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Multiscale modeling of viscoelastic fluids: an up-to-date CONNFFESSIT

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Abstract

The present communication introduces an up-to-date version of the CONNFFESSIT method in the field of micro-macro simulations of non-Newtonian fluids. The 'macro' section employs a semi-Lagrangian method in order to reduce the Navier-Stokes equations to a Stokes-like subproblem. Linear systems arising from the finite element formulation are solved via the 'Incomplete Cholesky Conjugate Gradient' iterative algorithm, wherein the sparsity pattern of the matrices is taking into account. As to the 'micro' part, the stochastic formulation simplifies the Fokker-Planck equations in the configuration space to stochastic differential equations for the internal degrees of freedom of the particles ('dumbbells') conveying the rheological information of the kinetic model, their integration being accomplished by means of a semi-implicit, Predictor-Corrector algorithm. The 'micro-macro' coupling involves the polymer stress tensor, which is computed through a mixed 'Finite Element / Natural Element' method. An extended, search-and-locate method for unstructured meshes and non-connected domains has been implemented. The robustness and efficiency of the method is highlighted on a benchmark problem (10:1 planar contraction).

1. Introduction.

The problem of viscoelastic flows is not a mild one: added to the complexity of the Navier-Stokes equations governing a Newtonian fluid, is the fact that viscoelastic materials

are exposed to a non-linear coupling among factors such as the history of the flow, their so-induced internal configurations, the macroscopic rheological properties or the geometry of the domain. However difficult it may seem, the outstanding number of applications for this sort of materials in fields as diverse as surgery, structural mechanics or nano-electronics more than make up for the effort that so tricky a flow may require.
The early days of research in non-Newtonian fluids can be traced back to late 1940's and mid 1950's, when pioneering work by Oldroyd ([14]) and Lodge ([13]) concerning the analytical solution of the so-called *order fluids* on simple geometries and low Weissenberg numbers, struck the scene. From that point on and for almost thirty years, the interest for this kind of flows grew up steadily. As it was, the progressive availability of computational tools during the 1960's and 1970's provided a prompt development of numerical models, starting with *viscometric flows*. But not until 1977 complex flows of viscoelastic fluids in two space dimensions were treated by a finite difference method proposed by Perera and Walters ([18]); although it caused a major breakthrough in the simulation of non-Newtonian fluids, boding all good for this field of research, a hindrance as yet not overcome would shortly appear: the 'high-Weissenberg number problem'. The decade of 1980's would continue to show advance in numerical simulation, but the initial momentum somewhat receded: higly convoluted, closed-form expressions of the constitutive equations for some of the simplest viscoelastic materials together with the inability to reach industrially significant Weissenberg numbers, proved rather discouraging. A novel approach that combined some of the molecular information provided by the extremely computer-wise expensive 'atomistic modelling' with the flexibility of coarse-grained kinetic theory models was shaped by the 'micro-macro' methods, being the original CONNFFESSIT by Öttinger and Laso ([12]) one of the foremost methods at the time (see, e.g., [11] for a more detailed revision on micro-macro methods).
In spite of the attactive properties of CONNFFESSIT, in which no closed-form constitutive equations are demanded, there were a number of drawbacks that spurred further research, such as the 'Brownian configuration fields' ([9]) or 'variance reduction' techniques ([16]) to palliate, up to a certain extent, the typical stochastic noise of this scheme; additional issues relate to needed stabilization techniques in the finite element implementation ([6], [7]), the location of the particles ('dumbbells') in complex geometries, or the size of the ensemble in the computation of the polymer stress tensor.
The present communication tries to address these situations, while introducing a robust and efficient implementation of the CONNFFESSIT approach.

2. Description of the model.

The structure of a CONNFFESSIT (Calculation of Non-Newtonian Flow:Finite Element and Stochastic SImulation Techniques) implementation may be divided into three different parts: a 'macro' part dealing with the conservation (Navier-Stokes) equations; a 'micro' part that passes the information from the kinematic model on to the particles scattered throughout the domain; and a 'micro-macro' interface which accounts for making up the polymer stress tensor. This procedure is to be iterated in time, so that transient processes come naturally to the internal structure of the method.
The next subsections introduces the semi-Lagrangian scheme for the Navier-Stokes equa-

tions, the stochastic processes involved as well as the algorithm employed for the location of particles on unstructured meshes, and the mixed Finite Element / Natural Element algorithm responsible for the calculation of the stress tensor.

2.1. Macroscopic part.

The Navier-Stokes equations for an incompressible, non-Newtonian fluid in an open bounded domain $\Omega \subset \mathbb{R}^d (d = 2, 3)$, with boundary $\Gamma = \Gamma_0 + \Gamma_1$, in absence of external forces and in a time interval [0,T], may be written as:

$$\rho \frac{D\boldsymbol{u}}{Dt} + \boldsymbol{\nabla} \cdot \boldsymbol{\tau} = \mathbf{0} \tag{1}$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0 \tag{2}$$

$\frac{D(\cdot)}{Dt} = \frac{\partial(\cdot)}{\partial t} + (\cdot)\boldsymbol{\nabla}(\cdot)$ accounts for the total derivative operator, $\boldsymbol{\tau} = \boldsymbol{\tau}_s + \boldsymbol{\tau}_p$ is the total stress tensor of the fluid, and the Newtonian solvent satisfies:

$$\boldsymbol{\tau}_s = \tilde{p}\boldsymbol{\delta} - \mu_s \left[\boldsymbol{\nabla u} + (\boldsymbol{\nabla u})^t\right] \tag{3}$$

where $\boldsymbol{\delta}$ is the unit tensor. Using (1),(2) and (3), the following system of equations result:

$$\begin{cases} \dfrac{D\boldsymbol{u}}{Dt} - \nu_s \Delta \boldsymbol{u} + \boldsymbol{\nabla} p &=& \dfrac{1}{\rho}\boldsymbol{\nabla} \cdot \boldsymbol{\tau_p} & \\ \boldsymbol{\nabla} \cdot \boldsymbol{u} &=& 0 & \\ \boldsymbol{u}(\boldsymbol{x}, 0) &=& \boldsymbol{u}_0(\boldsymbol{x}) & \text{in } \Omega \\ \boldsymbol{u}(\boldsymbol{x}, t) &=& \boldsymbol{g}_0(\boldsymbol{x}, t) & \text{on } \Gamma_0 \\ -p\boldsymbol{n} + \nu_s \dfrac{\partial \boldsymbol{u}}{\partial \boldsymbol{n}} &=& \boldsymbol{g}_1(\boldsymbol{x}, t) & \text{on } \Gamma_1 \end{cases} \tag{4}$$

This system is tackled via a two step Lagrangian-Eulerian procedure: the feet of the characteristic curves are calculated for all the computational nodes in the mesh and the equations are integrated along the trajectories of the fluid particles, thus obtaining a Stokes problem to be solved thereafter. The 'Method of Characteristics' deals with the first step, and its implementation follows that of Allievi and Bermejo (see [3] for a detailed description in a finite element framework). Schematically, $\boldsymbol{X}(\boldsymbol{x}, t_{n+1}; t)$ represents the position at time t of a fluid particle which reaches the mesh point $\boldsymbol{x} \in \overline{\Omega}$ at time t_{n+1}, so that the trajectory of such particle is ruled by:

$$\frac{D\boldsymbol{X}}{Dt}(\boldsymbol{x}, t_{n+1}; t) = \boldsymbol{u}(\boldsymbol{X}(\boldsymbol{x}, t_{n+1}; t), t) \tag{5}$$

$$\boldsymbol{X}(\boldsymbol{x}, t_{n+1}; t_{n+1}) = \boldsymbol{x} \tag{6}$$

The momentum and conservation equations (4) are integrated along these trajectories, employing the trapezoidal rule for the velocity and an the rectangular upper limit quadrature rule for both pressure and polymer stress tensor. As regards the computation of the feet of the characteristic curves (see, e.g. [19]), a mid-point approximation combined with an iterative fixed point algorithm is used.

Upon the resulting Stokes-like problem, the Galerkin formulation is applied; P2-P1 Taylor-Hood polynomials are used for velocity and pressure, respectively, and a first degree polynomial approximation is considered for the polymer stress tensor. This election of working spaces satisfies the Inf-Sup Babuska-Brezzi condition [10] whence any further stabilization technique is spared. The preconditioned form of the Conjugate Gradient Algorithm for incompressible, viscous flows as described in [5], is utilized to numerically reach the solution of the Stokes problem, with all lineal systems derived from the Galerkin formulation being solved by a preconditioned Incomplete Cholesky Conjugate Gradient iterative algorithm. Since the involved stiffness and mass matrices are sparse, *ad-hoc* data structure and code were devised to take advantage of that fact.

2.2. Microscopic part.

As previously stated, one of the relevant features of the CONNFFESSIT approach falls on its ability to cope with viscoelastic fluids lacking a closed-form constitutive equation, by the transformation of the Fokker-Planck equations into a stochastic equivalent [15]. The viscoelastic fluid chosen in the simulations presented in this communication is the FENE (Finite Extensible Nonlinear Elastic) fluid, for which an analytical constitutive expression cannot be written [4]. Basically, it may be described as buoyant, non-interacting 'dumbbells' carrying the polymeric information though their internal degrees of freedom (configuration field $\boldsymbol{Q}$), diluted in a Newtonian fluid. The elastic behaviour of the fluid is close to a Hookean when slight elongation is applied, whereas the spring-like force grows unbounded as one approaches to the maximum elongation $\boldsymbol{Q}_0$.

$$\boldsymbol{F}^{\mathrm{FENE}} = \frac{H\boldsymbol{Q}}{1 - \left(\frac{|\boldsymbol{Q}|}{|\boldsymbol{Q}_0|}\right)^2} \tag{7}$$

The Fokker-Planck diffusion equations for the FENE fluid adopt the form [15]:

$$\frac{\partial \psi}{\partial t} = \frac{2}{\zeta}\left(\frac{\partial}{\partial \boldsymbol{Q'}} \cdot \boldsymbol{F}^{\mathrm{FENE}}\psi\right) - \left(\frac{\partial}{\partial \boldsymbol{Q'}} \cdot \left[\boldsymbol{\kappa} \cdot \boldsymbol{Q'}\right]\psi\right) + \frac{2kT}{\zeta}\left(\frac{\partial}{\partial \boldsymbol{Q'}} \cdot \frac{\partial}{\partial \boldsymbol{Q'}}\psi\right) \tag{8}$$

where ζ is the friction coefficient, related to the relaxation time typical of any viscoelastic fluid according to

$$\lambda_H = \frac{\zeta}{4H} \tag{9}$$

ψ is the distribution function in the original configuration space, and $\boldsymbol{\kappa} = (\boldsymbol{\nabla u})^t$ is the transposed of the velocity gradient. The stochastic equivalent may be expressed as:

$$d\boldsymbol{Q} = \left(\boldsymbol{\kappa} \cdot \boldsymbol{Q} - \frac{1}{2\lambda_H}\frac{\boldsymbol{Q}}{1 - \frac{Q^2}{b}}\right)dt + \sqrt{\frac{1}{\lambda_H}}\partial\!\!\!^{-}\boldsymbol{W} \tag{10}$$

with $\boldsymbol{Q} = \boldsymbol{Q'}\sqrt{\frac{H}{kT}}$, and $\boldsymbol{W}$ a Wienner process. As it entails a generation of random numbers, we follow Öttinger ([15]) substituting the Gaussian distributions of the Wienner

process by far cheaper uniform distributions, with the adequate arrangements being performed.
The stochastic equation (10) is integrated by means of a semi-implicit Predictor-Corrector scheme which consits of an Euler-Forward algorithm for the 'prediction' plus a Crank-Nicolson algorithm applied at any time interval $[t_n, t_{n+1}]$ for the 'correction' step, whereas the $\boldsymbol{\kappa}$ tensor in the forward step is approximated by an Euler-Backward scheme.

As for the trajectories of the 'dumbbells', a time-adaptive version of the mid-point plus fixed-point iterative algorithm has been implemented for those particles not meeting the convergence criteria, shortening the integration step and the pseudo-foot of the characteristic to be computed.

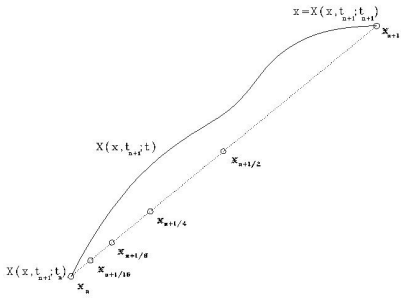


Figure 1: Time-adaptive scheme for the computation of the trajectories of the dumbbells.

Since this particles are moving within a domain, a search-and-locate algorithm must be provided. An extended, more robust version of the original algorithm proposed by Allievi and Bermejo [2] has been implemented for unstructured bidimensional meshes, and it is sketched below:

- The method may be divided into two modes: the so-called 'standard' and 'angular' modes.

  1. Standard mode: this mode should work in most conventional, connected domains, lacking acute angles. Following the theory in [2], additional (secondary, tertiary) criteria based on the value of the elemental basis functions are developed, and recurrent backwards behaviour used to detect possible wrong selection of element.
  2. Angular mode: a number of succesive angular incrementes are allowed in order to turn round possible hollows and corners.

- All in all, the algorithm is as fast as the original one for conventional meshes, and capable of detecting particles on unstructured non-connected domains.

2.3. Micro-Macro Coupling.

The computation of the polymer stress tensor by means of a fitting equation considering the internal degrees of freedom of the kinematic model occupies this section. For the FENE

model, that relation may be expressed in terms of second moments of the configuration of the 'dumbbells' as:

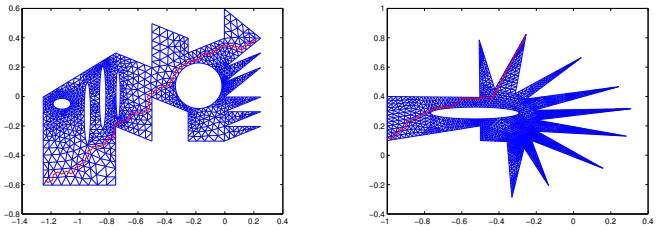
$$\boldsymbol{\tau}_p = -nk_BT\left(\frac{\boldsymbol{QQ}}{1-\dfrac{Q^2}{b}} - \boldsymbol{\delta}\right) \tag{11}$$

An implementation of the mixed 'Finite Element / Natural Element' computation method, similar to that recently proposed in [1] is herewith presented (see figure 3):

1. Each element is divided into three zones: for every node, a sub-elemental zone is defined containing the current node, the centroid of the element as well as the midpoints of the sides common to that node.

2. An average of the configurations of all particles belonging to each sub-elemental zone is performed, and the resulting value is assigned to the center of gravity of the sub-elemental zone.

3. A weighted average of the configurations of every sub-elemental zone belonging to each node provide the final value for the stress tensor at each node. The weights are the ratio between the areas of the sub-elemental zone and the total 'mixed-element' area.



(a) 'Tool Mesh' (b) 'Hedgegoh Mesh'

Figure 2: Two non-connected domains for the test of the search-and-locate algorithm.

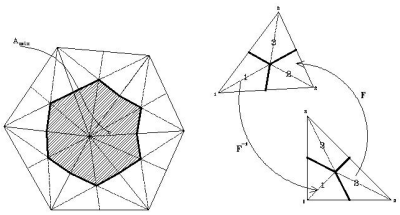


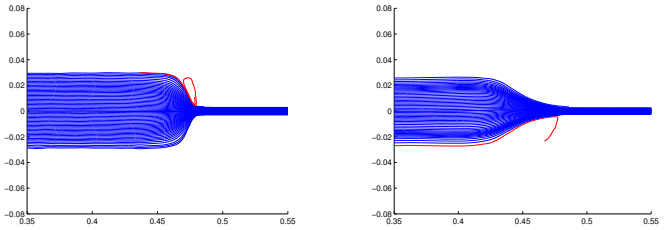
Figure 3: Finite/Natural Element computation method for the polymer stress tensor.

3. Benchmark problem. Planar contraction 10:1.

The current implementation was tested in a severe die-entry flow, 10 to 1 contraction, with a FENE fluid. Beforehand, the computation method for the stress tensor was checked in pure shear and elongational flows, and its results successfully compared to those showed in [8]. Free-stress boundary conditions were implemented instead of the more commonly imposed velocity profile at the outlet ([6],[7]) as to improve the flexibility of the method should complex domains be used.
The robustness of the method was additionally tested rising the Weissenberg number, which is defined [17] as:

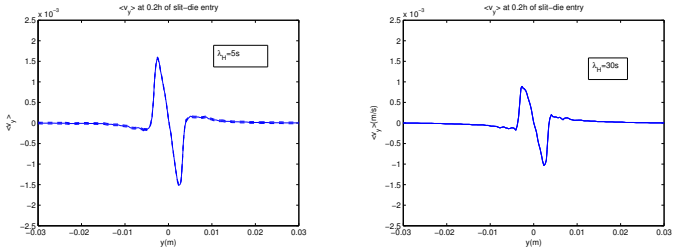
$$We = 2\lambda_H \frac{U}{D} \tag{12}$$

where U, D are the mean velocity and diameter at the outlet, respectively. For this purpose, elastic effects were to be highlighted so that only a gain in the relaxation time was considered. Appropriately reducing the time step, a maximum Weissenberg number of $We = 200$ has been achieved so far.



(a) $\lambda_H = 5$s (b) $\lambda_H = 90$s

Figure 4: Streamlines for increasing Weissenberg number. Notice the vortex size.



(a) $\lambda_H = 5$s (b) $\lambda_H = 30$s

Figure 5: Vertical component of the velocity, close to the die-entry.

4. Conclusions.

An improved, more robust version of the original CONNFFESSIT approach has been presented. New features include the method of characteristics for the integration of the

macroscopic equations, an extended 'search-and-locate' algorithm or the computation of a first degree polymer stress tensor. The results show remarkable ability of the method to achieve high Weissenberg numbers, with no stabilization techniques being employed.

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