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A NEW BOUNDARY CONDITION FOR RATE-TYPE NON-NEWTONIAN DIFFUSIVE MODELS AND THE STABLE MAC SCHEME *

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Abstract

We present a new Dirichlet boundary condition for the rate-type non-Newtonian diffusive constitutive models. The newly proposed boundary condition is compared with two such well-known and popularly used boundary conditions as the pure Neumann condition [1] and the Dirichlet condition by Sureshkumar and Beris [2]. Our condition is demonstrated to be more stable and robust in a number of numerical test cases. A new Dirichlet boundary condition is implemented in the framework of the finite difference Marker and Cell (MAC) method. In this paper, we also present an energy-stable finite difference MAC scheme that preserves the positivity for the conformation tensor and show how the addition of the diffusion helps the energy-stability in a finite difference MAC scheme-setting.

Mathematics subject classification: 15A15, 15A09, 15A23
Key words: Boundary Conditions, Diffusive Complex Fluids models, Positivity preserving schemes, Stability of the MAC schemes.

1. Introduction

The benchmark computation of the Oldroyd-B model at relatively large Weissenberg number has for decades been elusive for numerical rheologists. While there has been significant progress toward resolving this issue [3, 4], beyond critical Weissenberg number, the mesh convergence is shown to be lost in numerical calculations. A local analysis of the stress behavior for the benchmark problem [5] presents some indication of the difficulty of simulating highly elastic flows of the Oldroyd-B model. Much attention is then drawn to include the stress diffusion in the model for the stability to tackle the high Weissenberg number problem posed for the Oldroyd-B model. The Oldroyd-B model is a generic viscoelastic model that has its origin in continuum mechanics [6–8], but it can be derived from a microscopic model as well [9]. As discussed in [10], a microscopic derivation [9, 11] of the Oldroyd-B model indicates that two regularizing terms can be introduced for the second moment equation as follows:

$$\mathsf{M}^\varepsilon + \mathsf{Wi}\left(\frac{D\mathsf{M}^\varepsilon}{Dt} - \nabla\mathcal{J}_\alpha(\boldsymbol{u}^\varepsilon)\mathsf{M}^\varepsilon - \mathsf{M}^\varepsilon\nabla\mathcal{J}_\alpha(\boldsymbol{u}^\varepsilon)^T\right) = \varepsilon^2\Delta\mathsf{M}^\varepsilon + \boldsymbol{\delta}, \tag{1.1}$$

where M^ε is the second moment, D/Dt is the material derivative, ε^2 is a positive diffusion coefficient, $\mathcal{J}_\alpha$ is a certain mollifier operator with a positive parameter α and $\boldsymbol{\delta}$ is the identity

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tensor. There are two stabilizing terms: the diffusion coefficient ε^2 and the mollified velocity. While the diffusion coefficient ε^2 is very small for dilute solutions of polymers, ranging from 10^{-7} to 10^{-9} in general, the contribution of the stress diffusion can increase up to 10^{-3} for narrow channels [12]. The role played by the mollifier can be found at [10, 13–15], in which the regularized model is proven to be well-posed even without the diffusion. In addition, a recent work by Constantin et al. [16] established the global regularity of the two dimensional diffusive Oldroyd-B model even if the theory may not cover the bounded domain. It is therefore anticipated that simulations of highly elastic flows can be performed for the regularized model. In fact, the addition of the diffusion term has been successfully demonstrated in [2, 17].

Simulations of such regularized models apparently induce an issue on how to impose accurate boundary conditions for M^ε [18]. A popular boundary condition in practice and theory [1, 10, 19] is the pure Neumann condition. Another boundary condition is the Dirichlet boundary condition introduced by Sureshkumar and Beris [2, 17]. It has been widely and successfully used for turbulent viscoelastic channel flows [20–23]. Some other boundary conditions have also been discussed in literature [12, 24–27]. In this paper, we propose a new boundary condition and demonstrate that the newly proposed condition is better in many test cases than the pure Neumann condition and the Dirichlet condition by Sureshkumar and Beris [2] in stability and robustness, thereby addressing successfully the boundary condition issue. It is worthy to note that our new boundary condition can be easily extended to such many relevant diffusive complex fluid models as liquid crystal polymers [28] or the diffusive Johnson-Segalman model [29–31]. The robustness of certain boundary condition has been made through the comparison between the result obtained by simulating the diffusive model with the boundary condition and that by simulating non-diffusive model ($\varepsilon^2 = 0$). Note that the diffusion coefficient is generally not too large. The stability will be measured in terms of the Weissenberg number that can be simulated.

A new Dirichlet boundary condition is implemented in the framework of the finite difference Marker and Cell (MAC) method. In this paper, we also present an energy-stable finite difference MAC [32,33] scheme that preserves the positivity for the conformation tensor and show how the addition of the diffusion helps the energy-stability in a finite difference MAC scheme-setting. To our best knowledge, it is the fist time in this paper to show the effect of the diffusion toward the enhancement of the stability. In addition, our result is shown to help achieve better mesh convergence. The mesh convergence is often very difficult to achieve for the simulation of the non-diffusive models at high Weissenberg number regimes [34, 35].

Throughout this paper, we use the standard notation for Sobolev spaces: $H^p(\Omega)$ denotes the classical Sobolev space of scalar functions on a bounded domain $\Omega \subset \mathbb{R}^d$ ($d = 1, 2$ or 3) whose derivatives up to order p ($1 \le p < \infty$) are square integrable, with the full norm $\|\cdot\|_p$ and the corresponding semi-norm $|\cdot|_p$. The symbol $H_0^1(\Omega)$ denotes the subspace of $H^1(\Omega)$ whose trace vanishes on the boundary $\partial\Omega$. The space $L^p(0, T; H^1(\Omega))$ for $1 \le p < \infty$ is the Hilbert space consisting of functions $f(x, t) : \Omega \times [0, T] \mapsto \mathbb{R}$ such that

$$\left(\int_0^T \|f(\cdot, \nu)\|_1^p \, d\nu \right)^{1/p} < \infty. \tag{1.2}$$

The symbols $\|\cdot\|_\infty$ and $\|\cdot\|_0$ denote the usual L^∞ and L^2 norms, respectively. The symbols $(\cdot, \cdot)$ and $\langle \cdot, \cdot \rangle$ denote the classical L^2-inner product and the dual pairing, respectively. The