## Title
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ABSTRACT

We address the outstanding problem affecting the numerical simulation of viscoelastic flows, namely the existence of a critical value of the elastic parameter beyond which no discrete solution can be obtained. An extensive mesh refinement analysis conducted on a CRAY X-MP supercomputer indicates that limit points observed in the discrete solutions have a numerical origin.

## 1. INTRODUCTION

During the last ten years, a number of research groups have undertaken the development of computational methods for solving complex flows of highly elastic fluids. Viscoelastic flows cannot be described by simple extension of the Navier-Stokes equations in cases where memory effects play a significant role. Although inertia terms are negligible in most applications, the equations governing the flow of a viscoelastic fluid are highly non-linear in view of the functional relationship between the stress experienced by the material and the history of its deformation. Most of the work thus far has been concerned with steady flows (but see [1] and [2]), and relatively simple constitutive models have been used. Although a few successful predictions have been reported in the literature, an outstanding problem affects current numerical simulations. Whatever be the flow problem under investigation, the discretization and iterative schemes used to solve it, and the constitutive model selected to describe the rheology of the material, one observes that the iterative scheme fails to converge beyond some critical value of the **Weissenberg number**, a dimensionless group that determines the elastic character of the flow. This critical value is (problem, method, model) dependent. An unfortunate selection of this "operating triplet" can lead to poor results, while a better one, based on some theoretical considerations and/or numerical experiments, can lead to numerical predictions of observed phenomena (see e.g., [3] and [4]). At any rate, a sound understanding of the origin of the so-called "high Weissenberg number problem" is lacking. Comprehensive reviews are presented in [5] and [6].

A number of possible reasons for the breakdown of viscoelastic computations have been proposed recently (see [7] for a critical evaluation of these conjectures). Recent work has clearly identified the occurrence of limit points in the **discrete** solution of an upper-convected Maxwell fluid, the simplest model for a polymer melt (see [8] and [9]). The crucial question as to whether these limit points are numerical artifacts or intrinsic features of the **continuous** solution, however, has not been unequivocally answered in view of the enormous computer resources involved and the intricacy of the mathematical problem. Our goal in the present paper is to address this question. We present new results for the steady two-dimensional flow of a Maxwell fluid through a planar contraction. Contraction flows have been standard test problems for those actively engaged both in numerical and experimental work with viscoelastic materials. The presence of a singularity at the re-entrant corner makes the problem very challenging for flow simulators. The nature of the singularity is only known for Newtonian fluids. We have conducted a systematic mesh refinement analysis leading to numbers of nodal unknowns that are significantly larger than in any previous investigation. The numerical technique used here is a mixed Galerkin/Finite Element method referred to as algorithm MIX1 in our previous publications (see e.g., [10]), implemented for this particular study on a CRAY X-MP supercomputer. The results lead us to conclude that limit points observed at the discrete level **are not** intrinsic properties of the continuous problem, but rather have a numerical origin. A numerical experiment indicates that the present Galerkin formulation is unable to produce a stable discretization of the non-self-adjoint operators that characterize viscoelastic equations. We refer the reader to [7] for an extension of this work to alternative constitutive models and problems devoid of singularities.

## 2. FORMULATION AND NUMERICAL METHOD

The equations governing the steady isothermal flow of an upper-convected Maxwell (UCM) fluid are

$$-\nabla p + \nabla\cdot\underline{T} = \underset{\sim}{0} \;, \qquad (1)$$

$$\nabla\cdot\underset{\sim}{v} = 0 \;, \qquad (2)$$

$$\underline{T} + \lambda\ [\underset{\sim}{v}\cdot\nabla\underline{T} - (\nabla\underset{\sim}{v})^T\cdot\underline{T} - \underline{T}\cdot(\nabla\underset{\sim}{v})] = \mu[\nabla\underset{\sim}{v}+\nabla\underset{\sim}{v}^T] , \qquad (3)$$

where p is the indeterminate pressure, $\underline{T}$ is the extra-stress tensor and $\underset{\sim}{v}$ is the velocity vector. The constitutive model (3) contains two material parameters: a relaxation time $\lambda$, and a shear viscosity $\mu$. We have neglected convective terms as well as body forces in the momentum equations (1), and have assumed that the fluid is incompressible.

In the present paper, we consider the flow of a UCM fluid through a 4:1 planar contraction. With the aforementioned assumptions, a single dimensionless group appears in the analysis, namely the Weissenberg number We, defined as

$$We = \lambda \frac{V}{H} , \qquad (4)$$

where V and H denote the average velocity and half-thickness of the downstream slit, respectively. The Newtonian solution (Stokes flow) corresponds to We = 0. The boundary conditions are: i) fully developed velocity and extra-stress fields at the entry section, ii) no-slip at the wall, iii) fully developed velocity field at the exit section, and iv) symmetry conditions at the plane of symmetry.

The numerical method is a mixed Galerkin/Finite Element technique where the unknown fields $\underline{T}$ and $\underset{\sim}{v}$ are interpolated by second-order polynomials, while the pressure p is given by first-order polynomials. Both approximated fields are of class $C^o$. This technique is referred to as method MIX1 in [10], and is detailed in [6]. Its extension to more complex constitutive equations is presented in references [3], [4] and [11].

The discretized version of equations (1-3) constitutes a set of non-linear algebraic equations depending on the parameter We; it has the form

$$\underset{\sim}{F}\ (\underset{\sim}{X}\ ;\ We) = \underset{\sim}{0} , \qquad (5)$$

where $\underset{\sim}{X}$ is the vector of nodal values of $\underline{T}$, $\underset{\sim}{v}$ and p. We solve (5) by Newton's method combined with a first-order continuation scheme to obtain initial guesses as the Weissenberg number is incremented. The presence of limit or bifurcation points in the solution family of (5) is indicated by a change in sign of the determinant of the Jacobian matrix $\partial\underset{\sim}{F}/\partial\underset{\sim}{X}$ when such a point is encountered. First-order continuation allows one to pass a bifurcation point along the original branch; it is, of course, useless at a limit point, where a special scheme is needed to compute the return solution (see e.g., [8]).

A partial view of the three finite element meshes used in this work is shown in Fig. 1.

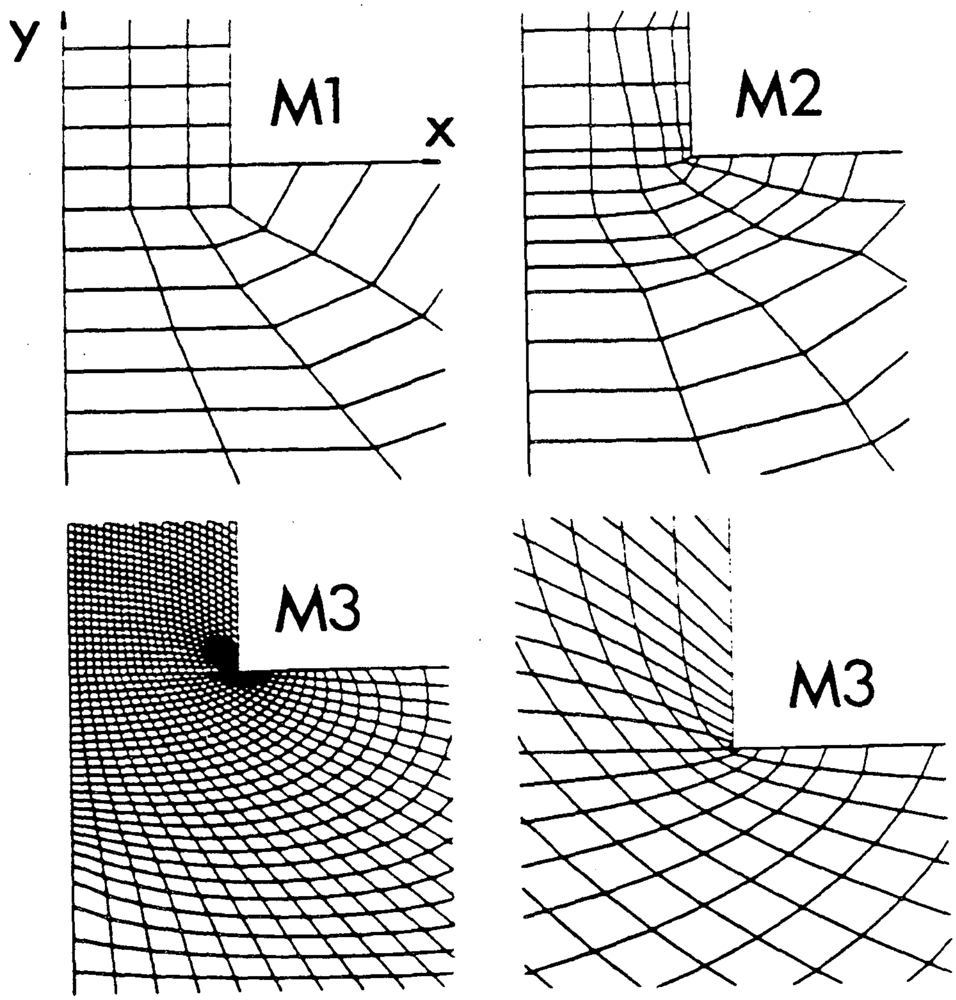


Fig. 1. Partial view of the three finite element meshes and magnification of M3 near the re-entrant corner.

Meshes M1 and M2 were used in [4] for the study of entry flows of a Phan-Thien-Tanner fluid. Mesh M3 is highly refined in the neighborhood of the re-entrant corner; we have exercised much care in the design of M3 so as to avoid sudden steps in element size as well as unfavorable element aspect ratios. Table 1 gives some characteristic dimensions for these grids. It is seen that M3 is an order of magnitude finer than M2, both in terms of number of degrees of freedom and size of the elements placed at the corner.

| | Nodes | Elements | Degrees of freedom | Size of corner elements |
|---|---|---|---|---|
| M1 | 594 | 130 | 3139 | 0.25 |
| M2 | 577 | 129 | 3046 | 0.05 |
| M3 | 7794 | 1912 | 40974 | 0.005 |

Table 1. Characteristic dimensions of the three finite element meshes.

The computations have been conducted on an IBM 3081/K, which is a scalar machine, and a CRAY X-MP, which is a vector supercomputer. To give the reader a feeling for the amount of computing resources needed here, we present in Table 2 the CPU cost for a single non-linear iteration on equation (5).

| | IBM 3081/K | CRAY X-MP | IBM/CRAY |
|---|---|---|---|
| M1 | 30 | 3.7 | 8 |
| M2 | 39 | 3.8 | 10 |
| M3 | 5040 | 167 | 30 |

Table 2. CPU time (in seconds) for a single non-linear iteration, and speed ratio between IBM and CRAY.

The third column of this table indicates the speed ratio between the scalar and vector machines. This ratio is not a constant, since it is related to the degree of vectorization achieved with any given grid. Needless to say, all simulations involving M3 were conducted with the CRAY, aside from the single iteration performed to provide the information in Table 2. We mention finally that the enormous size of M3 calls for special i/o procedures during the frontal elimination process. We have developed a "buffered" i/o routine which optimizes the amount of disk access. In so doing, the time spent in writing (reading) the triangulated Jacobian matrix to (from) disk is reduced to 30 seconds per iteration, which is quite acceptable for the transfer of about 96 Megabytes of data.

## 3. RESULTS

With each of the three finite element meshes, solutions of the discrete set (5) have been obtained up to a critical value $\overline{We}$ beyond which the iterative scheme failed to converge, whatever be the magnitude of increments of We in the continuation procedure. This fact, together with the associated singularity of the Jacobian matrix at $\overline{We}$, indicates a limit point of the discrete set (5). We find, however, that i) the location of the limit point is highly mesh-dependent, ii) the quality of the discrete solution degenerates dramatically before the limit point is reached.

Table 3 gives the values of $\overline{We}$ for the three grids. They correlate with the degree of refinement near the re-entrant corner.

| | M1 | M2 | M3 |
|---|---|---|---|
| $\overline{We}$ | 0.87 | 0.56 | 0.11 |

Table 3. Location of the limit point as a function of the mesh.

We observe that $\overline{We}$ decreases when the degree of refinement increases; it attains a very frustrating value of 0.11 with the highly refined grid M3. Solutions for We sufficiently smaller than $\overline{We}$ are smooth and will not be shown here. When We is incremented towards $\overline{We}$, however, spurious oscillations appear in the stress and velocity fields. Fig. 2 shows velocity and extra-stress contour lines obtained with M3 at the limit point. The Newtonian (mixed) solution is also shown for the sake of comparison. Although the velocity is devoid of large-amplitude oscillations at We = 0.11, the extra-stress field is highly oscillating downstream of the re-entrant corner. The numerical values of $T_{yy}$ in the corner elements are two orders of magnitude larger than those plotted in Fig. 2. The Galerkin technique fails to accurately resolve such large stress gradients. It is known that the combination $[\underline{T}+\mu\underline{I}/\lambda]$ must be definite-positive in the interior of the flow domain (see e.g., [12]). We have observed in the present study that the discrete solution loses this property at a few nodes in the corner elements. The loss of the definite-positive property **precedes** the occurrence of the limit point (it occurs at We = 0.05 with M3, for example).

From what we have presented above, it is clear that the loss of convergence of the iterative scheme is associated with the breakdown of the discretization scheme. A possible cause is the failure of the Galerkin method to produce stable approximations of the non-self-adjoint operators that characterize viscoelastic constitutive equations. This can be tested by solving the constitutive equation (3) alone, for a given well behaved velocity field. The reduced problem becomes linear in $\underline{T}$ and can thus be solved for any value of We. The velocity field chosen here is the finite-element Newtonian (u-v-p) solution for the flow in the contraction. The constitutive equation (3) is solved by the Galerkin method with the same basis functions used in the coupled problem (1-3).

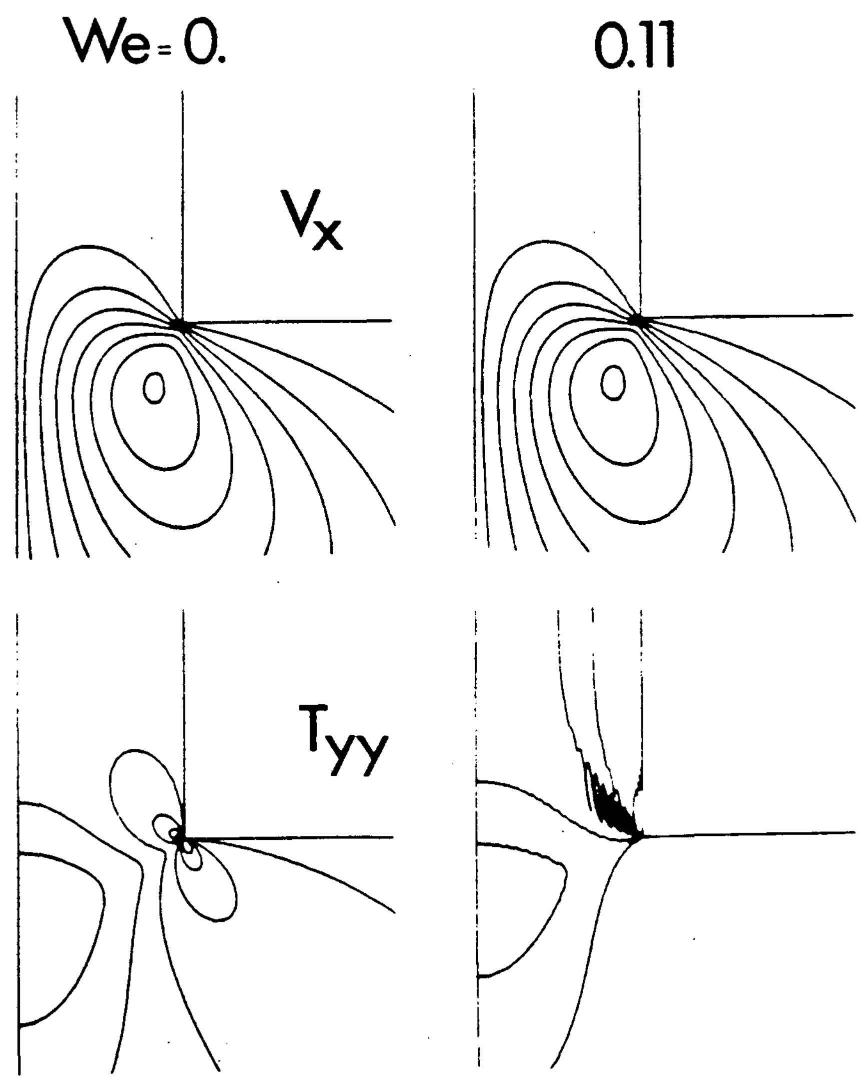


Fig. 2. Contour lines of the velocity $v_x$ and the extra-stress $T_{yy}$; We = 0. and 0.11; M3.

Fig. 3 shows extra-stress contour lines obtained with M3 for We = 0.03, 0.11 (the limit point of the coupled problem) and 1. As in the coupled problem, results for low We are quite smooth, but they degenerate when We increases. At We = 0.11, contour lines of the extra-stress $T_{yy}$ calculated on the basis of the Newtonian velocity field are indeed very similar

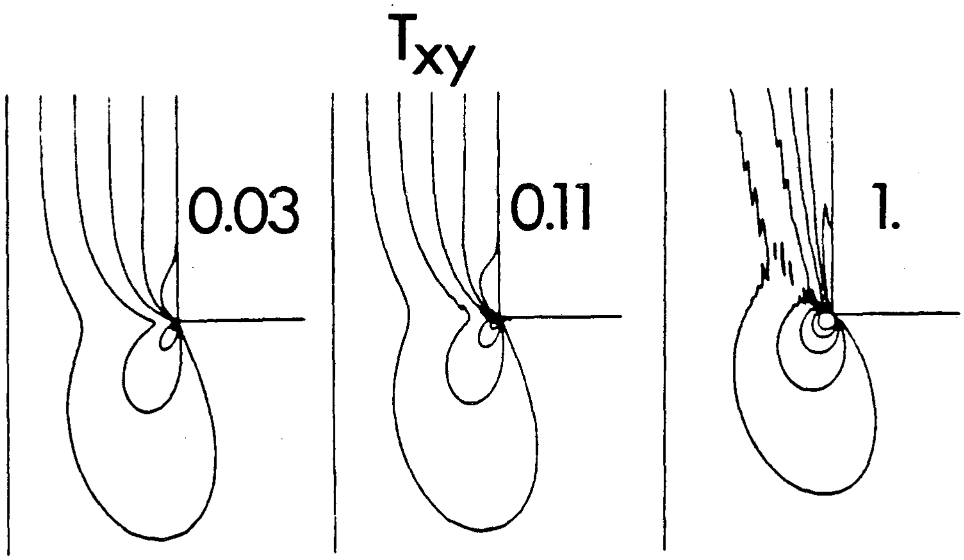


Fig. 3. Contour lines of the shear stress $T_{xy}$; We = 0.03, 0.11 and 1.; calculations based on the Newtonian velocity field; M3.

to those of the coupled problem (Fig. 2). The solution for We = 1. is extremely poor; it exhibits a loss of the positive-definite character of $[\underline{T}+\mu\underline{I}/\lambda]$ far away from the corner and inside the flow domain. Similar observations have been made with M1 and M2.

## 4. CONCLUSIONS

The main observations of this **particular** study can be summarized as follows:

A. The loss of convergence of the iterative scheme is due to the presence of a limit point of the discrete solution,

B. The location of the limit point is highly mesh-dependent,

C. The quality of the discrete solution degenerates when the Weissenberg number is increased up to the critical value,

D. The critical value of the Weissenberg number monotonically decreases when the mesh is refined; in other words, intensive mesh refinement is not the solution to the high Weissenberg number problem.

These observations lead us to conclude that **limit points observed at the discrete level are not intrinsic properties of the continuous problem, but rather are the consequence of discretization errors.** Our conclusion is based on a very intensive mesh refinement analysis of a single flow problem, using a single discretization procedure and a single constitutive model. We show in [7], however, that statements A, B, and C appear to hold quite generally with **currently available numerical methods.** Statement D is fortunately not as general; we show in [7] that it has to be amended when the flow problem does not contain a singularity or when the constitutive equations allow for shear thinning effects.

Finally, our numerical experiments on the solution of the Maxwell constitutive equations alone indicate the failure of the Galerkin principle to produce a stable approximation of a non-self-adjoint operator in regions of high solution gradients. The recent development of consistent Petrov/Galerkin formulations for first-order hyperbolic systems ([13], [14]) should provide useful guidelines in the search for improved numerical techniques for viscoelastic flows.

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