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Short communication

Constitutive laws for the matrix-logarithm of the conformation tensor

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Abstract

We show how to transform a large class of differential constitutive models into an equation for the (matrix) logarithm of the conformation tensor. Under this transformation, the extensional components of the deformation field act additively, rather than multiplicatively. This transformation is motivated by numerical evidence that the high Weissenberg number problem may be caused by the failure of polynomial-based approximations to properly represent exponential profiles developed by the conformation tensor. The potential merits of the new formulation are demonstrated for a finitely-extensible fluid in a two-dimensional lid-driven cavity at Weissenberg number $Wi = 5$.
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1. Introduction

Polymeric fluids are governed by momentum equations supplemented with a constitutive law: a relation between the state of stress of a fluid element—a second-order tensor $\boldsymbol{\tau} = \boldsymbol{\tau}(\boldsymbol{x}, t)$—and the deformation experienced by that element. This relation is in general nonlocal in time; the stress in a fluid element may depend on the entire deformation history. The constitutive law is often formulated in terms of the conformation tensor $\boldsymbol{\sigma}(\boldsymbol{x}, t)$, which is an approximate measure of the micro-structural state of the liquid. The eigenvalues and eigenvectors of the conformation tensor provide information on the local expectation value of the state of strain of an ensemble of flowing polymer molecules.

Most differential constitutive models are of the following general form:

$$\frac{\partial \boldsymbol{\sigma}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{\sigma} - (\nabla \boldsymbol{u})\boldsymbol{\sigma} - \boldsymbol{\sigma}(\nabla \boldsymbol{u})^{\mathrm{T}} = \frac{g(\boldsymbol{\sigma})}{Wi} P(\boldsymbol{\sigma}), \qquad (1)$$

where $\boldsymbol{u} = \boldsymbol{u}(\boldsymbol{x}, t)$ is the velocity field, $g(\boldsymbol{\sigma})$ is a scalar function, and $P(\boldsymbol{\sigma})$ is a polynomial. The left-hand side is the upper-convected time derivative, which accounts for the advection and the deformation of the conformation tensor by the flow field. The right-hand side accounts for sources and relaxation, both being possibly nonlinear. The dimensionless parameter Wi is the Weissenberg number, which is a ratio between the elastic relaxation time and a time associated with the local rate of deformation. A high Weissenberg number means that the history dependence of the conformation, or the stress is manifest. The Oldroyd-B, Giesekus, and the finitely-extensible Chilcott–Rallison models, for example, are instances of (1) [1–3].

Together with the momentum equations and the incompressibility constraint, (1) constitutes a highly nonlinear model. Much of its usefulness relies on numerical solvers, which, however, are severely limited by the high Weissenberg number problem (HWNP)—a numerical breakdown that occurs at moderately large values of the Weissenberg number. Numerical evidence relates this breakdown to the emergence of large stress gradients, i.e., to a loss of resolution. There is growing evidence that this breakdown may be related to the inappropriateness of polynomial-based approximations to represent the stress (or conformation) tensor profiles, which are exponential in regions of high deformation rate, or near stagnation points.

An important property of (1) is that it preserves the positive definiteness of the tensor $\boldsymbol{\sigma}$ (the simplest way to see it, is through the equivalent integral formulation, where the

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conformation tensor is expressed as a convolution of the positive-definite Finger tensor and a positive exponential kernel). This observation suggests that some of the difficulties associated with exponential stress profiles can be remedied by operating instead on the (matrix) logarithm of the conformation tensor, $\log \boldsymbol{\sigma}$ (recall that any symmetric positive-definite matrix A can be diagonalized, $A = R\Lambda R^{\mathrm{T}}$, and that $\log A = R \log \Lambda R^{\mathrm{T}}$; numerical algorithms for the computation of matrix-logarithms can be found in [6]). Moreover, the manifestation of the HWNP was seen in many cases to coincide with the loss of positivity of the conformation tensor [4,5]; positivity is guaranteed by a formulation based on $\log \boldsymbol{\sigma}$.

In general, knowing the rate of change of a second-order tensor does not imply that a simple explicit equation can be written for its logarithm. It turns out that equations of the form (1) have a simple enough structure to allow for such a transformation. The gist of this transformation is an appropriate decomposition of the velocity gradient, $\nabla \boldsymbol{u}$, into extensional and rotational components. The rotational component operates on $\log \boldsymbol{\sigma}$ in the same way as it operates on $\boldsymbol{\sigma}$; the extensional component operates on $\log \boldsymbol{\sigma}$ additively. The transformation of the advection and the source terms is relatively straightforward. Our result is summarized by Theorem 1. The potential power of a log-based formulation is demonstrated by a numerical example at $Wi = 5$. A detailed account of a numerical scheme as well as an extensive numerical validation will be presented in a subsequent article.

2. A matrix decomposition theorem

We start by deriving some facts about the decomposition of tensor fields.

Lemma 1. *Let Λ be a non-degenerate $n \times n$ diagonal matrix with distinct non-zero entries. Then, any $n \times n$ matrix $\tilde{M}$ has a unique decomposition*:

$$\tilde{M} = \tilde{\Omega} + \tilde{B} + \tilde{N}\Lambda^{-1}, \tag{2}$$

where $\tilde{\Omega}$ and $\tilde{N}$ are anti-symmetric and $\tilde{B}$ is diagonal.

Proof. We denote by $\mathcal{S}$ the subspace of symmetric matrices, by $\mathcal{A}$ the subspace of anti-symmetric matrices, and by $\mathcal{D}$ the subspace of diagonal matrices. Separating (2) into symmetric and anti-symmetric parts, we need to show the existence of $\tilde{\Omega}, \tilde{N} \in \mathcal{A}$, $\tilde{B} \in \mathcal{D}$, such that:

$$\tilde{B} + \tfrac{1}{2}(\tilde{N}\Lambda^{-1} - \Lambda^{-1}\tilde{N}) = \tfrac{1}{2}(\tilde{M} + \tilde{M}^{\mathrm{T}}),$$
$$\tilde{\Omega} + \tfrac{1}{2}(\tilde{N}\Lambda^{-1} + \Lambda^{-1}\tilde{N}) = \tfrac{1}{2}(\tilde{M} - \tilde{M}^{\mathrm{T}}).$$

Clearly, we only need to establish the existence and uniqueness of $\tilde{B}, \tilde{N}$, as $\tilde{\Omega}$ is then determined by the second equation. This is guaranteed if:

$$\mathcal{S} = \mathcal{D} \oplus \{\tfrac{1}{2}(\tilde{N}\Lambda^{-1} - \Lambda^{-1}\tilde{N}) : \tilde{N} \in \mathcal{A}\}.$$

This can be proved by a dimensional argument. The mapping $\tilde{N} \mapsto \frac{1}{2}(\tilde{N}\Lambda^{-1} - \Lambda^{-1}\tilde{N})$ is a linear mapping $\mathcal{A} \mapsto \mathcal{S}$, with:

$$\tfrac{1}{2}(\tilde{N}\Lambda^{-1} - \Lambda^{-1}\tilde{N})_{ij} = \tfrac{1}{2}(\Lambda_{jj}^{-1} - \Lambda_{ii}^{-1})\tilde{N}_{ij}.$$

Since, by assumption, all the diagonal elements of Λ are non-zero and distinct, this transformation has a null kernel, and its range has dimension $\dim \mathcal{A} = \frac{1}{2}n(n-1)$. Moreover, its range consists of matrices that have vanishing diagonal elements, from which we conclude that:

$$\dim \mathcal{D} \oplus \{\tfrac{1}{2}(\tilde{N}\Lambda^{-1} - \Lambda^{-1}\tilde{N}) : N \in \mathcal{A}\}$$
$$= \tfrac{1}{2}n(n-1) + n = \dim \mathcal{S}.$$

Note that this proof is constructive as:

$$\tilde{N}_{ij} = \frac{\tilde{M}_{ij} + \tilde{M}_{ji}}{\Lambda_{jj}^{-1} - \Lambda_{ii}^{-1}}, \qquad \tilde{B}_{ii} = \tilde{M}_{ii}.$$

□

Lemma 2. *Let S be an $n \times n$ symmetric positive-definite* (SPD) *matrix. Then, any $n \times n$ matrix M has a decomposition*:

$$M = \Omega + B + NS^{-1},$$

where $\Omega, N \in \mathcal{A}$ and $B \in \mathcal{S}$ commutes with S.

Proof. Since S is SPD it assumes a decomposition $S = R\Lambda R^{\mathrm{T}}$, where R is orthogonal. We will prove this lemma for the generic case where Λ has n distinct eigenvalues; the other cases require some adaptation. Note, however, that in the extreme case where S is proportional to the unit matrix this lemma is satisfied trivially with $N = 0$.

Let $R^{\mathrm{T}}MR = \tilde{\Omega} + \tilde{B} + \tilde{N}\Lambda^{-1}$ satisfy the decomposition of Lemma 1, then setting:

$$\Omega = R\tilde{\Omega}R^{\mathrm{T}}, \qquad B = R\tilde{B}R^{\mathrm{T}}, \qquad N = R\tilde{N}R^{\mathrm{T}},$$

it is easily verified that:

(1) $M = \Omega + B + NS^{-1}$.
(2) $\Omega, N \in \mathcal{A}$.
(3) B is symmetric and commutes with S.

This completes the proof. □

Since for incompressible flows the velocity gradient, $\nabla \boldsymbol{u}$, is a traceless second-order tensor, we immediately obtain the following decomposition rule.

Corollary 1. *Let $\boldsymbol{u}$ be a divergence-free velocity field and let $\boldsymbol{\sigma}$ be the positive-definite conformation tensor. Then, the velocity gradient $\nabla \boldsymbol{u}$ can be* (*locally*) *decomposed as*:

$$\nabla \boldsymbol{u} = \Omega + B + N\boldsymbol{\sigma}^{-1}, \tag{3}$$

where $\Omega = \Omega(\nabla \boldsymbol{u}, \boldsymbol{\sigma})$ and $N = N(\nabla \boldsymbol{u}, \boldsymbol{\sigma})$ are anti-symmetric (*pure rotations*)*, and $B = B(\nabla \boldsymbol{u}, \boldsymbol{\sigma})$ is symmetric, traceless, and commutes with the conformation tensor $\boldsymbol{\sigma}$.*

Example. Consider the two-dimensional case. If $\boldsymbol{\sigma}$ is proportional to the unit tensor then simply set $B = \frac{1}{2}[(\nabla \boldsymbol{u}) + (\nabla \boldsymbol{u})^{\mathrm{T}}]$ and $\Omega = 0$. Otherwise, calculate the diagonalizing transformation:

$$\boldsymbol{\sigma} = R \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} R^{\mathrm{T}},$$

and set

$$\begin{pmatrix} \tilde{m}_{11} & \tilde{m}_{12} \\ \tilde{m}_{21} & \tilde{m}_{22} \end{pmatrix} = R^{\mathrm{T}}(\nabla \boldsymbol{u})R.$$

Then,

$$N = R \begin{pmatrix} 0 & n \\ -n & 0 \end{pmatrix} R^{\mathrm{T}}, \qquad B = R \begin{pmatrix} \tilde{m}_{11} & 0 \\ 0 & \tilde{m}_{22} \end{pmatrix} R^{\mathrm{T}},$$

$$\Omega = R \begin{pmatrix} 0 & \omega \\ -\omega & 0 \end{pmatrix} R^{\mathrm{T}},$$

with $n = (\tilde{m}_{12} + \tilde{m}_{21})/(\lambda_2^{-1} - \lambda_1^{-1})$, and $\omega = (\lambda_2 \tilde{m}_{12} + \lambda_1 \tilde{m}_{21})/(\lambda_2 - \lambda_1)$.

When the decomposition (3) is substituted into the constitutive relation (1), the $N\boldsymbol{\sigma}^{-1}$ term vanishes. Exploiting the fact that B and $\boldsymbol{\sigma}$ commute we get:

$$\frac{\partial \boldsymbol{\sigma}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{\sigma} - (\Omega \boldsymbol{\sigma} - \boldsymbol{\sigma} \Omega) - 2B\boldsymbol{\sigma} = \frac{1}{Wi} g(\boldsymbol{\sigma}) P(\boldsymbol{\sigma}), \quad (4)$$

which represents the action of the deformation field on $\boldsymbol{\sigma}$ as a composition of a pure rotation Ω, and a symmetric volume-preserving deformation B aligned with the principal axes of $\boldsymbol{\sigma}$. Note that Ω is in general *not* the vorticity tensor; it contains an additional component arising from the deformation not being aligned with the principal axes of the conformation tensor.

3. Constitutive equation for log σ

Let $\boldsymbol{\psi} = \log \boldsymbol{\sigma}$. Our goal is to derive from (4) an evolution equation for $\boldsymbol{\psi}$. To do so, we decompose (4) into its four constituents:

(1) *Advection*: if $\boldsymbol{\sigma}$ is advected by an incompressible flow field, so is every continuous function of $\boldsymbol{\sigma}$, and in particular its logarithm:

$$\frac{\partial \boldsymbol{\sigma}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{\sigma} = 0 \quad \text{implies} \quad \frac{\partial \boldsymbol{\psi}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{\psi} = 0. \quad (5)$$

(2) *Rotation*: if the velocity gradient is a pure rotation, then any tensor-valued function of $\boldsymbol{\sigma}$, in particular its logarithm, rotates together with $\boldsymbol{\sigma}$:

$$\frac{\partial \boldsymbol{\sigma}}{\partial t} = (\Omega \boldsymbol{\sigma} - \boldsymbol{\sigma} \Omega) \quad \text{implies} \quad \frac{\partial \boldsymbol{\psi}}{\partial t} = (\Omega \boldsymbol{\psi} - \boldsymbol{\psi} \Omega). \quad (6)$$

Indeed, the solution for $\boldsymbol{\sigma}(t)$ is:

$$\boldsymbol{\sigma}(t) = \mathrm{e}^{\Omega t} \boldsymbol{\sigma}(0) \mathrm{e}^{-\Omega t} \quad \text{hence} \quad \boldsymbol{\psi}(t) = \mathrm{e}^{\Omega t}\, \boldsymbol{\psi}(0)\, \mathrm{e}^{-\Omega t},$$

and (6) follows.

(3) *Extension:* if the velocity gradient commutes with $\boldsymbol{\sigma}$, then it operates additively on its logarithm:

$$\frac{\partial \boldsymbol{\sigma}}{\partial t} = 2B\boldsymbol{\sigma} \quad \text{implies} \quad \frac{\partial \boldsymbol{\psi}}{\partial t} = 2B. \quad (7)$$

Here, we have:

$$\boldsymbol{\sigma}(t) = \mathrm{e}^{2Bt} \boldsymbol{\sigma}(0) \quad \text{hence} \quad \boldsymbol{\psi}(t) = \boldsymbol{\psi}(0) + 2Bt,$$

where we have used the fact that $\boldsymbol{\sigma}(0)$ and B commute.

(4) *Sources*: the source term is assumed to commute with $\boldsymbol{\sigma}$, hence

$$\frac{\partial \boldsymbol{\sigma}}{\partial t} = g(\boldsymbol{\sigma}) P(\boldsymbol{\sigma})$$

implies that:

$$\begin{aligned} \boldsymbol{\psi}(t) &= \log\{\boldsymbol{\sigma}(0) + t\, g(\boldsymbol{\sigma}(0)) P(\boldsymbol{\sigma}(0))\} + \mathrm{O}(t^2) \\ &= \log\{\boldsymbol{\sigma}(0)\{\boldsymbol{I} + t\, g(\boldsymbol{\sigma}(0))\boldsymbol{\sigma}^{-1}(0) P(\boldsymbol{\sigma}(0))\}\} + \mathrm{O}(t^2) \\ &= \boldsymbol{\psi}(0) + t\, g(\boldsymbol{\sigma}(0))\boldsymbol{\sigma}^{-1}(0) P(\boldsymbol{\sigma}(0)) + \mathrm{O}(t^2), \end{aligned}$$

from which we conclude that:

$$\frac{\partial \boldsymbol{\sigma}}{\partial t} = g(\boldsymbol{\sigma}) P(\boldsymbol{\sigma}) \quad \text{implies} \quad \frac{\partial \boldsymbol{\psi}}{\partial t} = g(\boldsymbol{\sigma}) \boldsymbol{\sigma}^{-1} P(\boldsymbol{\sigma}). \quad (8)$$

Since the time derivative of $\boldsymbol{\psi}$ is a linear transformation of the time derivative of $\boldsymbol{\sigma}$ (it is the Lie derivative of the matrix-logarithm evaluated at $\boldsymbol{\sigma}$ in the $\frac{\partial \boldsymbol{\sigma}}{\partial t}$ direction [6]), then the contributions (5)–(8) can be added up, which leads us to our main theorem.

Theorem 1. *Let $\boldsymbol{\sigma}$ be governed by a constitutive law of the form* (4) *with $\Omega \in \mathcal{A}$, $B \in \mathcal{S}$, and $B\boldsymbol{\sigma} = \boldsymbol{\sigma} B$, then $\boldsymbol{\psi} = \log \boldsymbol{\sigma}$ satisfies the following equation*:

$$\frac{\partial \boldsymbol{\psi}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{\psi} - (\Omega \boldsymbol{\psi} - \boldsymbol{\psi} \Omega) - 2B = \frac{g(\mathrm{e}^{\boldsymbol{\psi}})}{Wi} \mathrm{e}^{-\boldsymbol{\psi}} P(\mathrm{e}^{\boldsymbol{\psi}}). \quad (9)$$

4. A numerical example

We propose (9) as a starting point for numerical simulations. To demonstrate the potential strength of our approach, we show simulation results for a finitely-extensible (FENE) Chilcott–Rallison fluid [3] in a two-dimensional lid-driven cavity. In the Chilcott–Rallison model, the functions $g(\boldsymbol{\sigma})$ and $P(z)$ are given by $g(\boldsymbol{\sigma}) = L^2/(L^2 - \mathrm{Tr}\, \boldsymbol{\sigma})$ and $P(z) = z - 1$. Eq. (9) is coupled to the momentum equation:

$$\begin{aligned} \frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} + \nabla p = \frac{(1-\beta)}{Re} \nabla^2 \boldsymbol{u} \\ + \frac{\beta}{Re\, Wi} \nabla \cdot g(\boldsymbol{\sigma})(\boldsymbol{\sigma} - \boldsymbol{I}), \end{aligned}$$

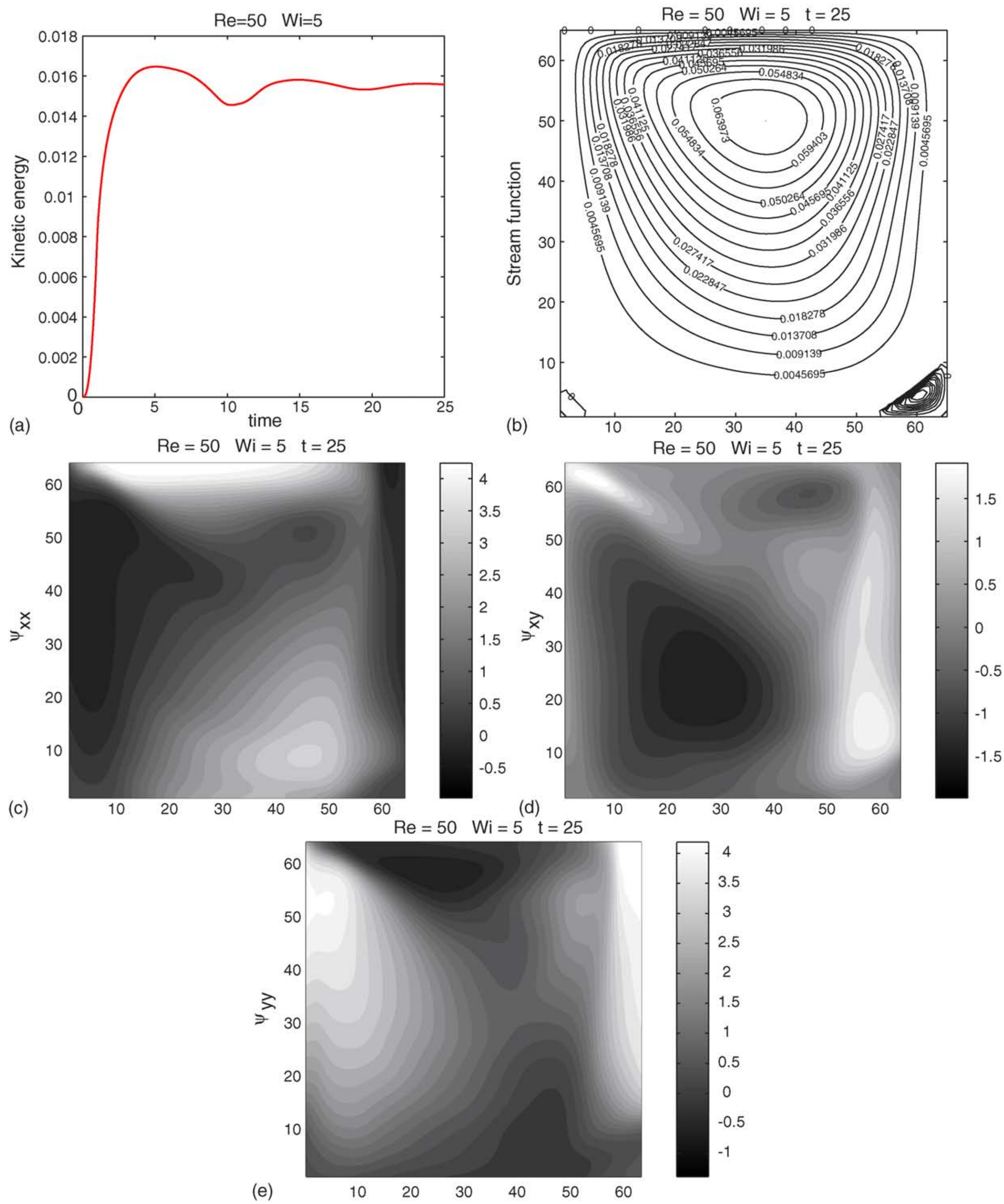

Fig. 1. Simulations results for a Chilcott–Rallison fluid in a lid-driven cavity with parameters $Re = 50$, $Wi = 5$, $\beta = 1/2$, and $L = 10$. (a) Time evolution of the kinetic energy; (b) contour lines of the stream function at time $t = 25$; (c–e) the fields ψ_{xx}, ψ_{xy}, and ψ_{yy} at time $t = 25$.

where p is the pressure and β is the ratio of polymeric and solvent viscosities. The displayed results are for a choice of parameters: $Re = 50$, $Wi = 5$, $\beta = 1/2$, and $L = 10$. The fluid is confined in a unit square, $x, y \in [0, 1]$, and the upper lid moves to the right with a velocity profile regularized both in space and time,

$$u_{\text{top}}(x, t) = 16x^2(1 - x)^2 \min(1, t).$$

This is an interesting test problem, as the fluid in the vicinity of the upper lid is subject to continual extension (due to the regularized boundary conditions), while being advected at very low speed near the upper corners (the stress may even grow unbounded in time for a model that does not limit extension). This calculation uses a finite-difference scheme based on the Kurganov–Tadmor discretization for the hyperbolic terms [7], and Chorin's projection method (also known as operator splitting) for the pressure [8].

The first graph in Fig. 1 shows the evolution of the kinetic energy, which after a transient exhibit decaying oscillations. The other images show the stream function and the three components of $\boldsymbol{\psi}$ at time $t = 25$. From the point of view of numerical *stability*, our numerical method does not seem limited at high Weissenberg numbers, which of course, does not guarantee that accuracy is preserved. A detailed description of the numerical scheme together with careful convergence analyses and comparisons with benchmark results will be presented in a subsequent publication.

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References

[1] R. Bird, R. Armstrong, O. Hassager, Dynamics of Polymeric Liquids, vol. 1, Wiley, New York, 1987.
[2] R. Larson, Constitutive equations for polymer melts and solutions, Butterworths Series in Chemical Engineering, 1988.
[3] M. Chilcott, J. Rallison, Creeping flow of dilute polymer solutions past cylinders and spheres, J. Non-Newton. Fluid Mech. 29 (1988) 381–432.
[4] M. Hulsen, A. van Heel, B. van den Brule, Simulation of viscoelastic flows using Brownian configuration fields, J. Non-Newton. Fluid Mech. 70 (1997) 79–101.
[5] T. Phillips, A. Williams, Comparison of creeping and inertial flow of an Oldroyd-B fluid through planar and axisymmetric contractions, J. Non-Newton. Fluid Mech. 108 (2002) 25–47.
[6] C. Kenney, A. Laub, A Schur–Frechét algorithm for computing the logarithm and exponential of a matrix, SIAM J. Matrix Anal. Appl. 19 (1998) 640–663.
[7] A. Kurganov, E. Tadmor, New high-resolution central schemes for nonlinear conservation laws and convection-diffusion equations, J. Comp. Phys. 160 (2000) 214–282.
[8] A. Chorin, On the convergence of discrete approximations to the Navier–Stokes equations, Math. Comp. 22 (1969) 745–762.