4. Existing Numerical Algorithms

This chapter provides a short overview of the algorithms developed so far to solve viscoelastic fluid flows. These methods may be divided into two classes: those which aim to solve the steady flows and those which try to simulate time dependent behaviour. Furthermore, a distinction can be made between the methods with which the problems are tackled: finite element methods, finite difference/volume methods and spectral methods. This chapter does not aim to give a historical overview, but merely presents, succinctly, some commonly accepted methods for solving viscoelastic flows. The most interesting point in this chapter is to figure out what the limitations of the methods are and how the methods have been improved over the past 10 or 20 years in order to reach higher Weissenberg numbers.

The first section is devoted to the algorithms which are designed to solve steady flows, whereas the second section addresses time-dependent flow calculations. In the last section some general principles may be subtracted from the ideas brought forth thus far.

4.1 Steady viscoelastic flow simulations

As mentioned in the first chapter, the first attempts to simulate viscoelastic flows numerically were restricted to very moderate Weissenberg numbers, but in the last 10 years rapid progress has been made in the numerical simulation of non-Newtonian fluids, especially in steady state calculations. The small Weissenberg numbers, which could be attained with central numerical methods, such as central finite differences or Galerkin finite elements, were overcome by the application of upwind schemes, such as the non-consistent streamline upwind scheme (SU) by Marchal and Crochet [39] and the streamline integration method, proposed by Luo and Tanner [37], [38], and Upadhyay and Isayev [57]. Furthermore, rewriting the set of partial differential equations in the explicit elliptic momentum equation (EEME) form allowed King et al. [34] to apply the streamline upwind Petrov-Galerkin (SUPG) method successfully, although this method is only applicable to smooth geometries.

4.1.1 The EEME formulation

As mentioned in the former chapter the creeping flow or Stokes approximation eliminates the velocity vector from the momentum equation and it was argued that, just as in the case of the incompressibility constraint, this equation has to be modified in order to be solved for the velocity. King et al. [34], following Renardy [49], rewrote the set of partial
differential equations in a form which is called the \textit{Explicit Elliptic Momentum Equation} (EEME). For the Maxwell model (non-dimensional) the constitutive equation is given by 
\((\partial / \partial t = 0)\)

\[\lambda \bar{\nabla} \bar{p} + \tau = 2D.\]

Taking the divergence of this equation and using the relations

\[-\bar{\nabla} p + \bar{\nabla} \cdot \tau = \bar{0},\]

and

\[\bar{\nabla} \cdot \bar{u} = 0,\]

leads to a momentum equation which now contains the velocity as unknown, just as the Poisson equation for the pressure replaces the incompressibility constraint for incompressible materials. This modified momentum equation is given by

\[\bar{\nabla} q - \bar{\nabla} \cdot (\chi \cdot \bar{\nabla} \bar{u}) - \bar{\nabla} \bar{u} \cdot (\bar{\nabla} \cdot \chi) = \bar{0},\] (4.1)

where

\[\chi = I + \lambda \tau,\]

and

\[q = p + \lambda \bar{u} \cdot \bar{\nabla} p.\]

The constitutive equation now becomes

\[\chi + \lambda \left( \bar{u} \cdot \bar{\nabla} \chi - L \cdot \chi - \chi \cdot L^T \right) = I.\]

The momentum equation is now (explicitly) elliptic in \(\bar{u}\) and may be solved for \(\bar{u}\), by a central method such as central differences or the Galerkin finite element method.

It is in fact better to perform these operations numerically and then to perform the manipulations described above. Just as the incompressibility constraint is first discretized and then by numerical means the Poisson equation is deduced from it.

This formulation of the momentum equation, Eq. (4.1), is equal to the wave equation described in section 3.5, where \(\rho\) is set to zero. If \(Re\) is non zero the momentum equation should be given by

\[\frac{D}{Dt} \left[ Re \frac{D\bar{u}}{Dt} + \bar{\nabla} p \right] - \left( \bar{\nabla} \cdot \tau A \bar{\nabla} \right) \bar{u} + \frac{1}{\lambda} \left[ Re \frac{D\bar{u}}{Dt} + \bar{\nabla} p \right] = \bar{0}.\]

If \(Re = 0\) and \(\partial / \partial t = 0\) and the equation is multiplied by \(\lambda\), then this equation reduces to Eq. (4.1)

### 4.1.2 The EVSS formulation

Another way of re-introducing the velocity in the momentum equation if the Stokes approximation is applied is called the Elastic Viscous Split Stress (EVSS) formulation, first introduced by Perera and Walters [44], in which the extra stress tensor is split into an elastic part and a viscous part.

\[\tau = S + 2\eta D,\]
in which \(2\eta D\) is called the viscous contribution to the extra stress tensor, while \(S\) represents the polymeric elastic part of the extra stress tensor. Insertion of this stress tensor in the momentum equation gives

\[
\nabla \cdot \mathbf{p} = \nabla \cdot \mathbf{S} + \eta \Delta \mathbf{u},
\]

so the velocity is reintroduced in the momentum equation. The constitutive equation is then given by

\[
\nabla \cdot \left[ \mathbf{u} (\mathbf{S} + 2\eta D) \right] - \mathbf{L} [\mathbf{S} + 2\eta D] - [\mathbf{S} + 2\eta D] \mathbf{L}^T + \frac{\mathbf{S}}{\lambda} = 0 .
\] (4.2)

In the paper by Sasmal [52] this form of the constitutive equation is supplemented by a pseudo-transient local time derivative, which acts as a relaxation parameter to converge to the steady state.

The finite difference approximation by Perera and Walters, which was concerned with the steady state solution in T- and L-shaped geometries, used a form of upwinding, which was chosen such that diagonal dominance was enhanced, without reference to direction of the characteristic equations. In the work by Sasmal only upwinding of the convective terms in the constitutive equation was applied in the direction of the fluid velocity. The additional terms in the convected time derivative were contained in the right hand side of the equations. In both papers a streamline-vorticity formulation was chosen. In Sasmal’s paper use is made of a staggered grid (see next chapter), whereas Perera and Walters define all variables at the same position in the computational domain.

The application of Eq. (4.2) in the finite element method is not straightforward. Since the velocity is usually only \(C^0\) between elements, the rate of deformation tensor, \(D\) is discontinuous at element boundaries, which gives problems when this discrete tensor is used in Eq. (4.2). It would be desirable to have \(D\) in the same vector space as \(\mathbf{r}\) and \(S\). This poses a compatibility relation between the discrete velocity space and the discrete tensor space (see subsection 4.1.3). Or one may try to approximate the discontinuous discrete rate of deformation tensor by an element of the discrete tensor space (see subsection 4.1.4).

### 4.1.3 Effects of the mesh size

The effect of the mesh size on the numerical solution is very intricate. The early algorithms were plagued by the fact that the maximum attainable Weissenberg number decreased with the mesh size. This may be explained by noting that the local Deborah number, as defined in the previous chapter, \(De_h = \lambda U / h\) goes to infinity, when \(h \to 0\). This means that the asymmetric terms in the constitutive equation dominate the (symmetric) source term, leading to uncoupling and wiggles in the numerical solution, which in turn may violate convergence. In the work by Keunings [33] it is shown that for the Maxwell and the Leonov fluid the attainable Weissenberg number ultimately reduces with mesh refinement. Keunings therefore concludes that this limiting Weissenberg number is not an intrinsic property of the viscoelastic fluid models, but a numerical artifact. Furthermore, it is shown in this paper that the stationary solution depends on the way this solution is obtained, either by using the Newtonian flow as an initial guess, or a stationary solution at a higher
Weissenberg number, which either means that these models are highly dependent on their initial value or the numerical errors present in his scheme ultimately leads to a completely different stationary solution. Application of upwind methods, whether first order or higher order, prevents the uncoupling between neighbouring variables and lead to converged solutions at higher Weissenberg numbers. However, in all the schemes upwinding in the direction of the streamlines is used. So far no schemes have been used based on the characteristic equations as described in chapter 3.

For incompressible fluids the velocity and the pressure field have to satisfy a certain compatibility relation, known as the inf-sup relation or the Babuska-Brezzi condition in weighted residual methods. It seems that also the velocity and the stress tensor fields have to be compatible in order to obtain a unique solution. In a very interesting analysis by Marchal and Crochet [39] the mixed method is presented, in which the (Newtonian) Stokes equation is solved by either a velocity-pressure formulation, given by

\[ \nabla \cdot \vec{u} = 0 , \]

and

\[ \nabla p = \eta \Delta \vec{u} , \]

or the mixed velocity-pressure-stress formulation given as

\[ \nabla \cdot \vec{u} = 0 , \]

\[ \nabla p = \nabla \cdot \tau , \]

and

\[ \tau = 2\eta D . \]

Analytically both sets of equations represent the same flow, but as the above mentioned paper demonstrates, the numerical results are completely different. The finite element approximation (Galerkin) to the first set of equation, applied to the stick-slip problem gives a smooth velocity field near the boundary, whereas the same approximation applied to the second set of equations leads to spurious oscillations in the velocity field. The finite element used consisted of biquadratic Lagrangian shape functions for the velocity and for the stress components and bilinear shape functions for the pressure. The reason for this difference in numerical solution is due to the fact that if the approximated stresses are in the linear space \( \mathcal{T}^h \) and the velocity vector in \( \mathcal{V}^h \), then the solution \( \tau^h = 2\eta D^h \) will in general not be in \( \mathcal{T}^h \). A sufficient condition would be

\[ \vec{u}^h \in \mathcal{V}^h \iff \nabla^h \vec{u}^h \in \mathcal{T}^h . \]

Instead of using the same meshes for both the velocity-pressure part and the stress part, each velocity-pressure element is subdivided into \( n^2 \) subelements, in which the stress is approximated by bilinear shape functions, where \( n \) is chosen sufficiently large, so that \( \tau^h \) will converge to \( 2\eta D^h \). The paper shows that using \( n = 4 \) leads to the same smooth solutions as the velocity-pressure formulation.

Obviously it would be more desirable to chose the unknowns such, that this so-called equivalence condition is fulfilled. One way of satisfying this condition, even for \( De \neq 0 \), will be given in the next chapter.
4.1.4 Smoothing of the velocity gradient

A procedure which is applied in many numerical codes is the smoothing of the velocity gradient \( L \). When a finite element method is used the tensor \( A = (L + L^T) \), the first Rivlin-Ericksen tensor, is approximated by

\[
0 = \int_\Omega (A - L - L^T : \phi) d\Omega.
\]  (4.3)

The reason to perform this smoothing is that, unless hermitian elements are used the velocity field is only continuous over element boundaries. The gradient of the velocity field \( L \) will therefore be discontinuous at the element boundaries. By using the smoothing operation Eq. (4.3) the tensor \( A \) will be a continuous approximation of \( L + L^T \). The thus obtained tensor \( A \) is then used in the constitutive equation. In fact the tensor \( A \) may be considered as a new tensor unknown for which Eq. (4.3) gives the additional equations to be solved. This procedure is also used in solving the EVSS method since in this case one wants to take partial derivative of \( 2D = A \) in the constitutive equation. However the characteristic equations presented in the previous chapter admit discontinuous velocity gradient, so the use of these extra unknowns and equations may give a too smooth picture of the actual flow.

A better way to circumvent these problems is to use either hermitian elements or to position the velocity and stress components such that no velocity gradients have to be evaluated at the boundary of the elements. The latter statement means that the velocity and the stress field have to satisfy a certain compatibility relation. In the next chapter it will be shown that the use of staggering circumvents these problems.

4.1.5 SU and SUPG methods

In a paper by Marchal and Crochet [39] the use of streamline upwind methods was advocated, following the ideas of Brooks and Hughes [15]. In their calculations the Oldroyd-B and the UCM model were used and the EVSS formulation was utilized and compared with un-split formulation. The use of the EVSS form is particularly stabilizing when \( S \) is small compared to \( 2\eta D \), but as soon as the elastic part of the extra stress tensor becomes large compared to the viscous part, this advantage is lost and \( \tau \) and \( S \) behave similarly. The latter is the case when the Deborah number increases and the use of the EVSS formulation is accordingly called a 'temporary relief'.

The idea in the Streamline Upwind Petrov Galerkin (SUPG) method is not to use a weighting function which belongs to the class of test functions, but to add a convection term to the weighting functions in the direction of the streamlines. When different function spaces are used for the test functions and the weighting function the method is called a Petrov-Galerkin method. This results in a first order upwind procedure in the direction of the streamlines only, thus reducing the amount of cross-wind diffusion. When the SUPG method is applied to the constitutive equation based on a given velocity field, the results are satisfactory, but when the same method is applied in conjunction with the conservation laws it fails. The reason for this failure is that in the decoupled approach the velocity vector and its derivatives act as variable coefficients in the constitutive equation. The constitutive equation only contains the extra-stress components as unknowns and it
is quite easy to verify that this set of equations is hyperbolic along the streamlines for all equations. However when the SUPG method is applied to the complete set of PDE’s, then the velocity is also an unknown and the coupling with the momentum equation leads to non-linear wave equations, which cannot be treated by streamline upwind or integration methods.

In order to remedy this, the streamline upwinding was only applied to the convective terms in the constitutive equation, whereas all the other terms were treated by a Galerkin method. This, in fact, is an inconsistent procedure of weighting the constitutive equation and is therefore termed the inconsistent Streamline Upwind (SU) method.

### 4.2 Time-dependent flow calculations

Recently the subject of time-dependent viscoelastic flow calculations has been addressed. Typical time-dependent problems are the start-up of a planar Posseuille flow, the settling of a sphere in a viscoelastic fluid and the time-dependent flow of viscoelastic fluids in a 4:1 contraction.

Usually the method of lines is used, in which the spatial derivatives are approximated by either finite element, finite difference or spectral methods and the resulting set of equations is integrated in time. For instance Sato and Richardson [53] used a decoupled approach for the system of PDEs. The conservation laws are solved explicitly in time and they use a finite element method to discretize the spatial derivatives. The UCM model was treated implicitly while a finite volume method has been used to discretize the spatial derivatives. This algorithm was applied to the 4:1 contraction and results are given up to \( De = \lambda \dot{\gamma} = 2 \). Beyond this Deborah number transient behaviour was found. In this paper it has been reported that a temporary lip vortex is formed when the Deborah number is increased instantaneously. This phenomenon has been reported by other numerical studies as well. The lip vortex disappears when the steady state solution is reached.

In a paper by Olsson [42] results are given for time-dependent simulations of the UCM model, the Oldroyd-B model and the Giesekus model. The spatial derivatives are approximated by second order accurate finite differences, while for the time integration a second order Runge-Kutta method, a second order Adams-Bashforth or a second order Adams-Moulton with Adams-Bashforth as predictor have been used. These calculations are performed on multiple overlapping meshes. In order to avoid singular solutions near the re-entrant corner, the corners in the contraction flows reported in this paper are rounded. Results for the planar 4:1 contraction are given for \( De = \lambda U/L = 5 \). Again the mechanism is shown that a lip vortex is formed which slides down the wall to form the salient corner vortex. Unfortunately, no stress characteristics are given in this paper and only the time dependent phase up to \( t = 2.4 \) is shown. So whether the solution ultimately becomes stationary and/or if this algorithm is capable of producing this result is not known.

A genuine time-dependent viscoelastic flow simulation is given by Bodart and Crochet [12]. In this paper the time-dependent settling of a sphere in a tube filled with a viscoelastic fluid is given. For the extra-stress tensor both the \( 4 \times 4 \) linear subelements of Marchal and Crochet and the biquadratic continuous representation are used. As time integrator
the Crank-Nicolson method with an Adams-Bashforth predictor is employed. Lack of convergence results in a decrease of the time step. Furthermore a mixed method is used in which all the equations are solved simultaneously. Stationary results are reported for the Oldroyd-B model with $\eta_2/(\eta_1 + \eta_2) = 1/9$ and $Re = 0.01$ up to $We \approx 1.3$, in which $\eta_2/\eta_1$ is the solvent viscosity, mentioned in chapter 2. Solutions are given on different meshes at different Weissenberg numbers for different values of $R_s/R_c$, in which $R_s$ is the sphere radius and $R_c$ the radius of the cylinder. The influence of the solvent viscosity and the Reynolds number have been investigated.

However the step from steady state algorithms to time-dependent algorithms may pose new restrictions on the attainable Weissenberg number. The reason is that in steady state algorithms one has to solve a system of the form

$$A \vec{x} = b.$$ 

This set of equations can be solved for $\vec{x}$ if $\det A \neq 0$, no matter what the eigenvalues of $A$ are. In time dependent simulations one has to solve a system of the form

$$\frac{\partial \vec{x}}{\partial t} + A \vec{x} = \vec{b}.$$ 

A steady state solution for this system exists if $Re(\xi) < 0$, ultimately, in which $\xi$ is an eigenvalue of $A$. In a paper by Keiller [31] it is shown that for the planar Couette flow this requirement depends on the grid aspect ratio $\Delta x/\Delta y$. If the wrong aspect ratio is chosen, eigenvalues may appear with $Re(\xi) \geq 0$ and no steady state solution will be reached. This phenomenon has been reported by others as well. One has to refine the grid in the cross stream direction with respect to the grid in the direction of the streamlines in order to obtain converged solutions. So the step from steady state algorithms to time dependent algorithms is not straightforward.

### 4.3 What happens beyond the limiting Weissenberg number?

The limit in the Weissenberg number may be due to the model used, which may loose well-posedness beyond a certain Weissenberg number, but it may also be due to improper discretization of the set of PDEs. The fact that the limiting Weissenberg number depends on the grid and the aspect ratio, suggests that the limit is due to an improper numerical treatment. Even rewriting the set of PDEs, which may be considered as a form of preconditioning, ameliorates the numerical results. Therefore it is interesting so see what happens when the solution diverges beyond a certain Weissenberg number. In a paper by Dupret et al. [20] it is shown that the solution behaves well as long as the tensor $\tau_A$ is positive definite. If this tensor becomes indefinite oscillations in the solution appear, although the algorithm still converges. If the Weissenberg number is increased even further the algorithm diverges, so it is believed that the appearance of a negative eigenvalue in $\tau_A$ is the source of a numerical ill-posed problem.

For time-dependent problems one has to decrease the time step considerably in order to reach a steady state solution when the limiting Weissenberg number is approached.
Ultimately the time step becomes very much smaller than the CFL condition on the time step. This may suggest that the time step acts more as an under relaxation parameter to solve the system, which in turn means that the system is ill-conditioned. This is confirmed by the fact that rewriting the set of equations improves the numerical solution, so proper preconditioning may lead to higher Weissenberg numbers, or may even remove the Weissenberg limit.

Furthermore in all the algorithms described in the literature only upwinding in the direction of the streamlines is performed, whereas the wave part of the set of PDEs is neglected. A proper treatment of the hyperbolic wave part and its boundary conditions may also lead to improved algorithms. An attempt to incorporate the wave part properly in the numerical scheme will be presented in the next chapter.

4.4 General conclusions

The general conclusions may be divided into those which can be drawn from the stationary algorithms and the time dependent algorithms. The conclusions based on the literature from the stationary algorithms can be summarized by

- In the case $Re = 0$, rewriting the equation in the EEME or EVSS formulation reintroduces the velocity vector in the momentum equation, but in the case of complex geometries this is temporary relief, because for higher Weissenberg number the direct approach, in which all equations are solved simultaneously, gives comparable results.

- The addition of a solvent viscosity term enables one to achieve higher Weissenberg numbers, i.e. a higher Weissenberg number is possible before the algorithms diverge.

- Smoothing of the first Rivlin-Ericksen tensor enhances the attainable Weissenberg number.

- Stationary algorithms reach converged solutions even if the positive definiteness of $\mathbf{\tau}_A$ is lost.

- Upwind methods, or more generally, hyperbolic discretization strategies, must be applied to the convective terms in the constitutive equation in order to overcome the very low Weissenberg limit of $O(10^{-1})$, encountered 10 years ago.

- A proper choice of the unknowns, both the velocity and the stress components, is necessary to satisfy the equivalence principle as mentioned by Marchal and Dupret. Specifically in regions where large gradients in the velocity occur, e.g. in the stick-slip problem and near re-entrant corners.

The general conclusion which may be drawn from the time dependent calculations in the literature are

- The stationary solutions for the 4:1 contraction problem obtained by stationary algorithms could not be reached by time dependent flow calculations, because the
time dependent algorithms diverged for Weissenberg numbers of order 5 (in case of the Maxwell and Oldroyd-B models).

- The use of more sophisticated models like the PTT-, Leonov- and Giesekus models, allowed time dependent flow calculations for higher Weissenberg numbers.

- As pointed out by Keiller [31] the limiting Weissenberg number in time dependent viscoelastic flows is a function of the grid aspect ratio, $\Delta x/\Delta y$.

- Near the limiting Weissenberg number the numerical time step required to obtain bounded solution decreases rapidly.

- The appearance of a negative eigenvalue in the tensor $\mathbf{\tau}_A$ at a certain Weissenberg number is usually followed by a divergent solution if the Weissenberg number is increased from there. Before the algorithm diverges the numerical solution is fraught with unphysical oscillations in regions where large changes in the flow take place.

These conclusions indicate that

- One has to design an algorithm which ensures the positive definiteness of the tensor $\mathbf{\tau}_A$.

- Rewriting the set of PDEs, using either the EEME or the EVSS formulation leads to more stable algorithms. In fact if the discrete system of equations could be rewritten in the wave form Eq. (3.4) the velocity is reintroduced in the momentum equation as well, which is in accordance with the type of the set of PDEs.

- If the hyperbolic part in the direction of the streamlines can be separated from the rest of the equations and treated with a proper hyperbolic scheme, the determinant of $\mathbf{\tau}_A$ remains strictly positive, which means that the system never becomes ill-posed.

- The coupled system, in which the velocity is determined for a large part by the constitutive equation should be discretized implicitly.

- The method of lines is usually adopted to integrate the discretized set of equations in time. However for a finite time step the difference quotient, which is approximated by these integration methods is not objective, (see section 2.2). Furthermore the discrete approximation of the deformation gradient does not satisfy the incompressibility constraint. In the next chapter a numerical scheme will be given in which the MCSH-approximation is used to approximate the deformation gradient. The results of this approach are given in chapter 6 where it is also shown that the approximation of $\mathbf{F}$ by $\mathbf{I} + \Delta t \mathbf{L}$ limits the attainable Weissenberg number.

In the next chapter a numerical scheme will be developed that satisfies the equivalence principle, stated by Marchal and Crochet, not only for $De = 0$, but also for $De > 0$. This consistent treatment of the velocity gradient and the extra stress tensor should prevent the loss of positive definiteness of the tensor $\mathbf{\tau}_A$ and guarantees time dependent convergent solutions at least up to $De \approx 11$. 