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A NEW MICRO-MACRO ALGORITHM FOR SIMULATION OF POLYMER FLOWS

*** J.L. Prieto[1], R. Bermejo[2] and M. Laso[3]**

[1] Dept. Matemática Aplicada
Universidad Politécnica de Madrid
José Gutiérrez Abascal,2
28006 Madrid
juanluis.prieto@upm.es

[2] Dept. Matemática Aplicada
Universidad Politécnica de Madrid
José Gutiérrez Abascal,2
28006 Madrid
rbermejo@etsii.upm.es

[3] Dept. Ingeniería Química
Universidad Politécnica de Madrid
José Gutiérrez Abascal,2
28006 Madrid
laso@diquima.upm.es

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ABSTRACT

We present a new micro-macro algorithm for the numerical calculation of polymer flows. The system being solved consists of the momentum and mass conservation equations from the continuum mechanics coupled with a microscopic-based rheological model for polymer stress.

Macroscopic part

The integration of the macroscopic part is carried out by combining a new semi-Lagrangian [1] Galerkin projection algorithm for the total derivative operator with a mixed finite element formulation of the linear Stokes problems that have to be solved at each time step of the integration process.
A two step Lagrangian-Eulerian procedure is employed, in which the so-called 'Method of the Characteristics' deals with the calculation of the feet of the characteristic curves for all the computational nodes in the mesh, and the resulting equations are integrated along the trajectories of the fluid particles. Schematically, $\boldsymbol{X}\left(\boldsymbol{x}, t_{n+1}; t\right)$ represents the position at time t of a fluid particle which reaches the mesh point $\boldsymbol{x}$ at time t_{n+1}, so that the trajectory of that particle is ruled by:

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

$$\boldsymbol{X}\left(\boldsymbol{x}, t_{n+1}; t_{n+1}\right) = \boldsymbol{x} \tag{2}$$

The momentum and conservation equations are integrated along these trajectories by means of the trapezoidal rule for the velocity and the rectangular upper limit quadrature rule for both pressure and stress tensor. As regards the computation of the feet of the characteristic curves, a mid-point approximation combined with an iterative fixed point algorithm is used.

The solution of the resulting Stokes problems is calculated by Taylor-Hood $P_2 - P_1$ elements, thus satisfying the Inf-Sup Babuska-Brezzi stability condition and sparing us any further stabilization technique.

Microscopic part

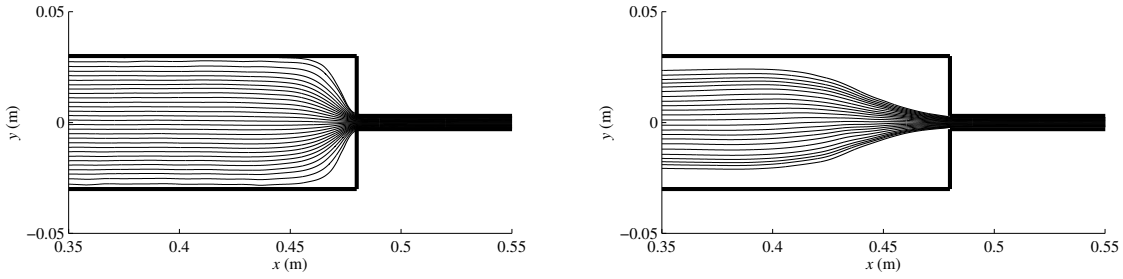
The microscopic part represents the polymer contribution to the stress tensor and is determined from a stochastic simulation [2] of an ensemble of model polymer molecules from whose configurations the polymer stress can be computed as an ensemble average. For a FENE (Finitely Extendable Nonlinear Elastic) model, the stochastic equivalent to the Fokker-Planck equation can be written as:

$$d\boldsymbol{Q} = \left(\boldsymbol{\kappa} \cdot \boldsymbol{Q} - \frac{1}{2\lambda_H} \frac{\boldsymbol{Q}}{1 - \dfrac{Q^2}{b}} \right) dt + \sqrt{\frac{1}{\lambda_H}} \eth \boldsymbol{W} \tag{3}$$

where $\boldsymbol{Q}$ is the configuration field, $\boldsymbol{\kappa} = (\boldsymbol{\nabla u})^t$ is the transposed of the velocity gradient, λ_H is the relaxation time of the polymer, and $\boldsymbol{W}$ is a Wiener process. The previous equation is integrated by a semi-implicit Predictor-Corrector scheme (Euler-Forward plus Crank-Nicolson).

Benchmark problem

The model is applied to study the flow in a complex geometry represented by an abrupt 10:1 axisymmetric contraction, assuming incompressibility and isothermal conditions, and the FENE kinetic model of polymeric fluids [3].



(a) $Wi = 11$ (b) $Wi = 444$

Figure 1: Stremlines for increasing values of the Weissenberg number $Wi = 2\lambda_H \frac{U}{D}$. Mean velocity U and width D are measured at the channel outlet.

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