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# FINITE ELEMENT METHODS FOR INTEGRAL VISCOELASTIC FLUIDS

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**ABSTRACT**

We review the field of finite element techniques for solving complex flows of viscoelastic fluids described by a constitutive model of the integral type. The focus is mainly put on mathematical formulations and numerical approaches. A short guide to published simulations of non-trivial flow problems is offered.

**KEYWORDS:** Viscoelastic fluids; Integral constitutive equations; Molecular theory; Numerical simulation; Finite elements.

## 1. INTRODUCTION

Numerical methods for simulating complex flows of viscoelastic liquids have been under development over the last twenty-five years. Progress during the first decade has been discussed in detail by Crochet et al [1] and Keunings [2]. Since the early days, the field has expanded considerably. Indeed, recent studies explore a wide spectrum of modeling and numerical approaches which go far beyond the framework of computational continuum mechanics. These exciting developments have been reviewed recently by Keunings [3] and Owens and Phillips [4]. It remains true, however, that a majority of published studies follows a macroscopic approach, wherein the rheological behaviour of the fluid is described by a differential constitutive equation and the governing equations are solved numerically by means of a suitable finite element method (Baaijens [5]). Use of an integral constitutive equation instead of a differential model has been comparatively scarce. The reason is certainly not one of lack of interest or relevance. In fact, molecular theories for memory fluids often yield constitutive equations of the integral type (Doi and Edwards [6]). For computational purposes, a differential approximation is usually sought, whose rheological response can be at odds with that of the original integral equation (Larson [7]). As the reader will soon find out, integral models present numerical challenges that call for truly creative ideas. Since the pioneering work of Viriyayuthakorn and Caswell [8], who devised the first finite element technique for integral viscoelastic models, progress has been steady but with a definite acceleration in recent years. It is our goal to describe these developments with enough technical detail for the motivated reader to appreciate the main issues involved.

 

## 2. GOVERNING EQUATIONS

Most numerical studies using integral viscoelastic models have been for isothermal, incompressible flows. Thus, the Cauchy stress tensor $\boldsymbol{\sigma}$ is determined up to an arbitrary isotropic tensor:

$$\boldsymbol{\sigma} = -p\boldsymbol{\delta} + \boldsymbol{\tau} \,, \qquad \text{..... (1)}$$

where $p$ is the pressure, $\boldsymbol{\delta}$ is the unit tensor, and $\boldsymbol{\tau}$ is the extra-stress tensor. Conservation of mass and linear momentum (body forces being neglected) is expressed as:

$$\nabla \cdot \boldsymbol{v} = 0 \,, \quad \nabla \cdot \boldsymbol{\sigma} = \rho \frac{D\boldsymbol{v}}{Dt} \,, \qquad \text{..... (2)}$$

where $\boldsymbol{v}$ is the velocity vector, $\rho$ is the fluid density, and $D/Dt$ is the material derivative $\partial/\partial t + \boldsymbol{v} \cdot \nabla$. This is the usual *Eulerian* formulation of the conservation equations, which relates the stress and velocity fields in the flow domain $\Omega$. For steady-state, creeping flows, the right-hand-side of the momentum equation vanishes.

A suitable constitutive equation that relates the extra-stress $\boldsymbol{\tau}$ to the deformation history closes the set of governing equations (2). Consider a fluid particle whose position at present time $t$ is given by $\boldsymbol{x}$; its position at some past time $t'$ is $\boldsymbol{x}'$. The particle motion is described by the displacement function $\boldsymbol{x}' = \boldsymbol{x}'(\boldsymbol{x}, t, t')$, while the deformation gradients $\boldsymbol{F}$ and $\boldsymbol{E}$, and Finger strain $\boldsymbol{B}$ are defined as:

$$\boldsymbol{F}(t,t') = \frac{\partial \boldsymbol{x}'}{\partial \boldsymbol{x}} \,, \qquad \boldsymbol{E}(t,t') = \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{x}'} = \boldsymbol{F}^{-1} \,, \qquad \boldsymbol{B}(t,t') = \boldsymbol{E} \cdot \boldsymbol{E}^{T} \,. \qquad \text{.....(3)}$$

Integral constitutive equations are usually formulated in a *Lagrangian* framework: they give the viscoelastic stress $\boldsymbol{\tau}$ at a moving fluid particle. Most numerical studies use a particular case of the *separable* single-integral model:

$$\boldsymbol{\tau}(t) = \int_{-\infty}^{t} m(t - t') \boldsymbol{f}(\boldsymbol{B}(t, t')) \, dt' \,, \qquad \text{.....(4)}$$

where the integral is taken along the past trajectory of the fluid particle, parameterized by the past time $t'$. The strain-independent factor $m(t - t')$ is the memory function of linear viscoelasticity, usually given as a sum of exponential functions involving the relaxation times $\lambda_k$ and viscosity coefficients $\eta_k$:

$$m(t - t') = \sum_{k=1}^{n} \frac{\eta_k}{\lambda_k^2} exp\left( \frac{-(t - t')}{\lambda_k} \right) , \qquad \text{.....(5)}$$

and $\boldsymbol{f}$ is an isotropic function of the form:

$$\boldsymbol{f}(\boldsymbol{B}) = \varphi_1(I_1, I_2)[\boldsymbol{B} - \boldsymbol{\delta}] + \varphi_2(I_1, I_2)[\boldsymbol{B}^{-1} - \boldsymbol{\delta}] \,. \qquad \text{.....(6)}$$

 

Here, $\varphi_1$ and $\varphi_2$ are scalar functions of the strain invariants $I_1 = tr(\boldsymbol{B})$ and $I_2 = tr\left(\boldsymbol{B}^{-1}\right)$.

It should be noted that the particle paths along which we need to compute the memory integral (4) are not known a priori. The problem is thus highly non-linear, even under creeping flow conditions. A second challenge is that the Lagrangian formulation of the constitutive model does not involve the Eulerian velocity field in an explicit manner. In fact, velocities and strains are related through the kinematic relation:

$$\frac{D}{Dt'}\boldsymbol{F}(t,t') = \nabla \boldsymbol{v}^T(t') \cdot \boldsymbol{F}(t,t'), \qquad \text{.....(7)}$$

which must in principle be integrated backward in time $t'$ along all particle trajectories, with the initial condition $\boldsymbol{F}(t,t) = \boldsymbol{\delta}$. Clearly, the task at hand is formidable.

The generic integral model (4-6) includes many well-known constitutive equations, whose rheological response is studied in the monographs by Bird et al [9], Larson [7], and Tanner [10]. For example, $\varphi_1 = 1$ and $\varphi_2 = 0$ yields the Lodge rubber-like liquid model, while the factorized K-BKZ equation is given by $\varphi_1 = \partial W(I_1, I_2)/\partial I_1$, $\varphi_2 = \partial W(I_1, I_2)/\partial I_2$, where $W$ is a suitable potential function. The reptation model of Doi and Edwards [6] for entangled linear polymers can also be written in the form (4-6) using Currie's approximation of the related potential function. *Non-separable* single-integral equations, such as the Rivlin-Sawyers model, also have the generic form (4), but with a strain-dependent memory function $m(t - t', I_1, I_2)$. Integral equations proposed recently on the basis of molecular theories for linear and branched polymers have a more complicated mathematical structure (e.g. Mead et al [11], McLeish and Larson [12], Ianniruberto and Marrucci [13], Wagner et al [14]). We shall devote a special section to their numerical implementation.

A Newtonian component $\boldsymbol{\tau}_N = \eta_N \dot{\boldsymbol{\gamma}}$ is sometimes added to the viscoelastic stress $\boldsymbol{\tau}$, where $\eta_N$ is a constant viscosity coefficient and $\dot{\boldsymbol{\gamma}}$ is the rate of strain tensor $\left(\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^T\right)$. It can be interpreted physically as the solvent contribution to the stress in polymer solutions, or as the stress response associated with fast relaxation modes. In other cases, the Newtonian component is added to correct the viscoelastic model itself (e.g., to eliminate the excessive shear-thinning of the Doi-Edwards model). The presence of a Newtonian component has a considerable impact on the mathematical nature of the governing equations (2-4). Indeed, viscoelastic fluid models *without* a Newtonian component can exhibit a variety of hyperbolic phenomena, including change of type and propagation of waves (Joseph [15]).

The set of governing equations is supplemented with appropriate boundary conditions. Since a complete mathematical theory of boundary conditions for viscoelastic flows is not available, the approach followed in numerical work is based

on physical considerations. Like in Newtonian fluid mechanics, one specifies components of either the velocity or the contact force at the boundary $\partial\Omega$ of the flow domain $\Omega$; the pressure is specified at one point of the flow domain if no normal contact forces have been specified anywhere at the boundary. For memory fluids, additional boundary conditions must be specified when the flow domain $\Omega$ contains an inlet boundary. Indeed, the flow inside $\Omega$ is affected by what happened to the fluid upstream of the inlet boundary. Specification of the *flow pre-history*, namely the deformation history experienced by the fluid elements prior to their entrance in the flow domain $\Omega$ , is readily achieved with the generic single-integral model (4). Indeed, the stress integral is split as follows:

$$\boldsymbol{\tau}(t) = \int_{-\infty}^{t_e} m(t-t')\boldsymbol{f}\left(\boldsymbol{B}(t,t')\right)dt' + \int_{t_e}^{t} m(t-t')\boldsymbol{f}\left(\boldsymbol{B}(t,t')\right)dt' \quad \text{.....(8)}$$

where $t_e$ is the time at which the fluid particle entered the flow domain $\Omega$. The flow pre-history is entirely taken into account in the first integral. In practice, one often specifies a flow pre-history corresponding to fully-developed flow upstream of the inlet boundary. For transient flows, initial conditions are also needed for the velocity and viscoelastic stress fields.

## 2. THE COUPLED STREAMLINE FINITE ELEMENT METHOD

We begin our survey of numerical methods with the coupled Eulerian technique advanced by Papanastasiou et al [16]. With integral models, it is a *tour de force* to devise a coupled scheme wherein the governing equations are solved simultaneously for the whole set of primary variables. A first difficulty is that the memory integral must be evaluated along particle paths that are unknown a priori. This feature is very much akin to free surface flows and can indeed be tackled with similar techniques. The second problem is related to the intrinsically Lagrangian formulation of integral models, which does not explicitly involve the Eulerian velocity field. As shown by Adachi [17, 18], among others, it is possible to derive an Eulerian formulation of integral models in the case of steady-state planar or axisymmetric flows. The coupled streamline finite element method (CSFEM) of Papanastasiou et al [16] makes use of this theoretical result, which we briefly present.

### Eulerian formulation

In steady-state planar or axisymmetric flows, fluid particles move along streamlines characterized by a constant value of the stream function $\psi$ . Use of a Protean coordinate system, in which one of the coordinate lines is the streamline, thus vastly simplifies the problem of tracking the motion of fluid particles. Consider the particular case of non-recirculating planar flows whose streamlines are single-valued functions of the coordinate $x$. At present time $t$, a fluid particle is located at $\boldsymbol{x}$ and has Protean coordinates $\bar{x}^1$ and $\bar{x}^2$ . A possible choice of Protean coordinates is defined by the transformation:

$$\bar{x}^1 = x\,, \qquad \bar{x}^2 = \psi(x,y)\,, \qquad \text{.....(9)}$$

 

where $(x,y)$ are the usual Cartesian coordinates. Recall that the stream function is related to the velocity components $(u,v)$ in Cartesian coordinates through:

$$\frac{\partial \psi}{\partial x} = -v\,, \qquad \frac{\partial \psi}{\partial y} = u\,. \qquad \text{.....(10)}$$

The particular choice (9) yields a system of non-orthogonal curvilinear coordinates whose $\bar{x}^1$ and $\bar{x}^2$ coordinate lines are respectively the streamlines and the $y$ coordinate lines. Adachi [17, 18] has shown that the kinematic relation (7) admits a closed form solution in the Protean coordinate system (9). The results can be expressed in the Cartesian coordinate system by means of standard tensor transformation rules. This yields the Eulerian formulation $\boldsymbol{B}(\boldsymbol{x}, \boldsymbol{x}')$ of the Finger strain tensor in Cartesian coordinates:

$$B_{xx} = \left(u^2U^2 + u^2V^2\right)I^2 - \left(2\frac{u^2V}{U}\right)I + \frac{u^2}{U^2}\,,$$

$$B_{xy} = uv\left(U^2 + V^2\right)I^2 + \left(U^2 + V^2 - 2\frac{uvV}{U}\right)I + \left(\frac{uv}{U^2} - \frac{V}{U}\right), \qquad \text{.....(11)}$$

$$B_{yy} = v^2\left(U^2 + V^2\right)I^2 + \left(-2\frac{v^2V}{U} + 2\frac{v}{u}\left[U^2 + V^2\right]\right)I + \left(\frac{v^2}{U^2} - 2\frac{vV}{uU} + \frac{U^2 + V^2}{u^2}\right),$$

where $(u,v)$ and $(U,V)$ are the velocity components at $\boldsymbol{x}$ and $\boldsymbol{x}'$, respectively, and $I$ is the streamline integral:

$$I = \int_{x'}^{x} \frac{\partial u}{\partial y}\frac{dx''}{u^3}\,. \qquad \text{.....(12)}$$

It is understood that the integrand of (12) is evaluated along the streamline passing through $\boldsymbol{x}'$ and $\boldsymbol{x}$. Since the streamline is parameterized by the single coordinate $x$, we can write formally $\boldsymbol{B}(\boldsymbol{x}, \boldsymbol{x}') = \boldsymbol{B}(x, x')$.

We are now able to write any single-integral viscoelastic model in Eulerian form. Consider for example the generic separable model (4). In view of the one-to-one correspondence between the coordinate $x$ and the particle travel time along the streamline, the Eulerian formulation of the constitutive equation is readily obtained:

$$\boldsymbol{\tau}(\boldsymbol{x}) = \int_{-\infty}^{x} m\left(\int_{x'}^{x} \frac{dx''}{u(x'')}\right) \boldsymbol{f}\left(\boldsymbol{B}(x, x')\right)\frac{dx'}{u(x')}. \qquad \text{.....(13)}$$

Using equations (11,12), this expression gives the viscoelastic stress at position $\boldsymbol{x}$ as an integral involving the Eulerian velocity field evaluated upstream along the streamline passing through $\boldsymbol{x}$. It is the key to the coupled numerical technique CSFEM proposed by Papanastasiou et al [16], which we describe next. The above result is valid for steady-state planar flows whose streamlines are single-valued functions of the coordinate $x$; it is readily adapted to axisymmetric flows [17]. In his second paper [18], Adachi has derived an extended result that holds for general two-dimensional steady-

state flows. This is achieved by selecting an orthogonal Protean coordinate system instead of the non-orthogonal system described in this section. To our knowledge, the general theory has not been exploited to devise a coupled numerical technique for integral models.

**Streamline finite elements**

The starting point of CSFEM is the Galerkin finite element formulation of the conservation equations. The velocity and pressure fields are approximated by means of the finite element interpolations:

$$\boldsymbol{v}^a = \sum_{i=1}^{N_v} \boldsymbol{v}^i \varphi^i \,, \quad p^a = \sum_{k=1}^{N_p} p^k \psi^k \,, \qquad \text{.....(14)}$$

where $\boldsymbol{v}^i$ and $p^k$ are unknown nodal values, $\varphi^i$ and $\psi^k$ are given shape functions, and $N_v$, $N_p$ are the number of velocity and pressure nodes, respectively. The Galerkin principle is then invoked to discretize the governing equations. Residuals obtained after substitution of the approximations (14) in the conservation laws (2) are made orthogonal to the set of shape functions, and an integration by parts is performed in the momentum equation. This yields the discrete Galerkin equations:

$$\int_\Omega \rho \, \boldsymbol{v}^a \cdot \nabla \boldsymbol{v}^a \varphi^j d\Omega - \int_\Omega p^a \nabla \varphi^j d\Omega + \int_\Omega \boldsymbol{\tau} \cdot \nabla \varphi^j d\Omega = \int_{\partial\Omega_T} \boldsymbol{t} \, \varphi^j d\partial\Omega \,, \qquad \text{.....(15)}$$

$$\int_\Omega \nabla \cdot \boldsymbol{v}^a \psi^l d\Omega = 0 \,, \qquad \text{.....(16)}$$

for $1 \le j \le N_v$, $1 \le l \le N_p$. Here, $\partial\Omega_T$ is part of the boundary with outward unit normal $\boldsymbol{n}$ where the contact force $\boldsymbol{t} = \boldsymbol{\sigma} \cdot \boldsymbol{n}$ is specified. Every term with the superscript $a$ denotes the corresponding finite element approximation obtained from (14). We now exploit the Eulerian formulation (13) of the integral model to evaluate the viscoelastic stress term in the left-hand side of equation (15):

$$\int_\Omega \boldsymbol{\tau} \cdot \nabla \varphi^j d\Omega = \int_\Omega \underbrace{\left[ \int_{-\infty}^{x} m\left( \int_{x'}^{x} \frac{dx''}{u^a(x'')} \right) \boldsymbol{f}\left( \boldsymbol{B}^a(x, x') \right) \frac{dx'}{u^a(x')} \right]}_{SI(\boldsymbol{x})} \cdot \nabla \varphi^j d\Omega \,. \qquad \text{.....(17)}$$

Here, $\boldsymbol{B}^a(x, x')$ is given by equations (11,12) in terms of the Eulerian velocity $\boldsymbol{v}^a$ along the streamline segment joining $\boldsymbol{x}'$ and $\boldsymbol{x}$. Upon substitution of equation (17) into equation (15), we thus obtain a set of Galerkin equations which only involves the Eulerian velocity and pressure unknowns.

In order to form the Galerkin equations, we must compute the streamline integral $SI(\boldsymbol{x})$ in equation (17) at the integration points of each element of the mesh. This is not a trivial task since the streamlines are themselves unknown. This difficulty is identical to that encountered in free surface flows wherein the governing equations must be solved over an a priori unknown computational domain. The approach proposed by Papanastasiou et al [16] is to discretize the flow domain $\Omega$ into streamline

 

elements. This approach generates a set of $N_s$ discrete streamlines whose location will be computed together with the velocity and pressure fields. At each iteration, it is then easy to identify the streamline passing through each individual integration point located at $\boldsymbol{x}_{int}$ . The upstream trajectory of the integration point $\boldsymbol{x}_{int}$ is thus readily constructed in each element, and the streamline integral $SI(\boldsymbol{x})$ can be evaluated in terms of upstream nodal velocities. In practice, few streamlines must be identified since many integration points share the same trajectory.

The location of the finite element nodes is of course unknown a priori in CSFEM, and must be computed as part of the solution. The methodology is identical to that developed in the early nineteen-eighties for solving free surface flows (e.g. Kistler and Scriven [19]). Each of the $N_s$ discrete streamlines is represented by a height function $h(x)$, which is approximated by means of the 1-d finite element interpolation:

$$h^a = \sum_{j=1}^{N_{st}} h^j \beta^j , \qquad \text{.....(18)}$$

where $h^j$ is an unknown nodal value, $\beta^j$ is a given shape function, and $N_{st}$ is the number of nodes defining the discrete streamline. The nodal values determine the $y$ coordinates of the finite element nodes lying on the streamline. In order to account for these additional unknowns, we impose in the Galerkin weak sense that the discrete streamline be tangent to the velocity field:

$$\int_{Str} \boldsymbol{v}^a \cdot \boldsymbol{n}^{Str} ds = 0 , \qquad \text{.....(19)}$$

for $1 \le j \le N_{Str}$. Here, the integral is computed along the streamline $Str$ with arc length $s$ and unit normal $\boldsymbol{n}^{\mathrm{Str}}$ .

Together with equations (15,16), the Galerkin equations (19) form a set of non-linear algebraic equations or the nodal velocities, pressures, and streamline coordinates. The total number of unknowns amounts to ($2N_v + N_p + N_s \times N_{st}$ ). In CSFEM, the Galerkin equations are solved by means of Newton's iterative scheme. This requires in particular the very tedious but straightforward evaluation of the derivatives of the Galerkin equations with respect to the nodal positions. It should be noted that the resulting Jacobian matrix is not sparse, as usually expected with finite elements, but rather has a lower-triangular form due to the non-local nature of the stress integral (17). The resulting storage requirements were certainly too high for most computers available at the time CSFEM was put forward. This perhaps explains why this elegant method has not been further developed by others. Papanastasiou et al [16, 20] have applied CSFEM to the analysis of die swell, using the Curtiss-Bird model and some of its particular cases.

## 3. THE DECOUPLED EULERIAN-LAGRANGIAN APPROACH

We now turn to decoupled techniques wherein the computation of the viscoelastic stress is performed separately from that of the flow kinematics. These techniques are based on an Eulerian-Lagrangian approach which combines the computation of Eulerian velocity and pressure fields with the Lagrangian evaluation of

the strain history along particle trajectories. Like CSFEM, the decoupled Eulerian-Lagrangian techniques are aimed at steady-state flows only. They have been under development since the end of the nineteen-seventies, and most of the fundamental ideas have been reviewed in detail by Crochet et al [1] and Keunings [2]. We shall thus present them collectively, and in a somewhat concise manner.

**Iterative strategy**

In most implementations of the Eulerian-Lagrangian approach, the basic iterative strategy is a simple Picard scheme typical of decoupled methods:

1. Using the velocity field computed at the previous iteration, integrate the constitutive equation to update the viscoelastic stress;
2. Using the viscoelastic stress computed in Step 1, update the kinematics by solving the conservation laws;
3. Check for convergence; if needed, return to Step 1 for another iteration.

A major difficulty with any decoupled method lies in the iterative procedure itself. Indeed, Picard (or simple substitution) iterations converge at best linearly. Moreover, convergence is sometimes difficult to assess, and it is never guaranteed even when the initial guess is chosen arbitrarily close to a solution. Among the available schemes, the most robust iterative strategy appears to be that proposed by Luo and Mitsoulis [21]. The extra-stress $\boldsymbol{\tau}$ in the momentum equation is replaced by:

$$\tilde{\boldsymbol{\tau}}(\omega) = \omega\boldsymbol{\tau} + (1-\omega)\eta_A\dot{\boldsymbol{\gamma}}, \qquad \text{.....(20)}$$

where $\eta_A$ is an arbitrary Newtonian viscosity, and $\omega$ is a control parameter between 0 and 1. For $\omega = 0$, the flow problem is purely Newtonian, while the original viscoelastic equations are recovered for $\omega = 1$. Let $\boldsymbol{\tau}^n$ denote the viscoelastic stress computed at the $n^{th}$ iteration. Then, for creeping flows, Step 2 amounts to solving:

$$\nabla\cdot\left(-p^{n+1}\boldsymbol{\delta} + \eta_A\dot{\boldsymbol{\gamma}}^{n+1}\right) = -\nabla\cdot\left(\omega\left[\boldsymbol{\tau}^n - \eta_A\dot{\boldsymbol{\gamma}}^n\right]\right), \qquad \text{.....(21)}$$

$$\nabla\cdot\boldsymbol{v}^{n+1} = 0, \qquad \text{.....(22)}$$

for the updated velocity and pressure fields $\boldsymbol{v}^{n+1}$ and $p^{n+1}$, respectively. During the iterative process, the control parameter $\omega$ is progressively increased from 0 to 1, so that a solution to the original viscoelastic equations is finally obtained. This strategy is similar to the incremental loading procedure used in non-linear elasticity.

Malkus and Bernstein [22] have implemented the Broyden iterative algorithm, which is closer to a Newton-Raphson scheme but does not require the exact evaluation of the Jacobian matrix. Like for the simple-substitution schemes, the viscoelastic stress must be computed once per iteration on the basis of the current velocity field. The relative merits of the Broyden algorithm and the incremental loading approach have not been studied in detail.

 

**Finite element equations**

Step 2 of the decoupled strategy is a *Newtonian* flow problem defined by equations (21-22), where $-\nabla\cdot\left(\omega[\boldsymbol{\tau}^n-\eta_A\dot{\boldsymbol{\gamma}}^n]\right)$ is treated as a pseudo-body force that is known from the previous iteration. The corresponding Galerkin finite element equations read:

$$\int_\Omega\left[-p^a\boldsymbol{\delta}+\eta_A\dot{\boldsymbol{\gamma}}^a\right]\cdot\nabla\varphi^j d\Omega=-\int_\Omega\omega\left[\boldsymbol{\tau}-\eta_A\dot{\boldsymbol{\gamma}}^a\right]\cdot\nabla\varphi^j d\Omega+\int_{\partial\Omega_T}\boldsymbol{t}\,\varphi^j d\partial\Omega\,,$$

$$\int_\Omega\nabla\cdot\boldsymbol{v}^a\psi^l d\Omega=0\,, \qquad \text{…...(23)}$$

where the velocity and pressure fields are approximated as in equation (14), and $1\le j\le N_v$, $1\le l\le N_p$. The pseudo-body force integral in the right-hand-side of the Galerkin momentum equations is computed using the viscoelastic stress and velocity fields known from the previous iteration. To this end, we must somehow evaluate the viscoelastic stress $\boldsymbol{\tau}^n$ at all integration points of the finite element mesh; this defines Step 1 of the decoupled strategy, which we discuss next.

**Integration of the constitutive model**

Computation of the viscoelastic stress $\boldsymbol{\tau}$ at each integration point of the mesh is performed in three basic steps, using the Lagrangian formulation of the constitutive model:

– Tracking: using the steady-state velocity field known from the previous iteration, compute the past (i.e. upstream) trajectory and the travel time of the integration point;

– Strain evaluation: at selected past times, compute the deformation gradient $\boldsymbol{E}$ and from it the integrand of the constitutive model;

– Stress evaluation: compute the memory integral numerically along the past trajectories, using the results of the first and second steps.

The last task is the simplest one. In a steady-state flow, the displacement function $\boldsymbol{x}'$ is independent of $t$ and may be written $\boldsymbol{x}'=\boldsymbol{x}'(\boldsymbol{x},s)$ where $s$ is the time-lapse $t-t'$ ($s\ge 0$). This implies that $\boldsymbol{B}=\boldsymbol{B}(s)$. With a single-exponential memory function, the generic integral model (4) then reads:

$$\boldsymbol{\tau}=\frac{\eta}{\lambda^2}\int_0^\infty exp\left(-s/\lambda\right)\boldsymbol{S}\left(s\right)ds\,, \qquad \text{…….(24)}$$

where $\boldsymbol{S}(s)=\boldsymbol{f}(\boldsymbol{B}(s))$. Following the early work of Viriyayuthakorn and Caswell [8], a possible approach is to use a Gauss-Laguerre integration rule to approximate the memory integral:

$$\boldsymbol{\tau}\approx\frac{\eta}{\lambda}\sum_{i=1}^{N}\omega_i^N\,\boldsymbol{S}\left(\lambda z_i^N\right), \qquad \text{…….(25)}$$

where $z_i^N$ are the roots of the $N^{th}$ Laguerre polynomial, and $\omega_i^N$ are the weights of the quadrature rule. In practice, $N$ is of order 10. This approximation implies that the deformation $\boldsymbol{S}$ need only be computed at the discrete time lapses $s_i = \lambda z_i^N$. Obviously, ever larger strains must be evaluated when the memory of the fluid increases. The Gauss-Laguerre approach has been extended to finite and infinite relaxation spectra by Malkus and Bernstein [22]; it has also been adapted to nonisothermal flows of thermorheologically simple materials by Goublomme and Crochet [23]. More flexible integration techniques, though also more expensive, have been introduced by Dupont et al [24] and Luo and Tanner [25]. The time integral (24) is transformed into a line integral along the past trajectory; the latter is subdivided into segments through which the fluid particle travels in a time shorter than the relaxation time $\lambda$, and a Gauss quadrature rule is used to compute the integral along each segment. The backward integration is stopped once the marginal contribution of a segment is less than some specified tolerance. Interestingly, small relaxation times require a finer segmentation in order to capture the recent deformation history.

In principle, tracking of past particle positions and computation of the strain history require the integration of the kinematic equations:

$$\frac{D}{Ds}\boldsymbol{x}'(s) = -\boldsymbol{v}(\boldsymbol{x}'(s)), \quad \frac{D}{Ds}\boldsymbol{F}(s) = -\boldsymbol{\nabla v}^T(\boldsymbol{x}'(s))\cdot\boldsymbol{F}(s), \qquad \text{.....(26)}$$

*backward* along each particle trajectory, with the respective initial conditions $\boldsymbol{x}'(0) = \boldsymbol{x}$ and $\boldsymbol{F}(0) = \boldsymbol{\delta}$. The early numerical schemes reviewed by Crochet et al [1] had severe numerical problems with these two tasks. A first satisfactory solution was advanced by Bernstein et al [26], for two-dimensional planar flows. Briefly, it consists in using a special low-order finite element made of four triangles to compute the velocity field. The velocity finite element approximation is such that both tracking and strain history calculations can be performed *analytically* within each triangle. The price to pay for this nice result is the relatively low accuracy of the computed velocity field, and also the fact that the special element has spurious pressure modes. Extension of this approach to axisymmetric flows is reported by Bernstein et al [27].

Luo and Tanner [25] introduced another approach based on the concept of streamline finite elements. These are quadrilateral elements which have a pair of opposed sides that are aligned with streamlines. From the computation of the stream function using the current velocity field, which amounts to solving the Poisson equation $\nabla^2\psi = (\partial u/\partial y - \partial v/\partial x)$, the mesh is updated at each iteration so that the nodes (and thus the integration points) always lie along selected streamlines. A parametric representation of past trajectories is thus readily available in each element. The authors then compute the deformation history by solving the kinematic equation (26b) backward along each discrete streamlines using a fourth-order Runge-Kutta method. This approach is both fast and accurate, but it cannot handle recirculation regions. Luo and Mitsoulis [28] integrate the tracking problem (26b) by means of a second-order scheme.

The tracking procedure developed by Goublomme et al [29] is independent of the type of element, and it defines, we believe, the current state of the art. Pathlines are

 

computed on an element-by-element basis, by means of a fourth-order Runge-Kutta integration of (26a) within the parent element. This eliminates most of the complicated geometrical problems of earlier tracking schemes. In order to compute the deformation history, the authors follow the work of Dupont et al [24], who showed that, for a steady-state flow, the deformation gradient $\boldsymbol{F}$ can be computed by means of the velocity vectors at Lagrangian times $t$ and $t'$ and values of a scalar quantity $\beta$ which obeys a first-order differential equation involving the velocity field along the pathline. (This theoretical result is in fact equivalent to that of Adachi [17, 18].) Like for the tracking itself, Goublomme et al [29] integrate the equation for $\beta$ in the parent element. Very efficient implementations of this method on message-passing parallel computers have been proposed by Aggarwal et al [30] and Henriksen and Keunings [31].

**A short guide to selected applications**

The decoupled Eulerian-Lagrangian techniques have been applied by several authors to a variety of isothermal, two-dimensional steady-state flows involving polymer solutions and melts: entry flows (Kiriakidis et al [32], Feigl and Öttinger [33, 34], Mitsoulis [35-37], extrusion flows (Goublomme et al [29], Barakos and Mitsoulis [38, 39]), sedimentation of a single sphere (Sun and Tanner [40], Mitsoulis [41]), and flow past a cylinder (Barakos and Mitsoulis [42]). Nonisothermal flows have been considered by Goublomme and Crochet [23], and Barakos and Mitsoulis [43]. Finally, we note that the paper by Bernstein et al [27] is one of the very few studies wherein different decoupled Eulerian-Lagrangian schemes are compared.

## 4. THE LAGRANGIAN INTEGRAL METHOD

It has long been thought impossible to devise a coupled method for integral models that has general applicability, until the development of the Lagrangian Integral Method (LIM) initiated by Hassager and Bisgaard [44]. As its name indicates, LIM is based on the Lagrangian formulation of the conservation laws. The primary kinematic variables are the time-dependent positions of the fluid elements, while the computational domain is a deforming material volume. The latter is discretized by means of a finite element mesh that deforms with the flow. A typical flow simulation with LIM amounts to solving a transient problem, given the initial particle positions and deformation pre-history. LIM is thus a coupled method capable of solving transient flow problems. Steady-state flows are computed as the long-time limit of a transient problem. As all Lagrangian techniques, LIM readily applies to flows with free surfaces. Over the years, the method has been refined and extended to treat three-dimensional flows (Rasmussen and Hassager [45, 46], Rasmussen [47, 48]).

**Lagrangian formulation**

In the Lagrangian formulation, the fluid particle positions $\boldsymbol{x}$ at present time $t$ are dependent kinematic variables and the computational domain is a deforming material volume $\Omega(t)$. The momentum equations reads:

$$\rho \frac{\partial^2 \boldsymbol{x}}{\partial t^2} = \boldsymbol{\nabla} \cdot \boldsymbol{\sigma} \,, \qquad \text{.....(27)}$$

where $\boldsymbol{\sigma}$ is the Cauchy stress ($-p\,\boldsymbol{\delta} + \boldsymbol{\tau}$) evaluated at the moving fluid particle. The inertia term thus reduces to a time derivative computed along the particle paths. We shall describe the main features of LIM for a particular case of the Rivlin-Sawyers model [9]:

$$\boldsymbol{\tau}(t) = -\int_{-\infty}^{t} m\left(t-t', I_1, I_2\right) \boldsymbol{\gamma}_{[0]}(t,t')\, dt' \,, \qquad \text{.....(28)}$$

where $\boldsymbol{\gamma}_{[0]} = \boldsymbol{\delta} - \boldsymbol{B}$. Finally, for an incompressible material, the Lagrangian formulation of the continuity equation reads:

$$det\left(\boldsymbol{E}^{-1}(t,t')\right) = 1 \,. \qquad \text{.....(29)}$$

The governing equations (27-29) are supplemented with boundary and initial conditions. In general, the boundary $\partial\Omega(t)$ is divided into $\partial\Omega_X(t)$ and $\partial\Omega_T(t)$ where particle positions and surface tractions are imposed, respectively. The initial particle positions $\boldsymbol{x}_0$ are specified at time $t_0$, and, for illustrative purposes, we assume that the fluid has been at rest until $t_0$.

**Lagrangian finite element discretization**

In LIM, the computational domain $\Omega(t)$ is discretized by means of a finite element mesh whose nodes are moving at the local fluid velocity. The particle position $\boldsymbol{x}$ at present time $t$ is thus approximated as:

$$\boldsymbol{x}^a = \sum_{i=1}^{N_x} \boldsymbol{x}^i(t)\, \varphi^i \,, \qquad \text{.....(30)}$$

where $N_x$ is the number of nodes, $\boldsymbol{x}^i(t)$ is the unknown position of node $i$ at time $t$, and $\varphi^i$ is a known shape function associated to node $i$. At this point, it is crucial to note that the shape functions are independent of time. In view of (30), the approximate deformation gradient $\boldsymbol{E}^a$ is given by:

$$\boldsymbol{E}^a(t,t') = \frac{\partial \boldsymbol{x}^a}{\partial \boldsymbol{x}'} = \sum_{i=1}^{N_x} \boldsymbol{x}^i(t) \boldsymbol{\nabla}' \varphi^i \,, \qquad \text{.....(31)}$$

where $\boldsymbol{\nabla}'$ is the del operator relative to $\boldsymbol{x}'$. Over each element $\Omega^e$, the gradient $\boldsymbol{\nabla}'\varphi^i$ can be computed as a function of the nodal positions at time $t'$ by means of:

$$\boldsymbol{\nabla}'\varphi^i = \left(\boldsymbol{J}'\right)^{-1} \cdot \boldsymbol{\nabla}_p \varphi_e^i \,. \qquad \text{.....(32)}$$

Here, $\boldsymbol{J}'$ is the Jacobian matrix of the element mapping at time $t'$, $\varphi_e^i$ is a local shape function defined over the parent element, and $\boldsymbol{\nabla}_p$ is the del operator in local coordinates.

 

**Galerkin weak formulation of conservation laws**

The next step in the development of LIM is the derivation of the Galerkin weak form of equations (27,29). We obtain the Galerkin weak form of the momentum equation (27) in the usual fashion, the integrals being taken over the deforming computational domain $\Omega(t)$:

$$\int_{\Omega(t)} \rho \frac{\partial^2 \boldsymbol{x}^a}{\partial t^2} \varphi^j d\Omega - \int_{\Omega(t)} p^a \nabla \varphi^j d\Omega + \int_{\Omega(t)} \boldsymbol{\tau} \cdot \nabla \varphi^j d\Omega = \int_{\partial \Omega_T(t)} \boldsymbol{t}\, \varphi^j d\partial\Omega \,, \qquad \text{.....(33)}$$

for $1 \le j \le N_x$,. For clarity, we shall drop the superscript $a$ in subsequent equations. Over a time step $\Delta t$ the inertia term is discretized as follows:

$$\frac{\partial^2 \boldsymbol{x}}{\partial t^2} \approx \frac{\boldsymbol{v}(t) - \boldsymbol{v}(t - \Delta t)}{\Delta t}, \quad \text{with} \quad \boldsymbol{v}(t) \approx \frac{\boldsymbol{x}(t) - \boldsymbol{x}(t - \Delta t)}{\Delta t}. \qquad \text{.....(34)}$$

In the current implementation of LIM, the pressure field $p$ is approximated by means of a constant within each element $\Omega^e$. Thus, the Galerkin weak form of the continuity equation (29) reduces to:

$$\int_{\Omega^e} \left[ det(\boldsymbol{E}(t,t')) )^{-1} - 1 \right] d\Omega^e = 0 \,, \qquad \text{.....(35)}$$

which implies that the volume of each finite element at time $t'$ is equal to that at time $t$.

In order to form the Galerkin equations (33), we must evaluate the extra-stress $\boldsymbol{\tau}$ carried at time $t$ by each integration point of the mesh. This delicate task we discuss next.

**Discretization of the memory integral**

Evaluation of the extra-stress integral in the Galerkin momentum equations (33) is a daunting task. Indeed, the constitutive model (28) yields:

$$\int_{\Omega(t)} \boldsymbol{\tau} \cdot \nabla \varphi^j d\Omega = -\int_{\Omega(t)} \left\{ \int_{-\infty}^{t} m(t - t', I_1, I_2)\, \boldsymbol{\gamma}_{[0]}(t,t') dt' \right\} \cdot \nabla \varphi^j d\Omega \,. \qquad \text{.....(36)}$$

Clearly, some form of temporal discretization is needed to compute the memory integral at each integration point of the mesh. Considering the present time $t$ as fixed, the temporal axis is discretized as follows: $t_{-1} = -\infty$, $t_0 = 0$, $t_T = t$ and $t_{l-1} < t_l$ for $l = 1, 2, \ldots, T$ . We thus have:

$$\boldsymbol{\tau} = -\sum_{l=0}^{T} \int_{t_{l-1}}^{t_l} m(t - t', I_1, I_2)\, \boldsymbol{\gamma}_{[0]}(t,t')\, dt' \,. \qquad \text{.....(37)}$$

The key idea now is to approximate $I_1$, $I_2$ and $\boldsymbol{\gamma}_{[0]}$, for $t'$ in $[t_{l-1}, t_l]$, by a Taylor expansion to first order in $(t' - t_l)$. As shown in [9], this yields:

$$\begin{aligned}
&\boldsymbol{\gamma}_{[0]}(t,t') \approx \boldsymbol{\gamma}_{[0]}(t,t_l) + (t'-t_l)\,\boldsymbol{\gamma}_{[1]}\,,\\
&I_1(t,t') \approx I_1(t,t_l) - (t'-t_l)\,tr\left(\boldsymbol{\gamma}_{[1]}\right) = I_{1,l}\,,\\
&I_2(t,t') \approx I_2(t,t_l) + (t'-t_l)\,tr\left(\boldsymbol{\gamma}^{[1]}\right) = I_{2,l}\,,
\end{aligned} \qquad \text{.....(38)}$$

where the kinematic tensors $\boldsymbol{\gamma}_{[1]}$ and $\boldsymbol{\gamma}^{[1]}$ are evaluated at $t' = t_l$ according to:

$$\begin{aligned}
&\boldsymbol{\gamma}_{[1]} = \boldsymbol{E}(t,t_l)\cdot\dot{\boldsymbol{\gamma}}(t_l)\cdot\boldsymbol{E}(t,t_l)^T\,,\\
&\boldsymbol{\gamma}^{[1]} = \boldsymbol{E}^{-T}(t,t_l)\cdot\dot{\boldsymbol{\gamma}}(t_l)\cdot\boldsymbol{E}^{-1}(t,t_l).
\end{aligned} \qquad \text{.....(39)}$$

Here, we have $\dot{\boldsymbol{\gamma}}(t_l) = \boldsymbol{\nabla}_l \boldsymbol{v}(t_l) + \boldsymbol{\nabla}_l \boldsymbol{v}(t_l)^T$ and $\boldsymbol{\nabla}_l$ denotes the del operator with respect to the position at time $t_l$. The discretization error implied in the approximations (38) is of order $(t_l - t_{l-1})^2$.

Next, we introduce the approximations (38) in the memory integral (37), taking the initial conditions into account. For a fluid that has been quiescent between $t_{-1} = \infty$ and $t_0 = 0$, we have $\boldsymbol{\gamma}_{[1]}(t,t') = \boldsymbol{\gamma}^{[1]}(t,t') = \mathbf{0}$ and $\boldsymbol{\gamma}_{[0]}(t,t') = \boldsymbol{\gamma}_{[0]}(t,0)$ for $t' < 0$. Moreover, $\boldsymbol{\gamma}_{[0]}(t,t) = \mathbf{0}$ , $\boldsymbol{\gamma}_{[1]}(t,t) = \dot{\boldsymbol{\gamma}}(t)$, $I_1(t, t) = I_2(t, t) = 3$, and $tr\left(\boldsymbol{\gamma}_{[1]}(t,t)\right) = tr\left(\boldsymbol{\gamma}^{[1]}(t,t)\right) = 0$. The memory integral (37) is thus approximated as follows:

$$\begin{aligned}
\boldsymbol{\tau} \approx &-\sum_{l=0}^{T-1} \underbrace{\left[\int_{t_{l-1}}^{t_l} m\left(t-t', I_{1,l}, I_{2,l}\right)dt'\right]}_{\boldsymbol{M}_{0,l}} \boldsymbol{\gamma}_{[0]}(t,t_l)\,,\\
&-\sum_{l=1}^{T-1} \underbrace{\left[\int_{t_{l-1}}^{t_l} m\left(t-t', I_{1,l}, I_{2,l}\right)\cdot(t'-t_l)dt'\right]}_{\boldsymbol{M}_{1,l}} \boldsymbol{\gamma}_{[1]}(t,t_l)\,,\\
&-\underbrace{\left[\int_{t_{T-1}}^{t} m\left(t-t',3,3\right)\cdot(t'-t)dt'\right]}_{\boldsymbol{M}_{2,t}} \dot{\boldsymbol{\gamma}}(t).
\end{aligned} \qquad \text{.....(40)}$$

We now need to substitute $\boldsymbol{\tau}$ into the Galerkin momentum equation (33). In so doing, a most welcome simplification is provided by the identity:

$$\boldsymbol{E}(t,t_l)^T \cdot \boldsymbol{\nabla}\varphi^i = \boldsymbol{\nabla}_l \varphi^i\,. \qquad \text{.....(41)}$$

The final Galerkin weak form of the momentum equation reads:

 

$$\int_{\Omega(t)} \rho \frac{\partial^2 \boldsymbol{x}}{\partial t^2} \varphi^j d\Omega - \int_{\Omega(t)} [p + \underbrace{\sum_{l=0}^{T-1} M_{0,l}}_{MI_1}] \boldsymbol{\nabla} \varphi^j d\Omega - M_{2,t} \int_{\Omega(t)} \dot{\boldsymbol{\gamma}}(t) \cdot \boldsymbol{\nabla} \varphi^j d\Omega$$

$$+ \int_{\Omega(t)} \sum_{i=1}^{N_x} \boldsymbol{x}^i(t) \underbrace{\left\{ \sum_{l=0}^{T-1} M_{0,l} C_l^{ij} - \sum_{l=1}^{T-1} M_{1,l} D_l^{ij} \right\}}_{MI_2} d\Omega = \int_{\partial\Omega_T(t)} \boldsymbol{t}\, \varphi^j d\partial\Omega \,, \qquad \text{.....(42)}$$

where $C_l^{ij}$ and $D_l^{ij}$ are symmetric matrix coefficients given by:

$$C_l^{ij} = \boldsymbol{\nabla}_l \varphi^i \cdot \boldsymbol{\nabla}_l \varphi^j \,, \qquad D_l^{ij} = \boldsymbol{\nabla}_l \varphi^i \cdot \left[ \boldsymbol{\nabla}_l \boldsymbol{v}(t_l) + \boldsymbol{\nabla}_l \boldsymbol{v}(t_l)^T \right] \cdot \boldsymbol{\nabla}_l \varphi^j \,. \qquad \text{.....(43)}$$

It should be noted that the discretized memory integrals $MI_1$ and $MI_2$ do generally depend on the particle positions $\boldsymbol{x}^i(t)$. A final approximation is now introduced in equation (43) in order to relate the $D_l^{ij}$ coefficients to the particle positions at past times $t_l$ and $t_{l-1}$:

$$\nabla_l \boldsymbol{v}(t_l) \approx \sum_{k=1}^{N_x} \left\{ \frac{\boldsymbol{x}^k(t_l) - \boldsymbol{x}^k(t_{l-1})}{t_l - t_{l-1}} \right\} \nabla_l \varphi^k \,. \qquad \text{.....(44)}$$

Equation (42) is the final Galerkin weak form of the momentum equation used in LIM. The last term of the left-hand side is a small Newtonian like contribution wherein $\dot{\boldsymbol{\gamma}}(t)$ is approximated using the discretized velocity (34). Even though the algebra is rather daunting, the task of assembling the Galerkin equations is conceptually simple. Indeed, knowledge of the stored history of nodal positions $\boldsymbol{x}^i(t_l)$ for $l = 0, 1\ldots..., T-1$, and $i = 1, 2, \ldots..., N_x$ allows the computation of the discretized time integrals $MI_1$ and $MI_2$ at all integration points of the mesh. Note that these integrals must be re-evaluated at each time step in the general case of a memory function $m$ that depends on the strain invariants $I_1$ and $I_2$. For strain-independent memory functions $m(t\text{-}t')$, $MI_1$ and $MI_2$ do not depend on the current nodal positions $\boldsymbol{x}^i(t)$. Furthermore, they do not need to be re-computed at each time step, but can merely be updated. So, the history of nodal positions should not be stored in principle with these simple models.

**Solution of the discrete equations**

At each time step, the Galerkin equations (35) and (42) form a set of non-linear algebraic equations whose unknowns are the nodal particle positions $\boldsymbol{X}(t) = \left[ \boldsymbol{x}^1(t), \boldsymbol{x}^2(t), \ldots..., \boldsymbol{x}^{N_x}(t) \right]^T$ and nodal pressures $\boldsymbol{P}(t) = \left[ p^1(t), p^2(t), \ldots..., p^{N_p}(t) \right]^T$. A solution is found by means of the Newton iterative scheme. This requires the evaluation of the derivatives of the Galerkin equations with respect to the unknowns, in particular the current particle positions $\boldsymbol{X}(t)$. The latter computation is lengthy but straightforward. Indeed, each term of the Galerkin equations is an integral of a certain

algebraic function $\boldsymbol{g}$ of the positions $\boldsymbol{X}(t)$, taken over the material volume $\Omega$ which itself also depends on $\boldsymbol{X}(t)$ and computed as a sum of integrals over each element $\Omega^e$:

$$\int_{\Omega(\boldsymbol{X}(t))} \boldsymbol{g}\left(\boldsymbol{X}(t)\right) d\Omega = \sum_e \int_{\Omega^e(\boldsymbol{X}(t))} \boldsymbol{g}\left(\boldsymbol{X}(t)\right) d\Omega^e \; . \qquad \text{.....(45)}$$

The derivative of equation (45) with respect to $\boldsymbol{X}(t)$ is then computed by transforming the integral over a particular element $\Omega^e$, which depends on $\boldsymbol{X}(t)$, into one over the parent element $\Omega_p$ , which does not depend on $\boldsymbol{X}(t)$:

$$\frac{\partial}{\partial \boldsymbol{X}(t)} \left\{ \int_{\Omega^e(\boldsymbol{X}(t))} \boldsymbol{g}\left(\boldsymbol{X}(t)\right) d\Omega^e \right\} = \int_{\Omega_p} \frac{\partial}{\partial \boldsymbol{X}(t)} \left[ \boldsymbol{g}\left(\boldsymbol{X}(t)\right) \cdot J \right] d\Omega_p \, , \qquad \text{.....(46)}$$

where $J$ is the Jacobian of the isoparametric transformation (30) at time $t$.

Our presentation of LIM would at this point be complete if the method could use the same finite element mesh during the course of the simulation. In most flow problems, this cannot be the case as the finite element mesh becomes overly distorted after a while. A remeshing procedure is thus in order. In view of the memory of viscoelastic fluids, remeshing is not a trivial task.

**Remeshing procedure**

Let us assume that the original finite element mesh used to start the simulation has become exaggeratedly distorted at time $\tilde{t}_1$ . A new mesh is then introduced in order to pursue the simulation. In order to compute the memory integrals $MI_1$ and $MI_2$ in the Galerkin equations (42), one basically needs to evaluate $\boldsymbol{\nabla}' \varphi^i$ at the integration points of the mesh, for all past times $t' = t_l$. As long as the same mesh is used, evaluation of $\boldsymbol{\nabla}' \varphi^i$ is performed in each element $\Omega^e$ by means of the identity (32). This identity does *not* hold, however, when a change of mesh is made. For $t' < \tilde{t}_1 < t$ we can use instead the relation:

$$\boldsymbol{\nabla}' \varphi^i = \boldsymbol{E}^a\left(\tilde{t}_1, t'\right)^T \cdot \boldsymbol{\nabla}_1 \varphi^i \; . \qquad \text{.....(47)}$$

Here, $\boldsymbol{\nabla}_1 \varphi^i$ is computed with respect to the coordinates at time $\tilde{t}_1$ by applying equation (32) on the new mesh. On the other hand, $\boldsymbol{E}^a\left(\tilde{t}_1, t'\right)$ is obtained using equation (31) on the original mesh. Since $\boldsymbol{\nabla}_1 \varphi^i$ must be computed at the integration points of the new mesh, evaluation of $\boldsymbol{E}^a\left(\tilde{t}_1, t'\right)$ there requires to find in which element of the old mesh and at what local coordinates in the parent element lies each integration point of the new mesh at time $\tilde{t}_1$ .

The above considerations are readily generalized to an arbitrary number of remeshing steps. Consider for example the case $\tilde{t}_{p+1} \le t' < \tilde{t}_p < ..... < \tilde{t}_1 < t$ , where new meshes have been introduced at times $\tilde{t}_k$ . The relation (47) becomes:

 

$$\nabla' \varphi^i = \boldsymbol{E}^a\left(\tilde{t}_p, t'\right)^T \cdot \prod_{k=p-1}^{1} \boldsymbol{E}^a\left(\tilde{t}_k, \tilde{t}_{k+1}\right)^T \cdot \nabla_1 \varphi^i \,, \qquad \text{.....(48)}$$

where

$$\boldsymbol{E}^a\left(\tilde{t}_k, \tilde{t}_{k+1}\right) = \sum_{j=1}^{N_x} \boldsymbol{x}^j\left(\tilde{t}_k\right) \nabla_{k+1} \varphi^j \,. \qquad \text{.....(49)}$$

In these expressions, all derivatives are well defined as they refer to the same mesh; the gradient $\nabla_{k+1}\varphi^i$, for example, corresponds to the mesh used between $\tilde{t}_{k+1}$ and $\tilde{t}_k$. Finally, we note that, whenever a new mesh is introduced, one must determine the element and local coordinates of its integration points in *all* previously used meshes. This is indeed necessary to apply the remeshing recipe (48).

For models with a strain-independent memory function $m(t-t')$, it is in principle not necessary to apply the above procedure. Indeed, all that is needed is to compute at the integration points of the new mesh the memory integrals $MI_1$ and $MI_2$ which have been accumulated until the remeshing time $\tilde{t}_k$. This could be achieved by means of an interpolation procedure between the old and new meshes, and the calculations could be pursued on the new mesh by updating the memory integrals. Thus, one would not need to store the history of nodal positions which is necessary to apply the remeshing rule (48). The problem with that approach is the interpolation step, which so far has not been achieved successfully. So, LIM treats strain-independent memory models like their strain-dependent counterparts, namely it applies the remeshing rule (48) and stores the history of past nodal positions.

**Applications of LIM**

The method has been applied in several studies of rheological interest: the transient sedimentation of a sphere in a viscoelastic liquid (Becker et al [49], Rasmussen and Hassager [50]), the stretching of viscoelastic filaments (Kolte et al [51], Rasmussen and Hassager [52, 53]), and the inflation of polymeric membranes (Rasmussen et al [54]).

## 5. THE METHOD OF DEFORMATION FIELDS

In this section, we present a new approach advanced recently by Peters et al [55] known as the Deformation Field Method (DFM). The basic idea behind DFM is that the deformation history is described by a finite number of deformation fields which are convected and deformed by the flow field. In fact, DFM is the first Eulerian technique for solving time-dependent flows with an integral constitutive equation. It thus combines the main advantage of an Eulerian technique, i.e. it does not need remeshing, with the intrinsic time-dependent character of Lagrangian simulat ions. Since its introduction, DFM has known several developments which we shall discuss in due course. It is useful to describe the original idea first.

**The concept of deformation field**

Consider a fluid particle located at position $\boldsymbol{x}$ at present time $t$, and at $\boldsymbol{x}'$ at some past time $t' < t$. The key idea behind DFM is to regard $t'$ as a fixed reference time. The Finger strain $\boldsymbol{B}$ is written as: $\boldsymbol{B}_{t'}(\boldsymbol{x},t)$ to make reference to $t'$ explicit. It is thus regarded as a *deformation field* that measures the deformation of a material element with respect to the reference time $t'$. For $t'$ fixed, the deformation field $\boldsymbol{B}_{t'}(\boldsymbol{x},t)$ can be thought of as having been created at time $t = t'$ with the initial condition:

$$\boldsymbol{B}_{t'}(\boldsymbol{x},t') = \boldsymbol{\delta} \; . \qquad \text{.....(50)}$$

The kinematic equation governing the evolution of $\boldsymbol{B}_{t'}(\boldsymbol{x},t)$ expresses that the upper-convected derivative of the deformation field vanishes:

$$\frac{\partial}{\partial t}\boldsymbol{B}_{t'}(\boldsymbol{x},t) + \boldsymbol{v}\cdot\nabla\boldsymbol{B}_{t'}(\boldsymbol{x},t) - \nabla\boldsymbol{v}^T\cdot\boldsymbol{B}_{t'}(\boldsymbol{x},t) - \boldsymbol{B}_{t'}(\boldsymbol{x},t)\cdot\nabla\boldsymbol{v} = \boldsymbol{0} \; , \qquad \text{.....(51)}$$

where $\boldsymbol{v} = \boldsymbol{v}(\boldsymbol{x},t)$. Together with the initial condition (50), equation (51) determines how a particular deformation field $\boldsymbol{B}_{t'}(\boldsymbol{x},t)$, labelled by its creation time $t'$, is convected and deformed by the flow. A crucial point is that the evolution equation for $\boldsymbol{B}_{t'}(\boldsymbol{x},t)$ involves the velocity field $\boldsymbol{v}$ at the present time_$t$ only. The deformation history is in fact contained in the deformation fields $\boldsymbol{B}_{t'}(\boldsymbol{x},t)$ for $t' < t$. In DFM, only a finite number of deformation fields will be computed to approximate the memory integral, as we now explain.

**Discretization of the memory integral**

For illustrative purposes, let us assume that the extra-stress $\boldsymbol{\tau}$ is given by the generic separable integral model (4). With the concept of deformation fields, the integral model is readily formulated in Eulerian fashion:

$$\boldsymbol{\tau}(\boldsymbol{x},t) = \int_{-\infty}^{t} m(t-t')\boldsymbol{f}\left(\boldsymbol{B}_{t'}(\boldsymbol{x},t)\right)dt' \; . \qquad \text{.....(52)}$$

In natural language, equations (50-52) thus read as follows: At each instant in time, a deformation field is created (as a unit tensor), and labelled by the time $t'$ of creation; the field is then convected and deformed by the flow according to equation (51). The stress field at current time $t$ is obtained by integrating the weighted contribution of all deformation fields that have been created so far.

In view of equation (52), the contribution of a particular deformation field to the stress at present time $t$ is weighted by the memory function $m(t-t')$. Thus, "old fields", with a large age $\tau = t-t'$, contribute less than "young" fields. Evaluation of the memory integral (52) requires in principle the knowledge of $\boldsymbol{f}\left(\boldsymbol{B}_{t'}(\boldsymbol{x},t)\right)$ for *all* $t' < t$. In DFM, only a finite number of deformation fields are computed. Moreover, deformation fields that become older than a user-specified cut-off age $\tau_c$ are discarded altogether and thus no longer contribute to the approximation of the memory integral. At all times $t$, the number of deformation fields used in DFM is thus a constant $N_{DF}$.

 

We can now detail the approximate evaluation of the memory integral (52). At present time *t*, DFM computes the evolution of the deformation fields $\boldsymbol{B}_{t-\tau_i}(\boldsymbol{x},t)$ with label $t_i' = t - \tau_i$ for $i$ = 0, 2, ..... , $N_{DF}$ −1. The ages of these fields are $\tau_0 = 0 < \tau_1 < \tau_2 < ..... < \tau_{N_{DF}-1} = \tau_c$. At this stage comes the second key idea behind DFM, namely the use of a finite element interpolation of $\boldsymbol{f}(\boldsymbol{B}_{t'}(\boldsymbol{x},t))$ in $\tau$-space:

$$\boldsymbol{f}(\boldsymbol{B}_{t-\tau}(\boldsymbol{x},t)) \approx \sum_{i=0}^{N_{DF}-1} \boldsymbol{f}\left(\boldsymbol{B}_{t-\tau_i}(\boldsymbol{x},t)\right)\varphi_i(\tau), \qquad \text{.....(53)}$$

where $\varphi_i(\tau)$ is a linear shape function associated to node $\tau_i$ in $\tau$-space. For $\tau > \tau_c$, DFM assumes in effect that $\boldsymbol{f}(\boldsymbol{B}_{t-\tau}(\boldsymbol{x},t)) = \boldsymbol{f}\left(\boldsymbol{B}_{t-\tau_c}(\boldsymbol{x},t)\right)$. In view of equation (53), the approximate stress integral (52) is obtained as:

$$\boldsymbol{\tau}(\boldsymbol{x},t) \approx \sum_{i=0}^{N_{DF}-1} W_i \boldsymbol{f}\left(\boldsymbol{B}_{t-\tau_i}(\boldsymbol{x},t)\right), \qquad \text{.....(54)}$$

where the weight $W_i$ of the deformation field of age $\tau_i$ is given by:

$$W_i = \int_0^\infty m(\tau)\varphi_i(\tau)\,d\tau\,. \qquad \text{.....(55)}$$

The weights decrease with age and are computed once and for all before the start of the simulation. In DFM, the memory integral (52) is thus approximated by the finite sum (54) which is second-order accurate in time. If $\boldsymbol{f}(\boldsymbol{B}_{t'})$ remains bounded and the cut-off age $\tau_c$ is several times the largest relaxation time of the fluid, then the error made by truncating the memory integral should be small since realistic memory functions decay exponentially at large $\tau$. Truncation can be problematic, however, in the simulation of strong flows with models that have an unbounded strain function $\boldsymbol{f}$. This difficulty arises for example with the upper-convected Maxwell model. One can of course argue that the possibility for $\boldsymbol{f}(\boldsymbol{B}_{t'})$ to grow without bound indicates a serious flaw in the constitutive model itself, in addition to causing numerical difficulties.

**Updating the deformation fields: implementation issues**

Let us now discuss some implementation issues related to the update of the deformation fields. We know that old fields contribute little to the stress. The idea of a cut-off age $\tau_c$ allows us to discard an old field at each time step. Memory space is thus freed to store the newly-created field labelled by the current time *t*. This approach keeps the number $N_{DF}$ of deformation fields constant during the course of the simulation.

The simplest implementation of DFM uses a uniform discretization in $\tau$-space, with a constant increment $\Delta t = t_i' - t_{i+1}' = \tau_{i+1} - \tau_i$ chosen equal to that used for solving the evolution equation (51) and the conservation laws. Updating the deformation fields then goes in three steps:

(i) update existing fields by solving for each the evolution equation (51):

$$\boldsymbol{B}_{t-i\Delta t}(\boldsymbol{x},t) \rightarrow \boldsymbol{B}_{t-i\Delta t}(\boldsymbol{x},t+\Delta t),$$

(ii) destruct the oldest field $\boldsymbol{B}_{t-\tau_c}$,

(iii) create a new field with label $t+\Delta t$ using memory space freed in step (ii):

$$\boldsymbol{B}_{t+\Delta t}(\boldsymbol{x},t+\Delta t) = \boldsymbol{\delta}.$$

Once updated, each deformation field is older by one time step $\Delta t$ and must therefore be assigned the next lower weight in the list. The updated deformation fields and their new weights are then used to compute the stress field $\boldsymbol{\tau}(\boldsymbol{x},t+\nabla t)$. A more sophisticated implementation of DFM uses a non-uniform discretization of the age axis, with small increments for young fields and larger ones for older fields. This enables DFM to capture the short time response of the fluid with more accuracy than the long time response whose weight is low.

In their early experiments with DFM, Peters et al [55] find that about $N_{DF} = 100$ deformation fields are sufficient to discretize the deformation history. It should be pointed out that the optimal choice of the cut-off time $\tau_c$ and of a particular distribution of age groups is expected to depend somewhat on the memory function, as well as on the actual flow problem (geometry, Weissenberg number) and its numerical discretization (time step and mesh refinement).

**Discretization of the governing equations**

In DFM, the governing equations are the conservation laws written in Eulerian form, supplemented by the evolution equation (51) for each of the $N_{DF}$ active deformation fields. The polymer stress is not a primary variable since it is directly related to the deformation fields through equation (54). Since $N_{DF}$ is of order 100 in actual simulations, the number of governing equations is rather large and a coupled method of solution is clearly not practical. Spatial discretization of the conservation laws is achieved by means of the Discrete Elastic-Viscous Split Stress (DEVSS) formulation of Guénette and Fortin [58], while the Discontinuous Galerkin (DG) method is used to solve the deformation field equations. The important point, as we shall see, is that the deformation fields can be updated at the element level, thus avoiding the solution of an inordinate number of coupled alegbraic equations. Following Baaijens et al [59], who introduced the combination of DG and DEVSS in the context of viscoelastic flows, Peters et al [55] have implemented DFM on two-dimensional quadrilateral elements using, in particular, discontinuous bi-linear deformation fields. Let us briefly examine a typical time step of DFM.

The DG weak formulation of equation (51) is expressed over each element $\Omega^e$ of the mesh: find $\boldsymbol{B}_{t'}$ over $\Omega^e$ such that for all admissible test functions $\boldsymbol{S}$ we have:

$$\left(\boldsymbol{S}, \frac{\partial}{\partial t}\boldsymbol{B}_{t'} + \boldsymbol{v}\cdot\nabla\boldsymbol{B}_{t'} - \nabla\boldsymbol{v}^T\cdot\boldsymbol{B}_{t'} - \boldsymbol{B}_{t'}\cdot\nabla\boldsymbol{v}\right)_{\Omega^e} - \left(\boldsymbol{S}, \left[\boldsymbol{B}_{t'} - \tilde{\boldsymbol{B}}_{t'}\right]\boldsymbol{v}\cdot\boldsymbol{n}\right)_{\partial\Omega^e_{in}} = 0. \quad \text{.....(56)}$$

 

Here, $(\cdot,\cdot)_{\Omega^e}$ denotes the $L^2$ inner product over the element $\Omega^e$, $\boldsymbol{n}$ is the outward unit normal at the boundary $\partial\Omega^e$ of the element, $\partial\Omega^e_{in}$ is the part of $\partial\Omega^e$ where $\boldsymbol{v}\cdot\boldsymbol{n} < 0$ and $(\cdot,\cdot)_{\Omega^e_{in}}$ is the corresponding inner product, and $\tilde{\boldsymbol{B}}_{t'}$ is the value of $\boldsymbol{B}_{t'}$ in the upstream neighbouring element (or the value specified at an inlet section of the computational domain). Peters et al [55] use an explicit Euler scheme to discretize equation (56) in time. At time $t_n$ , one knows the velocity field $\boldsymbol{v}^n \approx \boldsymbol{v}(\boldsymbol{x},t_n)$ and deformation fields $\boldsymbol{B}^n_{t'} \approx \boldsymbol{B}_{t'}(\boldsymbol{x},t_n)$ for $N_{DF}$ discrete values of the past time $t'$. The updated fields $\boldsymbol{B}^{n+1}_{t'} \approx \boldsymbol{B}_{t'}(\boldsymbol{x},t_{n+1}=t_n+\Delta t)$ are then computed at the element level with the explicit recurrence:

$$\left(\boldsymbol{S},\boldsymbol{B}^{n+1}_{t'}\right)_{\Omega^e} = \left(\boldsymbol{S},\boldsymbol{B}^{n}_{t'}\right)_{\Omega^e} - \Delta t\cdot\left(\boldsymbol{S},\boldsymbol{v}^n\cdot\nabla\boldsymbol{B}^n_{t'} - \nabla\left(\boldsymbol{v}^n\right)^T\cdot\boldsymbol{B}^n_{t'} - \boldsymbol{B}^n_{t'}\cdot\nabla\boldsymbol{v}^n\right)_{\Omega^e} + \Delta t\cdot\left(\boldsymbol{S},\left[\boldsymbol{B}^n_{t'}-\tilde{\boldsymbol{B}}^n_{t'}\right]\boldsymbol{v}^n\cdot\boldsymbol{n}\right)_{\partial\Omega^e_{in}}. \qquad \text{.....(57)}$$

Once the updated fields $\boldsymbol{B}^{n+1}_{t'}$ have been obtained, the stress $\boldsymbol{\tau}^{n+1} \approx \boldsymbol{\tau}(\boldsymbol{x},t_{n+1})$ is computed at the integration points of each element by means of equation (54). Its $L^2$ - projection on the space of discontinuous bi-linear polynomials is then computed, again in each element.

We now turn to the momentum and continuity equations to determine the velocity $\boldsymbol{v}^{n+1} \approx \boldsymbol{v}(\boldsymbol{x},t_{n+1})$ and pressure $p^{n+1} \approx p(\boldsymbol{x},t_{n+1})$. In the original implementation by Peters et al [55], inertia terms are neglected. The DEVSS weak formulation of the conservation laws reads: find $\left(\boldsymbol{v}^{n+1},\boldsymbol{e}^{n+1},p^{n+1}\right)$ such that for all admissible test functions ($\boldsymbol{u}$, $\boldsymbol{g}$, $q$) we have:

$$\begin{aligned}
&\left(\nabla\boldsymbol{u},2\eta\boldsymbol{D}^{n+1}-\boldsymbol{e}^{n+1}\right)_\Omega - \left(\nabla\cdot\boldsymbol{u},\,p^{n+1}\right)_\Omega = -\left(\nabla\boldsymbol{u},\boldsymbol{\tau}^{n+1}\right)_\Omega + \left(\boldsymbol{u},\boldsymbol{t}\right)_{\partial\Omega},\\
&\left(\boldsymbol{g},\left[2\eta\boldsymbol{D}^{n+1}-\boldsymbol{e}^{n+1}\right]\right)_\Omega = 0, \qquad \text{.....(58)}\\
&\left(q,\nabla.\boldsymbol{v}^{n+1}\right)_\Omega = 0,
\end{aligned}$$

where $(\cdot,\cdot)_\Omega$ and $(\cdot,\cdot)_{\partial\Omega}$ are the inner product over $\Omega$ and $\partial\Omega$, respectively, $\boldsymbol{t}$ is the contact force, and $\eta$ is taken as the zero-shear rate viscosity of the fluid. Note that the term involving the updated stress $\boldsymbol{\tau}^{n+1}$ is treated as a pseudo-body force. Values of $\boldsymbol{\tau}^{n+1}$ at the integration points are provided in each element by the $L^2$ - projection alluded to above. This completes a single time step of the original DFM.

**An alternative formulation of deformation fields**

In the original DFM, the deformation fields are labelled by the *absolute* reference time $t'$. This has several important consequences. First, a particular

deformation field $\boldsymbol{B}_{t'}(\boldsymbol{x},t)$ never attains a steady-state regime, even for steady flow kinematics. Second, implementation of DFM is somewhat difficult due to the creation and deletion of deformation fields. Finally, discretization of the $t'$-axis is not very flexible, being linked to the time step $\Delta t$ used to solve the governing equations. Hulsen et al [57] have recently proposed an alternative approach which addresses these issues. The basic idea is to select as independent variable the age $\tau = t - t'$, which is measured *relative* to the current time $t$:

$$\boldsymbol{B}(\boldsymbol{x},t,\tau) = \boldsymbol{B}_{t-\tau}(\boldsymbol{x},t). \qquad \text{.....(59)}$$

Since

$$\frac{\partial}{\partial t}\boldsymbol{B}_{t'}(\boldsymbol{x},t) = \frac{\partial}{\partial t}\boldsymbol{B}(\boldsymbol{x},t,\tau) = \frac{\partial \boldsymbol{B}}{\partial t} + \frac{\partial \boldsymbol{B}}{\partial \tau}\frac{\partial \tau}{\partial t} = \frac{\partial \boldsymbol{B}}{\partial t} + \frac{\partial \boldsymbol{B}}{\partial \tau}, \qquad \text{.....(60)}$$

the evolution equation for $\boldsymbol{B}(\boldsymbol{x},t,\tau)$ is readily obtained from equation (51):

$$\frac{\partial \boldsymbol{B}}{\partial t} + \frac{\partial \boldsymbol{B}}{\partial \tau} + \boldsymbol{v}\cdot\nabla\boldsymbol{B} - \nabla\boldsymbol{v}^T\cdot\boldsymbol{B} - \boldsymbol{B}\cdot\nabla\boldsymbol{v} = \boldsymbol{0}. \qquad \text{.....(61)}$$

Here, the velocity field $\boldsymbol{v}$ is a function of $(\boldsymbol{x},t)$ but is independent of $\tau$. Thus, by changing the reference time from absolute to relative, we have increased by one the dimensionality of the evolution equation. Also, the initial condition (50) becomes the boundary condition:

$$\boldsymbol{B}(\boldsymbol{x},t,0) = \boldsymbol{\delta}. \qquad \text{.....(62)}$$

A suitable initial condition must also be specified, such as $\boldsymbol{B}(\boldsymbol{x},t,0) = \boldsymbol{\delta}$ for a fluid that has been quiescent prior to $t = 0$.

In order to discretize equation (61) along the age axis, Hulsen et al [57] use the discontinuous Galerkin (DG) method. The $\tau$-axis is divided into $N$ elements:

$$I_j = [\tau_j, \tau_{j+1}], \qquad j = 0, 1, \ldots, N-1 \qquad \text{.....(63)}$$

with $\tau_0 = 0$ and $\tau_N = \tau_c$. Note that the age discretization is independent of $(\boldsymbol{x},t)$. The DG weak formulation is then: find $\boldsymbol{B}$ over each element $I_j$ such that for all admissible test functions $\boldsymbol{w}$ we have:

$$\int_{\tau_j}^{\tau_{j+1}} \left( \frac{\partial \boldsymbol{B}}{\partial t} + \frac{\partial \boldsymbol{B}}{\partial \tau} + \boldsymbol{v}\cdot\nabla\boldsymbol{B} - \nabla\boldsymbol{v}^T\cdot\boldsymbol{B} - \boldsymbol{B}\cdot\nabla\boldsymbol{v} \right) : \boldsymbol{w}\, d\tau + [\boldsymbol{B}]_j : \boldsymbol{w}(\tau_j) = 0, \qquad \text{.....(64)}$$

where $[\boldsymbol{B}]_j = \boldsymbol{B}^+(\tau_j) - \boldsymbol{B}^-(\tau_j)$ is the jump in $\boldsymbol{B}$ at the boundary $\tau = \tau_j$ between elements $I_{j-1}$ and $I_j$ [#]. The boundary condition (62) gives $\boldsymbol{B}^-(\tau_0) = \boldsymbol{\delta}$. Now, over each element $I_j$, the deformation is approximated by:

$$\boldsymbol{B} \approx \sum_{k=1}^{2} \boldsymbol{B}_j^k \varphi_j^k(\tau), \qquad \text{.....(65)}$$

[#] Compare with the analogous DG formulation (56) in $\boldsymbol{x}$-space.

 

where $\varphi_j^k$ is a linear shape function and $\boldsymbol{B}_j^k$ is an unknown nodal value. A two-point Gauss integration rule computes the integral in equation (64) exactly. By locating the nodes of element $I_j$ at the two integration points $\tau_j^k$ so that $\varphi_j^k\left(\tau_j^m\right)=\delta_{km}$, we obtain the evolution equation:

$$\frac{\partial \boldsymbol{B}_j^k}{\partial t}=-\boldsymbol{v}\cdot\boldsymbol{\nabla}\boldsymbol{B}_j^k+\boldsymbol{\nabla}\boldsymbol{v}^T\cdot\boldsymbol{B}_j^k+\boldsymbol{B}_j^k\cdot\boldsymbol{\nabla}\boldsymbol{v}-\sum_{m=1}^{2}\boldsymbol{B}_j^m\frac{\partial\varphi_j^m}{\partial\tau}\left(\tau_j^k\right)-[\boldsymbol{B}]_j\frac{2\varphi_j^k\left(\tau_j\right)}{\tau_{j+1}-\tau_j}. \quad \ldots.(66)$$

Thus, discretization of the age axis using DG yields the evolution equation (66) for the deformation field $\boldsymbol{B}_j^k\approx\boldsymbol{B}\left(\boldsymbol{x},t,\tau_j^k\right)$ of *constant* age $\tau_j^k$. The total number of unknown fields is $N_{DF} = 2N$. Although the last two terms of equation (66) induce a *coupling* between deformation fields which is absent in the original DFM, advantages of the alternative DFM are clear: the discrete fields $\boldsymbol{B}_j^k$ do become steady for steady-state kinematics, no difficult bookkeeping related to creation and deletion of fields is necessary, and discretization of the age axis is flexible and independent of the time step used to solve the governing equations.

Once the deformation fields are known, evaluation of the memory integral (52) is easy. Indeed, the stress is approximated as:

$$\boldsymbol{\tau}(\boldsymbol{x},t)\approx\int_0^{\tau_c}m(\tau)\boldsymbol{f}\left(\boldsymbol{B}(\boldsymbol{x},t,\tau)\right)d\tau+\int_{\tau_c}^{\infty}m(\tau)\boldsymbol{f}\left(\boldsymbol{B}(\boldsymbol{x},t,\tau_c)\right)d\tau, \quad \ldots\ldots\ldots(67)$$

and $\boldsymbol{f}(\boldsymbol{B})$ is computed over each element $I_j$ of $[0, \tau_c]$ using the finite element interpolation:

$$\boldsymbol{f}(\boldsymbol{B})\approx\sum_{k=1}^{2}\boldsymbol{f}\left(\boldsymbol{B}_j^k\right)\varphi_j^k(\tau). \quad \ldots\ldots\ldots(68)$$

This relates the stress to the deformation fields through:

$$\boldsymbol{\tau}(\boldsymbol{x},t)\approx\sum_{j=0}^{N-1}\sum_{k=1}^{2}W_j^k\,\boldsymbol{f}\left(\boldsymbol{B}_j^k(\boldsymbol{x},t)\right), \quad \ldots\ldots\ldots(69)$$

where the weights are given by:

$$W_j^k=\begin{cases}\int_{\tau_j}^{\tau_{j+1}}m(\tau)\varphi_j^k(\tau)\,d\tau, & j=0,1,\ldots..,N-2;\ k=1,2,\\ \int_{\tau_{N-1}}^{\tau_N}m(\tau)\varphi_{N-1}^k(\tau)\,d\tau+\varphi_{N-1}^k(\tau_c)\int_{\tau_c}^{\infty}m(\tau)\,d\tau, & j=N-1;\ k=1,2.\end{cases}$$

$\ldots\ldots\ldots(70)$

Finally, we note that Hulsen et al [57] discretize the evolution equation (66) in *t*-space by means of the explicit Adams-Bashforth scheme, which is second-order accurate. Discretization of the governing equations in $\boldsymbol{x}$-space and overall time-stepping is like in the original DFM.

**Applications of DFM**

The first version of DFM has been validated by Peters et al [55] in the numerical benchmark of the flow of an upper-convected Maxwell (UCM) fluid past a sphere. Extension to the Doi-Edwards model is reported by van Heel et al [56], who considered flow past a cylinder. Hulsen et al [57] validated the second version of DFM in the sphere benchmark using various K-BKZ models.

## 6. INTEGRO-DIFFERENTIAL MODELS DERIVED FROM MOLECULAR THEORY

Over the last few years, the development of molecular-based constitutive equations for entangled polymers has known exciting advances. Several extensions of the classical reptation theory (Doi and Edwards [6]) have been suggested for both linear and branched architectures. Notable examples are the proposals made by Mead et al [11], McLeish and Larson [12], Ianniruberto and Marrucci [13], and Wagner et al [14]. The resulting constitutive equations have an *integrodifferential* form that is considerably more complex than the generic integral model (4) considered so far in this review.

For illustration purposes, let us briefly consider the so-called double-convection-reptation (DCR) model proposed recently by Ianniruberto and Marrucci [13] for linear polymers. In addition to reptation, the DCR model accounts for convective constraint release and chain stretch effects. The polymer stress $\boldsymbol{\tau}$ is computed through an *algebraic* function $\boldsymbol{q}$ of two microstructural quantities, namely the average orientation of tube segments $\boldsymbol{S}$ and the average chain stretch $\lambda$:

$$\boldsymbol{\tau}(t) = \boldsymbol{q}(\boldsymbol{S}, \lambda). \qquad \text{.....(71)}$$

The orientation $\boldsymbol{S}$ is given by a memory integral which at first sight looks similar to equation (4):

$$\boldsymbol{S} = \int_{-\infty}^{t} \mu(\boldsymbol{S}, t, t')\, \boldsymbol{f}(\boldsymbol{B}(t, t'))\, dt' \ . \qquad \text{.....(72)}$$

The main difference, however, is that the memory function $\mu$ depends on past values of the orientation $\boldsymbol{S}$. Indeed, it obeys a differential equation of the form:

$$\frac{D\mu}{Dt} = g(\mu, \boldsymbol{S}, \boldsymbol{\nabla v}). \qquad \text{.....(73)}$$

Finally, the stretch $\lambda$ evolves according to a differential equation of the form:

$$\frac{D\lambda}{Dt} = h(\boldsymbol{S}, \lambda, \boldsymbol{\nabla v}). \qquad \text{.....(74)}$$

Recent extensions of DFM and LIM have made it feasible to simulate complex viscoelastic flows using integro-differential constitutive equations as intricate as the DCR model. Using DFM, Peters et al [60] report simulations with the Mead-Larson-Doi model [11], while various versions of the DCR theory are studied by Wapperom and Keunings [61] and Wapperom et al [62]. Wapperom and Keunings [63] also

 

extend DFM to the pom-pom model [12] for branched molecules. Finally, Wagner's molecular stress function model [14] is investigated by Rasmussen [64] using LIM.

## CONCLUSIONS

The numerical simulation of viscoelastic flows using an integral constitutive equation has long been considered considerably more difficult than similar studies with a differential constitutive model. Moreover, transient flows could not be computed with integral models until the development of the Lagrangian Integral Method (LIM) and the Deformation Field Method (DFM).

We feel that LIM and DFM define the current state of the art. In benchmark flow simulations with simple constitutive equations that have an equivalent differential form (e.g. the UCM model), LIM and DFM enjoy a similar degree of numerical stability as that of the best available techniques for differential models. The main point, however, is that recent extensions of LIM and DFM enable the investigation of a much wider constitutive space. Indeed, the way is now open for the critical evaluation in complex flows of molecular-based constitutive theories.

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