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STABILIZATION OF FLUID FLOW OLDROYD-B SIMULATIONS BASED ON EIGENVALUES OF CONFORMATION TENSOR

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Abstract. *From a physical point of view, the molecular strain tensor can be represented at continuous level in viscoelastic fluids by the conformation tensor. This symmetric tensor should always be positive definite, however the positive-definiteness is sometimes lost in numerical simulations of non-Newtonian viscoelastic fluids flows at larger values of the Weissenberg number. This problem known as the High Weissenberg Number Problem (HWNP) and is characterized by the breakdown of numerical solutions. In some cases the HWNP can be avoided (or at least delayed) by adding a stress diffusion term to the transport equations for viscoelastic tensors. In this work, numerical tests are presented, demonstrating the HWNP problem and its possible cure based on stabilization method employing local addition of an artificial stress diffusion term to the transport equations, in the regions of the computational domain where the positive-definiteness of the conformation tensor can be violated.*

1 INTRODUCTION

The numerical simulation of non-Newtonian viscoelastic fluids flows is a challenging problem. One of the issues is the instability of numerical solutions resulting from the increase in the value of the parameter that describes the effect of elasticity, called High Weissenberg Number Problem. As a result, the positive-definiteness of the conformation tensor is lost. There is a wide range of approaches described of literature trying to resolve this issue, as for example, our previous works [7, 8].

One of the possible approaches is to add an (artificial) stress diffusion term into the transport equations for viscoelastic stress tensor. As a consequence, the solution will be more stable, however the added term will also modify the whole solution. In order to keep the modified model consistent with the original problem, we propose a modified stabilization method employing local addition of an artificial stress diffusion term just locally, in the regions where positive-definiteness of the conformation tensor can be violated. This localized artificial diffusion minimizes the spurious effects of the added term on the numerical solution.

2 MATHEMATICAL MODEL

Over a finite time interval $\left[0, T_f\right]$ $(T_f > 0)$ and in a bounded domain $\Omega \subset \mathbb{R}^d$ $(d = 2, 3)$, the governing system of dimensionless equations of the unsteady, incompressible, isothermal viscoelastic flow of homogeneous Oldroyd-B fluid can be summarized as

$$\begin{cases} \mathcal{R}e\left(\dfrac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u}\cdot\nabla\boldsymbol{u}\right) + \nabla p = 2(1-\eta_p)\nabla\cdot\mathbf{D} + \nabla\cdot\boldsymbol{\tau} + \mathbf{f} \\ \nabla\cdot\boldsymbol{u} = 0 \\ \boldsymbol{\tau} + \mathcal{W}e\left(\dfrac{\partial \boldsymbol{\tau}}{\partial t} + \boldsymbol{u}\cdot\nabla\boldsymbol{\tau} - \nabla\boldsymbol{u}^T\cdot\boldsymbol{\tau} - \boldsymbol{\tau}\cdot\nabla\boldsymbol{u}\right) = 2\eta_p\mathbf{D} \end{cases} \tag{1}$$

where the Reynolds and Weissenberg numbers are defined, respectively by $\mathcal{R}e = \dfrac{\boldsymbol{U}L}{\mu}$ and $\mathcal{W}e = \dfrac{\lambda\boldsymbol{U}}{L}$, being μ the dynamic viscosity, λ the relaxation time parameter, U the characteristic velocity and L the characteristic length. Depending on the stress model adopted, μ_s can either represents the viscosity of the solvent (for the polymer solution) or part of the total (apparent) stress viscosity of the system. In this work, $\eta_p \in [0, 1]$ is the dimensionless polymer viscosity such that the total (dimensionless) kinematic viscosity is $1 = \eta_s + \eta_p$. The extra stress tensor is defined by $\mathbf{T} = 2\eta_s\mathbf{D} + \boldsymbol{\tau}$ is the sum of the contributions given by the viscoelastic tensor $\boldsymbol{\tau}$ and the strain rate tensor (symmetric part of velocity gradient) $\mathbf{D} = \dfrac{1}{2}\left(\nabla u + \nabla u^T\right)$. The body force is denoted by $\mathbf{f}$.

To complete the problem (1) the boundary conditions need to be prescribed along the

boundary $\partial\Omega = \Gamma_{in} \cup \Gamma_w \cup \Gamma_{out}$ and initial conditions to be given in the domain Ω:

$$\begin{cases} \boldsymbol{u} = 0 & \text{on } \Gamma_w \\ \boldsymbol{u} = u_{in} & \text{on } \Gamma_{in} \\ \boldsymbol{\tau} = \boldsymbol{\tau}_{in} & \text{on } \Gamma_{in} \\ \boldsymbol{u}_{|t=0} = u_0 \end{cases} \tag{2}$$

3 DISCRETE OLDRYD-B - LIKE SYSTEM

3.1 Semi-descritization

To discretize the momentum and constitutive equations with respect to time, the implicit Euler scheme was associated with Characteristic Galerkin Method, to evaluate time derivatives of (velocity) vector and (stress) tensor field in a Lagrangian frame. In this method, the characteristic lines describe a material particle trajectories describing the motion given by the corresponding advection velocity field, as described e.g. in [9].
Consider a set of points (time instants) $t_n = n\Delta t = n\frac{T_f}{N}$, $n = 0, \ldots, N$, defined over the time interval $[0, T_f]$. The v^n denotes the approximation of velocity v at the time instant t_n, i.e., $v^n \approx v(t_n, \cdot)$, t_n, $\mathrm{x} \in \Omega$. Hence, the convective time derivative is approximated as:

$$\frac{Dv}{Dt} = \frac{\partial v}{\partial t} + \boldsymbol{u} \cdot \nabla v \approx \frac{v^n - v^{n-1} \circ X^{n-1}}{dt},$$

where X is the convecting field defined by $X(\mathrm{x}) = \mathrm{x}_{dt}$ with the particle path x_t in the steady state velocity field $\boldsymbol{u}$, being the solution of $\dot{\mathrm{x}}_t = \boldsymbol{u}(\mathrm{x}_t)$, $\mathrm{x}_{t=0} = \mathrm{x}$ and $v \circ X(\mathrm{x}) = v(\mathrm{x} - v(\mathrm{x})dt) = v^{n-1}(\mathrm{x}^\star) \equiv v_\star^{n-1}$, with $\mathrm{x}^\star$ the position at time at time t_{n-1} of the particle located at x at time t_n.

To variational problem of (1-2), we associate the following semi-discretized problem:

$$\begin{cases} \boldsymbol{u}^0 = u_0 \\ \displaystyle\int_\Omega 2(1-\eta_p)\mathbf{D}^n : \nabla \mathbf{v} + \mathcal{R}e \int_\Omega \frac{\boldsymbol{u}^n - \boldsymbol{u}_\star^{n-1}}{\Delta t} \cdot \mathbf{v} - \int_\Omega p^n \nabla \cdot \mathbf{v} = \int_\Omega (\nabla \cdot \boldsymbol{\tau})\, \mathbf{v}, & \forall \mathbf{v} \in \mathbf{H}_0^1(\Omega) \\ \displaystyle\int_\Omega (\nabla \cdot \boldsymbol{u}^n)\, q = 0, & \forall q \in L_0^2(\Omega) \\ \displaystyle\int_\Omega \left(\boldsymbol{\tau}^n + \mathcal{W}e \frac{\boldsymbol{\tau}^n - \boldsymbol{\tau}_\star^{n-1}}{\Delta t} \right) : \mathbf{S} = \int_\Omega \left[2\eta_p \mathbf{D} + \mathcal{W}e \left(\nabla \boldsymbol{u}^T \cdot \boldsymbol{\tau}^n + \boldsymbol{\tau}^n \cdot \nabla \boldsymbol{u} \right) \right] : \mathbf{S}, & \forall \mathbf{S} \in \mathcal{S} \end{cases} \tag{3}$$

3.2 Finite element method

Over the $\mathbb{T}_h$, a family of triangulations, consider the following finite element spaces

$$X_h = \left\{ \mathbf{v}_h \in C(\overline{\Omega}) \cap \mathbf{H}^1(\Omega) : \mathbf{v}_h = 0 \text{ on } \Gamma_h, w,\ \mathbf{v}_h = u_{in} \text{ on } \Gamma_{h,in} \text{ and } \mathbf{v}_{h|_\mathcal{T}} \in \mathbb{P}_2(\mathcal{T}), \forall \mathcal{T} \in \mathbb{T}_h \right\},$$

$$M_h = \left\{ q_h \in C(\overline{\Omega}) \cap L^2_0(\Omega) : q_{h|_\mathcal{T}} \in \mathbb{P}_1(\mathcal{T}), \forall \mathcal{T} \in \mathbb{T}_h \right\} \text{ and}$$

$$\mathcal{S}_h = \left\{ \mathbf{S}_h \in \mathbf{C}(\overline{\Omega}) \cap [L^2(\Omega)]^{2\times 2} : \mathbf{S}_h^T = \mathbf{S}_h \text{ and } \mathbf{S}_{h,ij_{|_\mathcal{T}}} \in \mathbb{P}_2(\mathcal{T}), \forall \mathcal{T} \in \mathbb{T}_h \right\}.$$

The pair of spaces $(X_h; M_h)$ corresponds to the so-called Hood-Taylor finite element method, and if $\mathbb{T}_h$ is non-degenerate and has no triangle with two edges on $\partial\Omega$, it verifies a compatibility condition known as the discrete LBB (or inf-sup) condition [1], which reads as follows:

There exists $\gamma^\star > 0$ (independent of h) such that

$$\inf_{q_h \in M_h \setminus \{0\}} \sup_{\boldsymbol{v}_h \in \mathbf{X}_h \setminus \{0\}} \frac{\left|(q_h, \nabla \cdot \mathrm{v_h})\right|}{\|\mathrm{v_h}\|_{\mathbf{X}_h} \|q_h\|_{M_h}} \geq \gamma^\star$$

As the classical Oldroyd-B model is a coupled problem for the three (in 2D) unknowns (extra stress tensor components) , discretized variational formulations are needed for both the Stokes-like system and the transport equations. We begin by introducing an equivalent (and more suitable) formulation for the continuous Stokes-like problem.
To variational problem of momentum equation and mass conservation law of (1) with the appropriated boundary conditions (2), we associate the following approximate problem For each $t \in [0, T_f],\ u_{0,h} \in X_h$ find $(\boldsymbol{u}_h, p_h) \equiv \big(u_h(t,\cdot), p_h(t,\cdot)\big) \in X_h \times M_h$ such that

$$\begin{cases} \displaystyle\int_\Omega 2(1-\eta_p)\mathbf{D}_h^n : \nabla \mathbf{v}_h + \mathcal{R}e \int_\Omega \frac{\boldsymbol{u}_h^n - \boldsymbol{u}_{\star,h}^{n-1}}{\Delta t} \cdot \mathbf{v}_h - \int_\Omega p_h^n \nabla \cdot \mathbf{v}_h = \int_\Omega (\nabla \cdot \boldsymbol{\tau}_h)\, \mathbf{v}_h, & \forall \mathbf{v}_h \in X_h \\ \displaystyle\int_\Omega (\nabla \cdot \boldsymbol{u}_h^n)\, q_h = 0, & \forall q_h \in M_h \end{cases} \tag{4}$$

The problem defined by (3) and (4) has a unique solution $(\boldsymbol{u}_h, p_h) \in X_h \times M_h$. Moreover,

$$\lim_{h\to 0} \|u - u_h\|_{H^1(\Omega)} + \lim_{h \to 0} \|p - p_h\|_{L^2(\Omega)} = 0$$

and

$$\|u - u_h\|_{L^2(\Omega)} \leq C(t)h^2, \qquad \|p - p_h\|_{L^2(\Omega)} = C(t)h.$$

Further details about the properties of the above finite element method and the rigorous convergence analysis of spatial discretization of the Navier-Stokes problem can be found in [4].

Discretisation of tensorial problem
For the constitutive equation of problem (1), the approximate finite element problem is defined as:

For each $t \in [0, T_f]$, $\mathbf{T}_{0,h} \in S_h$ find $\mathbf{T}_h \equiv \mathbf{T}_h(t, \cdot) \in \mathcal{S}_h$ such that

$$\int_\Omega \left(\boldsymbol{\tau}_h^n + \mathcal{W}e \frac{\boldsymbol{\tau}_h^n - \boldsymbol{\tau}_{\star,h}^{n-1}}{\Delta t} \right) : \mathbf{S}_h = \int_\Omega \left[2\eta_p \mathbf{D}_h + \mathcal{W}e \left(\nabla \boldsymbol{u}_h^T \cdot \boldsymbol{\tau}_h^n + \boldsymbol{\tau}_h^n \cdot \nabla \boldsymbol{u}_h \right) \right] : \mathbf{S}_h, \ \forall \mathbf{S_h} \in \mathcal{S}_h \tag{5}$$

3.3 Solution algorithm

The steady solution is obtained by a time-marching method when $t \to \infty$ for the unsteady system solved with a stationary boundary conditions. The steady state is obtained as the converged limit solution in time. The problem formed by (3) and (4) is solved by the decoupled iterative algorithm of Picard. The Crout scheme is used to solve the linear system associated to discrete Stokes problem while the linear system associated with the discrete equation for the elastic tensor is solved by a multi-frontal Gauss LU factorization implemented in the FreeFem++ [5] package UMFPACK.

4 NUMERICAL RESULTS

The conformation tensor

$$\boldsymbol{c} = \boldsymbol{\tau} + \frac{\eta_p}{\mathcal{W}e} \boldsymbol{\delta} \tag{6}$$

where $\boldsymbol{\delta}$ is identity tensor, corresponds to a kind of elastic stretch tensor. Its eigenvalues can be interpreted as a level of the stretch applied on material with the directions of maximal stretch given by the respective eigenvectors. From the physical point of view, it is reasonable to require that the corresponding eigenvalues are positive, i.e. the symmetric conformation tensor is positive definite.
However, numerically, when the effect of elasticity increases, this property is often lost, which would correspond to a some kind of material collapse. This issue is know as High Weissenberg Number Problem (HWNP).
To guarantee the physicality of the numerical solution it is very important to verify that the eigenvalues and consequently the determinant of the conformation tensor $\boldsymbol{c}$ will remain positive. In order to achieve this objective it is possible to introduce an artificial diffusive term of the type $\alpha \Delta \boldsymbol{\tau}$ in the constitutive equation, with a positive (as small as possible) tuning coefficient α. Although this procedure helps to stabilize the algorithm, the added artificial term affects the numerical solution for any value of α because the smoothing of the solution is applied in the whole domain.
To stabilize the algorithm and minimize the adverse effects of the artificial diffusion introduced, in this work we propose a local addition of an artificial stress diffusion term only

in the regions where the positive definiteness of the conformation tensor can potentially be violated. For this, we define a variable (in space) coefficient α whose values depend on the determinant (in general invariants) of tensor $\boldsymbol{c}$. This allows to introduce the artificial diffusion just locally, in the nodes of the computational mesh, where at least one of the eigenvalues of $\boldsymbol{c}$ is negative (or close to become negative).

4.1 Setup of the simulations

Boundary conditions
The simulations are performed for a corrugated tube which has a length of straight inlet and outlet sufficiently long to obtain a fully developed Poiseuille flow upstream and downstream which allows to consider on the respective boundaries the fully developed flow. This way we impose on the inlet boundary the analytical Poiseuille solution for the fully developed flow (for both the velocity and stress tensor). On the solid walls are is applied the no-slip conditions for velocity.

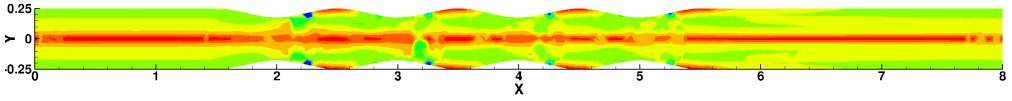
Simulations parameters
We set the dimensionless polymeric viscosity $\eta_p = 0.01$, the time-step $\Delta t = 0.025$, the Reynolds number $\mathcal{R}e = 1000$. The Weissenberg number is increased incrementally by the continuation method, while takes the converged solution obtained for lower $\mathcal{W}e$ as an initial condition for the next, higher Weissenberg number simulation.
The simulations are done with three different values of the diffusive parameter α. We take $\alpha \in \{0, \alpha_0, \propto \alpha_0 \operatorname{arctg}(\varepsilon Det(\boldsymbol{c}))\}$, being the $\alpha_0 = 1.0e^{-4}$ the asymptotic value and ε is an ad-hoc chosen parameter.
The non-uniform conforming mesh was generated by the FreeFem++ software.

4.2 Results

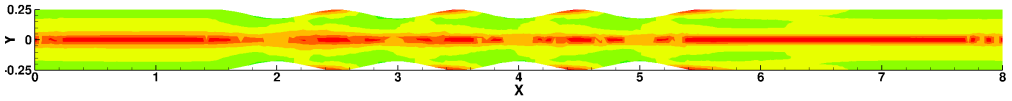
The figures below illustrate the behavior of the smallest eigenvalue of the tensor $\boldsymbol{c}$ with and without diffusion, for the cases where the numerical instabilities of the Oldroyd-B model (without diffusion) start to appear. The $\mathcal{W}e = 0.48$ is the higher value of the Weissenberg number for which we are able obtain the converged solution before the breakdown occurs. From the presented results it is clear that the artificial diffusion helps to keep the conformation tensor positive definite for higher values of $\mathcal{W}e$ (see Figures 1, 2 and 3,). It seems that the variable in space local artificial diffusion works well at least till $\mathcal{W}e = 0.4$ (see Figure 4). However results also show that the definition of the local diffusion parameter needs to be improved to remain efficient also for higher Weissenberg numbers (where the constant diffusion still works well).

$\mathcal{W}e = 0.3$

$\alpha = 0$



$\alpha = 1.0e-4$



$\alpha \equiv \alpha(Det(\boldsymbol{c}))$

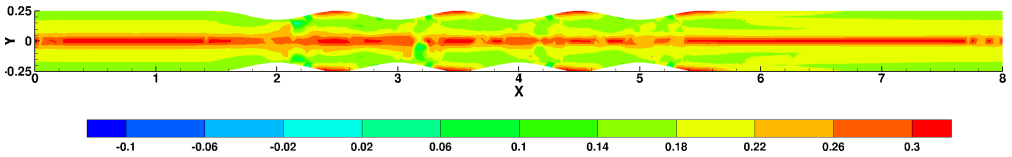
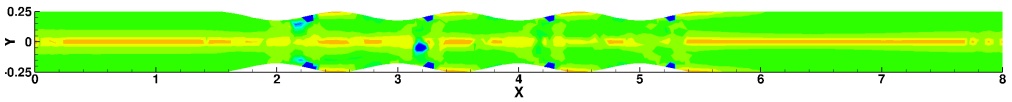


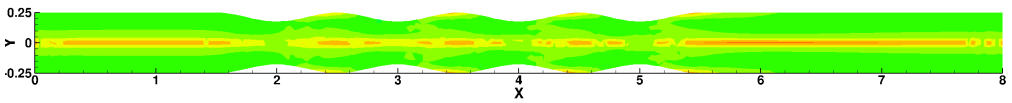
Figure 1: Comparison of the smallest eigenvalue of the conformation tensor contour plots $\mathcal{W}e = 0.3$.

$\mathcal{W}e = 0.4$

$\alpha = 0$



$\alpha = 1.0e-4$



$\alpha \equiv \alpha(Det(\boldsymbol{c}))$

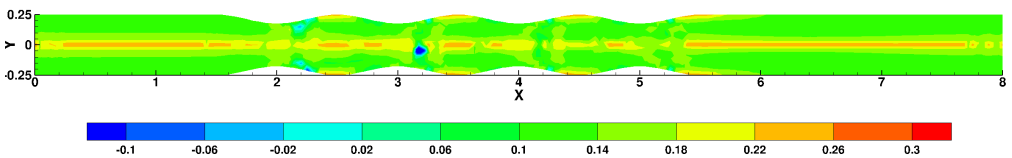


Figure 2: Comparison of the smallest eigenvalue of the conformation tensor contour plots $\mathcal{W}e = 0.4$.

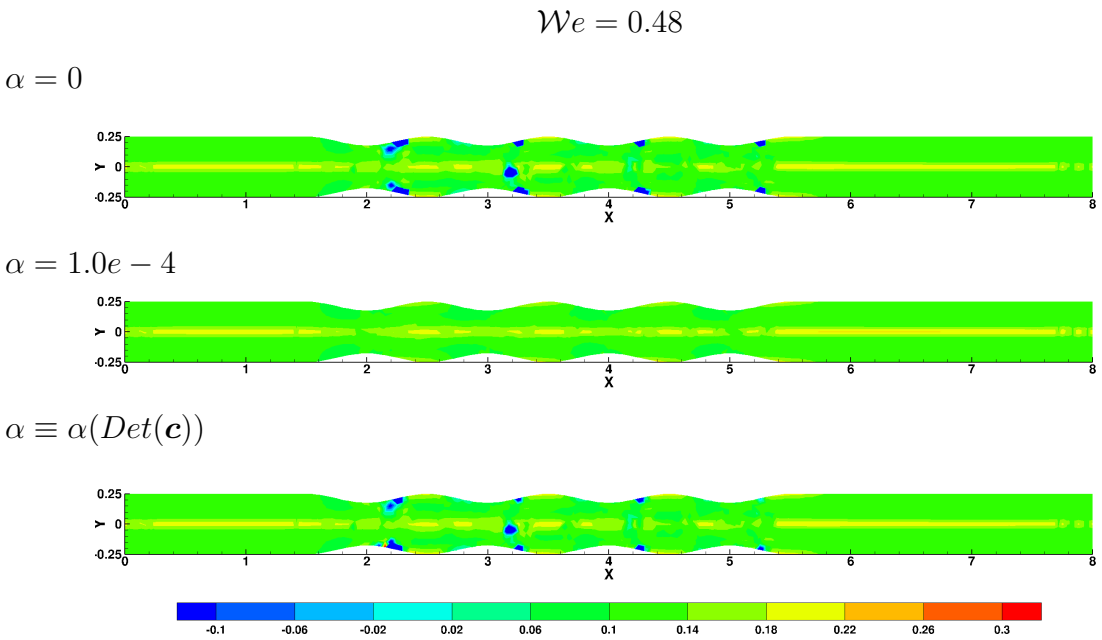


Figure 3: Comparison of the smallest eigenvalue of the conformation tensor contour plots $\mathcal{W}e = 0.48$.

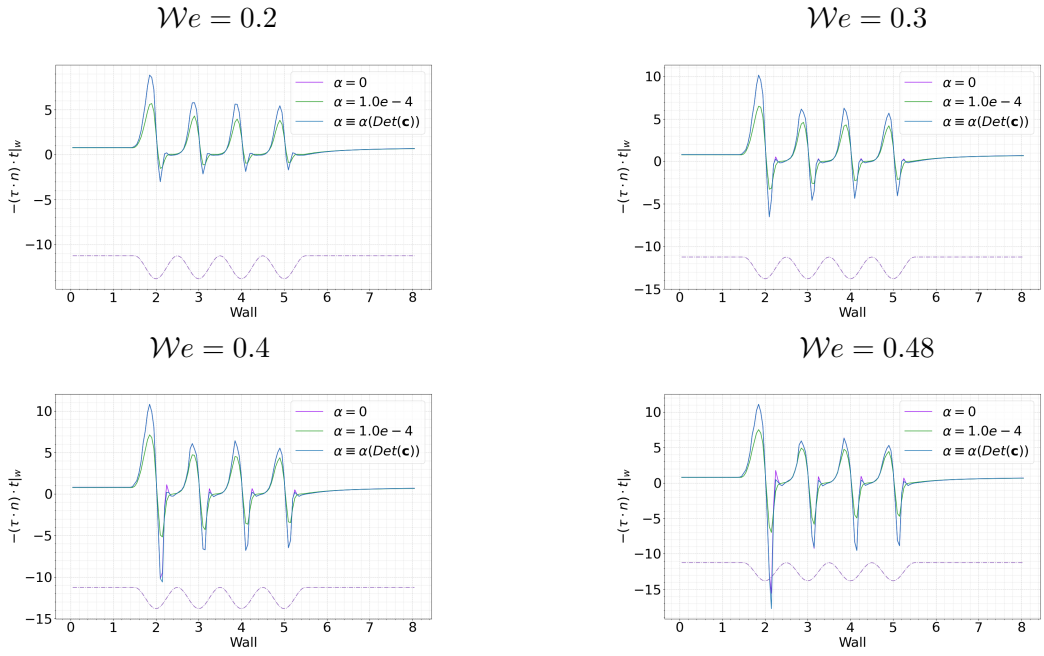


Figure 4: Comparison of the profile of the elastic stress tension on the wall for different values of the Weissenberg number.

5 CONCLUSIONS

The original formulation of the numerical method (without stabilization) becomes unstable (for given computational test case) for Weissenberg number $\mathcal{W}e > 0.2$.
The numerical stability is improved using an artificial diffusive stress term in the constitutive equation for extra stress.
The standard (constant) artificial stress diffusion term of the form $\alpha \cdot \alpha(Det(\boldsymbol{c}))$ visibly affects the solution for any value of α.
The the local diffusion coefficient $\alpha \equiv \alpha(Det(\boldsymbol{c}))$ still helps to stabilize the solution, without over-smoothing it in the whole domain.
The main problem, and challenge for the future research, is to chose and tune properly the function $\alpha(Det(\boldsymbol{c}))$. Moreover, the rigorous mathematical analysis of the underlying model is significantly more complicated, and some additional assumptions and restrictions will be needed to control the diffusion coefficient $\alpha(Det(\boldsymbol{c}))$.

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