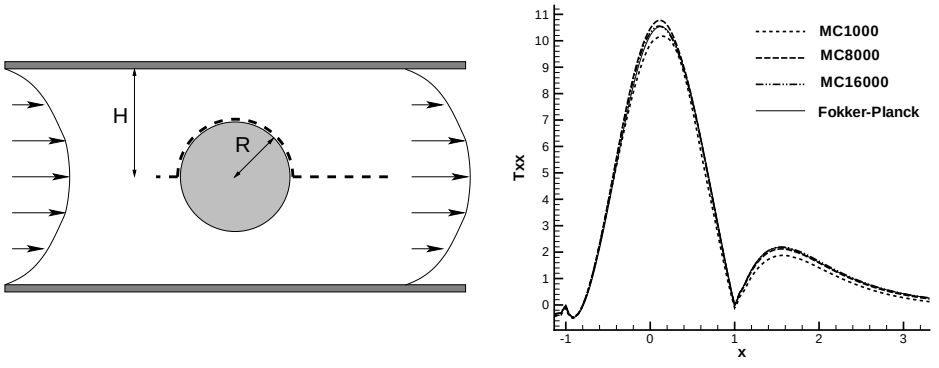

Fig. 1. Left: Schematic of a cylinder having radius R placed on the axis of symmetry of a uniform channel of half-width H. Right: Brownian configuration method (MC1000, MC8000 and MC16000) and Fokker-Planck method predictions of the extensional stress τ_{xx} for the FENE model along the dashed curve shown on the lefthand figure. $R/H = 0.5$, $b = 10$, $De = 0.5$, $\eta_s/\eta = 0.59$, $\Delta t = 0.025$, # iterations = 200. MC1000: 1000 configuration fields, MC8000: 8000 configuration fields, MC16000: 16000 configuration fields, Fokker-Planck: $N_F = 6$, $N_R = 12$.

azimuthal direction and by a degree 12 polynomial in the radial direction. The labels MC1000, MC8000 and MC16000 correspond to results from a Brownian configuration fields method[17] with, respectively, 1000, 8000 and 16000 configuration fields. The MC16000 and FP predictions may be seen to be in excellent agreement. However, the CPU times per time step Δt on a Pentium IV 1.5 GHz machine for the stochastic and FP calculations were very different: whereas the simulations MC1000, MC8000 and MC16000 required 8.6s, 70s and 140s, respectively, the FP method of Section 2 took only 9.6 CPUs per time step.

The FP method outlined in Section 3 was used for calculating the normal stress difference $N_1 = \tau_{zz} - \tau_{xx}$ for the uniaxial extensional flow $\mathbf{v} = (-\dot{\varepsilon}x/2, -\dot{\varepsilon}y/2, \dot{\varepsilon}z)$ of a UÖ fluid. λ_{max} was taken equal to 10 and τ_d/τ_s was set equal to 60. The results are compared in Fig. 2 with those of the stochastic method of Fang et al.[15] for an extensional rate $\dot{\varepsilon} = 200/\tau_d$. In the work of Fang et al. the simulations were performed in N_{block} independent blocks, in each of which N_{sample} trajectories of the stochastic processes $\mathbf{u}$ and s were allowed to propagate. The time steps used varied between $2 \times 10^{-4}/\dot{\varepsilon}$ and $2 \times 10^{-2}/\dot{\varepsilon}$. N_u and N_s in the figure caption refer to the discretization levels taken in the polynomial approximation to ψ in configurational space[16]. The high extensional rate was chosen in order to try to favour the stochastic simulation technique: the variance is smaller and it is difficult to adequately resolve the highly localized configuration pdf ψ. Despite this, however, the FP run labelled (c) required only 1.5min total CPU time on a Pentium III 800MHz machine, whereas the stochastic runs took between 3.5min and 5hr 48min.

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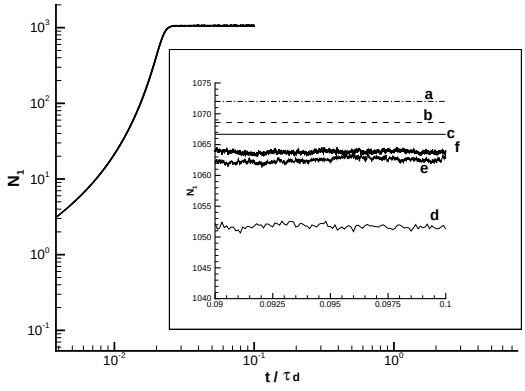

Fig. 2. The stress difference $N_1 = \tau_{zz} - \tau_{xx}$ for start-up uniaxial extensional flow. $\dot{\varepsilon} = 200.0/\tau_d$, $\lambda_{max} = 10.0$, $\tau_d/\tau_s = 60.0$. Fokker-Planck method: (a) $N_u = N_s = 24$, $\Delta t = 0.01/\dot{\varepsilon}$, (b) $N_u = N_s = 28$, $\Delta t = 0.01/\dot{\varepsilon}$, (c) $N_u = N_s = 32$, $\Delta t = 0.005/\dot{\varepsilon}$. Stochastic simulation with $N_{sample} = 10000$ and $N_{block} = 10$: (d) $\Delta t = 0.02/\dot{\varepsilon}$, (e) $\Delta t = 0.002/\dot{\varepsilon}$, (f) $\Delta t = 0.0002/\dot{\varepsilon}$.

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