

## Computing transient flows with high elasticity

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### Abstract

Although much progress has been made in the computation of Eulerian steady flows with high viscoelasticity, less work has been done for the case of transient flows. Because of their importance in injection moulding, blow moulding and other forming processes, as well as their intrinsic interest, we believe more attention should be focussed in this area. Hence in this paper we review progress in unsteady flow computations with high elasticity, and show some new results in this area.

**Keywords** : viscoelasticity, computation, transient or unsteady flow

### 1. Introduction

The mathematical complexity of rheology often forces one to use computation for the effective solution of many problems arising in practice. In response to this demand, the relatively new field of computational rheology (see Tanner and Walters, 1998) has developed two branches:

a) Given the mass, momentum and energy balances, and a choice of constitutive equation and initial/boundary conditions appropriate to the problem of interest, find a numerical solution of the problem;

b) Beginning with a microstructural concept, use computation to avoid the use of a constitutive relation, while still observing mass, momentum and energy conservation.

Subfield (a) has been used in rheology since 1964, but (b) is much younger, and has mainly developed since 1990. We shall not address (b) here, concentrating the review on solutions to initial/boundary problems with a chosen constitutive relation.

Hence we assume that a constitutive relation and initial/boundary conditions have been chosen. The choice (Tanner, 2000) between differential and integral models has a profound effect on the computing strategy adopted, and for viscoelastic materials the question of boundary and initial conditions also needs careful scrutiny.

The computation of highly elastic rheological flows has not proved to be straightforward, even for the case of Eulerian steady flows (Tanner, 2000). This is largely because of the mixed elliptic-hyperbolic nature of the set of equations formed by the conservation laws and the constitutive equa-

tions governing the rheological behaviour of the fluids. Often it has been difficult to secure convergence of the computations for flow conditions as severe as those occurring in practical processing situations. There are now signs that this problem has been at least partially solved for Eulerian steady flows.

Yet many processing situations (injection moulding, blow moulding, for example) are essentially unsteady, or transient, flows in an Eulerian frame and less progress has been made in this area and hence it forms the subject of our review. With increasing elastic effects, experimental rheological visualizations have demonstrated that a flow of a viscoelastic fluid often tends to develop into a time-dependent, three-dimensional (3D) complex flow even in very simple geometries, for example, swirling flow in an enclosed cylinder (see, for example, Xue *et al.*, 1999a). Therefore, investigations of the behaviour of viscoelastic fluids in transient flows are very important in studying the rheological properties of viscoelastic materials and their processing, as well as evaluating the predictive capability of the constitutive equations used to model the materials. To begin, we will describe the basic system of equations and boundary/initial conditions we need to solve, and classify the various methods that have been used, both for steady and transient flows.

Thermal effects and compressibility may be of importance in many problems, but they do not add greatly to the difficulty of the computations. Therefore, this review will consider only isothermal, incompressible flows; gravity body forces will also be ignored.

### 2. Equations to be solved

One can set up the problems in either the traditional

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Eulerian (fixed) coordinate system or the so-called Lagrangian (particle-following) system. The latter has been rarely used, but it has shown some spectacular successes (Rasmussen, 1999; 2000; Rasmussen and Hassager, 1993; 1995; 1999; 2000) in both steady and unsteady flows and deserves more attention, we believe. Rasmussen (2000) and co-workers (Rasmussen *et al.*, 2000; Rasmussen and Hassager, 2000) have shown that they are able to compute the 3D, unsteady flow which occurs when a cylindrical filament fixed to endplates is elongated. They used a finite element method and an integral-type constitutive model. They also showed how to predict the inflation of a polyisobutylene “bubble”, beginning from a flat sheet (Rasmussen *et al.*, 2000). The method offers second-order accuracy both in space and time. The Lagrangian method requires extensive remeshing, because of the extreme distortion of the mesh during flow, and so may be difficult to implement, for example, where a sharp solid boundary corner intrudes into the flow, as discussed by the pioneering paper in this area (Hassager and Bisgaard, 1983). Also, the entire past deformation history has to be stored, which renders the method expensive in terms of memory demanded.

Wapperom *et al.* (2000) applied a backward-tracking Lagrangian particle method (BLPM) for viscoelastic transient contraction flows using the differential FENE-P model. They demonstrated that accurate simulations on transient flow can be obtained by tracking backward in time over one single step only, thus the method is quite efficient, and particularly attractive to use with kinetic theory models, for which CPU time and memory requirements are very demanding.

Harlen *et al.* (1995) used a split Lagrangian-Eulerian method, and Yamaguchi *et al.* (2000) have a hybrid method, but there appear to be few other papers using the Lagrangian system, and henceforth we consider the more common Eulerian system of coordinates. In this case a fixed coordinate system ( $x$ ) is used, and the conservation laws are written in the form (no gravity):

• Continuity equation for the incompressible case,

$$\nabla \cdot \mathbf{v} = 0 \quad (1)$$

• Momentum equation,

$$R_e \left( \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = -\nabla p \mathbf{I} + \nabla \cdot \boldsymbol{\tau} \quad (2)$$

where  $\mathbf{v}(x, t)$  is the velocity vector,  $\nabla$  is the divergence operator,  $p$  the hydrostatic pressure,  $\mathbf{I}$  the unit tensor, and  $\boldsymbol{\tau}$  is the extra stress tensor. Length has been scaled with a characteristic value  $L$ , velocity with the characteristic value  $V$ . The Reynolds number is defined as  $R_e = \rho LV/\eta$ , where  $\rho$  is the density and  $\eta$  is the viscosity of the fluid.

$\boldsymbol{\tau}$  is computed via the constitutive equation, connecting  $\boldsymbol{\tau}$  to the history of the motion. There are many forms of constitutive equation in use (Tanner, 2000, p.278), which may

be broadly described as being either integral or differential forms. While the integral forms have been used successfully in steady flows, we are not aware of many such uses in transient flows except the notable work of Rasmussen and Hassager discussed above and also the work of Peters *et al.* (2000). Integral models have their advantages especially since improving the relaxation function, by adding more relaxation times, for example, is extremely easy. Here we shall concentrate on differential models. The kind of model to be used is written as

$$\lambda \frac{\Delta \boldsymbol{\tau}}{\Delta t} + f(\boldsymbol{\tau}, \mathbf{d}) \boldsymbol{\tau} = 2\eta \mathbf{d} \quad (3)$$

where the upper convected derivative  $\Delta \boldsymbol{\tau} / \Delta t$  is described by

$$\frac{\Delta \boldsymbol{\tau}}{\Delta t} = \frac{\partial \boldsymbol{\tau}}{\partial t} + \mathbf{v} \cdot \nabla \boldsymbol{\tau} - \boldsymbol{\tau} \mathbf{L}^T - \mathbf{L} \boldsymbol{\tau} \quad (4)$$

and the velocity gradient tensor  $\mathbf{L}$  is  $(\nabla \mathbf{v})^T$ , so that the component  $L_{ij} \equiv \partial v_i / \partial x_j$  and  $\mathbf{d} \equiv 1/2(\mathbf{L} + \mathbf{L}^T)$ .  $\lambda$  is a relaxation time. Generally, it has been found that a single relaxation time is insufficient to cover the range of shear rates involved in polymer processing. Often, 3-10 relaxation times are used with each time constant ( $\lambda_i$ ) developing its own partial stress field ( $\boldsymbol{\tau}_i$ ) and the sum of  $\boldsymbol{\tau}_i$  is the total stress  $\boldsymbol{\tau}$ . Clearly this increases the number of unknowns to be found greatly. In the present article we shall mainly deal with a single relaxation time, but advanced applications will generally need multiple times.

The form of the function  $f$  in Eq. (3), and possibly the variation of  $\lambda$  and  $\eta$  with  $\boldsymbol{\tau}$  and/or  $\mathbf{d}$  allows a variety of choices. The ones we will mention here are:

a)  $\lambda$  and  $\eta$  are constants,  $f=1$ . This is the well-known (Tanner, 2000) Upper Convected Maxwell (UCM) model, which is difficult to compute with and shows a constant shear viscosity. Addition of a Newtonian viscosity term  $2\eta_s \mathbf{d}$  to the stress gives the Oldroyd-B model.

b)  $\lambda$  and  $\eta$  are constants,  $f\boldsymbol{\tau} = \boldsymbol{\tau} + \alpha \boldsymbol{\tau} \boldsymbol{\tau}$  gives the Giesekus model ( $\alpha$  is a constant), more realistic than the UCM model.

c)  $\lambda$  and  $\eta$  are constants,  $f$  is a function of  $tr \boldsymbol{\tau}$ , giving various special PTT models. Sometimes  $\lambda$  and  $\eta$  have been allowed to depend on  $\mathbf{d}$ , but we shall not do this here. As a further ramification, a so-called “slip” coefficient ( $\xi$ ) may be used in the PTT model, so that a term  $\xi(\mathbf{d}\boldsymbol{\tau} + \boldsymbol{\tau}\mathbf{d})$  is added to the left-hand side of Eq. (3).

The most successful forms of  $f$  that have been used are ( $\eta, \lambda$  are constants)

(i)  $f = 1 + \frac{\lambda \varepsilon}{\eta} tr \boldsymbol{\tau}$  Linear PTT;  $\varepsilon$  is a constant governing the elongational behaviour.

(ii)  $f = \exp\left(\frac{\lambda \varepsilon}{\eta} tr \boldsymbol{\tau}\right)$  Exponential PTT;  $\varepsilon$  is constant.

The latter has been found to be more suitable for melts (Tanner, 2000).

d) The XPP model of Verbeeten (2001) gives, in dimensionless form,

$$\frac{\Delta \tau}{\Delta t} + \xi(d\tau + \tau d) + \alpha \tau^2 + F\tau + (F-1)I = 2d \quad (5)$$

where  $F$  is a function of  $tr\tau$  and  $tr\tau^2$ . The form of  $F$  given by Verbeeten is

$$F = 2r \exp(v(\wedge - 1))(1 - 1/\wedge) + \wedge^2 \left(1 - \frac{\alpha}{3} tr\tau^2\right) \quad (6)$$

where  $\wedge = \sqrt{1 + \frac{1}{3} tr\tau}$ .

(To make the equations dimensionless, the equations have been rewritten so that  $t \rightarrow t/\lambda$ ,  $\tau \rightarrow \tau \frac{\lambda}{\eta}$ ,  $d \rightarrow \lambda d$ ,  $L \rightarrow \lambda L$ , and  $\mathbf{v} \cdot \nabla \rightarrow \lambda \mathbf{v} \cdot \nabla$ ). In this case a PTT-form with the slip coefficient  $\xi$  and a Giesekus term ( $\alpha \tau^2$ ) are incorporated into the model. The model aims to describe branched polymers as well as linear polymers. A coefficient  $v$  (Eq. (6)) describes the number of branches on the molecules, and  $r$  is another coefficient, the ratio of two relaxation times, associated with different processes.

It is interesting to note the close relations between all the above models. For high stress level elongational flows, one can show that the XPP model reduces to ( $\|\mathbf{d}\| \gg 1$ ).

$$\lambda \frac{\Delta \tau}{\Delta t} + \left(1 - 2r + 2rv \exp\left(\frac{tr\tau}{3}\right)\right) \tau = 2\eta d \quad (7)$$

where  $r$  is a positive number.

Eq. (7) is another special case of the PTT model. The term  $1-2r$  merely ensures  $f = 1$  when  $tr\tau \rightarrow 0$ , and is negligible for high stress levels. In view of this similarity at high stresses we will mainly concentrate on the PTT/OldroydB/UCM family of models.

For the UCM model damped wave propagation may occur, as shown in the Rayleigh (suddenly started plate) problem (see Tanner, 2000, pp.334-5). With the Oldroyd-B model wave propagation does not occur. Thus the generation of waves may need to be considered in transient flows.

In real viscoelastic flows, a viscoelastic fluid may behave more or less like a viscous material (at small deformation), or like an elastic material (at larger deformation). To characterize the elastic level in a given flow, dimensional numbers, the so-called Deborah number ( $D_e$ ), and/or, the Weissenberg number ( $W_i$ ), defined by the ratio of the material time scale (relaxation time) to some appropriate time scale of the deformation, are used.

### 3. Boundary and initial conditions

In addition to the equations outlined above, boundary conditions are needed for steady flows. Also, transient flows require initial conditions. For Newtonian incompressible steady flows we have an elliptic problem, and we

require, on each portion of the boundary, that the velocities or tractions are given. Sometimes the direction of the flow is given, which gives a relation between the velocity components, and sometimes one traction and one velocity component are given. In cases where slip occurs, a relation between traction and slip speed could be given (Tanner, 2000).

When free surfaces are present, and the flow is steady, then the (normal) velocity boundary condition  $\mathbf{v} \cdot \mathbf{n} = 0$  must also be enforced, as well as the traction boundary conditions on the free surface; the position of the free surface becomes another unknown.

For unsteady free surface flows, if  $h(\mathbf{x}, t)$  is the free surface location, then one has (Stoker, 1957):

$$\frac{\partial h}{\partial t} + \mathbf{v} \cdot \nabla h = 0 \quad (8)$$

plus appropriate traction conditions. When surface tension is important, then the normal traction is related to the two principal curvatures  $1/R_1$  and  $1/R_2$ , so that  $\sigma(1/R_1 + 1/R_2)$  is the jump in normal traction on the surface. In cases where the surface tension coefficient  $\sigma$  varies on the free surface, then an effective shear traction proportional to  $\nabla \sigma$  is applied to the surface (Leal, 1992).

Thus in the case of inelastic flows, the relevant boundary conditions are that on the boundary of the body of fluid ( $S$  in Fig. 1) velocities or tractions (forces/unit area) or a mixture of the two, need to be specified everywhere. If velocity boundary conditions are applied to an incompressible fluid over the entire surface, then one must make sure that the net influx across the boundary is zero; usually it will be necessary to fix the pressure at some arbitrary value at a single point to fully determine the pressure field in these cases.

For viscoelastic fluid models, either of the differential or the integral type, further boundary conditions on the inlet section AB in Fig. 1 are needed. Consider the UCM fluid (Eq. (3), with  $f = 1$ ) as an example. For steady flows the equations can be written as

$$v_k \frac{\partial \tau_{ij}}{\partial x_k} = f_{ij}(\mathbf{L}, \boldsymbol{\tau}). \quad (9)$$

Given a known velocity field, this is a set of six first-

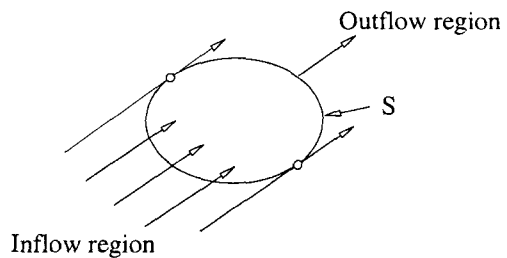


Fig. 1. Inflow and outflow regions on the boundary S of a body.

order hyperbolic partial differential equations for the extra stresses  $\tau_{ij}$ . The characteristics of Eq. (9) are the streamlines. Such equations (Courant, 1972) need initial conditions on the inflow boundary. Hence one expects that all six of the stress components should be specified on AB (Fig. 1) or, for plane and axisymmetric flow, three and four components respectively.

If one elects to solve Eq. (3) together with the momentum and mass conservation equations, then Renardy (1990) has shown that prescription of all stress components at the entry surface for the UCM model may lead to an over-determined problem. No simple resolution of the boundary data has been proposed, and some ingenuity is needed to generate a correct, compatible set of stresses at the entry surface. In many cases, this problem is absent, either because the exact solution is known on the entry plane, or the problem has a periodic character. Another approach is to add time-dependent terms to the problem and solve as an initial-value problem, with all extra stresses at zero values in the rest state or as known values at some time  $t_0$ .

For other models of the form of Eq. (3), for example the PTT and Giesekus models, similar problems arise. However, addition of a solvent viscosity, as in the Oldroyd-B model, removes the Renardy over-determination dilemma.

The above discussion has been in terms of differential viscoelastic models, but clearly the same problems occur with integral constitutive models; a complete (or compatible) set of stresses on the inlet region is needed.

A further discussion of the boundary data problem is given by Huilgol and Phan-Thien (1997), together with a clear discussion of the complex elliptic-hyperbolic nature of the mathematical problems being solved. Often it is better to treat the flows involving viscoelastic fluids as unsteady initial value problems even when one is concerned with equilibrium steady-state solutions.

In the case of slip at the solid surfaces another form of boundary condition is generated, needing special attention in the setting-up phase (Tanner, 2000). In other problems it may be necessary to prescribe thermal and other boundary conditions, but these are usually classical in nature and present no unknown problems.

#### 4. Discretization schemes

Numerical solution entails the discretization of the fields for  $\mathbf{v}$ , the stresses  $\tau_{ij}$  and  $p$ , and any other required variables. In all cases the object of the discretization is to reduce the partial differential equations of the problem to a set of (generally non-linear) simultaneous equations for a known finite number of nodal variables. There are many schemes: only a selection of methods is discussed. First, temporal discretization schemes will be reviewed, followed by spatial discretization schemes.

#### 4.1. Temporal discretization schemes

When we talk about the temporal discretization, it is more convenient to express the system of the governing equations given in the previous section as a purely hyperbolic system in time:

$$\frac{\partial \mathbf{U}}{\partial t} = \mathbf{F}(t, \mathbf{U}(t)) \quad (10)$$

where the function  $\mathbf{F}(t, \mathbf{U})$  represents the sum of convective, diffusive and source terms:

$$\mathbf{F}(t, \mathbf{U}(t)) = \mathbf{A}_c(t, \mathbf{U}) + \mathbf{A}_d(t, \mathbf{U}) + \mathbf{S}_U \quad (11)$$

with operators having the following forms:

$$\begin{aligned} \mathbf{A}_c &= \mathbf{v} \cdot \nabla \mathbf{U} \\ \mathbf{A}_d &= \Gamma \nabla^2 \mathbf{U} \end{aligned} \quad (12)$$

and  $\mathbf{S}_U$  contains all the terms that are not included in the convection term  $\mathbf{A}_c$  and diffusion term  $\mathbf{A}_d$ .

For an initial value problem, we need to find the solution  $\mathbf{U}$  a short time  $\Delta t$  after the initial point  $t_0 = 0$  with an initial condition  $\mathbf{U}_0$ . Then, the solution  $\mathbf{U}_1$  at  $t_1 = t_0 + \Delta t$  can be regarded as a new initial condition and the solution can be advanced to  $t_2 = t_1 + \Delta t$  and so on.

The basic schemes for temporal discretization can be constructed by using the Taylor series expansion of  $\mathbf{U}$ ,

$$\mathbf{U}(t_{n+1} + \Delta t) = \mathbf{U}(t_n) + \frac{\partial \mathbf{U}(t_{n+\theta})}{\partial t} \Delta t + \frac{\partial^2 \mathbf{U}(t_{n+\theta}) \Delta t^2}{\partial t^2} \frac{1}{2} + \dots \quad (13)$$

and by neglecting the higher order terms, we get the discretized time derivative:

$$\mathbf{U}(t_{n+1} + \Delta t) \cong \mathbf{U}(t_n) + \mathbf{F}(t_{n+\theta}, \mathbf{U}) \Delta t \quad (14)$$

where  $\mathbf{F}(t_{n+\theta}, \mathbf{U})$  means the weighted average of  $\mathbf{F}(t, \mathbf{U})$  over successive time levels  $n$  and  $n+1$ :

$$\mathbf{F}(t_{n+\theta}, \mathbf{U}) = \theta \mathbf{F}(t_{n+1}, \mathbf{U}) + (1 - \theta) \mathbf{F}(t_n, \mathbf{U}) \quad (15)$$

for a fixed blending factor  $\theta$  ( $0 \leq \theta \leq 1$ ).

The temporal accuracy and numerical stability will be determined by  $\theta$  for this kind of two level methods in which only the values of the unknown at two successive times are involved.

When  $\theta = 0$ , the value at time level  $n + 1$  is explicitly determined by the value at level  $n$ , which produces first-order accuracy with respect to time, and the Courant-Friedrichs-Lewy (CFL) condition (Wood, 1990) has to be satisfied for numerical stability. This stability condition places a severe restriction on the time step allowed, especially for mesh refinement because the stable time step is limited by the smallest mesh size and the highest velocity in the computational domain. More importantly, it is unconditionally unstable for hyperbolic constitutive equations with zero physical diffusion due to the requirement for the spatial stability (Xue *et al.*, 2001).

When  $\theta = 1$ , the value at time level  $n + 1$  is implicitly

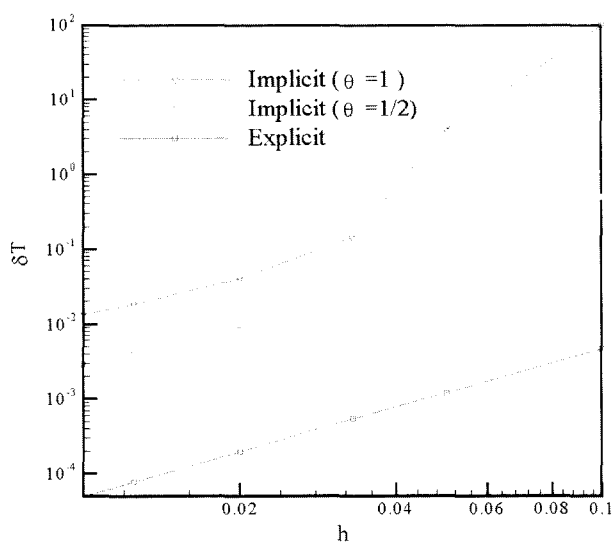


Fig. 2. Allowable non-dimensional time steps for a given non-dimensional mesh size  $h$  when three different temporal discretization methods are used.

determined by the value at level  $n$  and its neighbouring node value at time level  $n + 1$ . Von Neumann stability analysis shows that it is unconditionally stable (no CFL stability restriction over time step). However, it only gives first-order accuracy with respect to time.

When  $0 < \theta < 1$ , the value at time level  $n + 1$  is implicitly determined by the value at level  $n$  and its neighbouring node values at both time level  $n$ , and time level  $n+1$ . When  $\theta = 1/2$ , it is known as the Crank-Nicolson method, which gives second-order accuracy in time and is unconditionally stable. With other blending factors, the method remains first order accurate. The stability will increase with increasing value of  $\theta$ , but the accuracy in time will be degraded.

For the three different temporal discretization methods, a typical difference in time step  $\delta T$  allowed for stable calculation for a given mesh size  $h$  in a quasi-one dimensional Newtonian flow is shown in Fig. 2 (Xue *et al.*, 2002).

The above two-level methods lay the foundation for the solution of a purely hyperbolic equation, but the highest accuracy possible is second order. Higher order accuracy is possible, but information at more points is needed, such as the second or third order Adams-Bashforth explicit methods, Adams-Moulton implicit methods (Gear, 1971) and Runge-Kutta methods (Butcher, 1987). For these higher order methods, there is a principal disadvantage: they cannot be started using only data at the initial time point. Therefore, a lower order method, such as the explicit Euler method, has to be used for starting the calculation. As a result, the efficiency of the method will be degraded due to limits on stability. This is also true for the so-called implicit three time level method (Ferziger and Peric, 2002). In this method, second-order accuracy in time is reached by using

a quadratic backward approximation over three time levels to the time derivative. Obviously, the coefficient for the variable value at time level  $t_{n-1}$  is always negative. As a result, oscillatory solutions may be produced if a large time step is used.

## 4.2. Spatial discretization schemes

For transient calculations, time is taken as an extra dimension compared to steady-state calculations where three space coordinates are involved. For a fixed time position, one is actually solving a steady-state problem with the influence on the solution by the information of the solutions from previous time positions. Therefore, the accuracy and stability of the methods used for spatial discretization are equally important to that in steady-state calculations. For accurate transient flow calculations, the accuracy of spatial discretization should match the accuracy of temporal discretization, and the boundedness of the discretized system should be ensured. Otherwise, time-dependent calculations may be spoiled due to an inaccurate and unstable spatial discretization.

As far as the spatial discretization is concerned, generally a mesh is set in the domain of solution based on the assumption that any continuous quantity can be approximated by a set of piecewise continuous functions defined over a finite number of subdomains identified as elements or control volumes, although some research on spectral and other meshless numerical schemes has been done. We now survey the principal methods of discretization. With scarcely an exception, they can be regarded as variants of the methods of weighted residuals.

In these methods the field equations are written as

$$\mathbf{L} \cdot \mathbf{U} - \mathbf{f} = 0 \quad (16)$$

where  $\mathbf{L}$  is an operator,  $\mathbf{U}$  is the solution vector, and  $\mathbf{f}$  is a driving function;  $\mathbf{U}$  is then expressed as a sum of  $N$  modes of the form  $\sum a_n g_n$ , where  $a_n$  are constants and  $g_n$  are modal functions. Eq. (16) is weighted over the space  $\Omega$  of interest with respect to each mode  $g_n$

$$\int_{\Omega} (\mathbf{L} \cdot \mathbf{U} - \mathbf{f}) g_n dV = 0 \quad (n = 1, \dots, N) \quad (17)$$

thereby producing a weak-form solution with a given number of unknowns. The  $g_n$  depend on the method chosen (Finlayson, 1972).

### • Finite difference methods (FDM)

It is the oldest discretization method and has been used since (at least) 1908. The basic concept utilized in the method is purely mathematical. The differential operators in the governing equations (Eq. (10)) are directly transferred into their algebraic equivalents using truncated Taylor series expansions for the variables localized to a small region of the overall computational domain so that a set of governing equations for entire domain is discretized into a set of algebraic equations which relates the node values

with the neighbouring node values and can be solved in a straightforward manner.

FDMs have been successfully applied to the solution of a wide range of problems in continuum mechanics. However, the difficulties of handling arbitrary geometry and incorporating some boundary conditions, and the larger truncation errors for non-linear problems (first-order for convection terms) restrict their wider applications. Since there are many books on FDMs and a comparatively small use of them in computational rheology, we shall be brief here; a comprehensive review and extended discussion for viscoelastic calculations can be found in Crochet *et al.* (1984). It is worthy mentioning that attempts at developing second-order accurate discretization methods for constitutive equations have been made by Choi *et al.* (1988). They used an upwind corrected scheme explained in Peyret and Taylor (1983) to obtain results up to higher values of  $W_i$  compared to those obtained by the simple upwind differencing scheme. However, the attainable value of  $W_i$  is 1.5 for contraction flow of a Giesekus fluid which is rather low compared to those obtained by using the streamline integration procedure in the context of FEMs.

#### •Finite element methods (FEM)

The computational domain is divided into finite non-overlapping elements with any desired shape, and a set of proper shape functions, usually polynomials, is selected to approximate the real response of the subdomain in which the weighted residual technique or variational principle is applied to the discrete representation. Generally, the resulting discretized system of equations leads to a very large system matrix, which although it can be banded, is too large to store and compute in the case of large scale problems (see, Betlers, 1981), such as 3D viscoelastic flow problems. This is particularly true when a direct solver based on Gaussian elimination is used for solving the resulting system for a transient flow. However, the method has an inherent ability to handle complex geometry with accuracy, particularly for elliptic type problems.

For the problems involving strong convection, how to treat the convection term so that calculations are relatively free of false diffusion is one of the challenges. A number of upwinding schemes have been proposed, of which the most popular one is the streamline upwind Petrov-Galerkin (SUPG) method due to Brooks and Hughes (1982). In this method, a perturbation is added to the standard Galerkin weighting function so that false diffusion normal to the flow direction is minimised. However, a side product is an artificial diffusion directed along the streamlines. Thus, the quest to develop better formulation methods is far from ended.

The FEM has expanded very fast in the area of applications to viscoelastic flows. Since the first paper about the finite element simulation of flows with memory appeared (Kawahara and Takeuchi, 1977), it has quickly become the

most popular method in computational rheology. However, by the late 1970s, many workers were becoming frustrated by what quickly became known as the "High Weissenberg Number problem" (HWNP) - there was an upper limit on the value of  $W_i$ , above which the numerical algorithms failed. In 1984, Crochet *et al.* referred to it as "the outstanding problem in the numerical simulation of non-Newtonian flow".

Solutions to the HWNP have gradually evolved since 1977 (Tanner and Walters 1998). An early idea of importance was that of Crochet and Keunings (1980), who used a system of coupled equations. Here, the unknown pressure, velocity and stress components were solved for simultaneously, using Gaussian elimination. This led to a considerable advance in the critical value of  $W_i$  attainable (Crochet and Keunings 1982). The solution method was coupled to a Newton-Raphson scheme, which enabled accurate solutions to be made, once divergence had been avoided. A clear recognition of the source of the convergence problems began to appear. The *hyperbolic* nature of constitutive equations of the differential type was pinpointed and it was recognized as an important factor in the instability. Marchal and Crochet's (1987) work with the streamline upwinding (SU) demonstrated the necessity to design methods tailored to the hyperbolic character of the constitutive equations and a higher-order approximation for the stresses. Since then, extensive efforts have been devoted in developing new schemes which take into account the mathematical structure of the coupled system so as to improve the convergence properties of the whole system. Thus, many subsequent attempts have been focused on

- ensuring the momentum equation remains elliptic, such as those including: EEME (explicit elliptic momentum equation) of Renardy (1985) (also see King *et al.* 1988), EVSS (elastic viscous split stress) of Perera and Walters (1977) (also see Rajagopalan *et al.* (1990)), AVSS (adaptive viscoelastic stress splitting) of Sun *et al.* (1996), and
- the use of some specific stabilizing schemes designed for hyperbolic constitutive equations, such as application of the SUPG method in discretizing the constitutive equation (Marchal and Crochet 1987); the use of upwinding, discontinuous Galerkin (DG) or Lesaint-Raviart (Lesaint and Raviart 1974) methods (Fortin and Fortin 1989; Baaijens 1994; Fan, 1997)

A review on the recent advances in this area has been given by Baaijens (1998). We will not repeat it here.

#### •Boundary element methods (BEM)

In the FEM and FDM, one finds the complete solution field in all of fluid-filled region whether or not this is of interest. In some problems only the domain shape and/or the pressure losses may be needed, and it is therefore interesting to look at the BEM and its derivatives which avoid evaluating all of the internal variables, at least for linear

creeping flow problems. Essentially, the techniques are derived from reciprocal theorems familiar in linear elasticity, combined with a knowledge of the relevant Green's function. While the scheme works very well for linear and mildly nonlinear problems, it does not cope well with highly nonlinear viscoelastic problems, steady or unsteady; see Tanner (2000) for a more extended discussion. Hence we shall not discuss it further.

•Spectral methods

In these methods the solution vector does not contain nodal values of the velocity and other variables. Gottlieb and Orszag (1977) describe the method using as an example the solution of the heat diffusion equation by a truncated Fourier series. Consider the equation [for  $u(x, t)$ ]

$$\frac{\partial u}{\partial t} = Lu + g(x, t), \tag{18}$$

where  $L(x, t)$  is a linear spatial differential operator and  $g$  is a known driving function. Appropriate boundary and initial conditions are also required. An approximate solution is sought in the truncated series form

$$u_N(x, t) = \sum_{n=1}^N a_n(t)\phi_n(x). \tag{19}$$

The  $\phi_n$  are linearly independent functions (Fourier components, polynomials, Chebyshev series, for example) and the Galerkin weighting process applied to Eq. (18) produces the results ( $n = 1, \dots, N$ )

$$\frac{d}{dt}(\phi_n, u_N) = (\phi_n, Lu_N) + (\phi_n, g), \tag{20}$$

where  $(\phi, u) = \int \phi u dx$ ; the integration is taken over the space of interest.

Eq. (20) can then be used to solve for the coefficient functions  $a_n$ . Non-linear problems can also be “discretized” by this method; in a steady flow situation this yields a set of (non-linear) simultaneous equations for the time-independent  $a_n$  which needs to be solved.

Pilitsis and Beris (1989) have used a mixed pseudo-spectral finite difference method to demonstrated the ability of this high-order approximation for non-Newtonian flow calculations, and Dimitropoulos *et al.* (1998) have used this method to investigate turbulent flow of elastic liquids, which is a fully three-dimensional unsteady flow. See also Atalík and Keunings (2002).

Van Kemenade and Deville (1994) applied a spectral method for simulating steady-state two dimensional (2D) creeping flows of a Maxwell fluid in corrugated geometries. They have demonstrated that the convergence of the method with respect to the polynomial degree is of high order. The Weissenberg number reached in their calculations was about 14.

A high degree of efficiency of convergence in computing time (exponentially rapid convergence) compared to lower

order FEMs is achieved by the hybrid spectral/FEM with high-order polynomial degree of the approximating functions (Beris *et al.*, 1987). Beris *et al.* (1992) has used the method to analyze Taylor-Couette flow instabilities with the Giesekus model. With the method, sufficiently accurate solutions can be reached without need of the use of an upwind scheme to ensure the stability (for example, Talwar *et al.*, 1994). However, with the method, the geometry of the flow domain is necessarily limited to be a smooth one. The use of the domain decomposition and the EVSS-like fractioning of stress tensor have widened the range of accessible problems with the technique (Talwar and Khomami, 1995).

The main advantage of spectral methods lies in their accuracy (for a given number of unknowns) but they are geometrically relatively inflexible and often do not work satisfactorily on problems with sharp boundary wall corners pointing into the flow (salient points).

•Finite volume methods (FVM)

These methods can also be regarded as variants of the methods of weighted residuals. First, the entire computational domain is subdivided into finite non-overlapping control volumes over which the weighted functions  $g_n$  ( $n = 1, 2, \dots, N$ ) are chosen so that they are assumed a value of one for a certain control volume  $\Delta V$  interested, and zero in the rest of control volumes. We have:

$$\int_{\Delta V} (LU - f) dV = 0 \tag{21}$$

over a control volume. By implementing the integration in which, instead of using directly truncated Taylor series expansions to the differential governing equations as in FDMs, the conservation laws expressed by the integral mass, momentum and energy equations are applied over a control volume. Therefore, the resulting linearized algebraic equation relating the centred value of each dependent variable  $\Phi$  for each control volume with the values at its neighbouring nodes  $nb$  can be cast as:

$$a_p \Phi_p = \sum_{nb} a_{nb} \Phi_{nb} + S_c \tag{22}$$

This has a physically meaningful interpretation, and thus, a more conservative solution is expected. Here, P denotes the centre of the control volume and  $S_c$  contains all the terms that are not explicitly related with  $\Phi$ . Another attractive feature in this formulation is that the resulting discretized system of equations leads to a well-structured system matrix, tridiagonal for a structured mesh, for example. For solving this type of system, some efficient iterative solvers can be used, such as TDMA (Tridiagonal Matrix Algorithm) in which the number of operation is proportional to the number of unknowns, rather than the cube of them in full matrix Gauss elimination, thus much less CPU time consumption is expected.

FVMs have been widely and successfully used in New-

tonian flow and heat transfer computations, particularly at high Reynolds numbers (Patankar, 1980).

However, their applications to viscoelastic flow computations only appeared in the 1990s, and early applications extended directly from Newtonian calculations were characterized either by poor accuracy or numerical instabilities due to the use of first-order upwinding schemes (Hu and Joseph 1990; Sasmal 1995) for discretizing the constitutive equation or due to violation of the criterion of boundedness (Na and Yoo 1991; Yoo and Na, 1991; Darwish *et al.* 1992).

A series of works based on an implicit finite volume formulation by Xue *et al.* (1995; 1997; 1998a, b; 1999a, b) for fully 3D viscoelastic complex flow simulation demonstrated that the formulation is indeed an efficient and stable method to carry out 3D viscoelastic calculations on ordinary work stations. However, as pointed out and assessed by Xue *et al.* (1998a; 2001; 2002), with a first-order upwinding scheme for discretization of convection terms, it is inevitable that severe false diffusion is introduced whenever the flow streamlines are not closely aligned with the grid lines, or localised high-convection is dominant. Thus, a higher order scheme should be used to eliminate numerical diffusion for enhancing spatial accuracy. This is particularly true for hyperbolic type constitutive equations with strong nonlinear sources or sinks involved. However, with higher order schemes, the boundedness of the solution is another important issue. In simulating plane 4 to 1 contraction flows of UCM and PTT fluids, Oliveira and Pinho (1999) showed that spatial accuracy of the solutions could be improved by using a second-order linear-upwind differencing (LUDS) compared to direct application of the first-order upwinding scheme for discretizing convective terms, but this is achieved at the expense of worse convergence with increasing  $W_i$ . As pointed by Xue *et al.* (2001; 2002): for a hyperbolic equation, such as the momentum equation in convection dominant Newtonian flows, or the constitutive equation, the first-order upwinding scheme guarantees bounded solutions, but yields poor accuracy; while a higher-order scheme enhances the accuracy, but may produce oscillations or numerical divergence. To ensure the boundedness of the solution as well as the same order accuracy over the entire domain whenever a higher-order scheme is used, one of the effective measures is to use the deferred correction. The criterion of Gaskell and Lau (1988) ensures the boundedness, but the global accuracy may be degraded due to the necessity of switching scheme locally from a higher-order one to a first-order one as experienced by Alves *et al.* (2000).

Indeed, with the use of high-resolution schemes, as demonstrated by Alves *et al.* (2001), the numerical performance of FVMs in terms of stability and accuracy can be comparable to those with highly accurate finite element techniques, such as h-p refinement techniques (Fan *et al.*,

1999). This was also found by Luo (1996) who used a finite volume formulation to discretize the field equations under creeping flow condition (free of convection); but a different formulation (the strain tensor tracking algorithm developed by Luo and Tanner (1989)) for the integral viscoelastic models. It was found that the method gave better computing stability and solution smoothness than its finite element counterpart when simulating the axisymmetric contraction flow problem.

So far, we have discussed the issues about efficiency, accuracy and stability of a finite volume formulation. Yet, there are some disadvantages of the formulation in treating complex geometry and traction boundary conditions. Some efforts have been made either by using an unstructured mesh (Huang *et al.*, 1996) for 2D and 3D (Xue, 1997), or using boundary-fitted non-orthogonal grids (Oliveira *et al.*, 1998). Further work is necessary in these areas.

## 5. Solution algorithms

In the previous section, we dealt with the review of the discretization schemes of a general conservation equation. However, as seen, the solution for coupled non-linear equations governing incompressible viscoelastic flows cannot proceed without finding an independent equation for the pressure by enhancing the mass conservation via the continuity constraint. In addition, how to treat the implicit and nonlinear coupling is of importance for efficient, accurate and stable calculations.

There are two types of methods to treat the coupling. In the first, the so-called coupled method in which all variables are solved simultaneously, using Gaussian elimination. In the other, each equation is solved for its dependent variable by successively substituting the other variables with their latest currently available values. The procedure is repeated until all equations are satisfied. This procedure is called the decoupled method. The two approaches may be mixed.

For time-dependent flow calculation, the above procedures will be repeated either implicitly or explicitly for each time step.

Each discretization method has its adherents. For example, finite difference and finite volume methods usually use decoupled methods and an iterative procedure (or at most, a tridiagonal algorithm) to solve the equations. In finite element procedures using differential models, the tendency has been to use coupled solution method (Crochet and Keunings, 1980; 1982).

One of the advantages of the coupled technique is that Newton's iterative scheme can be used, which gives a quadratic convergence rate for the solution if the initial estimates are chosen sufficiently close to the solution, and if the system matrix is non-singular (Keunings, 1989). With the coupled technique, however, a larger global matrix and



longer solution vector for a given number of elements (containing an extra three stress variables for a 2D problem and six for a 3D problem) have to be constructed so more core memory and CPU time are required, thus obstructing its applications to 3D transient flow problems with available computer resources.

To improve the efficiency and stability of FEMs in terms of fast convergence rate and less number of degrees of freedom (DOF) as well as accuracy, several attempts have been made. Among others, it is worth mentioning an iterative method proposed by Fortin and Fortin (1990) based on the GMRES (Generalized Minimal RESidual) method developed by Saad and Schultz (1986). The advantage of the method is that the construction and factorization of a global matrix are not required and only the residual has to be computed and stored. The method has been refined by Fortin and Zine (1992) and modified by Gu enette and Fortin (1995) for other types of models. The method is efficient compared to the direct schemes based on a modified frontal method for the stick-slip problem and contraction flow problem as shown by Tsai and Liu (1996) in their comparison work.

The time-dependent EEME (the explicitly elliptic momentum equation) formulation for the UCM model was first used by Northey *et al.* (1990; 1992) by combining finite element discretizations in space with the implicit Euler finite-difference approximations for time derivatives. The start-up of flow of a UCM fluid between concentric and eccentric rotating cylinders has been calculated and numerical results demonstrated that this method has excellent stability characteristics. The linear stability analysis carried out with the method for axisymmetric Taylor-Couette flow of viscoelastic fluids between parallel cylinders was able to reproduce the oscillatory linear instability beyond a critical Deborah number  $De_c$  as analyzed by Larson *et al.* (1990). However, many fully-coupled methods are computationally expensive because a larger system of linear equations has to be solved at every Newton iteration for each time step.

An alternative is to solve the two types of equation separately. One can find a velocity field either by coupled methods (Sun *et al.*, 1996) or decoupled methods (Xue *et al.*, 1995) for a Newtonian flow, then compute the stresses, and iterate back and forth between the sets of equations by treating the viscoelastic stress in the momentum equation as a pseudo-body force acting on the Newtonian fluid. This leads to smaller matrices at each step for coupled method, thus much less expensive than its fully-coupled counterpart. It was found (Harlen *et al.*, 1995) that if a coupled method is used for velocity and pressure calculations, and a Lagrangian method for stress calculations, the computational cost of each time-step is greatly reduced, and it was found that 95% computational effort is in the solution of the FEM for the velocity and pressure.

With a decoupled strategy, convergence can be a prob-

lem. But, it allows the constitutive equation to be solved by using some more suitable method, such as the method of characteristics (Kabanemi *et al.*, 1994; Petera, 2002). For integral models, one is forced to use this iterative (Picard) procedure.

Therefore, it seems that for transient viscoelastic flow calculations, decoupled methods are more feasible than fully-coupled methods. Hence, we will concentrate our review on the solution strategies based on decoupled methods.

Methods to solve the linear set of algebraic equations resulting from the fully-coupled Newton method by preconditioned, preferably matrix-free, iterative solvers like GMRES have received little attention yet, but could be useful in solving three-dimensional steady and unsteady viscoelastic flow problems: see Tsai and Liu (1995).

#### •Explicit time advance schemes

Two of the most widely used methods in computational fluid dynamics (CFD) are the Marker and Cell (MAC) method proposed by Harlow and Welch (1965), and the so-called artificial compressibility method due to Chorin (1967). In both methods, the integration in time is carried out explicitly either with the first-order Euler method (for the former) or a higher-order Runge-Kutta method (for the latter), and the resulting discretized equations are solved in a time-marching manner.

The former was originally developed for solving an unsteady free-surface flow of incompressible fluid. A Poisson equation for the pressure is derived by taking the divergence of the momentum equation and fulfilling the continuity constraint. This method has been used for time-dependent viscoelastic flows by Sato and Richardson (1994a) for solving momentum and continuity equations in the context of a FEM and by Mompean and Deville (1997) for solving the whole set of the governing equations in the context of a FVM.

The Chorin scheme is a pseudo-transient formulation method. In this method, by assuming the fluid to be slightly compressible, a dynamic equation for the pressure is created by substituting the density as a function of the pressure. In this way, a system of parabolic-hyperbolic equations governing the flow has been changed to a purely hyperbolic system as

$$\frac{\partial \Phi}{\partial t} = F(\Phi) \quad (23)$$

where  $\Phi$  is the field variable vector which includes three velocity components, six stress components and the pressure for 3D cases. As a result, it is not necessary to solve a Poisson equation for the pressure at each time step, and the steady state solution is considered as the asymptotic solution of time-dependent problems. This method is very commonly used in CFD dealing with high Reynolds number flows. However, this method is more suitable for the calculations

where the purpose is to obtain an asymptotic steady solution, since the true transient equations are not solved.

Phelan *et al.* (1989) have developed this method to predict the velocity and stress fields in a square cavity of a UCM fluid; the convergent solutions with mesh refinement were limited to  $D_e = 4$  due to heavy computational expenses associated with the method (not numerical instability).

A similar scheme was used by Jin *et al.* (1994) in the context of a finite volume formulation with unstructured grids for spatial discretization, and a standard fourth-order Runge-Kutta algorithm was used in the explicit time-stepping scheme for solving each of the hyperbolic equations. The performance of the scheme was investigated by carrying out the stick-slip problem for the modified UCM fluid. The  $W_i$  number attainable was only 2.2 due to the poor spatial accuracy used.

Olsson (1994) used a similar strategy to develop a solver for computing time-dependent 2D viscoelastic flows based on second-order finite differences on composite overlapping grids. We note that in this formulation, the first-order operators (convection terms) were discretized using a centred difference scheme, and for the time integration, a second-order explicit method was used, which may cause numerical instability problems. Some interesting transient phenomena were presented including a numerical study of a channel flow with a cylinder, a contraction flow and a paper-coating flow with the fluid modelled by UCM, Oldroyd-B and Giesekus constitutive equations.

The explicit time-marching method is expensive for large scale problems with acceptable accuracy because time steps are constrained by the CFL condition, although some measures have been developed to accelerate the convergence rate, such as the adaptive step size control scheme of Press *et al.* (1986). More importantly, as analyzed by Xue *et al.* (2002), from the numerical stability point of view, the explicit time-marching method is not suitable for solving the hyperbolic constitutive equation.

**•Implicit pressure-correction methods**

Due to their unconditional stability (less stringent time step restrictions), implicit schemes seem frequently favoured over their explicit counterparts, particularly if one is looking for steady and slow-transient flows in which larger time steps are usually used for efficient calculations.

Like the MAC method, most of the implicit algorithms were based on pressure correction procedures. That is, the continuity of the flow field at each time step (each outer iteration for steady solvers) is enforced via a pressure correction so that the resulting pressure relation, which couples the pressure and the velocities, replaces the continuity relation; and the momentum equations retain their role for determining the velocity field.

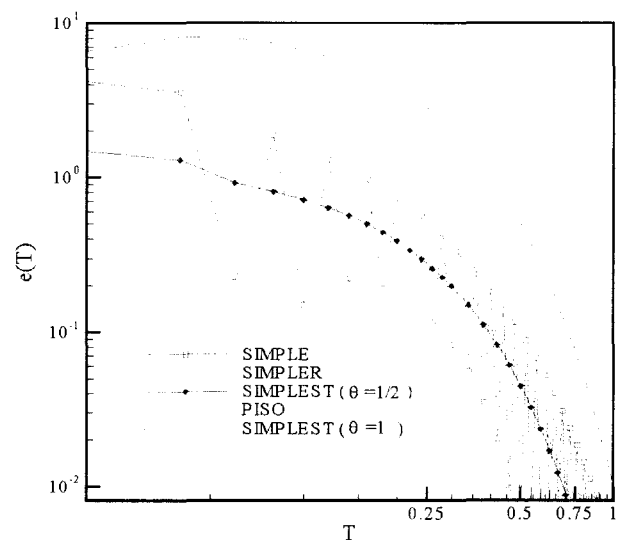
The two most popular implicit algorithms for solving the pressure-velocity coupled system are SIMPLER (Semi-Implicit Method for Pressure-Linked Equations Revised)

due to Patankar (1980) and PISO (Pressure-Implicit with Splitting of Operators) of Issa (1985).

Gervang and Larsen (1991) used the PISO algorithm to simulate the secondary flows in straight ducts with rectangular cross section of a CEF fluid (see, Criminale *et al.*, 1958).

After analyzing the shortcomings existing in the above two algorithms, Xue *et al.* (1995) proposed a more efficient and stable implicit algorithm called SIMPLEST (SIMPLE with Splitting Technique), and have applied it successfully to both steady and transient computations of 3D viscoelastic flows by a decoupled technique.

The method adds an additional step to the SIMPLER algorithm so that the velocity and pressure fields are made to satisfy one and the same momentum equation at the end of each time-step, and the pressure correctors are used to correct the velocity field only. As a result, an improved temporal accuracy for time-dependent problems is ensured even for large time steps; and iterations for convergence and the need for under-relaxation for steady-state problems are greatly reduced. Xue *et al.* (2002) have compared the numerical performance in terms of efficiency and accuracy for four different implicit algorithms, namely, SIMPLE, SIMPLER, SIMPLEST and PISO. They found that in calculating the start-up of plane Poiseuille flow of a Newtonian fluid at  $Re = 0.05$  over a given mesh size, a time step for stable calculations is  $4.65 \times 10^{-3}$  according to the CFL condition if an explicit method is used. For the four implicit algorithms, they are 0.02, 0.11, 0.5 and 0.56, respectively. With the allowable time steps, the numerical accuracy with respect to time is clearly demonstrated in Fig. 3 where the evolution of relative error  $e(T)$  of cen-



**Fig. 3.** Evolution of relative error  $e(T)$  of the centreline velocity over time  $T$  for Newtonian calculations for different implicit solution algorithms

time velocity over non dimensional time  $T$  for the four different implicit algorithms is shown.

An implicit iteration pressure correction procedure used by Oliveira (2001) is more or less like the SIMPLE algorithm with 3 to 5 extra outer iterations used in each time step to meet a convergence criterion.

#### •Operator splitting (OS) methods

Operator splitting methods (Glowinski and Pironneau, 1992) treat nonlinearity and incompressibility in Navier-Stokes equations separately by 'splitting' operators  $A_c(t, U)$  and  $A_d(t, U)$  in Eq. (11) with a fractional time stepping strategy. As a result, the problem of solving a system of equations is broken into much simpler sub-problems: one of convection-diffusion type and one close to the steady Stokes problem, which can be solved accurately and efficiently by applying dedicated solvers designed for the specific type of the sub-problem at each fractional time step.

The three-step  $\theta$ -method (Glowinski and Pironneau, 1992) is the most popular one in terms of accuracy and convergence. It is possible for the method to produce the results with second-order accuracy in time if the splitting parameters are properly chosen.

This method was first used by Singh and Leal (1993) for simulating the start-up of viscoelastic fluids in eccentric rotating cylinders. Saramito (1994; 1995) used the method (also see, Saramito and Piau, 1994) to simulate steady-state planar contraction flow calculations of a PTT fluid, and demonstrated that the method is much more efficient than other algorithms: the Picard method (50 times faster) and the GMRES method (5 times faster) (Fortin and Zine, 1992). The flow of a UCM fluid around a sphere in a tube was calculated by Luo (1996; 1998) with this method, and steady state solutions with  $W_i$  up to 2.8 were obtained. Recently, Sureshkumar *et al.* (1999) used the method for time integration combined with finite element spatial discretization to explore the linear and non-linear dynamics of UCM/Oldroyd-B fluids in 2D Couette flow and flow past a linear, periodic array of cylinders in a channel. Somasi and Khomami (2000) applied this method to the CONFFESSIT (calculation of non-Newtonian flow: finite elements and stochastic simulation techniques).

Besides the three-step  $\theta$ -method, Glowinski and Pironneau (1992) also described a two-step operator splitting method forming the basis of a number of ODE-type methods for time dependent viscoelastic flows. Essentially, this operator splitting method is a method of characteristics. In this method either a discrete particle is traced back in time and space or a pure convection problem is solved. However, this method only has first-order accuracy in time.

#### •Hybrid schemes in terms of discretization and solution methods

In order to solve time-dependent viscoelastic flow problems accurately and efficiently in terms of computation

time consumption and memory storage requirement as well as numerical stability, the above discretization methods and solution algorithms may be mixed according to the features of the equation to be solved. The operator splitting methods are examples.

A split Lagrangian-Eulerian method was developed by Harlen *et al.* (1995). In this method, the solution for the velocity and pressure from the momentum equation is split from the solution for the stresses from the constitutive equation. A standard mixed FEM for a Stokes flow subject to a body force was used for solving the momentum equation in an Eulerian frame. The constitutive equation is solved in a co-deforming frame in which the axes move and stretch with the fluid so that stress tensor can be found by solving an ordinary differential equation by the explicit forward time-stepping way or an implicit scheme.

To circumvent the stability problems associated with upwind biased interpolation schemes, and the difficulties introduced by Lagrangian methods due to large deformation of a set of fluid particles, a semi-Lagrangian approach in the context of FVM has been developed by Phillips and Williams (1999) for time-dependent viscoelastic flow problems. In their method, they adopted the splitting idea to decouple the treatment of the convection terms from the remaining terms, and the remaining terms in the governing equations are treated implicitly and discretized by integrating over the control volume modified after tracing particles on a regular grid of points backwards over a single time-step to their departure points based on the Lagrangian approach. The method is only first-order accurate in time, and the  $W_i$  attained for 4 to 1 planar contraction flow of an Oldroyd-B fluid was  $W_i = 2.5$  with a very small time-step ( $8 \times 10^{-5}$ ).

Sato and Richardson (1994a) developed a hybrid FE/FV method in which a time-explicit FE method for momentum and time-implicit FV for pressure and stress of cell-centred type. The method was tested by carrying out the start-up of planar Poiseuille flow of UCM and Oldroyd-B fluids. However, because the method is explicit and first-order accuracy in time, the time-step allowable is constrained by the CFL stability condition.

A Taylor-Petrov-Galerkin algorithm (a semi-implicit time-stepping Taylor-Galerkin/pressure-correction method (Donea, 1984) in conjunction with the consistent SUPG scheme for spatial discretization) was proposed by Carew *et al.* (1993) for solving both transient and steady state viscoelastic flow problems. In this method, in each time step, a Lax-Wendroff time-stepping scheme based on a Taylor series expansion in time was employed as a predictor-corrector, followed by a two-step pressure-correction approach (Van Kan, 1986) to handle the incompressibility constraint. Thus, the coupled equation system in each time step is segmented into a number of fractional-staged equations to be solved in sequence. The Galerkin test function for the

momentum equations and Petrov-Galerkin test function for the constitutive equations were adopted for spatial discretization. This time-stepping scheme has a predominantly explicit form, yet incorporates a semi-implicit Crank-Nicolson treatment for diffusion terms only. The method was claimed to have second-order accuracy in time for the momentum equation, but only first-order accuracy for the constitutive equation due to its explicit features. The method was extended to 3D viscoelastic 40:3:3 expansion flow calculations (Baloch *et al.*, 1996) with the PTT model.

Based on the two methods above, a new hybrid FE/FV scheme for spatial discretization was proposed by Wapperom and Webster (1998). In this method, like Sato and Richardson's hybrid strategy, a cell-vortex FV scheme is used for the constitutive equation, but a FE discretization (semi-implicit Taylor-Galerkin/pressure correction) is used for both continuity and momentum equations. They carried out calculations for three test flows which are ultimately becoming steady-state for an Oldroyd-B fluid: smooth start-up channel flow, flow past a cylinder with steep gradients and non-smooth contraction flow with a sharp corner (Wapperom and Webster, 1999; Aboubacar and Webster, 2001). It was reported that a considerable gain in efficiency per time step can be obtained compared to an alternative pure FE implementation, but it is more stable than the pure FE alternative for smooth flows, and less for non-smooth flows. It seems that the method is not very promising because they could only reach a value of  $W_i$  of order of  $O(1)$ . They attributed the instability to the coupling process, not the spatial discretization schemes, but it could be due to the overestimation of the pressure in the SIMPLE-like solution algorithm, and the explicit method for constitutive equations.

### 6. Transient viscoelastic flow calculations

Although a number of methods have been reported for numerical simulation of time-dependent viscoelastic flows, most of them used temporal discretization as a means of obtaining an asymptotic solution of a flow which is ultimately steady. That is, the time term is functioning as an underrelaxation factor to help the calculations.

There are a few works in which the evolution of the solution with the time is presented.

#### •Start-up flows

For an initial problem, truly transient behaviour is determined by its initial conditions. Therefore, it is inappropriate to assess the accuracy of a numerical method by comparing with experimental observations in a complex flow. However, with one dimensional or quasi-one dimensional simple flows where base flow solutions are available in closed form, the numerical accuracy with respect to time can be easily evaluated by investigating the start-up or

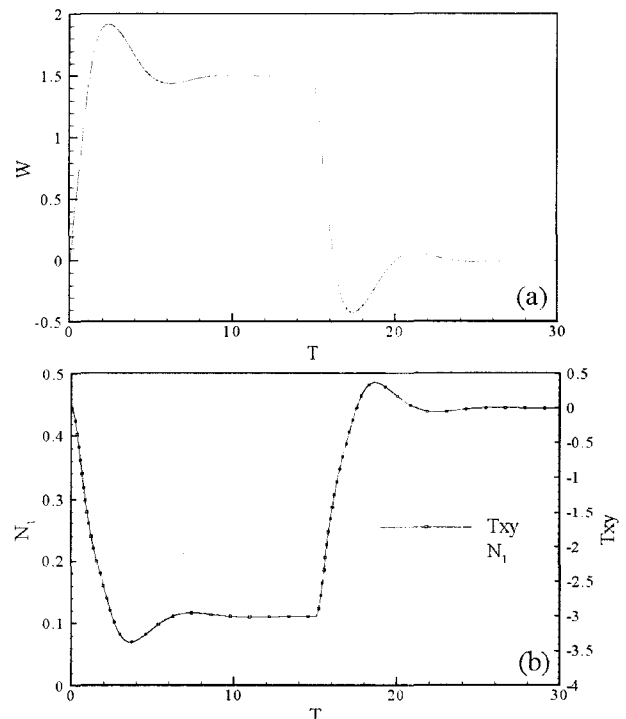
decay process of a flow for which both numerically and experimentally, initial conditions can be specified as quiescent.

The start-up or decay of planar Poiseuille flow of Oldroyd-B or UCM fluids is an excellent test problem for evaluating the accuracy of transient numerical methods because it is one of the few transient viscoelastic flow problems for which analytic solutions are available under some conditions.

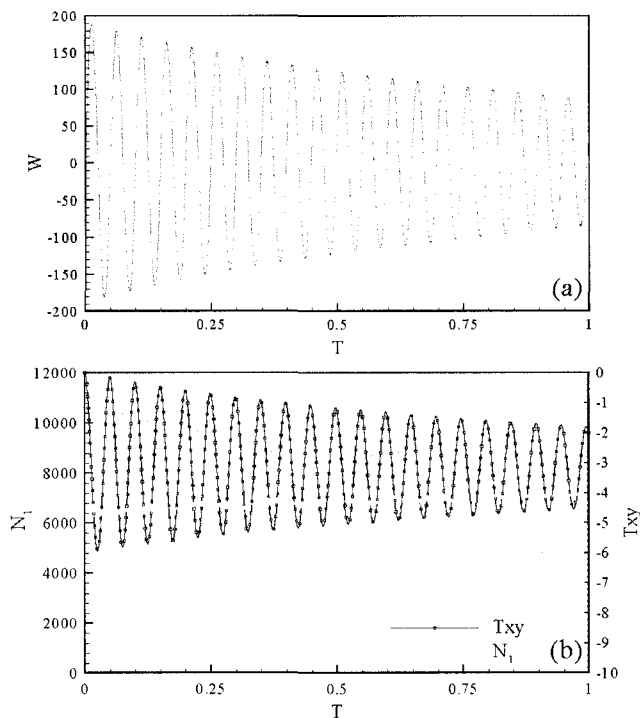
Serdakowski and Caswell (1988) accurately predicted the start-up of planar Poiseuille flow of UCM and Oldroyd-B fluids by using their Eulerian-Lagrangian implicit time marching scheme. However, due to the improper decoupling (Northey *et al.*, 1990), the calculations were limited to a very low value (order of 1) of  $W_i$ .

Sato and Richardson (1994) tested their hybrid FE/FV method with the same problem. They did not experience an upper limit on  $W_i$ , but the numerical results were not very smooth.

Very smooth results were obtained by Xue *et al.* (2002) with a time-dependent implicit finite volume formulation which is third-order accurate in space and second-order accurate in time. The evolution of the centreline velocity (Fig. 4(a)) and the first normal stress difference and shear stress (Fig. 4(b)) on the solid wall over time during start-



**Fig. 4.** Evolution of (a) centreline velocity, (b) first normal stress difference (left), and shear stress (right) on the solid wall with time during start-up and decay of planar Poiseuille flow of a UCM fluid at  $R_e = 0.05$  and  $W_i = 0.02$  ( $T$  is non-dimensional time  $t/\lambda$ ).



**Fig. 5.** Evolution of (a) centreline velocity, (b) first normal stress difference (left), and shear stress (right) on the solid wall with time during start-up of planar Poiseuille flow of a UCM fluid at  $R_e = 0.05$  and  $W_i = 300$ .

up and decay of planar Poiseuille flow of a UCM fluid at  $R_e = 0.05$  and  $W_i = 0.02$  is presented in Fig. 4 (non-dimensional time step used is  $10^{-2}$ ). As seen, compared to the results presented by Sato and Richardson (1994) in their figure 2, there are no localized oscillations near the peaks at all.

Also, no limitation on the value of  $W_i$  was experienced in those calculations. In Fig. 5, the numerical predictions for a UCM fluid at  $W_i = 300$  and  $R_e = 0.05$  are presented. This represents a relaxation time  $\lambda = 1500$  (s) for the fluid at the non-dimensional mean velocity  $W_m = 0.1$  in the channel with height being 1. A non-dimensional time step  $10^{-5}$  is used for this calculation, which indicates the non-dimensional time step for solving the momentum equation is  $1.5 \times 10^{-2}$ .

Here we must point out that one-dimensional or quasi-one dimensional simple flows can only be used for testing the accuracy with respect to time of a solution algorithm. The numerical performance may be degraded in multi-dimensional complex flows, such as spatial oscillations due to improper spatial discretization for a particular solution algorithm.

#### •Sphere falling in a tube

A sphere falling along the axis of a cylindrical tube (with a blockage ratio of 2) filled with a viscoelastic liquid is one of the benchmark problems for transient viscoelastic flow

calculations. It was reported that even at rather low Deborah numbers, instabilities in flow field may occur (Bisgaard, 1983).

With an integral model, Rasmussen and Hassager (1993), and Rasmussen (1999) applied a Lagrangian method to study the start-up of the flow. A smooth temporal development of drag coefficients up to  $W_i = 0.8$  was obtained with a UCM fluid. Recently, by using a time dependent Eulerian technique for implementing integral model, Peters *et al.* (2000) obtained smooth solutions with the value of  $W_i$  up to 1.8.

However, with a differential model, the results are not so promising. Bodart and Crochet (1994) applied a fully coupled implicit FEM. They presented the time-dependent sphere velocity in a UCM and Oldroyd-B fluid. Overshoots and oscillations about the terminal value are predicted as observed by Becker *et al.* (1994) with a larger blockage ratio. In their calculations, the time needed to reach the steady-state increases with  $W_i$  and the maximum value of  $W_i$  reached with the UCM model is less than 1. Similarly, Harlen *et al.* (1995) applied a split Lagrangian-Eulerian method for the same problem, but numerical noise increases dramatically when  $W_i$  is beyond 0.6.

Interestingly, the critical values of  $W_i$  reached in most of the steady state calculations with a differential model on this problem are over 2.0 (see Warichet and Legat, 1997; Fan *et al.*, 1999 and the review by Baaijens, 1998) although mesh convergence of solutions at Weissenberg numbers beyond 2.0 has not been convincingly demonstrated. Recently, Petera (2002) used a time-stepping algorithm in which the momentum equation is solved in the Eulerian framework, and the Lagrangian approach is applied for the solution of hyperbolic constitutive equations. A stable solution with the values of  $W_i$  up to 6.6 was obtained. But, judging from the patterns of the velocity vector near the downstream stagnant point presented, we cannot say the results are convincing.

#### •Contraction flow

Sato and Richardson (1994a) applied their hybrid FE/FV method to carry out planar 4 to 1 contraction flow of an Oldroyd-B fluid with the value of  $W_i$  up to 2 at which the flow is supposed to be ultimately steady. In order to investigate the vortex-behaviour mechanism in this flow, they demonstrated the transient vortex behaviour near the sharp corner. However, the transient behaviour was induced by instantaneous increase of  $W_i$  from 1 to 2, which cannot be regarded as truly transient simulations.

Olsson (1994) used a time-dependent solver based on an artificial compressibility method to simulate the flow of a Giesekus fluid in a planar 4 to 1 contraction with a rounded re-entrant corner. The results shown for different times indicated that the vortex builds up from just below the re-entrant corner, then grows until it occupies the corner.

Recently Bishko *et al.*, (1999) applied the split

Lagrangian-Eulerian method (Harlen *et al.*, 1995) to simulate the transient flow of branched polymer melts in a planar 4 to 1 contraction using the pom-pom model (McLeish and Larson, 1998). The streamline patterns at different times for  $W_i$  up to 3 were presented.

#### •Flow past a cylinder

Olsson (1994) presented some interesting transient phenomena of an unstable character for a Giesekus fluid in a channel flow past a cylinder located near one of the walls. It was demonstrated that for the flow conditions under which the flow converges to a steady state immediately after the startup time for Newtonian fluid, pronounced unstable behaviour in a flow for the viscoelastic fluid is in evidence.

Oliveria (2001) applied a finite volume formulation with a second-order backward difference scheme for the time derivatives to simulate the flow around a cylinder in the range of higher  $R_c$  (50-120) where the flow becomes time periodic with vortex shedding. The viscoelastic fluid is described by the modified Chilcott-Rallison model (see Coates *et al.*, 1992). The numerical results agree with experimental observations. That is, the frequency of vortex shedding is attenuated by elasticity of the fluid, and the size of the formation zone behind the cylinder is elongated.

#### •Free surface flows

To our knowledge, the first paper dealing with the simulation of transient viscoelastic flows with free surface is due to Keunings (1986). The numerical technique is based on a Galerkin/Finite Element discretization of the governing equations combined with a first-order implicit (Euler backward) scheme for the integration in time. At each time step, the flow field and the location of the free surface are first predicted explicitly by means of a first-order extrapolation, and then corrected by implicitly solving the discretized governing equations with the Newton-Raphson iterative technique. The method was applied to the simulation of jet breakup into droplets caused by capillary forces for a fluid described by the Oldroyd-B model.

The MAC method has been extensively used for transient Newtonian and generalized Newtonian flows (Tomé *et al.*, 1996) involving free surfaces. However, we have not seen any application in the cases involving viscoelastic fluids, which may mainly be due to the difficulty of boundary treatment for the free surfaces.

The so-called fringe element generation method was developed by Sato and Richardson (1994b) to treat moving free surface problems. By generating new fringe elements at the fringe of the free surface temporarily at each time step, the element faces coincide with the edge of the fluid. As a result, the boundary conditions for the free surface are accurately satisfied along the whole surface in the finite element formulation for the momentum equation. With this treatment incorporated into their hybrid FE/FV method, they are able to simulate filling flow in injection moulding

for viscoelastic fluids.

To close, we may also note that Taylor-Couette instabilities were numerically investigated by Beris *et al.* (1992) and Northey *et al.* (1992).

## 7. Conclusions

For a long time it was difficult to achieve *stability* in computations with highly viscoelastic flows, as detailed in this review. Now the HWNP has been at least partially solved, particularly in steady state calculations. However, accurate predictions are still not always guaranteed, especially in transient flow simulations for which one must not confuse computational instability with a real physical instability occurring in flows.

It seems very straightforward to extend the formulations for steady state calculations to the case of transient flows in confined geometries by discretizing the partial time derivatives over time by means of standard techniques. However, a convergent solution may be obtained in a method for steady state calculations, but it could be divergent for a transient calculation if the temporal discretization scheme or the time advancing solution method used is improper. Numerical stabilities can be determined by the time step chosen according to the stability condition and the spatial discretization method as well as the solution method.

As far as numerical accuracy in space is concerned, generally, in the limit of an infinitesimal mesh size, the algebraic equations produced numerically should reduce to the exact partial differential equations. The accuracy of a solution can usually only be judged by reducing the mesh size, adding more modes in the spectral method, or by using more complex interpolations in the elements. Usually, one plots some measure of the change in variables against mesh size. The convergence rate can then be seen, and accurately established. Richardson extrapolation (Roache, 1998) can also be useful.

One should not confuse accuracy with the iterative convergence obtained by iteration on a fixed grid, which is necessary to solve the non-linear equations. Often iterative convergence can be driven down to machine accuracy ( $10^{-15}$ ) and is not related to the overall accuracy of the computation.

For a transient flow calculation, the long time accuracy is determined by the spatial accuracy, but the short time numerical accuracy is determined by the temporal discretization method. Therefore, to accurately and efficiently capture a transient process, the techniques used for temporal discretization should be at least second order. For spatial discretization, the features inherent in the governing equations must be considered. The major challenge is how to ensure the boundedness of the resulting system of discretized equations without numerical diffusion.

In order to predict the flow instabilities observed exper-

imentally in many apparently steady 2D viscoelastic flows (McKinley *et al.*, 1996; Stokes *et al.*, 2001), it is necessary to perform 3D transient viscoelastic flow calculations with more realistic constitutive models. For doing this, decoupled methods are more realistic from the feasibility point of view, and an implicit method is a better choice than its explicit counterpart from the numerical stability point of view. However, unless we can attain *numerical stability* with accuracy in transient computations (stable numerical results under experimental conditions) we cannot tell whether or not the mathematical model is adequate for describing the real flow system.

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