Mathematical problems in mechanics

From the free surface flow of a viscoelastic fluid towards the elastic deformation of a solid

La déformation d’un solide élastique à partir de l’écoulement à frontière libre d’un fluide viscoélastique

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A R T I C L E   I N F O

Article history:
Received 28 November 2014
Accepted after revision 5 February 2016
Available online 21 March 2016
Presented by the Editorial Board

A B S T R A C T

The free surface flow of an Oldroyd-B viscoelastic fluid is considered, following A. Bonito, M. Picasso, and M. Laso (2006) [1]. When removing a term in the extra-stress constitutive relation, the description of an elastic incompressible solid is obtained, in Eulerian coordinates, with the velocity field as the unknown, rather than the usual deformation field. Two simulations are proposed, a bouncing ball and an oscillating beam.

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R É S U M É

L’écoulement à frontière libre d’un fluide viscoélastique d’Oldroyd-B est considéré, selon A. Bonito, M. Picasso et M. Laso (2006) [1]. En supprimant un terme dans la loi constitutive de l’extra-contrainte, nous décrivons un solide élastique incompressible, en coordonnées eulériennes, avec le champ de vitesse comme inconnue, plutôt que le champ de déformation. Deux simulations sont proposées, le rebond d’une balle et une poutre vibrante.

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1. Introduction

The numerical simulation of fluid flow coupled with deformable solids is a difficult task, mainly because i) the unknowns are different, velocity in the liquid region, deformation in the solid region, ii) the velocity is expressed in Eulerian coordinates, whereas the deformation is in Lagrangian coordinates. In [3], the solid deformation is expressed in Eulerian coordinates in order to solve a fluid–structure interaction problem, thus removing difficulty ii) listed hereabove. However, difficulty i) is still present.

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http://dx.doi.org/10.1016/j.crma.2016.02.001
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In this paper, we propose to formulate the elastic deformation of a solid in Eulerian coordinates, with the velocity as unknown instead of the usual deformation. This formulation is obtained starting from a viscoelastic fluid with free surface. Large deformations are naturally included in the formulation.

2. The model

We follow [1]. Consider a cavity $\Lambda$ of $\mathbb{R}^d$, $d = 2$ or 3, partially filled with a viscoelastic incompressible fluid, for instance a Newtonian solvent with non-interacting polymer chains. We are interested in computing the fluid shape between time $0$ and time $T$. Let $\Omega(t) \subset \Lambda$ be the liquid region at time $t$ and let $\Omega_T$ be the space–time domain containing the fluid. The velocity $\mathbf{v} : \Omega_T \to \mathbb{R}^d$, pressure $\mathbf{p} : \Omega_T \to \mathbb{R}$ and extra-stress $\sigma : \Omega_T \to \mathbb{R}^{d \times d}$ satisfy the mass and momentum equations

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \rho(\mathbf{v} \cdot \nabla)\mathbf{v} - 2\eta_s \nabla \epsilon(\mathbf{v}) + \nabla \cdot \mathbf{p} = \rho \mathbf{g},$$

$$\nabla \cdot \mathbf{v} = 0,$$

supplemented with the Oldroyd-B constitutive equation

$$\sigma + \lambda \left( \frac{\partial \sigma}{\partial t} + (\mathbf{v} \cdot \nabla)\sigma - \nabla \mathbf{v} \sigma - \sigma \nabla \mathbf{v}^T \right) = 2\eta_p \epsilon(\mathbf{v}).$$

Hereabove $\rho$ is the fluid density, $\eta_s$ the solvent viscosity, $\epsilon(\mathbf{v}) = \frac{1}{2}(\nabla \mathbf{v} + (\nabla \mathbf{v})^T)$ the symmetric part of the velocity gradient, $\mathbf{g}$ the gravity, $\lambda$ the polymer relaxation time, $\eta_p$ the polymer viscosity. Let $\varphi : \Lambda \times (0, T)$ be the characteristic function of the liquid. Then, the domain containing the fluid at time $t$ is defined by

$$\Omega(t) = \{ x \in \Lambda ; \varphi(x, t) = 1 \}.$$

Assuming the fluid particles move with the fluid velocity, $\varphi$ must satisfy

$$\frac{\partial \varphi}{\partial t} + (\mathbf{v} \cdot \nabla)\varphi = 0 \quad \text{in} \quad \Lambda \times (0, T)$$

so that

$$\varphi(x(t), t) = \varphi(x(0), 0) \quad 0 \leq t \leq T,$$

with $\dot{x}(t) = \mathbf{v}(x(t), t)$ and $x(0) \in \Omega(0)$. Concerning the initial conditions, $\varphi(0)$ or equivalently $\Omega(0)$ must be provided at time $0$, so as $\mathbf{v}(0)$ and $\sigma(0)$ in $\Omega(0)$. Concerning the boundary conditions, it is assumed that no external force applies on the fluid’s free surface (the set of points where $\varphi$ jumps from 0 to 1), thus

$$\left( -p I + 2\eta_s \epsilon(\mathbf{v}) + \sigma \right) n = 0,$$

where $n$ is the unit outer normal of the free surface. On the boundary of the fluid being in contact with the walls, either slip, imposed or no-slip boundary conditions apply.

3. The elastic limit

In order to consider the elastic limit of the Oldroyd-B constitutive equation, we shall replace (3) by

$$\alpha \sigma + \lambda \left( \frac{\partial \sigma}{\partial t} + (\mathbf{v} \cdot \nabla)\sigma - \nabla \mathbf{v} \sigma - \sigma \nabla \mathbf{v}^T \right) = 2\eta_p \epsilon(\mathbf{v}),$$

where $\alpha = 0$ or 1. Three cases can be considered:

- $\alpha = 1$, $\lambda = 0$, $\eta_s \geq 0$, $\eta_p \geq 0$: an incompressible Newtonian fluid with viscosity $\eta_s + \eta_p$;
- $\alpha = 1$, $\lambda > 0$, $\eta_s \geq 0$, $\eta_p > 0$: an incompressible Oldroyd-B viscoelastic fluid;
- $\alpha = 0$, $\lambda > 0$, $\eta_s = 0$, $\eta_p > 0$: an incompressible elastic solid formulated in Eulerian variables, with velocity $\mathbf{v}$ as unknown, instead of the usual deformation field.

The integral formulation corresponding to (6) is the following, see also [5]. Let $x(t; X)$ be the position at time $t$ of the fluid particle that left $X \in \Omega(0)$ at time 0, that is the solution to $\dot{x}(t) = \mathbf{v}(x(t), t)$, $x(0) = X$, or equivalently

$$x(t; X) = X + \int_0^t \mathbf{v}(x(s; X), s) \, ds.$$
Let $F$ be the deformation tensor defined by $F(X, t) = \nabla x(t; X)$, i.e.

$$F_{ij}(X, t) = \frac{\partial x_i}{\partial X_j}(t; X) \quad i, j = 1, \ldots, d.$$ 

Taking the derivative of (7) with respect to $X$ and $t$, we have

$$\frac{\partial F}{\partial t}(X, t) = \nabla v(x(t; X), t) F(X, t).$$

We can then check (taking the derivative of the below formula with respect to $t$) that

$$\sigma(x(t; X), t) = \frac{\eta_p}{\lambda} \left( \int_0^t e^{-(t-s)/\lambda} F(X, t) F^{-1}(X, s) F^{-T}(X, s) X F(X, t) \ ds + \lambda \left( e^{-t/\lambda} F(X, t) F^T(X, t) - I \right) \right)$$

satisfies (6) when $\alpha = 1$ (Oldroyd-B), whereas

$$\sigma(x(t; X), t) = \frac{\eta_p}{\lambda} \left( F(X, t) F^T(X, t) - I \right)$$

satisfies (6) when $\alpha = 0$ (elastic solid). This model ($\alpha = 0$) coincides with the Eulerian formulation of an incompressible Neo–Hookean material described in [3]. It should be stressed that in [3] the unknown is the deformation $x(t; X) - X$, whereas here the unknown is the velocity $v$.

### 4. The numerical method

The numerical method is the one presented in [1] for viscoelastic fluids; it stems from the one advocated in [2,6] for Newtonian flows. An implicit, order one, splitting method [4] is used for the time discretization, in order to decouple advection and diffusion phenomena. Let $N$ be a positive integer, $\tau = T/N$ the time step, $t^n = n \tau$, $n = 0, 1, \ldots, N$. For each $n$, given approximations of $\psi$, $v$ and $\sigma$ at time $t^n$, advection:

$$\frac{\partial \psi}{\partial t} + (v \cdot \nabla) \psi = 0, \quad \frac{\partial v}{\partial t} + (v \cdot \nabla) v = 0, \quad \frac{\partial \sigma}{\partial t} + (v \cdot \nabla) \sigma = 0,$$

is performed between $t^n$ and $t^{n+1}$ using a forward characteristics method on a structured grid of size $h$. This provides a new liquid domain at time $t^{n+1}$, so as predictions of $v$ and $\sigma$ in this new liquid domain.

$$\rho \frac{\partial v}{\partial t} - 2 \eta_s \text{div} \ v + \nabla p - \text{div} \ \sigma = \rho g, \quad \text{div} \ v = 0, \quad \alpha \sigma + \lambda \left( \frac{\partial \sigma}{\partial t} - \nabla v^T \sigma - \sigma \nabla v \right) = 2 \eta_p \varepsilon(v),$$

is then solved between $t^n$ and $t^{n+1}$ on this new liquid domain using a fixed finite element mesh with larger size $H$. In order to reduce the numerical diffusion of the volume fraction of liquid $\phi$, the size $h$ of the structured grid is three to five times smaller than the finite element mesh size $H$. The CFL number is between one and ten. The method is of order one with respect to $H$, $h$, and $\tau$.

### 5. Numerical experiments

#### 5.1. Bouncing ball

All physical data are given in the International system of units. Consider the cavity $\Lambda = [-0.2, 0.2] \times [-0.2, 0.2] \times [0, 0.3]$ partially filled with a viscoelastic fluid in the elastic limit – $\alpha = 0$ in (6) and $\eta_s = 0$ in (1) – having density $\rho = 1000$, polymer viscosity $\eta_p = 0.1$, elastic coefficient $\lambda = 0.005$ and subject to gravity $g = (0, 0, -9.81)$ in the vertical direction. In order to allow bouncing when the ball touches the bottom wall of the cavity, Signorini-like boundary conditions are enforced, see Section 2.2 in [6] for details.

At the initial time, the fluid is the ball centered at $(0, 0, 0.15)$ with radius 0.1 and has velocity $(0, 0, -0.1)$. The finite element mesh is uniform, the requested mesh size is $H = 0.005$, has 485,485 vertices and 2,823,660 tetrahedra. The size of the cells is $h = 0.001$, the time step is 0.025. As reported in Fig. 1, the ball bounces on the bottom wall of the cavity.

The convergence of the numerical method at time 2.9 is checked as follows. Three finite element meshes of typical size $H = 0.01$, $H = 0.005$, $H = 0.0025$ are considered, the number of nodes being 56,723, 485,485, 3,933,299, respectively. The ratio between $H$ and $h$ is kept constant, thus the size of the cells is $h = 0.002$, $h = 0.001$, $h = 0.0005$, respectively. The CFL number is also kept constant, thus the time step is $0.05$, 0.025, 0.0125, respectively. The shape of the deformed ball at time 2.9 in the plane $x = 0$ is reported in Fig. 2. The CPU time (in seconds) required to run the computations is 177, 3569, 196,844, respectively. The first two computations have been carried out on an Intel i7-2820QM 2.30 GHz processor with 16 Gb memory, while the last computation was done on a Intel Xeon X5675 3.06 GHz with 192 Gb memory.
Fig. 1. Ball bouncing. Shape of the deformed ball at time steps 30, 60, 90, ..., 540 (time 0.75, 1.50, 2.25, ..., 13.5).

Fig. 2. Convergence with mesh size. Shape of the deformed ball at time 2.9 in the plane $x = 0$ with three meshes of typical sizes $H = 0.01$, $H = 0.005$, and $H = 0.0025$.

We have checked the conservation of the total energy

$$\frac{1}{2} \int_{\Omega} \left( \rho (v \cdot v) + \frac{\lambda}{2\eta_p} (\sigma : \sigma) \right) \psi \, dx$$

as a function of time with these three meshes, in the case when the gravity $g$ is set to zero, and when the nonlinear terms $\nabla v \sigma + \sigma \nabla v^T$ are omitted in (6). The results indicate that a discrepancy of 10% still occurs on the finest mesh, thus showing that more accurate numerical strategies should be investigated. This is not surprising, since the method is only order-one accurate in space and space.
5.2. Oscillating beam

The same fluid is considered with the same numerical parameters ($H = 0.005$, $h = 0.001$, time step 0.025) but with a different initial condition. At initial time, the fluid is a beam located at $[-0.2, 0.1] \times [-0.05, 0.05] \times [0.1, 0.2]$ and still has velocity $(0, 0, -0.1)$. At the plane $x = -0.2$, the fluid is in contact with the cavity and has zero velocity, thus zero deformation. As reported in Fig. 3, the beam bends towards the bottom of the cavity, bounces, and finally reaches a stationary position.

6. Conclusion

The description of an elastic incompressible solid is proposed, in Eulerian coordinates, with the velocity field as the unknown, rather than the usual deformation field. Large deformations are naturally included in the model. The next step would be to couple this elastic incompressible solid with an incompressible Newtonian fluid in order to simulate fluid–structure interactions with large deformations, with velocity as the unknown in both the solid and the liquid.

Acknowledgements

All the simulations were performed using the cfsFlow software developed by EPFL and Ycoor Systems SA (ycoorsystems.com). The author would like to thank Alexandre Masserey and Gilles Steiner for support.
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