## A NEW COUPLED METHOD FOR VISCOELASTIC FLOW SIMULATION

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## ABSTRACT

A new coupled method for finite element viscoelastic flow simulation is presented. Although the method is not free of instabilities, it allows high Weissenberg number flows to be modeled with a simpler mixed element than that of Marchal and Crochet. Numerical results for the planar four-to-one contraction are included that illustrate the good performance of our scheme.

## 1. INTRODUCTION

This work is based upon the fundamental contributions made by M.J.Crochet and J.M.Marchal [10,11] to the finite element modeling of viscoelastic flow (see also [6]. To say it in just a few words, MJC and JMM proposed that a numerical method for viscoelastic fluids should work if:

(i) The three-fields (stress-velocity-pressure) discrete formulation is stable in the zero-elasticity limit.

(ii) A streamline diffusivity (SU) proportional to the local mesh size is added to the equations expressing extra-stress transport.

(iii) The resulting non-linear system is solved using fully-coupled techniques, such as Newton-Raphson schemes.

As a result of these ideas, in [11] they propose a new method involving a non-standard mixed element which interpolates velocity components biquadratically, pressure bilinearly, and extra-stress components bilinearly on a  $4 \times 4$  subdivision of each element. This element was later proved convergent in the zero-elasticity case by M.Fortin and R.Pierre [8].

*Remark:* In what concerns condition (i), replacing the extra-stress approximation of the JMM-MJC element by simply  $Q_3$  would still yield a convergent scheme [8]. However, the piecewise bilinear approximation seems to match particularly well the SU upwinding.

To our knowledge, the method of Marchal and Crochet remains as one of the very few that do not exhibit the so-called *High Weissenberg Number Problem (HWNP)*, i.e., lack of convergence of the nonlinear algorithm at a moderate amount of fluid elasticity.

In a previous paper [1], we have shown that the decoupled method of M.Fortin and A.Fortin [7] with low-order interpolation could be an alternative, as we reached a *Deborah number* of 18 in the 4-to-1 contraction problem. However, a decoupled approach needs far more nonlinear iteration than a coupled one, so that as far as differential constitutive laws are considered the latter should be prefered. Also, coupled methods seem to be more robust in what concerns the *HWNP*.

In this paper, we present a new coupled method for viscoelastic flow simulation, involving much simpler elements than that of Marchal and Crochet. The underlying ideas have not changed, we try to fulfill (i)-(iii) above, but discontinuous interpolation of the pressure allows us to use more standard extra-stress spaces.

## 2. GOVERNING EQUATIONS

We consider the Johnson-Segalman model with additional viscosity, also used in [1]. The governing equations are the following:

$$\tau + \lambda \, \ddot{\tau} = 2\mu_1 \mathbf{D} \mathbf{u} \tag{1}$$

$$\rho(\mathbf{u} \cdot \nabla)\mathbf{u} - div \ \tau - \mu_2 \nabla^2 \mathbf{u} + \nabla p = \mathbf{f}$$
<sup>(2)</sup>

$$div \mathbf{u} = 0 \tag{3}$$

Above,  $\tau$  is the extra-stress tensor,  $\lambda$  is a characteristic time related to elastic effects, **u** is the velocity field and *p* the pressure. **Du** stands for the symmetric part of the velocity gradient, which we will also call **d** (the antisymmetric part will be denoted by **r**). Also,  $\rho$  stands for the density, **f** for the volumetric force, and  $\mu_1, \mu_2$  for the polymer and solvent viscosities, respectively.

Finally, the objective time derivative  $\frac{1}{\tau}$  is defined as:

$$\overset{\mathbf{O}}{\tau} = \mathbf{u} \cdot \nabla \tau + \tau \cdot \mathbf{r} - \mathbf{r} \cdot \tau - \theta (\mathbf{d} \cdot \tau + \tau \cdot \mathbf{d})$$
(4)

where  $\theta$  is a real parameter  $\in [-1, 1]$ .  $\theta = 1$  corresponds to the upper-convected derivative.

In the following, we will concentrate on the inertia-less flow ( $\rho = 0$ ) of an upper-convected fluid with  $\mu_1 = 0.89$  and  $\mu_2 = 0.11$ . These are standard values used to test numerical methods, in particular because the inertia term scems to have an stabilizing effect on the discrete problem [7]. A more exhaustive study will be presented in [4].

## 3. ABOUT EQUAL-ORDER STRESS INTERPOLATION

In a recent paper [2] (see also [3]), we have studied stress-velocity-pressure mixed finite elements for newtonian flows ( $\lambda = 0$ ) in which we used the same interpolants for velocity and extra-stress components. At first glance, this procedure could be cast into equal-order schemes framework and thus be presumed to yield unstable approximations in the  $\mu_2 = 0$  limit. However, we numerically showed that, if the incompressibility constraint is strong enough, or equivalently the pressure space rich enough, some stable approximations can be obtained. In fact, the discrete incompressibility constraint reduces the space of admissible velocity fields, and thus the approximation is no longer of equal order.

Let us denote a given three-fields mixed element by "Extra-Stress / Velocity / Pressure interpolants". As an example, the element of Crochet and Marchal would be labeled  $(16 \times Q_1)/Q_2/Q_1$ . In [2], we found that  $P_2^+/P_1^+/P_1$ ,  $Q_2/Q_2/P_1$  and  $Q_1/Q_1/P_0$  elements exhibited stable numerical behaviour.  $P_2^+$  stands for quadratic triangles plus the usual cubic bubble-function, and all pressure interpolants are discontinuous across interelement boundaries.

*Remark:* Recently, M.A.Hulsen used a variant of the  $P_2^+/P_2^+/P_1$  (namely the  $P_2/P_2^+/P_1$ ) element within a decoupled method, with quite successful results [9].

As an application of the observations above about the importance of the discrete incompressibility constraint, let us compare the  $Q_2/Q_2/Q_1$  element (known to be unstable [8]) with the  $Q_2/Q_2/P_1$ one (stable in our tests). Asymptotically, the former has one pressure freedom per element, while the latter has three times this number. On the other hand, an element with discontinuous pressure interpolants with one pressure unknown per element is the  $Q_2/Q_2/P_0$ , which in fact is unstable [2]. To overcome this difficulty, JMM and MJC enriched the discrete-stress space. Our proposal is to reduce the admissible velocities space by enriching the discrete-pressure space. Of course, the limit for this is the compatibility between velocity and pressure interpolants (the well-known Babuška-Brezzi condition).

The results in [2] concerning  $P_2^+/P_2^+/P_1$  element, which performs best in the newtonian limit, are extended to viscoelastic flows in the following sections. Although this extension proved to be far from obvious, we expect the reader to keep in mind that condition (i) of Section 1 is fulfilled by our elements (this assertion is up to now only based upon strong numerical evidence), which are simpler than that of Marchal and Crochet. In a forthcoming paper, we investigate the  $Q_2/Q_2/P_1$  and  $Q_1/Q_1/P_0$  in viscoelastic simulation. We expect that other simple elements can be found that are stable in the newtonian limit, perhaps one involving continuous pressure interpolants, the  $P_1^+/P_1^+/P_1$  (natural extension of the mini-element) being a good candidate.

## 4. THE NUMERICAL METHOD

We implemented a coupled scheme based on Newton-Raphson's algorithm. The incompressibility constraint is treated by iterative penalization, allowing the elimination of pressure unknowns at element level. In fact, our iterative scheme can be viewed as the viscoelastic version of the method introduced by R.Codina for the Navier-Stokes equations [5].

Let  $\Sigma_h, V_h, L_h$  be the discrete linear manifolds of extra-stress, velocity and pressure, respectively. For simplicity, we will assume in this section that the boundary conditions are such that these manifolds are vector spaces, so that we can identify the space of test functions with that of weight functions. The discrete variational formulation of (1)-(3) corresponding to the SU mixed method of Marchal and Crochet thus reads:

**Discrete variational problem:** Find  $(\tau_h, \mathbf{u}_h, p_h) \in \Sigma_h \times V_h \times L_h$  such that

$$\int_{\Omega} (\tau_h + \lambda \ \overline{\tau}_h) : \chi +$$

$$+ \sum_{T \in \mathcal{T}_h} h_f \int_T \frac{\lambda}{|\mathbf{u}_h|} (\mathbf{u}_h \cdot \nabla \tau_h) : (\mathbf{u}_h \cdot \nabla \chi) = \int_{\Omega} 2\mu_1 \mathbf{D} \mathbf{u}_h : \chi \qquad \forall \chi \in \Sigma_h$$
(5)

$$\int_{\Omega} \rho(\mathbf{u}_{h} \cdot \nabla \mathbf{u}_{h}) \cdot \mathbf{w} +$$
$$+ \int_{\Omega} (\tau + 2\mu_{2} \mathbf{D} \mathbf{u}_{h} - p\mathbf{1}): \mathbf{D} \mathbf{w} = \int_{\Omega} \mathbf{f} : \mathbf{w} \quad \forall \mathbf{w} \in V_{h}$$
(6)

$$\int_{\Omega} q \, div \, \mathbf{u}_h = 0 \qquad \forall q \in L_h \tag{7}$$

where  $\Omega$  is the domain under consideration, over which a finite element mesh  $\mathcal{T}_h$  has been specified. Once  $\mathcal{T}_h$  is given,  $\Sigma_h$ ,  $V_h$  and  $L_h$  become defined by the  $P_2^+/P_2^+/P_1$  (or some other to be introduced later) interpolation inside each triangular element, together with the boundary conditions.  $h_f$  stands for the local mesh size in the flow direction and 1 for the unit tensor.

A lengthy explanation would be needed to completely describe our iterative scheme, so we will only sketch the most relevant features:

- The whole system (5)-(7) is solved by classical Newton-Raphson iterations. As usual, the characteristic time for SU  $h_f/|\mathbf{u}_h|$  is updated after each iteration in a Picard-like manner.
- At each iteration, the incompressibility equation (7) is replaced by

$$\int_{\Omega} (\epsilon p_h^{n+1} + div \ \mathbf{u}_h^{n+1}) q = \int_{\Omega} \epsilon p_h^n q \qquad \forall q \in L_h$$
(8)

so that, upon convergence  $(p_h^{n+1} = p_h^n)$ , (7) is satisfied exactly.

- At each iteration, equation (8) allows the elimination of pressure unknowns at element level, so that these unknowns do not enter the Jacobian matrix.
- In order to obtain a solution at a certain elasticity value  $\lambda$ , we performed several steps beginning with the solution at  $\lambda = 0$ . Usually, we performed a linear extrapolation of the results obtained with two previously computed  $\lambda$ 's to generate the initial guess for the iterative algorithm.

#### 5. THE FOUR-TO-ONE CONTRACTION PROBLEM

It has become usual to test viscoelastic flow methods in the so-called 4-to-1 contraction problem, which for this reason is only briefly described in this section.

We consider the planar flow of an inertia-less upper-convected fluid which enters the domain through a channel of half-width 4, with a parabolic vertical velocity profile of mean value 0.25. At  $x_2 = 0$ , there is a sudden contraction into a narrower channel of half-width 1, its downstream end being imposed a parabolic vertical velocity profile of mean value 1.

At the entry section, it is customary to impose fully-developed conditions for  $\tau$ , but we instead prefered to specify  $\tau$  to vanish there. This causes no serious trouble, as the stress field soon develops, well before reaching the region perturbed by the contraction.

The lengths of the upstream and downstream channels  $(l_{up} \text{ and } l_{down})$ , for the boundary conditions not to perturb the flow, depend upon the elasticity time  $\lambda$ . We have performed some test with the same values of [1]  $(l_{up} = 16, l_{down} = 20)$ , and some others with  $l_{up} = 30$  and  $l_{down} = 50$ . Symmetry conditions are imposed at  $x_1 = 0$ , while no-slip ones at the solid walls.

With the above definitions, the Deborah number of the flow is defined as  $De = 3\lambda$ , because the shear rate at the downstream wall is 3 in fully developed flow. The methods exhibiting the HWNP usually fail to converge at a limit De of  $\sim 2$  to  $\sim 7$ , so that we will regard Deborah numbers greater than 7 as high (also, numerical results will show that for De > 7 the elastic effects significantly modify the flow).

## 6. FINDING A NEW MIXED ELEMENT

Let us begin by introducing three meshes that will be referred to in the sequel.  $T_1$  is a structured mesh with 194 elements, involving 3185 stress-velocity unknowns.  $T_2$  has 248 elements, which results in 3985 unknowns, and  $T_3$  contains 492 elements (7905 unknowns) (see Fig. 1).  $T_1$  and  $T_2$  have  $l_{up} = 16$  and  $l_{down} = 20$ , while  $T_3$  has  $l_{up} = 30$  and  $l_{down} = 50$ .

## **6.1 The** $P_2^+/P_2^+/P_1$ element

Encouraged by the good behaviour of the  $P_2^+/P_1^+/P_1$  element in newtonian flow, we tested it in the viscoelastic situation. We considered three treatments of equation (1): Galerkin, full SUPG, and the SU method of (5). The first two yielded oscillatory results for  $\tau$  on mesh  $T_1$  at *De* as low as 3, confirming that these methods do not work for viscoelastic fluids.

More promising were the results of the SU method. With mesh  $\mathcal{T}_1$ , we were able to reach De = 9 with no convergence difficulties. Although the pressure and velocity fields at this De were smooth, the  $\tau$  field exhibited strong oscillations downstream of the contraction. In Fig. 2 we plot  $\tau_{22}$  along the vertical line  $x_1 = 1$  for De = 1 to 9. These results are clearly unacceptable.

To see if these oscillations could be removed by mesh refinement, we performed an analogous study on  $T_2$ . On this mesh we could not find a converged solution for De > 5.5. Moreover, comparing the results of both meshes the method seems to be unstable. In Fig. 3 we plot  $\tau_{22}$  along  $x_1 = 1$  for both meshes at De = 3, 4 and 5. It can be seen that the first oscillation behind the peak at  $x_2 \sim 0$ becomes *stronger* on the finer mesh.



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Figure 1: Finite element meshes (detail near the contraction): (a)  $T_1$ , (b)  $T_2$ , (c)  $T_3$ .



Figure 2:  $\tau_{22}$  viscoelastic stress along the line  $x_1 = 1$  for De = 1 to 9.  $P_2^+/P_2^+/P_1$  element. Mesh  $\mathcal{T}_1$ 

We think that the above numerical evidence is enough to justify the sake of a new element, although the  $P_2^+/P_2^+/P_1$  allowed us to reach high Deborah numbers on quasi-regular meshes. It should be kept in mind that any existing method for viscoelastic flow is sensitive to abrupt mesh-size changes.

#### 6.2 A new element

Turning back to conditions (i) to (iii) in Section 1, the three of them were fulfilled by the previous method, which nevertheless does not behave satisfactorily. The explanation we conjecture for this deduces from the apparent bad behaviour of SU with quadratic interpolants already remarked.

Let us now turn to consider a modification of the  $P_2^+/P_2^+/P_1$  element. We keep pressure and velocity interpolants as before, but replace the quadratic interpolation by a *piecewise linear* one, obtained by subdividing each triangle into four equal ones (joining the midpoints of each side) and interpolating stresses linearly *inside each sub-triangle*. This modification is obviously inspired in the work of Marchal and Crochet, but, as we only perform one subdivision, the stress nodes still coincide with the velocity ones. Furthermore, we will keep the bubble function for stresses so that, except for boundary conditions, the discrete spaces are the same for each velocity and stress component. This new element will be labeled  $(4 \times P_1)^+/P_2^+/P_1$  hereafter.

Our numerical tests have shown that this element is stable for newtonian flow. In the viscoelastic case, and using the SU method, we reached without difficulty De = 12 with meshes  $T_1$  and  $T_2$ . In Figs. 4 and 5 we include plots similar to the previous ones for De = 4,8 and 12, as obtained with the new element on  $T_1$  and  $T_2$  respectively. It can be seen there that the oscillations not only do not propagate as far downstream as with the previous element, but also decrease with mesh refinement. We believe this to be an evidence of h-convergence of the method.

As meshes  $T_1$  and  $T_2$  are not long enough to carry out simulations at De > 12, we conducted a last test on mesh  $T_3$ . We found no convergence difficulty up to the high De value of 19 (for De > 15 the mesh proved to be inadequate). In Fig. 6 we plot  $\tau_{22}$  along  $x_1 = 1$  for De = 3, 7, 11, 15 and 19. At the highest values some oscillations appear, that we attribute to two facts: First, that this mesh has similar element sizes near the contraction as  $T_2$ . Second, the oscillations near  $x_2 \sim 10$  occur where a sudden mesh-size change occurs (see Fig. 1 (c)), and thus can probably be removed by making this transition smoother. We stopped the calculations here because this pathology where the mesh-size abruptly changes strongly deteriorates the results (see also Fig. 7 below).

As we have already said, the stress field is the most sensitive field of the flow, particularly at the downstream wall, and for this reason it has strong numerical interest. Some other flow features serve better for comparison and for the visualization of the effect of elasticity on the fluid behaviour. In Fig. 7, we plot the vertical velocity along the symmetry axis for De = 3, 7, 11, 15 and 19. These were obtained with mesh  $T_3$  but do not differ substantially from mesh to mesh. The results at De = 19 clearly show that the mesh is not appropriate for De > 15. Also notice the substantial modifications to the flow introduced by elastic effects.

As a final remark, it is clear that neither theoretical nor numerical proofs of convergence in mesh are contained in this article. We believe that, considering that the four-to-one contraction problem has proved to be a highly challenging test for the model considered, and that we have tested the method on quite different meshes (some of them are not shown here), our conjecture that the proposed method converges is quite reasonable. Further analyses are under way to better assess these important questions.

# 7. CONCLUSIONS

A new mixed element has been presented that performs satisfactorily for viscoelastic flow simulation and is much simpler than that of Marchal and Crochet. In fact, in planar flow the  $(4 \times P_1)^+/P_2^+/P_1$ element yields meshes containing 9 stress unknowns per element (asymptotically), while the 16 ×



Figure 3:  $\tau_{22}$  viscoelastic stress along the line  $x_1 = 1$ . A comparison of the results obtained with meshes  $T_1$  and  $T_2$  at De = 3, 4 and 5.





Figure 4:  $\tau_{22}$  viscoelastic stress along the line  $x_1 = 1$ , for De = 4,8 and 12 as obtained with the  $(4 \times P_1)^+/P_2^+/P_1$  element on mesh  $T_1$ .



Figure 5: Idem Fig. 4 , on mesh  $\mathcal{T}_2$  .



Figure 6:  $\tau_{22}$  viscoelastic stress along the line  $x_1 = 1$ , for De = 3, 7, 11, 15 and 19 as obtained with the  $(4 \times P_1)^+/P_2^+/P_1$  element on mesh  $T_3$ .

 $Q_1/Q_2/Q_1$  raises this number to 48. If condensable unknowns are eliminated at element level our element is still less costly by a factor 6/21.

This should not be taken as an argument against Marchal and Crochet's work. Very much on the contrary, the development of this new method was inspired and based upon their ideas, which we briefly summarized in conditions (i)-(iii) of Section 1 and the subsequent remark. This is of course a personal interpretation of their work, and is confirmed by the results shown in this paper. We believe that some other appropriate elements for this problem can be found following the same methodology that was used here. We are now studying two of them, and the results will be the subject of a forthcoming paper. It should be remarked that the presence of limit points in our calculations was thoroughly investigated, and some current results indicate that limit points indeed exist near De = 12 for several meshes.

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Figure 7: Vertical velocity along the symmetry axis as obtained with the new method, for De = 3, 7, 11, 15 and 19.

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