IMPLICATIONS OF BOUNDARY SINGULARITIES IN COMPLEX GEOMETRIES

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Summary

Viscoelastic flow problems are singular in Weissenberg number whenever the stress for the corresponding Newtonian flow becomes infinite at a boundary point (a re-entrant corner, for example); this is the apparent reason that the critical Weissenberg number in numerical computation decreases with increasing refinement for sufficiently fine meshes. The explicit form of the singularity for the second order fluid shows that viscoelastic stresses reach physically-unrealistic values over length scales at which the continuum hypothesis remains valid, and non-integrable stresses can result. The present study points to the need for new formulations (constitutive models and/or boundary conditions) for the description of viscoelastic flows near boundary discontinuities.

1. Introduction

The failure of numerical algorithms for viscoelastic liquids to converge in complex geometries beyond a critical Weissenberg number is generally conceded to be an artifact of the discretized equations, but the underlying causes of this failure have not been unambiguously identified. The propagation of numerical errors associated with the computation of large stresses near boundary discontinuities (re-entrant corners, for example) is undoubtedly a major contributing factor. The stresses are known to be singular at such discontinuities, but the nature of the singularity for common viscoelastic models has not been established; thus, it has not been possible to employ specialized techniques that account for the structure of the singularity in seeking solutions at moderate and high Weissenberg numbers.
The stress singularity can be computed explicitly for two-dimensional flows of the second order fluid (SOF); the SOF is the lowest order approximation to viscoelastic fluid flow beyond the Newtonian fluid in Simple Fluid theory. The computation establishes several characteristics that we believe generalize to more widely-applicable constitutive equations and which have far-reaching numerical and physical implications. First, the viscoelastic fluid flow problem is singular in Weissenberg number whenever the stress for a Newtonian fluid becomes infinite at any point on the boundary; that is, for any non-zero Weissenberg number there is a region containing the singular point in which the viscoelastic fluid stress differs from that in a Newtonian fluid by an arbitrarily large amount. It is apparently for this reason that the critical Weissenberg number decreases with increasing mesh refinement for sufficiently fine meshes. (This conclusion can be extended to more complex models such as the Maxwell and Giesekus fluids through a perturbation analysis, although the exact singularity cannot be computed for the latter liquids.) Second, in contrast to the Newtonian liquid, the stresses in the SOF reach physically unrealistic values over length scales at which the continuum hypothesis remains valid, and they can be non-integrable (i.e., lead to infinite forces); numerical experiments indicate that this latter result may be applicable to more complex models. We believe that there is a need for new formulations of constitutive models and/or boundary conditions for the description of viscoelastic flow near a boundary discontinuity.

2. Second order fluid

2.1 Singularity

The second order fluid is given in dimensionless form as

\[ \tau_{\text{SOF}} = 2D + We \left( v \cdot \nabla D + D \cdot \nabla v + \nabla v^\top \cdot D + \left( \alpha_2/\alpha_1 \right) D^2 \right), \tag{1} \]

where \( \tau \) is the extra-stress and \( 2D = \nabla v + \nabla v^\top \). This equation approximates all Simple Fluids in the limit of slow flows (small Weissenberg number \( We \)). It is thus a convenient vehicle for gaining insight into viscoelastic flow in complex geometries as long as appropriate care is taken to avoid generalizations to situations where the SOF is not a valid approximation (c.f. the discussion below) This is particularly so as a consequence of theorems by Giesekus [1], Tanner [2], and Huilgol [3]. The Giesekus–Tanner theorem applies to the two-dimensional creeping planar flow of Newtonian and second order fluids that are subject to the same specified boundary conditions in terms of velocity and velocity gradients, establishing that the
Newtonian velocity field \( v_N \) is also a solution to the SOF equations, with the (dimensionless) extra-stress and pressure for the latter given by

\[
\tau_{\text{SOF}} = 2D_N + We\left[v_N \cdot \nabla D_N + D_N \cdot \nabla v_N + \nabla v_N^\top \cdot D_N + \left(\frac{\alpha_2}{\alpha_1}\right) D_N^2\right],
\]

\[
p_{\text{SOF}} = p_N + We\left[v \cdot \nabla p_N + \left(\frac{\alpha_2}{2\alpha_1} + \frac{3}{4}\right) \text{tr} D_N^2\right],
\]

where \( 2D_N = \nabla v_N + \nabla v_N^\top \), and \( p_N \) is the Newtonian pressure field corresponding to \( v_N \).

Hulgoł's theorem establishes that the velocity field \( v_N \) is the unique solution to the second order fluid equations in domains \( \Omega \) satisfying the boundary constraint

\[
\int_{\partial \Omega} \left(\nabla^4 \varphi\right)^2 v \cdot n \; ds \leq 0
\]

\( \varphi \) is the stream function; \( n \) is the outward-pointing normal on the domain boundary \( \partial \Omega \). Boundary elements where the velocity vanishes or is parallel to the boundary do not contribute to the integral in eqn. (4), nor do boundaries crossed by a fully-developed rectilinear flow (for which \( \nabla^4 \varphi = 0 \)).

The general result that we shall subsequently develop in detail for two specific flows now becomes transparent. Consider a flow satisfying the Giesekus–Tanner and Hulgoł theorems in which the Newtonian stress field exhibits a singularity at a boundary discontinuity; i.e.,

\[
\tau_N = 2D_N \sim r^{-n},
\]

where \( r \) is a dimensionless distance from the boundary discontinuity and \( n > 0 \). Flow through a plane contraction and extrusion from a plane slit are such flows. It then follows immediately from eqn. (2) that

\[
\| \tau_{\text{SOF}} - \tau_N \| \sim We \: r^{-2n}.
\]

Equation (6) establishes the important result that the limit \( We \to 0 \) (the Newtonian fluid) is singular; i.e. there always exists some region \( r \ll We^{1/2n} \) of the boundary discontinuity such that the stress fields differ by an arbitrarily large amount.

We believe that the numerical implications of eqn. (6) are far reaching. First, numerical resolution on a length scale of order \( We^{1/2n} \) will of necessity lead to stresses that are so large as to cause uncontrollable discretization error. For a given Weissenberg number there is therefore a limit to the spatial resolution obtainable before degeneration of the numerical solution. For a given spatial resolution, characterized by a scale \( r_0 \) in the neighborhood of the boundary discontinuity, we speculate that there is a critical Weissenberg number

\[
We_c \sim r_0^{2n}
\]
beyond which the numerical solution must degenerate because of the numerical inability to resolve arbitrarily large stress gradients. \( \text{We}_c \) decreases with increased spatial resolution.

The singular nature of the limit \( \text{We} \to 0 \) constitutes a second difficulty, for it means that the exact viscoelastic solution close to the boundary singularity cannot be obtained by a continuation scheme starting from the Newtonian solution. Current numerical methods for solving viscoelastic flows always lead to discrete problems that are regular in \( \text{We} \), however, because none of the current techniques implements the exact form (6) of the singularity [4]. The continuation process is thus possible at the discrete level, despite the properties of the continuous system, until a critical value of \( \text{We} \) at which the discrete Jacobian matrix becomes singular (a turning point; see, e.g., [5]). We again expect that the critical value \( \text{We}_c \) will decrease with increased spatial refinement near the singularity, since the improved refinement will allow the numerical solution to mimic the singular nature of the exact solution more accurately.

We shall return to the computational and physical implications following discussion of two specific flows for which the explicit form of the SOF singularity can be obtained.

2.2 Contraction flow

Consider flow through a planar contraction, as shown in Fig. 1. This flow field has generally been employed as a test of numerical algorithms for viscoelastic liquids (c.f. [4]). The flow is taken to be fully-developed plane Poiseuille flow at the up- and downstream boundaries, in which case the Huilgol theorem establishes the Newtonian fluid velocity field as the unique solution for the flow of the second order fluid.

Flow of a Newtonian fluid near the re-entrant corner (shown as the origin of the coordinate system in Fig. 1) has been analyzed by Moffatt [6], who

![Fig. 1 Schematic of flow in a planar contraction](image)
Fig 2. Schematic of stick-slip flow

gives the stream function as an eigenfunction expansion having a dominant term
\[ \phi_N = r^\lambda \left[ \cos \frac{3\pi}{4} (\lambda - 2) \cos \lambda \theta - \cos \frac{3\pi \lambda}{4} \cos (\lambda - 2) \theta \right], \tag{8} \]
where \( \lambda = 1.5445 \). We then have \( n = 0.4555 \); the shear stress for the SOF is given, for example, as
\[ \tau_{r\theta} = r^{-0.4555} f_1(\theta) + We r^{-0.9110} f_2(\theta). \tag{9} \]
The functions \( f_1(\theta) \) and \( f_2(\theta) \) are given in the Appendix. The critical Weissenberg number would then be expected to decrease with mesh spacing as \( r_0^{-0.9110} \), where \( r_0 \) is characteristic of the spatial resolution near the reentrant corner.

2.3 Stick-slip flow

Stick-slip flow, shown schematically in Fig. 2, has been used as an analog of extrusion from a slit die. The no-slip boundary condition is applied up to \( x = 0 \), after which the boundary condition is changed to zero shear stress and zero normal velocity. The extrudate width is maintained constant, however. If the upstream boundary condition in a plane stick-slip flow is taken to be plane Poiseuille flow, and the downstream velocity is taken to be uniform in the flow direction, then the Hulugol theorem is satisfied and the Newtonian velocity \( u_N \) is the unique SOF solution. (Coleman [7] has already noted that \( u_N \) is a possible solution for the SOF in this flow.)

Richardson [8], following Moffatt [6], has shown that the leading term in the stream function for a Newtonian fluid near the boundary discontinuity is
\[ \phi_N = r^{1.5} \sin \frac{\theta}{2} \sin \theta. \tag{10} \]
It then follows that
\[ \tau_{r\theta} = r^{-0.5} f_1(\theta) + We r^{-1.0} f_2(\theta), \tag{11} \]
where \( f_1(\theta) \) and \( f_2(\theta) \) are given in the Appendix. (The \( r^{-1} \) term does not arise in the stress normal to the boundary.) This stress is non-integrable for any \( We > 0 \), leading to infinite forces parallel to the surface. The problem of numerical resolution is thus particularly severe, since the exact integrated force is infinite over any finite region containing the boundary discontinuity.

### 2.4 Physical boundary conditions

The singular nature of the SOF near a boundary discontinuity raises significant physical questions that are independent of the numerics. Non-integrable stresses are physically inadmissible; indeed, stresses greater than some value corresponding to the strength of the continuum (typically of order \( 10^9 \) Pa) are inadmissible. Inadmissibly large stresses are reached in a Newtonian liquid only over length scales where the continuum hypothesis is itself inapplicable, and the effects of (integrable) stress singularities do not propagate into the bulk. In contrast, because of the \( We r^{-2n} \) dependence, the integrable stress singularity for a SOF propagates over a length scale that is physically meaningful in the context of continuum theory.

We illustrate this point with a physical example, to which we shall return subsequently. We consider a fluid with the physical properties of a linear low density polyethylene at \( 215^\circ C \) and a shear rate of \( 300 \) s\(^{-1} \) in a 2 mm channel, with viscosity \( \eta \sim 10^3 \) Pa s and relaxation time \( \lambda = (\alpha_2/\alpha_2) \sim 1 \) s. These are approximately the conditions under which extrudate distortions are first observed [9,10]. The dimensional stress in a Newtonian fluid near the point of departure from a slit die, using the stick-slip approximation, is of order \( \eta Q/\sqrt{rw^3} \), where \( Q \) is the flow rate per unit of channel width, \( w \) is the half-thickness, and \( r \) is the distance from the singularity. The corresponding dimensional SOF stress, calculated from the second term in eqn (11), is of order \( \lambda \eta Q^2/rw^3 \) Hence, a shear stress of \( 10^8 \) Pa, which is somewhat greater than the stress at which failure is typically observed at a polymer-solid interface, will penetrate a distance of order several Ångstroms from the singularity into a Newtonian liquid, the continuum hypothesis is clearly inapplicable over this length scale. The penetration length in the second order fluid, on the other hand, is of the order of one-fourth \( w \). The corresponding distances for a stress of \( 10^9 \) Pa, which is of the order of the ultimate strength of the material, are much less than 1 Å for the Newtonian fluid and 100 \( \mu m \) for the SOF.

### 3. Simple fluids

#### 3.1 Singular perturbation

The SOF is not a valid approximation to a Simple Fluid in regions in which the fluid elements experience large accelerations, and such could be
the case close to boundary points at which a stress singularity exists for a Newtonian fluid. The question thus arises as to which of the conclusions from the preceding analysis for the SOF are applicable to more complex viscoelastic models.

For the sake of illustration, consider the Giesekus model [11] in dimensionless form,

\[ [I + \alpha \text{We} \tau] \cdot \tau + \text{We} [v \cdot \nabla \tau - \tau \cdot \nabla v - \nabla v^\tau \cdot \tau] = 2D, \]

(12)

where \( \alpha \) is Giesekus' mobility parameter. The upper-convected Maxwell model is obtained when \( \alpha = 0 \). The kinematics in the neighborhood of the singularity are not known \textit{a priori} for this fluid model, hence, determination of an explicit form of the stress singularity would be a formidable task, requiring the solution of the full nonlinear set of constitutive and conservation equations. A perturbation solution suffices, however, to establish that the flow of a Giesekus fluid also constitutes a singular perturbation in \( \text{We} \) in the presence of a boundary singularity.

For small \( \text{We} \), we seek a solution for the stress in the form

\[ \tau = \tau_0 + \text{We} \tau_1 + \text{We}^2 \tau_2 + \ldots \]

(13)

Similar expansions are defined for the velocity and pressure fields. Substitution of these expressions into the governing equations reveals immediately that the zeroth-order term is the Newtonian solution, while the first-order truncation obeys the SOF model. (This result follows directly from the fact that a perturbation in \( \text{We} \) is equivalent to a slow flow expansion, but we believe that the explicit demonstration is useful.) The series (13) is expected to converge, of course, only for sufficiently smooth deformation histories. Close to a boundary point at which the Newtonian singularity goes like \( r^{-n} \), we obtain

\[ \tau = O(r^{-n}) + \text{We} O(r^{-2n}) + \ldots \]

(14)

As for the case of the SOF, the limit \( \text{We} \to 0 \) is singular, since the Newtonian solution is not uniformly valid as \( r \to 0 \).

An alternative way to arrive at the same conclusion is simply to substitute the Newtonian velocity and stress fields into the Giesekus model (12). One then obtains

\[ O(r^{-n}) + \text{We} O(r^{-2n}) = O(r^{-n}) \]

(15)

It is always possible to find a value \( r_0 \) for any small but non-zero \( \text{We} \) such that eqn (15) cannot be satisfied in the region \( 0 \leq r \leq r_0 \). As with the SOF, we believe that the singular perturbation nature of the solution for a Giesekus fluid implies that the critical Weissenberg number must decrease with increasing spatial resolution near the singularity. This conclusion is
consistent with the numerical findings of Keunings [5], but it must always be recalled that the form of the singularity for the Giesekus fluid remains unknown.

3.2 Numerical observations

Keunings [5] has described calculations for planar entry flow of a Maxwell fluid using a series of finite-element meshes of increasing resolution. For the finest mesh, comprising 40,974 degrees of freedom, the critical Weissenberg number was 0.108. This is within a range where one might normally expect the SOF to provide a reasonable approximation to the Maxwell fluid, except perhaps near the singular corner. The computed normalized stress difference \( (\tau_{yy} - \tau_{yy,N})/We \) is shown in Figs. 3(a) and 3(b) as a function of dimensionless distance from the corner.

![Normalized stress difference](image)

**Fig. 3** Normalized stress difference \( (\tau_{yy} - \tau_{yy,N})/We \) at \( \theta = \pi/4 \) for a Maxwell fluid in a plane contraction (a) \( We = 0.03 \), (b) \( We = 0.06 \)
Fig 4 Normalized velocity difference \((v_y - v_{y,N})/We\) at \(\theta = \pi/4\) for a Maxwell fluid in a plane contraction (a) \(We = 0.03\), (b) \(We = 0.06\)

Dimensionless distance \(r\) at \(\theta = \pi/4\) for \(We = 0.03\) and 0.06, respectively. The sharp break at \(r = 5 \times 10^{-3}\) occurs at the edge of the first element. The computed normalized velocity difference, \((v_y - v_{y,N})/We\), is shown in Figs. 4(a) and (b), respectively, for the same values of \(We\).

Two points are apparent in Figs. 3 and 4. First, except in the element adjacent to the corner, the asymptotic \(r^{-0.911}\) stress dependence predicted by the SOF is followed, and the velocity is nearly that of the Newtonian fluid. Second, the stress dependence is linear in \(We\), in accordance with the expected behavior of the SOF. Thus, the SOF is representative of the Maxwell fluid at the level of the discrete numerical equations for this flow and at these Weissenberg numbers. The averaging effect of the first element
on the numerical solution is evident here; indeed, while the continuous problem is singular in $W_e$, the "smearing" inherent in the discretization regularizes the numerical problem.

In anticipation of the subsequent discussion of constitutive equations and boundary conditions, we describe here a further set of calculations. We have repeated the calculations in Figs. 3 and 4 using the finest resolution (40,974 degrees of freedom) with a single change; the relaxation time was set to zero in the element incorporating the re-entrant corner, thus controlling the magnitude of the singularity. The results outside the corner element were indistinguishable from those shown in Figs. 3 and 4; now, however, the critical Weissenberg number was increased to 0.6. It is clear, therefore, that the bulk flow is insensitive to the details of the stress right at the corner, but that the degeneration of the solution is directly related to the propagation of numerical error emanating from the large stresses at the corner. (The stress singularity in this latter calculation is that of a Newtonian fluid, and the use of singular elements implementing the Newtonian stress singularity near the re-entrant corner could resolve these numerical difficulties.)

4. Conclusions and speculations

We have established that second order fluid theory leads to unphysical (and sometimes non-integrable) stresses in a macroscopic neighborhood of a boundary discontinuity where the Newtonian solution is singular, and that the limit $W_e \to 0$ is singular at the discontinuity. Furthermore, the latter result has been shown to be true for the Giesekus fluid and all special cases, including the Maxwell fluid, and it appears to hold in fact for any viscoelastic fluid within Simple Fluid theory. The numerical implications are, we believe, far reaching. Our results suggest that for sufficiently fine discretization the critical Weissenberg number must decrease with increased resolution, consistent with the numerical evidence in [5]. As a result, we cannot expect current numerical techniques to provide high Weissenberg number solutions that can be checked by mesh refinement when a boundary discontinuity is present. (This situation must be contrasted with flow problems that admit smooth velocity and stress fields, for which successful and reliable simulations have been described; e.g., Beris [12], Keunings and coworkers [13–15].)

We believe that the underlying difficulty is physical, and lies with existing descriptions of viscoelastic flow that are inadequate to describe the true physical behavior near a boundary discontinuity. We cannot establish this belief as fact, because the exact form of the singularity is unknown for any but the SOF; we do feel, however, that such speculation is warranted on the basis of the observations made in this paper. The numerical experiments
show that there is a region away from the singularity \((r > r_0)\), but still close to the corner in physical dimensions, where the stresses in a Maxwell fluid at low \(We\) grow at the same rate as in the SOF. The Maxwell fluid is a consistent constitutive equation for "fast" flows, and at least qualitatively approximates the rheological behavior of real polymer melts. The unphysical stresses computed for the SOF for parameters characteristic of LLDPE (though at much higher \(We\)) are then plausible for the Maxwell fluid as well.

There appear to be two ways within the context of continuum theory in which unphysical stresses can be avoided in flows with boundary discontinuities. One is by relaxing the no-slip condition at the boundary. (The need to relax the no-slip condition near a moving contact line in order to avoid non-integrable stresses is a well-known result in Newtonian fluid mechanics [16].) Indeed, such a relaxation is likely to be consistent with the real physical behavior near a region of high stress; recent observations of extrudate flow by Ramamurthy [9] and Kalika and Denn [10], following many earlier observations (cf. [17,18]), suggest wall slip, for example. Lau and Schowalter [18] have correlated existing data with a powerlaw modification of the Navier boundary condition (slip velocity proportional to wall stress), and Kalika and Denn [10] have shown that the onset of melt fracture in linear low density polyethylene occurs at a value predicted by a stability analysis of Pearson and Petrie [19] based on a Navier boundary condition. A Navier boundary condition is difficult to implement in a numerical algorithm near a corner, since it seems that no-slip must be imposed at the corner point to avoid flow through the boundary walls.

The second possible change in the physical description is to employ a constitutive model in which structure breakdown at high stresses is so severe that the viscoelastic contribution vanishes in the neighborhood of the singularity. In network models of the type discussed by Acerno and coworkers [20] and Mewis and Denn [21], this would require that the structural parameter go to zero at a finite stress; the current formulation of such models has the structural parameter approach zero asymptotically with increasing stress. The numerical experiment described above for the Maxwell fluid, in which the relaxation time was set to zero in the corner element, can be viewed as an ad-hoc (and mesh dependent) way of implementing a constitutive equation with complete structure breakdown. Such a structural breakdown is unlikely to be distinguishable experimentally from slip.

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Appendix

The stream function in eqns. (8) and (10) is of the form $r^\lambda f(\theta)$. The functions $f_1(\theta)$ and $f_2(\theta)$ are defined as follows:

$$f_1(\theta) = -\frac{1}{2}[\lambda(2-\lambda)f + f''],
$$

$$f_2(\theta) = \frac{1}{2}[\lambda(2-\lambda)f + f''] + \lambda f \left[ \frac{\lambda^2}{2} (3\lambda + 2) f' - \frac{1}{2} f'' \right]$$

$$+ (2-\lambda)f' (\lambda^2 f + f'').$$

The prime denotes differentiation with respect to $\theta$. 