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A third order accurate Lagrangian finite element scheme for the computation of generalized molecular stress function fluids

Andrea Fasano, Henrik Koblitz Rasmussen*

Department of Mechanical Engineering, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark

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ABSTRACT

A third order accurate, in time and space, finite element scheme for the numerical simulation of three-dimensional time-dependent flow of the molecular stress function type of fluids in a generalized formulation is presented. The scheme is an extension of the K-BKZ Lagrangian finite element method presented by Marín and Rasmussen (2009).

1. Introduction

The modelling of the flow behavior of polymer melts is needed to evaluate the design of polymer processing operations. These involve shaping molten polymers into plastic products, enabling a production of key importance for our way of life. The insight into the fluid dynamics of entangled liquids and polymer melts was initiated by phenomenologically based differential constitutive equations such as the Giesekus (1962) [1] and Phan-Thien and Tanner (1977) [2] models, whereas integral constitutive equations started with the K-BKZ [3,4] model. A mathematical generalization of nonlinear elasticity to viscoelasticity. All these models are versatile constitutive equations that are still used to model the flow of entangled polymer systems.

The understanding of the fluid dynamics of polymer melts still evolves [5–14]. This is a consequence of the developments in extensional rheometry [15–17]. In particular, the theoretical interpretation of measured extensional viscosities of idealized polymer systems [18–20] has represented a challenging task. At least two of the previously referred constitutive equations seem to contain concepts capable of explaining the fluid mechanics of idealized entangled melt systems. Either considering monomeric friction [11,12,21,22] or interchain pressure [14]. These theoretical efforts have been made aiming to predict the complex flow behavior of entangled polymer systems in general, but particularly for polymer melts, driven by a need for accurate design of polymer production processes. Accurate design indeed requires knowledge of the flow behavior of polymer melts. Moreover, polymer processing is geometrically complex, time dependent, and mostly complicated by the presence of moving melt surfaces or interfaces in three dimensions (3D). In the formulation of a numerical method for polymer melt flow, the choice of the particular constitutive equation to be implemented is important. Here we focus on the type of constitutive equation originally introduced by M.H. Wagner [6,14]. This molecular stress function constitutive equation is of the integral type.

Computationally the Lagrangian finite element method [23–26] is currently the only implemented technique for solving 3D time dependent flow problems with integral constitutive equations [27–30]. The formulation in [30] is capable of handling the molecular stress function constitutive equation, whereas all previous formulations are based on the K-BKZ model. Other steady [31] or unsteady [32–38] 2D formulations for the flow of K-BKZ fluids have been published with a variety of numerical concepts. Especially for the molecular stress function type of constitutive equation, the only other published method is the 2D steady code by P. Olley and M.H. Wagner [39]. Note that, in a Lagrangian method, interface or surface movement is a natural boundary condition due to the particle formulation. Such a formulation is able to handle large displacements of surfaces or interfaces.

In this work, the purpose is to develop a more accurate implementation of the three dimensional Lagrangian finite element method for the flow of molecular stress function constitutive equations. The previously published papers concerning the time-dependent flow of this type of fluid are in 2D [40–43], although they are all performed with a 3D code [30], actually second or-

* Corresponding author.
E-mail addresses: andreafasano.af@gmail.com (A. Fasano), hkra@mek.dtu.dk (H.K. Rasmussen).

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der convergent in both the time and spatial discretization. For the more simplified constitutive equation of the K-BKZ type, the first fully 3D time dependent study was published seventeen years ago [44]. The lack of published 3D computations is a consequence of insufficient computational speed. An increase in convergence order is one way to enhance the computational accuracy and efficiency. The latter is related to the possibility of reducing the number of nodes and increasing the time step size. The method in [30] converged second order with respect to the spatial and time discretizations. They are both increased to third order accuracy in the new numerical method presented here.

2. The stress tensor

The stress tensor is described by a generalized molecular stress function model. This is an extension of the well established factorized K-BKZ model.

In the continuum mechanical analysis the deformation gradient field is defined - in Cartesian coordinates - by the components of the displacement gradient tensor as

$$E_{ij}(\boldsymbol{x}, t, t') = \frac{\partial x_i}{\partial x'_j}, \qquad i = 1,2,3 \text{ and } j = 1,2,3. \tag{1}$$

The coordinates $\boldsymbol{x} = (x_1, x_2, x_3)$ and $\boldsymbol{x}' = (x'_1, x'_2, x'_3)$ are the particle positions of the same particle at the present time t and (all) the past times t', respectively. In a Lagrangian kinematics specification the independent variables are the initial particle positions of the particles $\boldsymbol{x}$ at the present time t. The dependent variables are consequently the positions of the particles $\boldsymbol{x}'$ at the past times t'. Bold symbols are used as matrix/vector notation in all formulae.

The Finger strain tensor is defined as follows

$$\mathbf{B}(\mathbf{x}, t, t') = \mathbf{E}(\mathbf{x}, t, t') \cdot \mathbf{E}(\mathbf{x}, t, t')^{\dagger} \tag{2}$$

where the symbol '†' denotes the transpose tensor operation.

Here we use the basic assumption of incompressibility allowing the third invariant of the Finger strain tensor to be unity: $I_3(\mathbf{x}, t, t') = \det[\mathbf{B}(\mathbf{x}, t, t')] = 1$. We can further write that:

$$\det[\mathbf{E}(\mathbf{x}, t, t_0)] = 1 \tag{3}$$

which represents the equation of continuity. Furthermore, the first and second invariants are given as

$$I_1(\mathbf{x}, t, t') = \operatorname{tr}\mathbf{B} \text{ and } I_2(\mathbf{x}, t, t') = \operatorname{tr}\mathbf{B}^{-1} = \frac{1}{2}\{[\operatorname{tr}\mathbf{B}]^2 - \operatorname{tr}[\mathbf{B}\cdot\mathbf{B}]\}. \tag{4}$$

The last equality is a consequence of the incompressibility and the Cayley–Hamilton theorem: $\mathbf{B}^{-1} = \mathbf{B}^2 - I_1\mathbf{B} + I_2\boldsymbol{\delta}$. The symbol '−1' denotes the inverse tensor operation and $\boldsymbol{\delta}$ is the unit tensor. Note that the dependence on ($\mathbf{x}$, t, t') is shortened in the notation.

The isotropic strain tensors, $\mathbf{S}_u$, are defined as [45]

$$\mathbf{S}_u(\mathbf{x}, t, t') = \psi_{1,u}(t - t', I_1, I_2)(\boldsymbol{\delta} - \mathbf{B}) + \psi_{2,u}(t - t', I_1, I_2)(\mathbf{B}^{-1} - \boldsymbol{\delta}) \tag{5}$$

with $u = 1, \ldots, U$. $\psi_{1,u}$ and $\psi_{2,u}$ are scalar functions that depend on the elapsed time and the invariants.

The stress tensor $\boldsymbol{\sigma}$ may be written as follows

$$\boldsymbol{\sigma} = -\sum_{u=1}^{U}\int_{-\infty}^{t} M_u(t - t') f_u(\mathbf{x}, t, t')^2 \mathbf{S}_u(\mathbf{x}, t, t')\mathrm{d}t' \tag{6}$$

in which $M_u(t - t')$ are the memory functions and f_u represent scalar quantities referred to as the molecular stress functions. In the case of f_u being unity, the above stress is identical to the well established factorized K-BKZ model [3,4].

The molecular stress functions f_u, with an initial value $f_u(\mathbf{x}, t', t') = 1$, are defined by using a set of differential equations in the present time t as

$$\frac{\partial}{\partial t} f_u(\mathbf{x}, t, t') = F_u\left(P_1, \ldots, P_V, \frac{\partial}{\partial t}P_1, \ldots, \frac{\partial}{\partial t}P_V, f_1(\mathbf{x}, t, t'), \ldots, f_U(\mathbf{x}, t, t')\right) \tag{7}$$

where $P_\nu(t - t', I_1(\mathbf{x}, t, t'), I_2(\mathbf{x}, t, t'))$, $\nu = 1, \ldots, V$, are scalar functions depending on the first and second invariants, $I_1(\mathbf{x}, t, t')$ and $I_2(\mathbf{x}, t, t')$, and the relative time $t - t'$.

3. Finite element discretization

Many of the details described in this section resemble the developments found in [30] and, most importantly, the present method is identical to the one in [29] for the case $f_u(\mathbf{x}, t, t') = 1$, i.e. the factorized K-BKZ model.

In the Lagrangian specification the equation of motion can be written in the following way [46]:

$$\rho\frac{\partial^2\mathbf{x}}{\partial t^2} = -\nabla\cdot\left(p\,\boldsymbol{\delta} - \boldsymbol{\sigma}\right) + \rho\,\mathbf{g} \tag{8}$$

where ρ is the fluid density, p is the pressure and $\mathbf{g}$ is the gravitational acceleration vector. The discretization of the continuity equation (3) and of the equation of motion (8) follow the mixed Galerkin finite element method [47]. The Galerkin weak forms of the continuity equation and the momentum balance multiplied by arbitrary weight functions ψ and ϕ, respectively, follow the procedure by Rasmussen [27,28]:

$$\int_\Omega [\det[\hat{\mathbf{E}}(\hat{\mathbf{x}}, t, t_0)] - 1]\psi^i \mathrm{d}\Omega = 0, \tag{9}$$

$$\begin{aligned}\mathbf{0} \;=\; & \int_\Omega \rho\left[\frac{\partial^2\hat{\mathbf{x}}}{\partial t^2} - \mathbf{g}\right]\phi^j\,\mathrm{d}\Omega - \int_\Omega \hat{p}\,\nabla\phi^j\,\mathrm{d}\Omega \\ & + \int_\Omega \widehat{\boldsymbol{\sigma}}\cdot\nabla\phi^j\,\mathrm{d}\Omega + \int_{\Gamma_n}\left[\mathbf{n}\cdot\left(\hat{p}\boldsymbol{\delta} - \widehat{\boldsymbol{\sigma}}\right)\right]\phi^j\,\mathrm{d}\Gamma_n,\end{aligned} \tag{10}$$

where i = 1,...,M and j = 1,...,N. M represents the total number of pressure nodes and N is the total number of coordinate nodes. Ω denotes the fluid domain, whereas Γ_n are the surfaces with natural boundary conditions. $\mathbf{n}$ is the outward unit vector to the referred surface and ∇ indicates the gradient operator. The approximated quantities of the exact variables are supplied with a hat.

The particular case of the particle positions at the present time, t, is

$$\hat{\mathbf{x}} = \sum_{i=1}^{N}\mathbf{x}^i\phi^i \tag{11}$$

where the particle positions at any time, t', are approximated as follows

$$\hat{\mathbf{x}}' = \sum_{i=1}^{N}\mathbf{x}'^i(\mathbf{x}^i)\phi^i. \tag{12}$$

Likewise, the pressure field can be described as:

$$\hat{p}(\hat{\mathbf{x}}) = \sum_{n=1}^{M} p^n(\mathbf{x}^n)\cdot\psi^n. \tag{13}$$

The approximation of the particle positions is introduced directly into the displacement gradient tensor required to define the spatial discretization of the stress:

$$\hat{\mathbf{E}}(\hat{\mathbf{x}}, t, t') = \sum_{i=1}^{N}\mathbf{x}^i\nabla'\phi^i \tag{14}$$