



# A mathematician's perspective on the Oldroyd B model: Progress and future challenges

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## ABSTRACT

We review progress and open challenges for a number of problems related to the Oldroyd B model which are of current interest to the mathematical community. We discuss existence results for initial value problems and steady flows, flow stability, and the problem of understanding the asymptotics of the high Weissenberg number limit. We also discuss efforts and challenges in numerical simulation, exemplified by three problems: extensional flow in a four roll mill geometry, flow past a confined cylinder, and locomotion of microorganisms in a viscoelastic fluid.

## 1. Introduction

This review article is intended to address a two-fold audience: mathematicians who are interested in working on viscoelastic flow problems, and rheologists who have a need for a deeper understanding of the underlying equations and for interactions with mathematicians. To the former, we wish to give a perspective of the state of current progress and the many open problems in the field; to the latter we hope to convey a sense of how mathematicians look at the field, what interests them and what they can accomplish.

We begin our review with a section on the physical background of the Oldroyd B model. Section 2 summarizes what we think a mathematician working on this subject needs to know about the underlying physics. Any mathematical analysis starts with the question of existence of solutions. The techniques used in analyzing this question lay the foundation for any study of further issues such as qualitative behavior of solutions, methods of approximation, etc. Sections 3 and 4 review the state of the art for initial value problems, and, respectively, steady flows. Generally speaking, the question of existence is at this point reasonably well understood “in the small”, i.e. for short time in initial value problems, and for small perturbations of the rest state or of Newtonian flows. On the other hand, the existence problem “in the large” is still open even for the Newtonian case, and it only becomes harder for viscoelastic flows. Little is known at this point.

Section 5 is concerned with flow stability. Flow instabilities in Newtonian flows are a rich subject, which has inspired much mathematical research in dynamical systems and asymptotics. Viscoelastic effects add new mechanisms of instability. Beyond that, fundamental mathematical questions arise. The standard approach to studying the

onset of instability links stability to eigenvalues and employs center manifold reduction and bifurcation theory. The rigorous justification of these methods is well understood in Newtonian fluid mechanics but still leaves open questions for viscoelastic flows.

Newtonian flows become increasingly complex as the Reynolds number increases. Something similar happens in viscoelastic flows at high Weissenberg number. The idea of separating the study of the high Reynolds number limit into near inviscid flow in the interior of the flow domain and a boundary layer where viscous effects are important is now more than a century old. But actually implementing this idea is far from straightforward or simple. Section 6 reviews efforts to formulate an analogous framework for high Weissenberg number flows.

In the latter part of our paper, we review numerical simulations of a number of flow problems. We have chosen a few specific topics which illustrate the importance of singular or near singular behavior at high Weissenberg number, instabilities, possible nonexistence of steady flows, and the impact of such mathematical difficulties on numerical simulations. Specifically, we discuss extensional flow generated in a four roll mill geometry (Section 8), flow past a cylinder (Section 9) and locomotion of microorganisms (Section 10).

## 2. Motivation of the Oldroyd B model

Oldroyd's article in 1950 [1] is the first systematic attempt to formulate constitutive models for viscoelastic fluids in a way that respects material frame indifference. This principle states that stresses in a continuous medium should arise from deformations only and

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should not change if the material is merely rotated. More specifically, consider a given motion where a particle initially at point  $\xi$  occupies position  $\mathbf{x}(\xi, t)$  and another where the same particle occupies position  $\mathbf{x}^*(\xi, t) = \mathbf{Q}(t)\mathbf{x}(\xi, t)$ , where  $\mathbf{Q}$  is a rotation. If the stress tensor in the first case is  $\mathbf{T}(\mathbf{x}, t)$ , then in the second motion the stress tensor should be  $\mathbf{T}^*(\mathbf{x}^*, t) = \mathbf{Q}(t)\mathbf{T}(\mathbf{x}, t)\mathbf{Q}^{-1}(t)$ , i.e. apart from a rotation of the principal axes the stress tensor is unchanged.

As a special case, Oldroyd considers the extension of a linear Jeffreys model to the nonlinear case. The Jeffreys model relates the stress tensor to the velocity gradient. Let  $\mathbf{v}(\mathbf{x}, t)$  denote the velocity of the fluid, and let  $\nabla \mathbf{v}$  be its gradient, with the convention that the  $ij$  component is  $\partial v_i / \partial x_j$ . We denote by  $\mathbf{D}$  the symmetric part  $\frac{1}{2}(\nabla \mathbf{v} + (\nabla \mathbf{v})^T)$ . The linear Jeffreys model postulates a relationship of the form

$$\mathbf{T} + \lambda_1 \frac{\partial \mathbf{T}}{\partial t} = 2\eta(\mathbf{D} + \lambda_2 \frac{\partial \mathbf{D}}{\partial t}). \quad (1)$$

Here  $\eta$  is the viscosity,  $\lambda_1$  is called the relaxation time, and  $\lambda_2$  is called the retardation time. All of these are presumed constant.

Naively, we might just replace the time derivative  $\partial/\partial t$  by the material time derivative  $d/dt = \partial/\partial t + (\mathbf{v} \cdot \nabla)$ , i.e. a time derivative following the same particle. However, this is wrong. To see this, let us consider how the various terms in (1) change under a superimposed rotation. We have

$$\begin{aligned} \frac{\partial \mathbf{x}(\xi, t)}{\partial t} &= \mathbf{v}(\mathbf{x}, t), \\ \frac{\partial \mathbf{x}^*(\xi, t)}{\partial t} &= \mathbf{v}^*(\mathbf{x}^*, t) = \mathbf{Q}(t)\mathbf{v}(\mathbf{x}, t) + \dot{\mathbf{Q}}(t)\mathbf{x} \\ &= \mathbf{Q}(t)\mathbf{v}(\mathbf{Q}^{-1}(t)\mathbf{x}^*, t) + \dot{\mathbf{Q}}(t)\mathbf{Q}^{-1}(t)\mathbf{x}^*. \end{aligned} \quad (2)$$

Consequently, we find

$$\nabla^* \mathbf{v}(\mathbf{x}^*, t) = \mathbf{Q}(t)\nabla \mathbf{v}(\mathbf{x}, t)\mathbf{Q}^{-1}(t) + \dot{\mathbf{Q}}(t)\mathbf{Q}^{-1}(t). \quad (3)$$

Since the latter term is antisymmetric, the symmetric part satisfies

$$\mathbf{D}^*(\mathbf{x}^*, t) = \mathbf{Q}(t)\mathbf{D}(\mathbf{x}, t)\mathbf{Q}^{-1}(t). \quad (4)$$

This confirms that the Newtonian fluid satisfies material frame indifference. Now, however, consider the behavior of a material time derivative. If  $\mathbf{T}^*(\mathbf{x}^*, t) = \mathbf{Q}(t)\mathbf{T}(\mathbf{x}, t)\mathbf{Q}^{-1}(t)$ , we find

$$\begin{aligned} \frac{d}{dt} \mathbf{T}^*(\mathbf{x}^*, t) &= \mathbf{Q}(t) \frac{d\mathbf{T}(\mathbf{x}, t)}{dt} \mathbf{Q}^{-1}(t) \\ &\quad + \dot{\mathbf{Q}}(t)\mathbf{Q}^{-1}(t)\mathbf{T}^*(\mathbf{x}^*, t) - \mathbf{T}^*(\mathbf{x}^*, t)\dot{\mathbf{Q}}(t)\mathbf{Q}^{-1}(t), \end{aligned} \quad (5)$$

which is not  $\mathbf{Q} \frac{d\mathbf{T}}{dt} \mathbf{Q}^{-1}$ . Oldroyd's paper presents two simple ways to fix this. We can replace (1) by

$$\mathbf{T} + \lambda_1 \frac{D\mathbf{T}}{Dt} = 2\eta(\mathbf{D} + \lambda_2 \frac{DD}{Dt}), \quad (6)$$

where either

$$\frac{D\mathbf{T}}{Dt} = \frac{\partial \mathbf{T}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{T} + (\nabla \mathbf{v})^T \mathbf{T} + \mathbf{T}(\nabla \mathbf{v}), \quad (7)$$

or

$$\frac{D\mathbf{T}}{Dt} = \frac{\partial \mathbf{T}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{T} - (\nabla \mathbf{v})\mathbf{T} - \mathbf{T}(\nabla \mathbf{v})^T. \quad (8)$$

He calls these two alternatives Model A and Model B. Oldroyd notes that experiments of Weissenberg [2], which show that polymeric fluids climb a rotating rod, favor Model B (Model A would predict the opposite effect). For a more systematic study of the rod climbing effect, we refer to [3]. For future reference, we note that (6) can be put in the alternative form

$$\mathbf{T} = \mathbf{T}_p + \mathbf{T}_s, \quad (9)$$

where

$$\begin{aligned} \mathbf{T}_p + \lambda_1 \frac{D\mathbf{T}_p}{Dt} &= 2\eta_p \mathbf{D}, & \mathbf{T}_s &= 2\eta_s \mathbf{D}, \\ \eta_p &= (1 - \lambda_2/\lambda_1)\eta, & \eta_s &= (\lambda_2/\lambda_1)\eta. \end{aligned} \quad (10)$$

The model is physically reasonable only if  $\lambda_2 \leq \lambda_1$ .  $\eta_p$  and  $\eta_s$  are referred to as the “polymer” and “solvent” viscosity. In the practical application of the model, however,  $\eta_s$  is often much larger than the viscosity of the solvent, except for very viscous solvents (polymeric fluids typically have more than one relaxation time, and the contribution of shorter relaxation times to the viscosity usually exceeds that of the solvent). The limiting case  $\lambda_2 = 0$  (i.e.  $\eta_s = 0$ ) of the Oldroyd B model is called the upper convected Maxwell model.

In the language of tensor analysis, the derivative appearing in the Oldroyd A model is called covariant or lower convected, while that in the Oldroyd B model is called contravariant or upper convected. We shall not go into this further, but give some simple heuristics which explains why one model might be preferred over the other. Let us consider a curve consisting of points which move with the material. If  $s$  is the curve parameter, and  $\mathbf{x}(s, t)$  is the position of a point on the curve, we have  $\frac{d\mathbf{x}}{ds} = \mathbf{v}(\mathbf{x}(s, t), t)$ . For the tangent vector  $\mathbf{u} = \frac{\partial \mathbf{x}}{\partial s}$ , we find

$$\frac{d\mathbf{u}}{dt} = (\nabla \mathbf{v}(\mathbf{x}, t))\mathbf{u}. \quad (11)$$

If we think of a polymer molecule as a linear object which is affinely stretched with the flow and carries a stress proportional to  $\mathbf{u}\mathbf{u}^T$ , then we find

$$\frac{D\mathbf{T}}{Dt} = \mathbf{0}, \quad (12)$$

with  $D/Dt$  denoting the upper convected derivative. This is indeed assumed in the neo-Hookean model of rubber elasticity [4]. This makes the Model B the more natural one for fluids like polymers. On the other hand, we may consider a family of surfaces moving with the medium, given by an equation  $\phi(\mathbf{x}(\xi, t), t) = g(\xi)$ . We have  $d\phi/dt = 0$ , which for the normal vector of these surfaces yields

$$\frac{d}{dt} \nabla \phi + (\nabla \mathbf{v})^T \nabla \phi = \mathbf{0}. \quad (13)$$

Materials in which stresses are carried by surfaces exist (indeed surface tension is the primary source of stresses in emulsions), but they are not adequately modeled by linear elasticity.

There are two quite distinct “molecular” theories of polymeric liquids which lead to the Oldroyd B model. One is motivated by the network theory of rubber elasticity, which visualizes rubber as a network of interconnected elastic strands. For a liquid, the connections are temporary and form and decay according to laws postulated ad hoc. Such a theory leading to the upper convected Maxwell model was formulated by Green and Tobolsky in 1946 [5]. A quite different theory visualizes a polymer molecule as a linear elastic spring subject to drag from the surrounding fluid (which is modeled as Newtonian) on its ends and also to Brownian motion. This theory is originally due to Kuhn [6]. We may regard the Oldroyd B model as the simplest model for the flow behavior of polymeric fluids which has some underpinning in the physics of the underlying microstructure. There are however, serious limitations:

1. It is not realistic to have a single relaxation time. Polymers do not usually consist of identical molecules, and, even if they do, molecules have internal modes of deformation which have shorter relaxation times than the dominant mode.
2. Both the rubberlike and dumbbell theories treat molecules as linearly elastic. This is, at the very least, inappropriate for large deformations. The elasticity of polymeric liquids is primarily associated with the decrease in entropy that results from stretching out a randomly coiled molecule. A different physics takes over once molecules are fully stretched.
3. The model does not adequately account for interactions between different polymer molecules. In most polymeric fluids, entanglements between molecules are essential, but unlike in a “rubber-like” network, molecules are not pinned at these entanglements, but slither through them.

For reasons like these, rheologists had to go to some length to even find a fluid that is well described by the Oldroyd B model. The search for such a fluid finally led to “Boger fluids;” these are polymer solutions in highly viscous solvents. The original Boger fluid [7] was a solution of polyacrylamide in corn syrup. The Oldroyd B model predicts a higher stress growth at large deformation rates than typical elastic fluids actually possess. This leads to more pronounced singular behavior in the limit of high deformation rates, which poses challenges for both mathematical analysis and numerical simulation.

The Oldroyd B model has an equivalent integral form. Let  $\chi(\mathbf{x}, t, s)$  denote the position at a prior time  $s$  of the particle which occupies position  $\mathbf{x}$  at time  $t$ , and let

$$\mathbf{F}_t(\mathbf{x}, s) = \nabla \chi(\mathbf{x}, t, s), \quad \mathbf{C}_t(\mathbf{x}, s) = \mathbf{F}_t(\mathbf{x}, s)^T \mathbf{F}_t(\mathbf{x}, s). \quad (14)$$

Then an equivalent form of the Oldroyd B model is

$$\mathbf{T}_p = \frac{\eta_p}{\lambda_1^2} \int_{-\infty}^t \exp(-(t-s)/\lambda_1) (\mathbf{C}_t^{-1}(\mathbf{x}, s) - \mathbf{I}) ds. \quad (15)$$

It is obvious from the integral form that  $\mathbf{T}_p + (\eta_p/\lambda_1)\mathbf{I}$  is positive definite. It can also be shown from the differential version of the model that this positive definiteness is preserved as long as it holds for the initial data [8]. Preservation of positive definiteness is an important concern for numerical simulations. If positive definiteness is lost, instabilities arise, and the upper convected Maxwell model even becomes ill-posed [9].

### 3. Existence for initial value problems

The basic existence problem consists in solving (6), together with the balance of momentum

$$\rho \left( \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right) = \operatorname{div} \mathbf{T} - \nabla p, \quad (16)$$

the incompressibility condition

$$\operatorname{div} \mathbf{v} = 0, \quad (17)$$

the boundary condition  $\mathbf{v} = \mathbf{0}$ , and initial conditions for  $\mathbf{v}$  and  $\mathbf{T}$ . Creeping flow problems (i.e. with inertia neglected) seem to have been the first to be solved; see [10] for an early reference. With the inclusion of inertia, an existence result locally in time was proved in [11] for a broad class of models including the Oldroyd B model. The method uses Lagrangian coordinates and is essentially based on a perturbation of the Newtonian case. The case  $\eta_s = 0$  is harder; the first existence result for a three-dimensional situation is due to Kim [12]; it concerns a class of integral models including the lower convected Maxwell model. The technique can be generalized to cover also the upper convected model [13]; a different method is developed in [14]. A result which proceeds directly from the differential form of the model is given in [15].

If the initial data are sufficiently small, we can expect a global existence result. Indeed, any reasonable model of fluid flow ought to predict that small perturbations of the rest state, in absence of a driving force, decay to zero. Kim’s result [12] and the result given in [13] include a result on global existence and decay for small perturbations of the rest state in addition to local existence. These results are for problems without boundaries. Guillopé and Saut [16] prove a global existence result for one-dimensional shearing motions for a class of models including the Oldroyd B model. This result is for large data, but is trivial for the Oldroyd B case, since this model is linear for shearing motions. In [17] they prove global existence for small data in the multidimensional setting, under the assumption that the retardation time is not too small. Hakim [18] also proves a result on existence of time-periodic solutions for small time-periodic data. The assumption of sufficiently large retardation time is disposed of by Molinet and Talhouk [19]. More recent further results concern the incompressible limit of compressible versions of the Oldroyd B model [20], the limiting

case of zero relaxation time [21], exterior domains [22], and the molecular version of the model, which includes additional “molecular” variables [23]. There are also improvements regarding function spaces in which data need to be small, which can be chosen to be critical Besov spaces; moreover, in two dimensions the known global existence result for the Newtonian case can be exploited if  $\lambda_2/\lambda_1$  is close to 1 [24].

Global existence for large initial data is a much harder and essentially unsolved problem. Even for the Newtonian case, only existence of weak solutions is known in the three-dimensional case. Lions and Masmoudi [25] show a global existence result for weak solutions of the corotational Oldroyd model; their result, however, relies on a cancellation of terms which is specific to this model and does not generalize to more physically realistic models. Chemin and Masmoudi [26] give necessary criteria for blow-up which need to be satisfied if global existence (of regular solutions) fails. Constantin and Kliegl [27] prove global existence in two space dimensions, provided an additional stress diffusion term is added to the constitutive law. (There is a physical rationale for such a term, but the coefficient is very small, and stress diffusion is in practice relevant only at submicron length scales). Barrett and Süli [28] prove a similar result for the molecular version of the Oldroyd B model. Masmoudi [29] proves global existence of weak solutions for the FENE-P, Phan-Thien Tanner and Giesekus models; all these models have slower stress growth at high deformation rates than the Oldroyd B model.

### 4. Existence results for steady flows

The first existence result for steady flows is due to Renardy [30]. The proof is based on taking the divergence of the constitutive law and using the result in the momentum equation; this combination leads to a Stokes-like problem. Solutions for small data can then be constructed by proving convergence of an iteration which alternates between solving a Stokes problem and integrating stresses along streamlines. Guillopé and Saut [31] prove existence of steady flows close to a stable Newtonian flow if the ratio of polymer to solvent viscosity is small. Existence for small data, also based on iteration between Stokes problems and integration along streamlines, has also been proved for exterior flows in three dimensions [32,33] and flows with outlets to infinity [34]. For exterior domains in two dimensions, the Newtonian case is already more complicated; Stokes solutions do not exist in general and an Oseen linearization has to be considered instead. This case does not seem to have been tackled for viscoelastic flows.

It is not clear if any large data global existence result should be expected. The Oldroyd B model leads to infinite stresses in steady elongation at a finite extension rate. In complex flows, this leaves us with three possibilities:

1. The flow arranges itself in such a manner that the limiting elongation rate is not reached.
2. Steady flows cease to exist.
3. Steady flows exist even when the limiting elongation rate is exceeded; they then have infinite stresses at the stagnation point and along the streamline emanating from it.

If velocity boundary conditions are inhomogeneous, the problem of additional boundary conditions at inflow boundaries arises. The integration of stresses along streamlines would require stresses at inflow boundaries to be prescribed. For the Oldroyd B model, a well-posed problem is indeed obtained if polymer stresses at inflow boundaries are prescribed in addition to velocities on all boundaries [35]. For the upper convected Maxwell model, however, this is an overdetermined problem. Correct choices of inflow boundary conditions were given in [36,37]. In real flow problems, inflow boundaries usually terminate at corners, and the issue of compatibility conditions to avoid singularities arises [38]. Of course, inflow boundaries can arise in time-dependent as well as steady flows. Work on this problem has so far been rather fragmentary [39].

## 5. Flow stability

Newtonian fluid flows display a rich variety of instabilities and bifurcations, which has inspired much mathematical work in dynamical systems, asymptotics and other fields. Viscoelastic effects modify these instabilities and can also lead to new mechanisms. We shall not attempt a comprehensive literature review, but merely outline some of the basic problems. The review articles of Larson [40] and Shaqfeh [41] can serve as a starting point for further reading.

Early work on stability of viscoelastic shear flows was motivated by the hope that a linear shear flow instability might explain extrudate instabilities known as melt fracture. The early literature is characterized by quite a bit of confusion, with reports of positive results which turned out to be based on faulty approximations or inaccurate numerics. More accurate numerical computations showed no evidence of linear instabilities in parallel shear flows of the upper convected Maxwell and Oldroyd B fluids [42,43]. One difference between Newtonian and viscoelastic flows is the appearance of continuous spectra, even in bounded geometries. Numerical methods are generally not very accurate in approximating these, which explains some of the early claims of instability. It would be of interest to know how to design numerical methods which approximate continuous spectra more faithfully, but there seems to be no literature on this topic. Elastic instabilities do, however, exist in shear flows with curved streamlines. This was first discovered by Larson, Shaqfeh and Muller [44], and there has been much subsequent work on this topic. In multilayer shear flows, there can be instabilities driven by a normal stress difference at the interface; this was first observed in [45] and [46].

In elongational flows, the strong resistance of viscoelastic fluids to stretching has a stabilizing influence. For the Rayleigh instability of jets, viscoelasticity actually has a destabilizing effect on the initial linear instability, where elongation is not yet important [47–49]. However, viscoelastic effects become stabilizing in the later evolution [50–52]. Indeed, the analysis of one-dimensional models shows that jet breakup is suppressed entirely for the Oldroyd B fluid [53]. The stabilizing effect of elasticity on elongation has also been found to be the dominant effect responsible for turbulent drag reduction; see [54] for a review.

From the mathematician's point of view, there are a number of fundamental questions which are largely unresolved for viscoelastic flows. First of all, stability is usually inferred from eigenvalue calculations. While this is well justified for Newtonian flows, it is well known that there are examples of evolution problems which are unstable even though the entire spectrum of the generator is in the left half plane. This can happen in examples as “applied” as a lower order perturbation of the wave equation, with the natural choice of function spaces [55]. Linear stability can be proved rigorously if, in addition to having a spectrum strictly in the left half plane, a resolvent bound on the imaginary axis can be established [56–59]. This is applied to parallel shear flows of a class of fluids including the Oldroyd B model in [55,60]. The idea is to first take advantage of separation of variables to reduce the stability problem to ODEs. Then the ODE problems are reduced to finite dimension by taking advantage of the correspondence between solutions and initial data. Doing this makes it possible to deduce resolvent bounds from the location of spectra.

In [31] it is shown that flows of weakly elastic fluids inherit stability characteristics from the Newtonian case. A somewhat larger perturbation is allowed in [61]; the result there is not that the flow inherits Newtonian stability, but that a resolvent estimate holds which allows inferring stability from the spectrum. These results also show nonlinear stability for small perturbations.

Another approach to the stability problem looks for conditions in addition to the location of the spectrum which guarantee stability. For some types of hyperbolic PDEs such conditions have been given which involve the stability of ODE systems along characteristics. Results along such lines [62] have been shown to be applicable to creeping flows of Maxwell fluids [63,64]. It should be emphasized, however, that the

actual application of such criteria in a complex flow would be a rather formidable task.

The continuous spectrum for the upper convected Maxwell fluid is analyzed in [65]. For the linearization at a steady flow in a bounded domain, the continuous spectrum consists of three parts: The first part always has real part equal to  $-1/\lambda_1$ , the second part is associated with the short wave limit of wall modes and has real part between  $-1/\lambda_1$  and  $-1/(2\lambda_1)$ , and the third part is associated with integrating stresses in the given velocity field of the base flow. If there are hyperbolic stagnation points, then this latter part will depend on the choice of function space. It will always be unstable in Sobolev spaces of sufficiently high order; this is because derivatives in a converging direction of the flow will grow by advection and stress relaxation cannot compensate for this if the order of the derivative is high enough. On the other hand, it is shown in [65] that in two dimensional flows without interior stagnation points the continuous spectrum is always stable.

If instabilities are associated with an isolated eigenvalue crossing the imaginary axis, we expect the usual methods of bifurcation theory to be applicable. This requires a version of the center manifold theorem which reduces the problem to finite dimensions. The versions available in the literature, however, are for parabolic PDEs and the equations of viscoelastic flow are always partly hyperbolic, which causes serious technical issues. A version of the center manifold theorem which is suitable for hyperbolic PDEs with periodic boundary conditions is proved in [66] and applied to the viscoelastic Bénard problem.

## 6. High Weissenberg number asymptotics

The study of Newtonian high Reynolds number flows has a long history. Formally, the high Reynolds number limit of the Navier–Stokes equations leads to the Euler equations. But the Euler equations do not allow imposition of zero velocity on the boundary. More than a century ago, Prandtl [67] advanced the idea that viscous effects are confined to a boundary layer: In the bulk of the flow the Euler equations apply, but in a thin layer near the boundary viscous effects need to be taken into account to allow transition to the right boundary condition. The actual implementation of this strategy, however, turns out to be far more complicated than the illustrative examples usually presented in textbooks, and the results remain fragmentary. Perhaps the most successful applications are for the technologically important problem of flow past bodies; on the other hand, such seemingly simple problems as determining the flow rate through a pipe elude a full analysis. There are a number of major obstacles. The Euler equations allow many solutions, and it is not clear which is the “right” one. For instance, there are infinite dimensional manifolds just of steady solutions. Most of these are unstable, and the dynamics resulting from instabilities is complex. The Prandtl equations are difficult to analyze, and in general not well-posed [68]. Similar considerations apply to high Weissenberg number flows of elastic fluids, and indeed we can expect the flow behavior to be just as complicated as high Reynolds number flows of Newtonian fluids [69].

There is a connection between viscoelastic high Weissenberg number flows and the Euler equations [70]. Recall that the source of elasticity in polymeric fluids is the stretching of polymer molecules by the flow. At high Weissenberg number, we can expect these stretched molecules to align in whatever direction the flow stretches them in, leading to a predominant component of the stress which is of rank 1. Let us write this component in the form

$$\mathbf{T} = \gamma \mathbf{u} \mathbf{u}^T, \quad (18)$$

where  $\mathbf{u}$  is a vector, and  $\gamma$  is a scalar. For given  $\mathbf{T}$  of this form, we can always choose  $\gamma$  and  $\mathbf{u}$  in such a way that

$$\operatorname{div}(\gamma \mathbf{u}) = 0. \quad (19)$$



If we now assume creeping flow and insert (18) into the equation of motion, we find

$$\operatorname{div} \mathbf{T} - \nabla p = \gamma(\mathbf{u} \cdot \nabla) \mathbf{u} - \nabla p = \mathbf{0}. \quad (20)$$

The Eqs. (19) and (20) are the steady compressible Euler equations. In contrast to compressible Newtonian flow,  $\mathbf{u}$  is not the velocity and  $\gamma$  is not the density, although  $p$  is the pressure. Moreover, the sign of the pressure term is opposite, reflecting the fact that elastic stresses in polymers are tensile while Reynolds stresses are compressive. Finally, there is no equation of state linking  $p$  to  $\gamma$ .

We note that so far we have neither invoked a specific constitutive law nor even mentioned the velocity of the fluid. All we have used is that the stress is one-dimensional. In the high Weissenberg number limit for steady flow of the Oldroyd B model, polymer stress dominates over solvent stress, and quadratic terms in the constitutive equation dominate over linear ones, so we have the following dominant balance:

$$(\mathbf{v} \cdot \nabla) \mathbf{T} - (\nabla \mathbf{v}) \mathbf{T} - \mathbf{T}(\nabla \mathbf{v})^T = \mathbf{0}. \quad (21)$$

It is shown in [70] that, in a two-dimensional flow, this leads to the following relationships between  $\mathbf{v}$  and  $\mathbf{u}$  and  $\gamma$  introduced above:

$$\mathbf{v} \cdot \nabla \gamma = 0, \quad \mathbf{v} \times (\gamma \mathbf{u}) = K \mathbf{e}_3. \quad (22)$$

Here  $\mathbf{e}_3$  is the out-of-plane unit vector and  $K$  is an arbitrary constant. The condition that  $\mathbf{v}$  be divergence-free leads to the “equation of state”

$$\operatorname{div} \mathbf{u} = \phi(\gamma). \quad (23)$$

In this equation,  $\phi$  is an arbitrary function. In particular,  $\phi$  can be zero, and  $\gamma$  can be constant; in this case we recover the incompressible Euler equations. We note that the velocity does not appear in (19), (20) and (23); it is determined by (22) once  $\gamma$  and  $\mathbf{u}$  are known.

We see that the indeterminacy in this problem is even greater than for the steady Euler equations, since the “equation of state” now involves an arbitrary rather than a specific function. The time dependent problem raises even more difficult problems. Basically, the high Weissenberg number limit of the Oldroyd B model is a neo-Hookean elastic solid with zero equilibrium stress modulus. A stress modulus arises as a result of flow, but it is in one direction only. This degeneracy of the stress modulus makes it impossible to determine both stresses and velocities in creeping flow. An analogous situation arises in simpler contexts: In a rigid body, we can fully determine the motion, but we know nothing about the stresses (other than that the divergence is zero), in contrast, in a vacuum, we know exactly what the stress is, but we cannot define a motion. Unlike these “obvious” and extreme cases, however, the high Weissenberg number limit of viscoelastic flow does not give us a “clean” way of separating knowable and unknowable variables. Lower order terms need to be considered to resolve the indeterminacy; this problem has not been resolved in a satisfactory manner [71,72].

A different limit arises if both Weissenberg and Reynolds number are large, and inertial terms are included in the equations. In that case, the limiting equations are well-posed [73]. Well-posedness for boundary layer equations can be shown as well [74,75]. Thus this problem is actually better behaved mathematically than the Newtonian case, due to a stabilizing effect of viscoelasticity on high Reynolds number shear flow instabilities [76]. This stabilization has previously been noticed in the mathematically equivalent situation of ideal magnetohydrodynamics [77].

In steady flows without inertia, boundary layers arise for a different reason than in the Newtonian case. High Weissenberg number means long memory, and as a result stresses depend on the velocity gradient along the entire streamline. On walls and at stagnation points, however, the velocity is zero, and hence stresses depend only on the local velocity gradient. The boundary layer equations resulting from

this are derived in [78]. The most successful application of matched asymptotics involving these boundary layer equations is in the analysis of the reentrant corner singularity. When it comes to corners between walls, there is a fundamental difference between corners with angle less than 180 degrees and “reentrant” corners of angle greater than 180 degrees. The former lead to zero velocity gradients and stresses at the corner and a dominant Newtonian behavior, see [79] for a rigorous result along such lines. For reentrant corners, on the other hand, stresses and velocity gradients are infinite, and the study of the stress singularity becomes a matter of high Weissenberg number asymptotics. A matched solution based on potential flow of the Euler equations [80] and similarity solutions of the boundary layer equations was suggested and partially constructed by Renardy [81] and completed by Rallison and Hinch [82]. In principle, the viscoelastic stresses always dominate near the corner, and Newtonian terms are subdominant. If the model is close to Newtonian (i.e.  $\lambda_2$  is close to  $\lambda_1$ ), this can only be the case very close to the corner. Evans [83] has given a partial analysis for this case. Rigorous results on existence of solutions with reentrant corners are not available at this point. Another flow with a point singularity that is amenable to boundary layer analysis is sink flow, which was analyzed by Evans and Hagen [84].

Little is known about the high Weissenberg number behavior along separating streamlines. The simpler problem of integrating the constitutive law in a given velocity field can be analyzed, see e.g. [85] for a study of flow past a cylinder. Numerical results for the same simplified problem agree with the analysis [86], but simulations of the full problem have not reached Weissenberg numbers where a meaningful comparison would be possible.

## 7. Mathematical analysis informing numerical methods

Understanding the nature of viscoelastic flows in complex geometries is important for many engineering and biological problems at the micro-scale, and numerical simulations are a key tool to developing theory. We continue the focus on the Oldroyd B model in the creeping flow regime and now turn to how mathematical analysis can help inform the use and design of numerical methods. Challenges in simulating the Oldroyd B model have a long history, going back to the early 1980's when the “high Weissenberg number problem” was first discussed [87,88]. We refer the interested reader to a recent review [89,90] and book dedicated to more of an overview of these issues; here we focus on a few simple flow geometries and related observations.

There is a need for high resolution numerical methods to handle the complex flows and dynamics for biological problems. Some of this was pointed out in [91]. The immersed boundary (IB) method is a popular method used for its flexibility [92] but its low order of convergence makes it ill suited for simulating problems in complex fluids. Some modifications to the stress tensor locally near boundaries have been proposed [93,94] as well as higher order versions of IB [95–97] but there are still significant limitations in the technology for numerical simulations of moving and deforming objects in viscoelastic fluids, especially in three spatial dimensions.

The Oldroyd B model is a good model to analyze mathematically because it is more tractable than models with lots of “bells and whistles” (aka parameters). Nevertheless it still captures key features of a nonlinear viscoelastic fluid, such as storage of memory from past deformation on a characteristic time-scale. We focus here on flows near extensional points, as they present the most notable challenges to the Oldroyd B model. Three settings are explored, a steady extensional point created by steady background forcing, flow around a cylinder in 2D, and flows near tips of waving filaments that create oscillating extension.

## 8. Flows at steady extensional points with periodic forcing

A relatively simple way to simulate a steady extensional point is by imposing a four-roll mill background force. In this section we discuss results from [98–101], which were obtained by simulating the following non-dimensional set of equations

$$-\nabla p + \Delta \mathbf{u} + \xi \nabla \cdot \mathbf{C} + \mathbf{f} = 0 \quad (24)$$

$$\operatorname{div} \mathbf{u} = 0 \quad (25)$$

$$\frac{D\mathbf{C}}{Dt} = -\frac{1}{Wi}(\mathbf{C} - \mathbf{I}) + \nu \Delta \mathbf{C}, \quad (26)$$

where the upper convected derivative  $\frac{D\mathbf{C}}{Dt}$  is defined in (8). The conformation tensor  $\mathbf{C}$  is related to the polymer stress tensor via

$$\mathbf{T}_p = \frac{\eta_p}{\lambda}(\mathbf{C} - \mathbf{I})$$

and the background force  $\mathbf{f}$  in Eq. (24) is given by

$$\mathbf{f} = \begin{pmatrix} -2 \sin x \cos y \\ 2 \cos x \sin y \end{pmatrix}. \quad (27)$$

The Weissenberg number is defined to be  $Wi = \frac{\lambda}{T_f}$  where  $T_f$  is the flow time scale. The coupling parameter  $\xi = \frac{\eta_p}{\lambda \eta_s}$  is related to the more familiar viscosity ratio  $\beta$  via

$$\beta = \frac{\eta_s}{\eta_s + \eta_p} = \frac{1}{1 + \lambda \xi}.$$

The system in Eqs. (24)–(26) is equivalent to the Stokes Oldroyd B model for  $\nu = 0$ . For  $\nu > 0$  the model has an additional polymer stress diffusion. We scale the diffusion  $\nu = \alpha dx^2$ , with the grid discretization, thus in the limit  $dx \rightarrow 0$  this model converges to the Oldroyd B model. In Section 8.1 we set  $\nu = 0$ , and we discuss the effects of this stress diffusion in detail in Section 8.2

### 8.1. Steady flow in the 4-roll mill geometry

To study the behavior of the Stokes Oldroyd B model near steady extensional points in [99] we simulated Eqs. (24)–(26) in a 2D periodic domain  $[-\pi, \pi)^2$  using a pseudo-spectral method. We did not use polymer stress diffusion, i.e.  $\nu = 0$  in Eq. (26). In a purely viscous fluid the solution to Eq. (24) with the forcing  $\mathbf{f}$  given in Eq. (27) would be  $\mathbf{u} = \frac{\mathbf{f}}{2}$ , resulting in a flow with 2 extensional stagnation points in the periodic domain. We focus on the extensional point at the origin in what follows.

One mathematical and numerical result from [99] was that the polymer stress field loses smoothness as a function of  $Wi$ . Previously there were analytical predictions along these lines [102,103], but in those analyses the stress and velocity were decoupled. In these simulations we demonstrate how the stress responds to an imposed background flow. The results reveal an algebraic structure of the solutions that depends critically on the Weissenberg number.

A local analysis near the origin finds that the velocity converges to an extensional flow of the form  $\alpha(x, -y)$  where  $\alpha$  is the local strain-rate at the origin. In this numerical framework  $\alpha$  does not remain order one as  $Wi$  increases. Rather, the flow slows down to compensate for the increasing stress at the origin and the product  $\epsilon \equiv \alpha Wi$  remains bounded by 1. Using this rescaled velocity one can solve for the components of the stress tensor directly along the characteristics of the local velocity. The  $xx$ -component of the conformation tensor is

$$C_{xx}(x, y, t) = \frac{1}{1 - 2\epsilon} + e^{(2\epsilon - 1)t} H(xe^{-\epsilon t}, ye^{\epsilon t}). \quad (28)$$

The structure of the function  $H$  cannot be derived without coupling to the background flow. The analysis and comparison with numerical simulations suggests that the steady-state structure of the conformation tensor is

$$C_{xx}^\infty = \frac{1}{1 - 2\epsilon} + A|y|^{\frac{1-2\epsilon}{\epsilon}}. \quad (29)$$

There are two significant transitions in the flow structure. First beyond  $Wi \approx 0.5$  ( $\epsilon = 1/3$ ) the stress approaches a cusp solution exponentially in time, meaning that the limiting (or steady state) stress is not differentiable. Second beyond  $Wi \approx 0.9$  ( $\epsilon = 1/2$ ) the stress exponentially approaches a divergent solution. The numerical validation of these analytical predictions relies on the use of the pseudo-spectral method which allows one to study the approach of a singularity via the Fourier spectrum of the solution [104–106].

The simulations also show that although the stress is diverging exponentially in time, the velocity (which is modified by the stress via the divergence of the stress tensor) converges. We can see this if we define the energy  $\mathcal{E} = \frac{1}{2} \int \int \operatorname{tr}(\mathbf{C} - \mathbf{I}) dx dy$ . This energy satisfies

$$\partial_t \mathcal{E} + \frac{1}{Wi} \mathcal{E} = -\frac{1}{\xi} \int \int |\nabla \mathbf{u}|^2 dx dy - \frac{1}{\xi} \int \int \mathbf{u} \cdot \mathbf{f} dx dy, \quad (30)$$

hence for bounded input power,  $\mathbf{u} \cdot \mathbf{f}$ , this integral will remain bounded. Thus although the stress may diverge at a point, the integral remains bounded, allowing for convergence of the velocity field. We demonstrate this via an asymptotic analysis in Section 8.2.

### 8.2. Polymer diffusion asymptotics

We saw above that the stress diverges for sufficiently large  $Wi$  so only a quasi-steady state exists without some regularization. The addition of polymer stress diffusion,  $\nu > 0$  in Eqs. (24)–(26), allows one to obtain steady state numerical solutions. Although polymer stress diffusion has microscopic justification [107,108], the size of numerical diffusion used in simulations is usually larger than can be justified by the kinetic theory. Polymer stress diffusion has been studied in the Oldroyd B model [98,109,110] and it has been shown that the addition of *any* amount of polymer stress diffusion appears to remove the singularity found in [99]. This is because for  $\nu > 0$  in Eq. (29) asymptotic analysis [98,109] finds that for sufficiently large  $Wi$  and small  $\nu$  we get a solution that has a Gaussian structure in  $y$  at steady state of the form

$$C_{xx}(0, y) \approx C_0 Wi \nu^{-1/2} e^{-y^2/2\nu}. \quad (31)$$

Numerical simulations support this analysis. Here we show simulations of Eqs. (24)–(26) with a fixed grid discretization  $dx = 2\pi/512 \approx 0.0123$ , and  $Wi = 5$ . Simulations are run to steady state at  $t \approx 10Wi$ . We vary the polymer stress diffusion of the form  $\nu = \alpha dx^2$ . To describe the results it is useful first to look at  $C_{xx}$  and the vorticity near the origin. The color map shown in Fig. 1(a) displays the first component of the conformation tensor  $C_{xx}(x, y)$  at steady state for the lowest diffusion level  $\alpha = 0.5$ . This shows that the stress is large at the origin, but also along the entire line of extension near  $y = 0$ . In Fig. 1(b) we show the vorticity at steady state for this same level of diffusion. The vorticity near the centers of the “rolls” is slaved to the background forcing, but near the line of extension at  $y = 0$  we find that there are vortical structures that rotate in the opposite direction.

Next we zoom in near the origin for the stress and near  $(\pi/2, 0)$  for the velocity and vorticity in Fig. 2, and examine how these structures depend on the diffusion. In Fig. 2(a) we demonstrate the effect of diffusion on the  $xx$ -component of the conformation tensor. The maximum is growing, but the maximum is growing as  $\max C_{xx} \sim \mathcal{O}(\nu^{-1/2})$  as predicted in Eq. (31). In Fig. 2(b) we also plot the best fit to a power-law function, and the best fit gives  $\nu^p$ , with  $p = -.43$ . As expected from the bound on the energy, we find that the integral or  $L^1$  norm of the conformation tensor is converging (not shown). We also examine how the velocity is effected by the highly concentrated stress. The largest differences in the velocity with high stress concentration arise near  $x = \pm\pi/2$ . We plot the horizontal velocity at  $(\pi/2, y)$  in Fig. 2(c) and the velocity gradient  $\partial_y u$  in Fig. 2(d). The velocity appears to be converging to a cusp which yields a jump in the velocity gradient across the line of extension. We emphasize that although the stress is diverging near the axis of extension, it is converging in average, and this is sufficient for

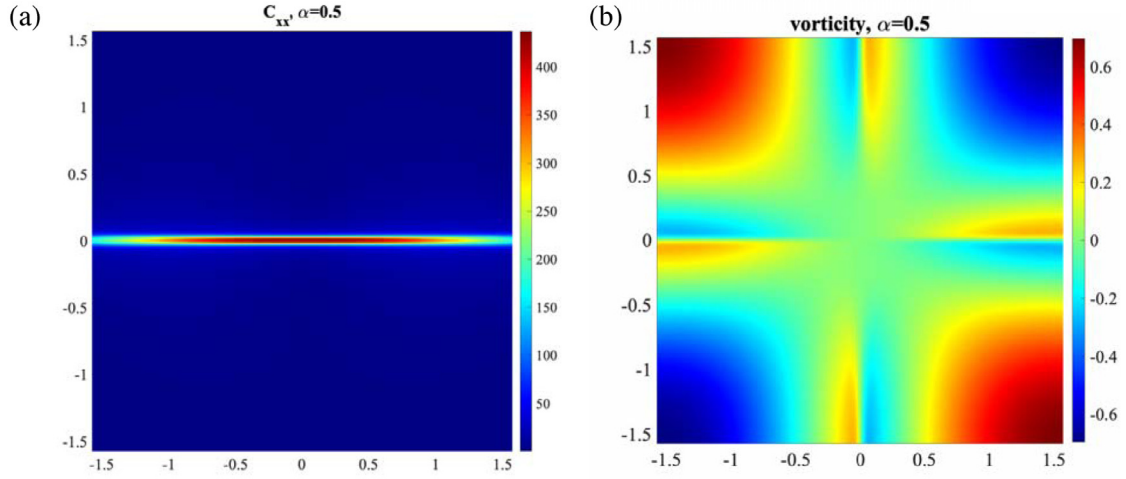


Fig. 1. Results of simulations for  $Wi = 5$  run to steady state. (a)  $C_{xx}(x, y)$  conformation tensor (b) Vorticity.

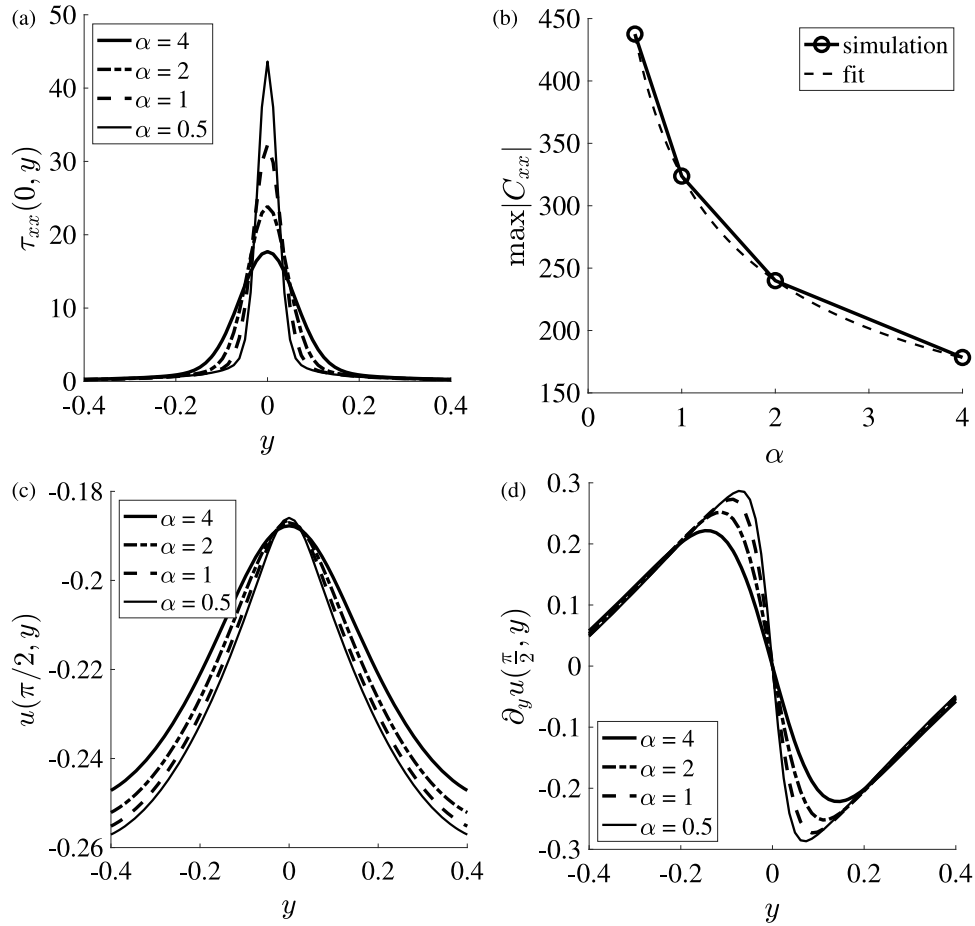


Fig. 2. Slices of stress and velocity for  $Wi = 5$  at steady state and a range of diffusion  $v = \alpha dx^2$  (a) Polymer stress (b) Maximum of conformation tensor (c) Velocity (d) Vorticity.

the velocity to converge, but the smoothness of the velocity is lower order resulting in what looks like a finite sized jump in the derivative across the stress near-singularity. The asymptotic analysis in [109] supports these conclusions.

On the one hand, polymer stress diffusion, used carefully and with consideration of the numerical artifacts it may create, can rescue the Oldroyd B model from the singularities it suffers at steady extensional points. And, the polymer stress diffusion term is not added without

physical justification, it can be justified from kinetic theory when including the effect of center of mass diffusion of polymer coils [107, 108]. To apply the asymptotic analysis we need only posit that  $v > 0$ , which is enough to obtain bounded solutions for the velocity and velocity gradients. On the other hand, simply adding polymer stress diffusion is not always sufficient to mitigate the challenges of the more complex geometries and flow dynamics that arise in engineering and biological applications.

### 8.3. Symmetry breaking in the 4-roll mill geometry

Experimental observations of symmetry breaking flow transitions near extensional points [111] motivated simulations of viscoelastic fluids in cross slot geometries [112–116]. In [111] a polymeric fluid in a cross-slot geometry exhibited two distinct symmetry breaking transitions as a function of the Weissenberg number. The first transition was characterized by the onset of a steady asymmetry in the flow near the extensional point. At a higher Weissenberg number the flow became aperiodic. Simulations in the four-roll mill geometry observed qualitatively similar results [100,101,117]. To obtain numerical steady states stress diffusion  $\nu = .001 \approx 5/3 dx^2$  is added to the Stokes Oldroyd B model. The symmetry breaking occurs first as the flow loses slaving to the background flow locally near the extensional point in the flow. A second instability that is characterized by the onset of quasi-periodic motion occurs for a larger critical Wi. These asymmetric steady states were found by numerically evolving the flow from small perturbations to the initial data. Here the loss of pinning of the centers of the “4-rolls” appears to be related to the onset of oscillatory motion. This oscillatory flow also leads to high levels of mixing in the flow.

It has been suggested that this second instability may arise due to the additional polymer stress diffusion, as simulations without diffusion found the first instability but not the second instability [118]. One must take care when using any numerical regularization as it may introduce unwanted artifacts. Stress diffusion as a method of regularization has the advantage that it makes the system well-posed [27,119] and we can quantify the effect via asymptotic analysis [98,109]. Regarding the second instability discussed above, it is interesting to note that in recent experimental work [120] the onset of the temporal aperiodicity coincided with a 3-dimensional instability along the  $z$ -axis, and simulations of a 3-dimensional 4-roll mill found a similar result [121].

## 9. Two dimensional flow around cylinder

One of the most challenging static flow geometries for the Oldroyd B model in simulations has been the flow around a cylinder in a planar channel. This geometry was introduced as a benchmark for the numerical simulations of viscoelastic fluids in the report from the VIIth international workshop on numerical methods in non-Newtonian flow [122] in 1992. Despite significant effort it has proven elusive to find numerical solutions to the Oldroyd B model in creeping flow in this geometry beyond  $Wi \approx 0.7$ . In the low Wi regime, this benchmark is a very popular geometry to test new numerical methods, but it is noteworthy that higher values of Wi are unattainable for numerical simulations. Here we will not attempt to review the state of numerical methods in this flow geometry, but we direct the interested reader to the extensive information in the book *Computational Rheology* [90] which reviews this material thoroughly up to its publication date, along with the recent review article that summarizes many subsequent developments [89]. Rather we take this opportunity to discuss some of the numerical challenges that are deeply connected to the mathematical challenges posed in the first half of this manuscript related to this flow geometry.

A standard benchmark flow for evaluating numerical solvers for polymeric flow problems is the confined flow of a fluid around a cylinder in a channel, studied in [123–132]. The behavior of the flow is well understood at low Weissenberg numbers but the behavior of the flow is unknown above  $Wi = 0.7$ . The typical computational setup is to solve the Stokes Oldroyd B system given in Eqs. (24)–(26) (with  $\mathbf{f} = 0, \nu = 0$ ) in a rectangular domain,  $[-20, 20] \times [-2, 2]$  with no-slip ( $\mathbf{u} = 0$ ) boundaries imposed on the bottom and top of the domain, the inflow condition  $u(-20; y) = (u_{in}(y), 0)$  with  $u_{in}(y) = \frac{3}{2} \left(1 - \frac{y^2}{4}\right)$ , and an outflow boundary condition (which may differ depending on the computational setup). The parameter  $\beta = \frac{\mu_s}{\mu_s + \mu_p}$  is fixed at 0.59.

It is quite reasonable to ask *What makes this flow geometry so challenging for numerical simulations?*, but the answer is unclear. As mentioned

at the end of Section 6 there are asymptotic results [85] for the decoupled problem (where the polymer stress is advected along fixed streamlines of the corresponding Newtonian flow) that indicate that for large Wi the maximum value of the stress in the wake of the cylinder should scale like  $Wi^5$  for large Wi. This scaling creates significantly large stresses and stress gradients in the wake of the cylinder that are numerically challenging to resolve. However, numerical simulations in a Lagrangian frame (i.e. evolving the stress along streamlines of the Newtonian flow) have been able to capture these large stress and stress gradients [86], and these numerical simulations confirm the asymptotic scaling for sufficiently large Wi ( $Wi \gtrsim 128$ .) In that work it is noted that to reach the regime where this scaling should be valid the stresses need to be fully convected around the cylinder. This does not occur for small Wi and thus for the decoupled problem one should not have these scalings for  $Wi \sim 1$ . However, it is important to note that it is not clear exactly how the coupling changes the dynamics of the flow and in particular does the coupling make the onset of this scaling occur at a smaller Weissenberg number? It was noted in [86] that when designing numerical simulations for this flow geometry one could use the fact that the decoupled problem is well-posed and can be resolved numerically at high Wi as a test of any numerical scheme. However, it appears that at least finite element method (FEM) [133] and unstructured grid methods [134] of the decoupled case are still unable to resolve large stress growth beyond  $Wi \approx 1$  indicating that this is still a very challenging numerical computation.

There is a range of possibilities that could explain what happens in the coupled problem for  $Wi \gtrsim 0.7$ . Experiments have indicated a wake instability [135] for  $Wi \sim 1$  and numerical simulations also indicate similar results [136,137]. In [126] the authors indicate that there are velocity fluctuations near the channel walls for  $Wi > 0.62$ , and suggest that these fluctuations will lead to the onset of an oscillatory state. It is also possible that underlying these numerical oscillations is a mathematical singularity and the system is not well-posed beyond a critical Wi. It would be nice to resolve this problem with either an analytical result or sufficiently convincing numerical simulations that determine a critical Wi for a transition to unsteady behavior, but neither solution appears readily available. It is likely that numerical simulations that accurately predict the dynamics observed in experiments [135] for high Wi will require 3D grids, making computations very expensive.

One candidate for potential singularities in the flow around a cylinder geometry is the stationary stagnation point at the front and rear of the cylinder. In Section 8.1 we discussed the nature of the coupled flow in the stationary stagnation point driven by a background forcing. In that case the de-coupled problem has singularities [102,103] but in the coupled problem as the Weissenberg number is increased the flow locally near the origin rearranges to maintain integrability of the polymer stress. This flow geometry is quite different and the flow is driven by an upstream in-flow condition. In addition we know that the decoupled case is well-posed. So in this case one can ask, does the flow coupling make the problem more singular?

In Fig. 3 we show the  $xx$ -component of the polymer stress tensor  $\tau$  on the centerline of the channel (when  $x \notin [-1, 1]$ ), and along the wall of the cylinder (for  $x \in [-1, 1]$ ), for  $Wi = 0.7$ . These solutions were computed using the immersed boundary smooth extension method [95–97], and the results for the coupled cases were compared with benchmarks from the literature [126]. These results show that there is a noticeable steepening of the gradient in the wake of the cylinder, and the maximum of the stress in the wake is increased by the coupling. However, the stress accumulation around the cylinder is much lower in the coupled case. Studying the differences between the coupled and decoupled cases may give us further insight into this challenging numerical benchmark for the Oldroyd B model.



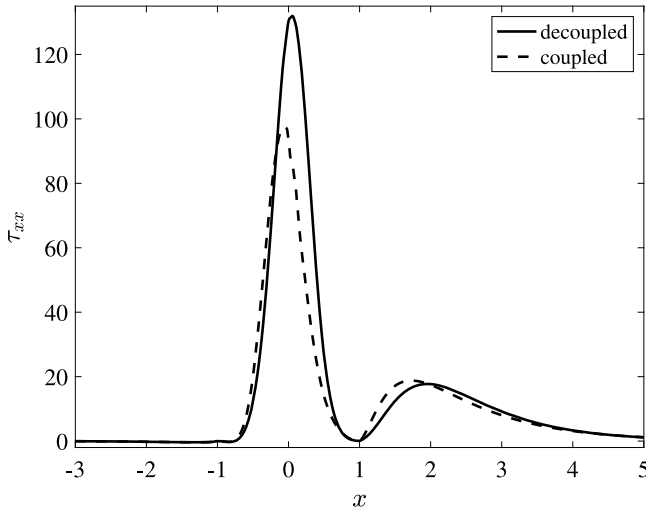


Fig. 3. The  $xx$ -component of the polymer stress tensor  $\tau$  on the centerline of the channel (when  $x \notin [-1, 1]$ ) and along the wall of the cylinder (for  $x \in [-1, 1]$ ), for  $Wi = 0.7$  for both the decoupled and coupled flow. Full domain is truncated for better visualization.

## 10. Microorganism locomotion in viscoelastic fluids

Many micro-organisms and cells move and function in complex materials and specifically in viscoelastic fluids. For example mammalian sperm must navigate through the cervical mucus in the female reproductive tract. Until relatively recently most theoretical studies of micro-scale locomotion have assumed a Newtonian background fluid, ignoring the effects of complex rheology on motion. A further challenge in biological systems is that the swimming gait depends on the physical properties of the surrounding fluid. For example, sperm are known to exhibit different gait characteristics (shape and frequency of the beat pattern) based on the fluid rheology and their activation state which is known to be necessary for fertilization [138–141].

There has been an intense effort over recent years to understand the effect of fluid elasticity on micro-organism swimming [93,142–161]. Experiments, analysis, and simulations of low-Reynolds number swimming of microorganisms in complex fluids, in particular viscoelastic fluids, has led to a variety of results on the effect of fluid elasticity on swimming speed. It has become clear that whether fluid elasticity increases or decreases swimming speed depends on the swimmer's gait. Swimming in viscoelastic fluids using small amplitude gaits has been analyzed [143,145–150,156], but both computational and experimental studies of the biologically relevant large amplitude gaits can show fundamentally different behavior than that predicted by small amplitude analysis [151,154,155,158,159]. In the large amplitude regime

the nonlinearities in the fluid produce elastic stress localization [151, 155,158,159], and the physical mechanism behind the formation of these localized stresses and their resulting impact on swimming remains unknown.

It has been noted that the immersed boundary method presents challenges for numerical simulations of structures moving in viscoelastic fluids, but it still remains one of the simpler ways to simulate large deformations and motions in fluid dynamics simulations. While convergence of the polymeric stress is poor near boundaries, quantifying average swimming speed and stress localization near but not on the boundaries of structures is still possible, though it requires a high level of resolution making computations expensive and especially so in three space dimensions. Some efforts to modify the immersed boundary method for complex fluids have been made by other groups [93,94], but there is still work to be done, and simulating complex fluids with many moving objects or active particles is still quite a challenge.

In recent work [151,159,162–164] the effect of polymer stress concentration near and in the wake of moving objects in both 2D and 3D has been shown to greatly affect the swimming speed and dynamics of motion at the micro-scale. One interesting observation is that oscillatory extensional flows arise near tips of thin filaments moving with undulatory motion in complex fluids [164].

In Fig. 4 we show an example of a “flexor” moving in a 2D simulation with the Stokes Oldroyd B model. In order to study the flows around the tips of undulatory swimmers we consider filaments of length  $L = 1$  oscillating through circular arcs with peak curvature  $A$ . Specifically, the curvature is

$$\kappa(s, t) = A \sin\left(\frac{2\pi}{T}t\right). \quad (32)$$

For  $A = \pi$  the fully bent shape is a semi-circle. By symmetry, this motion does not result in any horizontal translation of the body.

It was observed in [164] that near the tips of such an object the flow is well approximated by an oscillatory extensional flow of the form

$$\mathbf{F} = 2\alpha \sin(\omega t)(x, -y) \quad (33)$$

Here we define the Deborah number  $De = \lambda/T$ , for  $T = 2\pi/\omega$ , and the Weissenberg number as  $Wi = 2\alpha\lambda$ . Analysis of the flow above concludes that there is a *Deborah number* dependent Weissenberg number transition, below which the stress is linear in  $Wi$ , and above which the stress grows exponentially in  $Wi$ . In Fig. 4 the stress concentration near the tips and in the wake of the tips for a large amplitude flexor at  $De = 3$  is shown; this figure shows the stress concentration in the exponential regime.

The strong concentration of elastic stress near tips of flexing objects seen here is likely important when studying how cells and flagella move in real fluids with elasticity such as sperm in cervical mucus. Experiments have shown that changes in fluid rheology are related to important changes in gait, but without careful experiments compared

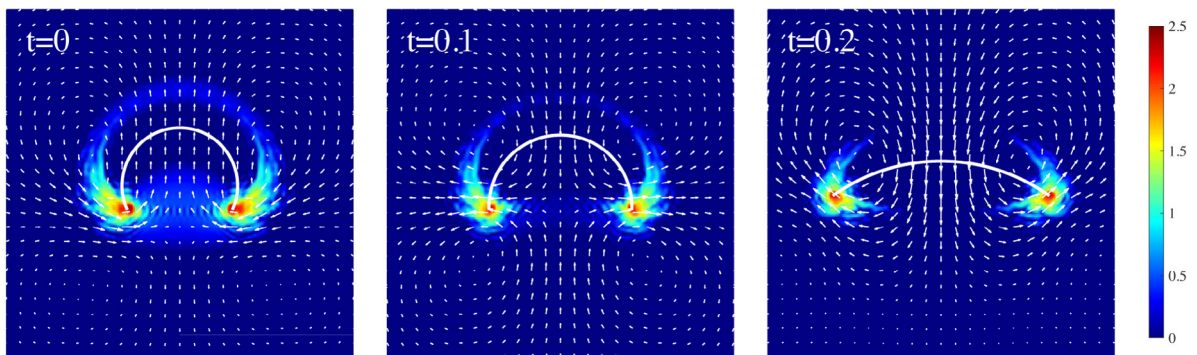


Fig. 4. Flexors at different phases in one period,  $A = 3.5$ ,  $De = 3$ , after the stress has equilibrated to a periodic state. The colors are contours of the trace of the polymer stress, note there is a logarithmic scale.

with simulations it is hard to unlock the complicated nonlinear interaction between gait and fluid changes. Given the highly nonlinear fluid responses seen in recent simulations, it is likely going to be important to resolve fluid effects in biologically relevant fluid rheologies. It is also important to look at the relevant length-scales for resolution, which are likely to require very fine grids. Coupling high resolution simulations with the complicated 3D gaits for realistic cell locomotion and flagellar motion is an important task for researchers to approach. In addition the complex nonlinear coupling between gait changes and fluid changes, and relevant biological modeling questions about internal motor activity in flagella remain to be investigated.

## Conclusions

Over the last four decades, there has been major progress on the mathematical analysis and numerical simulation of viscoelastic flows. We are beginning to understand the complexities arising at high Weissenberg numbers, such as instabilities, singularities and steep stress gradients. There remains significant potential for further work, and this promises to remain an active area for some time to come.

## Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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