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New formulations, positivity preserving discretizations and stability analysis for non-Newtonian flow models ☆

Young-Ju Lee [a], Jinchao Xu [b,*]

[a] *Department of Mathematics, UCLA, 520 Portola Plaza, CA 90095, USA*

[b] *Department of Mathematics and Center for Computational Mathematics and Application of Pennsylvania State University, PA, USA*

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Abstract

We propose a class of new discretization schemes for solving the rate-type non-Newtonian constitutive equations. The so-called conformation tensor has been known to be symmetric and positive definite in a large class of constitutive equations. Preserving such a positivity property on the discrete level is believed to be crucially important but difficult. High Weissenberg number problems on numerical instabilities have been often associated with this issue. In this paper, we present various discretization schemes that preserve the positive-definiteness of the conformation tensor regardless of the time and spatial resolutions. Moreover, the robustness of the algorithm has been also demonstrated by the stability analysis using the discrete analogue of energy estimates. New schemes presented in this paper are constructed based upon the newly discovered relationship between the rate-type constitutive equations and the symmetric matrix Riccati differential equations.

Keywords: Conformation tensor; Non-Newtonian models; Constitutive equation; Positivity preserving scheme; Riccati differential equation; Lie derivative

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* Corresponding author. Address: Department of Mathematics, The Pennsylvania State University, 332 McAllister Building, PA 16802, USA. Tel.: +814 865 1110; fax: +814 865 3735.

E-mail address: xu@math.psu.edu (J. Xu).

URLs: http://www.math.ucla.edu/~yjlee (Y.-J. Lee), http://www.math.psu.edu/xu (J. Xu).

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1. Introduction

Fluids comprised of large macromolecules, known as viscoelastic fluids, can produce a great variety of new phenomena. The better known examples of this richness, among many others, include the rod climbing Weissenberg effect [9], die swell [8], extrusion instabilities [4], and the oscillation of falling sphere [21]. While most of these effects are qualitatively understood to some extent, there has not been much understanding on proper mathematical models that are responsible for such phenomena. It is widely acknowledged that numerical simulations play a crucial role in mathematical modelling for such experimental results.

In the last two decades, there have been rapid advances in the development of numerical algorithms for simulating viscoelastic flows. However, the developments are hampered by various difficulties. One of most notable examples of such difficulties is the breakdown in convergence of the algorithms at critical values of the Weissenberg or Deborah numbers, which was first observed in the late 1970s [33]. Since then it has been called the high Weissenberg number problem. Despite extensive efforts in the search for suitable methods, the high Weissenberg number problem still remains elusive. It has been widely believed that such a problem is attributed to the lack of positivity preserving property of the so-called conformation tensor $\mathscr{C}$ on the discrete level.

The conformation tensor $\mathscr{C}$, from the molecular theories, denotes the ensemble average of the dyadic product of end-to-end vector $\mathbf{Q}$ of the dumbbell (see e.g. [3]). The positive-definite (non-negative) character of $\mathscr{C}$ is then necessary for making meaningful microscopic interpretation and so it is known to give rise to a criteria for the physical admissibility of the models (see [3, p. 281]). Indeed, the positivity of the conformation tensor has been proved to be valid for various models, including UCM (upper convected Maxwell model) and the Oldroyd-B model. These models are known to be mathematically stable in the classical sense of Hadamard, namely the solution for such models depends continuously on the initial data (see e.g. [15,22–24]). Moreover, the stability analysis depends crucially on the fact that the conformation tensor $\mathscr{C}$ remains positive definite while it evolves in time. Another observation is that the trace of the conformation tensor $\mathscr{C}$ can be considered to be an elastic energy. Indeed, from the positive-definiteness of the conformation tensor, one can derive an energy estimate (see [27,30] and also Section 7 in this paper, where an energy law has been driven in a more general context and the discrete analogue of energy estimates has also been driven). Such a property is also valid for other models including Giesekus, Phan-Thien and Tanner, Leonov and Larson models (see [3,19] for detailed descriptions) for a wide range of parameters and the local loss of this property on the discrete level causes the onset of oscillation of solutions and leads to disastrous effects (see [3,11,18,24,33]).

Clearly, it is significant to develop numerical schemes that preserve the positive definiteness of the conformation tensor. It is in fact believed that the aforementioned numerical difficulty can be overcome in time-dependent calculations with positivity preserving schemes (see [33, p. 197]) and a loss of the positivity has long been known to be due to the fact that the constitutive equation has not been discretized properly (see also [3,11,18,24]). Such improper discretization may result from a lack of understanding on the mathematical models. It is well-known that mathematical analysis for models describing complex fluids is quite challenging. We would like to refer readers to the following articles [7,27,29,28] for the state of the art mathematical analysis on certain viscoelastic models.

Apparently, finding positivity preserving discretization scheme is not an easy task. In a recent (2002) book "Computational Rheology" written by Owens and Phillips (see [33, p. 59]), authors noted that "although the continuous system possesses the property that $\mathscr{C}$ is positive definite, this may *not* be carried over to the corresponding discrete problem".

The only attempt known to the authors for obtaining positivity preserving scheme is a very recent (2003) work [30]. Their main idea was to set $\mathscr{C} = AA^{\mathrm{T}}$ and then try to write down equations for A approximately on the discrete level. Hence, the positivity of $\mathscr{C}$ is forced with such an approach. One may argue that this is an unnatural approach since, judging from the integral expression of $\mathscr{C}$ (see (3.6) below), the artificially introduced A has no apparent physical meaning. Moreover, this approach seems to be restricted to Oldroyd-B models and its extension to other models does not seem to be obvious and also the scheme is only first-order accurate.

In this paper, we will develop a unified numerical discretization framework that can be used for simulating most existing constitutive equations in a way that the positivity of the conformation tensor in continuous level can be naturally extended to its discrete counterpart. We also demonstrate the stability of the algorithm based on the discrete analogue of energy estimates. Our main observation in this paper is that the constitutive equation from most of the existing models can be recast, in terms of certain Lie derivative, into an ''ordinary'' differential equation which closely resembles the well-known symmetric Riccati differential equations. The Riccati equation arises in many fields of applied mathematics, engineering and economic sciences, especially in the domains such as, just to cite a few, linear optimal control and filtering problems with quadratic cost functionals, differential geometry and singular perturbation theory. Moreover, there are well-developed theory of symmetric (or Hermitian) Riccati equation. For basic theory of the matrix Riccati differential equations, we refer interested readers to the monograph of Reid [36]. For the state of the art of the theory of symmetric matrix Riccati equations, readers refer to the recent monograph by Abou-Kandil et al. [1].

Using a semi-Lagrangian approach and finite element method [20,35], we obtain a class of positivity preserving discretization schemes whose accuracies are of up to second-order both in space and in time under some mild conditions. In proposing positivity preserving schemes, we shall begin our discussion on the simplest model, so-called the Oldroyd-B model and we then take steps to extend the idea to a wide spectrum of models including various non-linear models as well as multi-mode models. Details of implementation and numerical experiments shall be reported in forthcoming papers.

The rest of the paper is organized as follows. In Section 2, we present some preliminaries together with various terminologies to ease our expositions. In Section 3, the Oldroyd-B model is given as an illustration. The general Riccati equation is then introduced in Section 4. In Section 5, the reformulation of various constitutive equations have been performed and in Section 6 we present several algorithms to solve viscoelastic models in a way that the positivity of the conformation tensor is preserved both in time and space discrete senses. We then show the stability analysis for the fully discrete systems via the discrete analogue of energy estimates in Section 7. We close the paper with some concluding remarks in Section 8.

2. Preliminaries

In this section, we shall introduce some preliminary materials and important identities, which shall be the building blocks for the algorithmic development. We begin this section with a basic review on kinematics of bodies.

2.1. Deformation tensor

To describe a particle moving in a fluid, we introduce two configurations, say Ω_t and Ω_s. The motion of a particle is then manifested by the following mapping:

$$y: \ \Omega_s \mapsto \Omega_t.$$

Let us denote $y(X,t,s)$ the position of particle X at time s and $y(X,t,t) = X$.

We shall now introduce a set of notation for ease of our presentation throughout this paper. For any given tensor σ, $\sigma(y(X,t,s),s)$ shall be denoted by $\sigma(t,s)$ and $\sigma(X,t)$ by $\sigma(t)$. The same notation also apply to any vector $\mathbf{u}$.

The velocity of the particle is given by $\mathbf{u} = \dot{y}$, where the dot indicates the partial derivative with respect to s with t fixed. In the Eulerian description (y, s), the chain rule gives the familiar material derivative defined as follows:

$$\frac{Dg}{Ds} = \frac{\partial g}{\partial s} = g_s + (\mathbf{u} \cdot \nabla)g,$$

where ∇ is the gradient for the y variables. Classical mechanics assumes that $y : \Omega_s \mapsto \Omega_t$ is a diffeomorphism and the relative deformation gradient is the matrix defined by (see [29,33] or [37])

$$F_{ij}(t,s) = \frac{\partial y_i(X,t,s)}{\partial X_j}.$$

We note that an application of the chain rule gives an Eulerian description,

$$\frac{DF(t,s)}{Ds} = \dot{F}(t,s) = \left(\frac{\partial}{\partial s}\frac{\partial y_i}{\partial X_j}(X,t,s)\right) = \left(\frac{\partial u_i}{\partial X_j}(X,t,s)\right) = \left(\frac{\partial u_i}{\partial y_k}\frac{\partial y_k}{\partial X_j}(X,t,s)\right) = \nabla\mathbf{u}(t,s)F(t,s).$$

Our convention for the gradient of a vector $\mathbf{u}$ is that the (i,j) component of $\nabla\mathbf{u}(t,s)$ is $\partial u_i/\partial y_j$, where $\mathbf{u} = (u_i)_{i=1}^d$ with $d = 2$ or 3. The inverse of F is often called the displacement gradient tensor. From the relation that $FF^{-1} = I$, we obtain

$$\frac{DF^{-1}(t,s)}{Ds} = -F^{-1}(t,s)\nabla\mathbf{u}(t,s). \tag{2.1}$$

We note that the following relations hold true:

$$F^{-1}(t,s) = F(s,t) \tag{2.2}$$

and

$$\frac{DF(s,t)}{Dt} = \nabla\mathbf{u}(t)F(s,t). \tag{2.3}$$

2.2. Two identities on upper convective derivatives

In this subsection, we shall introduce two main identities related to the upper convective time derivative of tensors. The upper convected derivative denoted by $\frac{\delta_F}{\delta_F t}$ for the tensor ζ is defined through:

$$\frac{\delta_F \zeta}{\delta_F t} = \frac{\partial \zeta}{\partial t} + (\mathbf{u} \cdot \nabla)\zeta - (\nabla\mathbf{u})\zeta - \zeta(\nabla\mathbf{u})^{\mathrm{T}}. \tag{2.4}$$

We introduce first identity for the upper convected derivative as follows: for any $(X,t) \in \Omega \times (0,\infty)$,

$$\frac{\delta_F \zeta}{\delta_F t}(X,t) = \lim_{s \to t} F(t,s)\frac{D(F(s,t)\zeta(t,s)F(s,t)^{\mathrm{T}})}{Ds}F(t,s)^{\mathrm{T}}. \tag{2.5}$$

This can be shown by a straightforward calculation based on the facts (2.1) and (2.2). This is often called the Lie derivative of ζ and also known as the Truesdell stress rate (see [40, p. 254]).

The second identity is on the upper convective derivative of the identity tensor (see e.g. [32]), namely

$$\frac{\delta_F I}{\delta_F t} = -2\mathscr{D}(\mathbf{u}). \tag{2.6}$$

This identity can be obtained by simply setting $\zeta = I$ in (2.4) and is crucial when we reformulate the constitutive equation in terms of the conformation tensor. It can also be viewed as a tool for approximating the rate of strain $\mathscr{D}(\mathbf{u})$.

The identity (2.5) has been used for developing objective time-stepping algorithm commonly called *incrementally objective discretization*, a nomenclature first introduced in Hughes and Winget [17]. Since then it has also been used for simulating some non-Newtonian models by Baaijens [2]. In their works, the direct discretization of the upper convected time derivative (2.4) has been performed along the particle trajectory based on the Lagrangian framework and the approximation for the rate of strain has been made based on the following identity:

$$\lim_{s\to t} F(s,t)^{\mathrm{T}} \frac{DC(t,s)}{Ds} F(s,t) = 2\mathscr{D}(\mathbf{u})(t), \tag{2.7}$$

where C is called the *Cauchy* strain tensor defined through:

$$C(y(X,t,s),s) = F^{\mathrm{T}}(t,s)F(t,s).$$

Our approach is subtle but fundamentally different from their algorithms from the following two aspects. Namely, we shall use the so-called semi-Lagrangian framework (see e.g. [20,35,38]) for the time discretization and shall use (2.6) to approximate the rate of strain. Indeed, the use of (2.6) is instrumental and necessary in that it allows us to view various constitutive models (e.g. the Oldroyd-B model) as the Riccati differential equation and leads to the positivity preserving scheme. More detailed time discretization scheme shall be described in Section 6 and we will see that the use of (2.7) may not lead to the positivity preserving discretization.

In the following section, to illustrate the basic form of viscoelastic models, the Oldroyd-B model is introduced. We then present its reformulated version by using the identity (2.6).

3. An illustration: the Oldroyd-B model

In this section, we shall give a brief description of the Oldroyd-B model [32] as an illustrative example for viscoelastic models.

3.1. The Oldroyd-B model

Let us consider the flow of the Oldroyd-B fluid occupying a bounded domain $\Omega \subset \mathbb{R}^d$. The equations of motion for unsteady incompressible flows are

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right) = -\nabla p + \operatorname{div}\sigma,$$

$$\mathbf{div}\,\mathbf{u} = 0,$$

respectively, where $\mathbf{u}$ is the velocity field, p the isotropic pressure, σ the extra-stress tensor and ρ is the density of the fluid. The extra-stress tensor is related to the rate-of-strain tensor $\dot\gamma = \nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}}$ by the following constitutive equation:

$$\sigma + \lambda_1 \frac{\delta_F \sigma}{\delta_F t} = \eta_0\left(\dot\gamma + \lambda_2 \frac{\delta_F \dot\gamma}{\delta_F t}\right), \tag{3.1}$$

where λ_1 and λ_2 are characteristic relaxation and retardation times of the fluid, respectively, η_0 is the constant shear viscosity. Furthermore, if the extra-stress tensor is expressed in terms of its solvent and polymeric contributions, τ

$$\sigma = \eta_{\mathrm{s}}\dot\gamma + \tau,$$

then the polymeric contribution of stress, τ satisfies

$$\tau + \lambda_1 \frac{\delta_F \tau}{\delta_F t} = \eta_p \mathscr{D}(\mathbf{u}).$$

The constants, η_s and η_p are the solvent and polymeric viscosities, respectively, where $\eta_0 = \eta_s + \eta_p$, and

$$\eta_s = \frac{\lambda_2}{\lambda_1}\eta_0 \quad \text{and} \quad \eta_p = \left(1 - \frac{\lambda_2}{\lambda_1}\right)\eta_0.$$

In dimensionless form, the governing equations can be given by

$$Re\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}\right) = -\nabla p + \operatorname{div} \tau + \eta_s \operatorname{div} \mathscr{D}(\mathbf{u}), \tag{3.2}$$

$$\mathbf{div}\,\mathbf{u} = 0, \tag{3.3}$$

$$\tau + We \frac{\delta_F \tau}{\delta_F t} = 2(1 - \eta_s)\mathscr{D}(\mathbf{u}) = 2\mu_p \mathscr{D}(\mathbf{u}), \tag{3.4}$$

where $\mathscr{D}(\mathbf{u}) = (\nabla \mathbf{u} + \nabla \mathbf{u}^T)/2$ and

$$\beta = \frac{\lambda_1}{\lambda_2}, \quad Re = \frac{\rho U L}{\eta_0} \quad \text{and} \quad We = \frac{\lambda_1 U}{L}.$$

In case $\eta_s = 0$, UCM (the upper convected Maxwell) model results and it is well-known that the model (3.1) or (3.4) is the simplest non-linear extensions of Maxwell's idea of formulating a system of ordinary differential equations which determines the stress in terms of the velocity gradient. As mentioned earlier, the Eqs. (3.2)–(3.4) are well-known to be stable in the sense of Hadamard (see e.g. [33]).

3.2. A reformulation of the Oldroyd-B model using the conformation tensor

One crucial technique used in this paper is based on the reformulation of the models in terms of the conformation tensor. The aforementioned model, the Oldroyd-B model has a property that the following tensor is positive-definite:

$$\tau_A(X, t) = \tau(X, t) + \frac{\mu_p}{We} I.$$

Thanks to (2.6), the constitutive Eq. (3.4) can be rewritten as follows:

$$\tau_A + We \frac{\delta_F \tau_A}{\delta_F t} = \frac{\mu_p}{We} I. \tag{3.5}$$

We also note that, for the Oldroyd-B model, it is well-known that the conformation tensor τ_A can be written as the following integral form:

$$\tau_A(X, t) = \int_{-\infty}^{t} \frac{\mu_p}{We^2} \exp\left(\frac{-(t - s)}{We}\right) F(s, t) F(s, t)^T \, ds. \tag{3.6}$$

From the integral expression for τ_A, it is immediate to see that τ_A is positive definite while the rate type model (3.5) does not show such a property immediately.

The positive-definiteness of τ_A appeared to be first established by Hulsen (see [19]) directly from the models such as (3.5) under certain conditions. This shall be revisited in Section 5 in terms of our new framework and shall be proved in a simpler way. Even though the model (3.6) is known to be equivalent to the rate-type model (3.5), it does not seem to have been fully clarified. Namely, the equivalent relation has been claimed by showing that the rate-type model (3.5) can be deduced from the integral model (3.6) without showing the other direction. So, if the integral model is not available a priori, the equivalent integral model for the corresponding rate-type model is not considered to be known (see e.g. [22, p. 15]). Indeed, to obtain the integral model from its rate-type model, one needs to find out the analytic solution to the rate-type model. It also seems to have been missing (see [37, p. 18]). We shall elaborate this issue and derive various integral models from their rate-type models in Section 5.

4. Generalized Riccati equations in terms of Lie derivatives

In this section, we shall prepare for our new framework to construct positivity preserving schemes by introducing a generalized Riccati differential equation in terms of a general Lie derivative.

The classic symmetric Riccati differential equation that we are interested in is of the following form:

$$\frac{\mathrm{d}\mathscr{C}(t)}{\mathrm{d}t} = A(t)\mathscr{C} + \mathscr{C}A(t)^{\mathrm{T}} - \mathscr{C}B(t)\mathscr{C} + U(t) \tag{4.1}$$

with a symmetric positive semidefinite initial condition $\mathscr{C}(0) = \mathscr{C}_0$.

This type of equations have been well studied in the literatures. Among others, there are two important properties of Riccati differential equation that are interesting to us in the current work. First of all, this equation has a certain closed-form solution, from which the solution $\mathscr{C}$ can be proved to be symmetric positive definite under certain conditions (see Proposition 4.1). Secondly, the positivity preserving schemes for such equations are easily devised, especially in time (see [10] and Section 6.3).

4.1. A general Lie derivative

The Riccati equation (4.1) will be generalized by replacing the ordinary derivative $\frac{\mathrm{d}}{\mathrm{d}t}$ by a general Lie derivative defined as follows:

Definition 4.1

$$\frac{\delta_L \tau}{\delta_L t} = \lim_{s\to t} L(t,s)\frac{D(L(s,t)\tau(t,s)L(s,t)^{\mathrm{T}})}{Ds}L(t,s)^{\mathrm{T}}, \tag{4.2}$$

where $L(s,t)$ is a smooth tensor.

The tensor L can be viewed as a transformation rule and in general satisfy the following ordinary differential equation:

$$\frac{DL(s,t)}{Dt} = R(t)L(s,t), \quad L(s,s) = I. \tag{4.3}$$

See for example (2.3), the case for the upper convected derivative, where $L = F$ and $R(t) = \nabla\mathbf{u}(t)$.

The tensor L determined by (4.3) is called *the transition matrix or* (*evolution matrix*) in the community concerning the Riccati differential equation (see [1, p. 2]). However, it is not known to the authors that the Riccati differential equation has ever been studied in terms of the Lie derivative.

Note that the choice of L shall change the rate of stress. The possible choices for L useful for our exposition in this paper are listed as follows:

$$L(t,s) = \begin{cases} I, & R(t) = 0 & \text{(material)}, \\ F(t,s), & R(t) = \nabla\mathbf{u}(t) & \text{(upper convected)}, \\ F(s,t), & R(t) = -\nabla\mathbf{u}^{\mathrm{T}}(t) & \text{(lower convected)}, \\ E(t,s), & R(t) = \dfrac{a+1}{2}\nabla\mathbf{u}(t) + \dfrac{a-1}{2}\nabla\mathbf{u}^{\mathrm{T}}(t) & \text{(Gordon–Schowalter)}. \end{cases}$$

A rate defined by the following relation is known to be objective (see e.g. [2, p. 1119]):

$$\frac{\delta_L \tau}{\delta_L t} = \frac{D\tau}{Dt} - (\omega + H)\tau - \tau(\omega + H)^{\mathrm{T}}, \tag{4.4}$$

where $\omega = \frac{\nabla \mathbf{u} - \nabla \mathbf{u}^{\mathrm{T}}}{2}$, H is some objective tensor (see e.g. [16] for the definition of the objectivity). The rate defined by (4.4) can be cast into the Lie derivative with the transition tensor $L(s,t)$ satisfying the following ODE:

$$\frac{DL(s,t)}{Dt} = (\omega + H)L(s,t), \quad L(s,s) = I.$$

With some appropriate choice of H, we can show that three cases except for $L = I$ are objective rates. We can also consider some other objective stress rates available in any literatures. Indeed, it has been addressed especially in Hughes [16], Simo and Hughes [40] that any possible objective stress rate is a particular case of a fundamental geometric object known as the Lie derivative and moreover under the tensor L, a transformation rule, a somewhat complicated expression e.g. (2.4) becomes a rather simple time derivative (2.5).

4.2. A generalized Riccati equation

A generalized Riccati differential equations in terms of the above general Lie derivative is as follows:

$$\frac{\delta_L \mathscr{C}(t)}{\delta_L t} = A(t)\mathscr{C}(t) + \mathscr{C}(t)A(t)^{\mathrm{T}} - \mathscr{C}(t)B(t)\mathscr{C}(t) + U(t). \tag{4.5}$$

In this formulation, we shall assume that the coefficient matrices are bounded and piecewise continuous and that the matrices B and U are symmetric and positive semidefinite.

Let us first consider a special case of the Eq. (4.5).

Lemma 4.1. *The solution to the following ordinary differential equation written in terms of a general Lie derivative*:

$$\frac{\delta_L \mathscr{C}(t)}{\delta_L t} = U(t) \tag{4.6}$$

can be given in the following closed-form:

$$\mathscr{C}(t) = L(s,t)\mathscr{C}(s)L(s,t)^{\mathrm{T}} + \int_s^t L(v,t)U(v)L(v,t)^{\mathrm{T}}\,\mathrm{d}v.$$

Proof. The ordinary differential equation (4.6) can be rewritten as followings:

$$\lim_{s\to t} L(t,s)\frac{D(L(s,t)\mathscr{C}(s)L(s,t)^{\mathrm{T}})}{Ds}L(t,s)^{\mathrm{T}} = U(t).$$

This expression can then be cast into the following form:

$$\lim_{s\to t} \frac{D(L(s,t)\mathscr{C}(s)L(s,t)^{\mathrm{T}})}{Ds} = \lim_{s\to t} L(s,t)U(s)L(s,t).$$

To distinguish the fixed variable in the above expression, we shall denote t by $\hat{t}$ for now. We then have the following ordinary differential equation for $L(t,\hat{t})U(t)L(t,\hat{t})$

$$\frac{D(L(t,\hat{t})\mathscr{C}(t)L(t,\hat{t})^{\mathrm{T}})}{Dt} = L(t,\hat{t})U(t)L(t,\hat{t})^{\mathrm{T}}.$$

Taking integration and changing $\hat{t}$ back to t, we obtain the desired results. □

Proposition 4.1. *The solution of (4.5) exists and it is symmetric and nonnegative for all $t \geqslant 0$. Further, if $\mathscr{C}(s)$ or $U(s)$ is positive for some $s \geqslant 0$, then $\mathscr{C}(t)$ is positive for all $t > s$.*

Proof. We begin with a reformulation of the general Riccati equation (4.5). Notice

$$\frac{\delta_L \mathscr{C}(t)}{\delta_L t} = \frac{D\mathscr{C}(t)}{Dt} - R(t)\mathscr{C}(t) - \mathscr{C}(t)R(t)^{\mathrm{T}}.$$

Now by a simple reformulation, we obtain that

$$\frac{D\mathscr{C}(t)}{Dt} = \left(A(t) + R(t) - \frac{1}{2}\mathscr{C}(t)B(t)\right)\mathscr{C}(t) + \mathscr{C}(t)\left(A(t) + R(t) - \frac{1}{2}\mathscr{C}(t)B(t)\right)^{\mathrm{T}} + U(t). \tag{4.7}$$

Let us set

$$G(t) = A(t) + R(t) - \frac{1}{2}\mathscr{C}(t)B(t)$$

and rewrite (4.7) as followings:

$$\frac{\delta_\Phi \mathscr{C}(t)}{\delta_\Phi t} = U(t),$$

where

$$\frac{D\Phi(s,t)}{Dt} = G(t)\Phi(s,t), \quad \Phi(v,v) = I. \tag{4.8}$$

By Lemma 4.1, we obtain that

$$\mathscr{C}(t) = \Phi(s,t)\mathscr{C}(s)\Phi(s,t)^{\mathrm{T}} + \int_s^t \Phi(v,t)U(v)\Phi(v,t)^{\mathrm{T}}\,\mathrm{d}v. \tag{4.9}$$

Since $\Phi(s,t)$ is non-singular for all s and t, the statement of the proposition follows as long as the solution exists. However, from the fact that $B(t)$ is semi positive-definite, we can deduce that with $\|\mathscr{C}(t)\| = \sup_{\|\chi\|=1}\chi^{\mathrm{T}}\mathscr{C}(t)\chi$,

$$\|\mathscr{C}(t)\| \leqslant \|\mathscr{C}(0)\| + \int_0^t (2\|A(v) + R(v)\|\|\mathscr{C}(v)\| + \|U(v)\|)\,\mathrm{d}v,$$

from which it follows by the Gronwall's inequality that $\|\mathscr{C}(t)\|$ is finite and hence $\mathscr{C}(t)$ exists for all $t > 0$. This completes the proof. □

5. Reformulating constitutive equations as generalized Riccati equations

In this section, we shall show that various interesting constitutive equations can be reformulated into the generalized Riccati equations (4.5) based on the Lagrangian frame.

Note that the reformulation will be made in terms of the conformation tensor denoted by τ_A (with abuse of notation) and τ_A is determined by the rate used in the model. Especially, the objective rate of our interest here is

$$\frac{\delta_E \tau_A}{\delta_E t} = \frac{D\tau_A}{Dt} - R(t)\tau_A - \tau_A R(t)^{\mathrm{T}}, \tag{5.1}$$

where

$$R(t) = \frac{a+1}{2}\nabla\mathbf{u}(t) + \frac{a-1}{2}\nabla\mathbf{u}(t)^{\mathrm{T}}. \tag{5.2}$$

In this case, the tensor τ_A will be of the following form:

$$\tau_A = \tau + \frac{\mu_{\mathrm{p}}}{aWe}I. \tag{5.3}$$

For models with the upper convected derivative, the conformation tensor τ_A is given with $a = 1$ and with $a = -1$ in case the lower convected derivative is used.

The objective rate (5.1) is often called the Gordon–Schowalter derivative [14]. This can be written as a Lie derivative (4.2) with the transition matrix $E(s,t)$ satisfying the following ordinary differential equation:

$$\frac{DE(s,t)}{Dt} = R(t)E(s,t), \quad E(s,s) = I. \tag{5.4}$$

The tensor $E(s,t)$ obeying (5.4) has been first introduced by Johnson and Segalman [25] as a deformation tensor for viscoelastic fluids having non-affine histories.

In this section, first we shall study some interesting properties of the following Riccati equation:

$$\frac{\delta_E\tau_A}{\delta_E t} = -\alpha\tau_A + \beta I, \tag{5.5}$$

where α, β may depend on τ_A. Second, we shall illustrate how various rate-type models including multi-mode FENE-PM model can be cast into the aforementioned special Riccati equation (5.5) (see Table 1).

In the end of this section, we shall extend this idea to some general single variable models with the property of the positive definiteness and present their reformulations into another type of Riccati equations.

Let us begin with an explicit solution of the Riccati equation (5.5).

Lemma 5.1. *The solution to* (5.5) *satisfies*

$$\tau_A(t) = \exp\left(-\int_s^t \alpha(\varsigma)\,\mathrm{d}\varsigma\right)E(s,t)\tau_A(t,s)E(s,t)^{\mathrm{T}} + \int_s^t \exp\left(-\int_v^t \alpha(\varsigma)\,\mathrm{d}\varsigma\right)\beta(v)E(v,t)E(v,t)^{\mathrm{T}}\,\mathrm{d}v. \tag{5.6}$$

Proof. By an argument similar to what was used in the proposition (4.1), we can solve the Eq. (5.5) to obtain

$$\tau_A(x,t) = \Phi(s,t)\tau_A(t,s)\Phi(s,t)^{\mathrm{T}} + \int_s^t \beta(v)\Phi(v,t)\Phi(v,t)^{\mathrm{T}}\mathrm{d}v, \tag{5.7}$$

where

$$\frac{D\Phi(s,t)}{Dt} = \left(\frac{a+1}{2}\nabla\mathbf{u}(t) + \frac{a-1}{2}\nabla\mathbf{u}(t)^{\mathrm{T}} - \frac{\alpha(t)}{2}I\right)\Phi(s,t), \quad \Phi(s,s) = I.$$

Now we shall show that $\Phi(s,t)$ can be expressed by the following form:

$$\Phi(s,t) = \exp\left(-\int_s^t \frac{\alpha(v)}{2}\,\mathrm{d}v\right)E(s,t). \tag{5.8}$$

To see this, note that $\Phi_1(s,t) = E(s,t)$ is the solution to the following ordinary differential equation:

$$\frac{D\Phi_1(s,t)}{Dt} = \left(\frac{a+1}{2}\nabla\mathbf{u}(t) + \frac{a-1}{2}\nabla\mathbf{u}(t)^{\mathrm{T}}\right)\Phi_1(s,t)$$

and the solution to the equation

$$\frac{D\Phi_2(s,t)}{Dt} = -\frac{\alpha(t)}{2}\Phi_2(s,t)$$

is given by

$$\Phi_2(s,t) = \exp\left(-\int_s^t \frac{\alpha(v)}{2}\,\mathrm{d}v\right)I. \tag{5.9}$$

A simple observation that $\Phi(s,t) = \Phi_1(s,t)\Phi_2(s,t)$ completes the proof. □

We shall now derive α and β corresponding to some interesting models such as the Oldroyd-B, the Johnson–Segamal, the Phan-Thien and Tanner, and the FENE-PM, respectively. Let us first summarize the result in the following table.

Here u and g are scalar functions given as (5.12) and (5.13) below, respectively. Some interesting results that can be deduced from the result (5.6) of Lemma 5.1 and Table 1 are in order. First, if $\alpha \geqslant c$ for some positive constant c, under the assumption that the transition matrix $E(s,t)$ is bounded for $s \leqslant t$, we obtain formally the following integral models by taking $s \to -\infty$:

$$\tau_A(t) = \int_{-\infty}^t \exp\left(-\int_v^t \frac{\alpha(v)}{2}\,\mathrm{d}v\right)\beta(v)E(v,t)E(v,t)^{\mathrm{T}}\,\mathrm{d}v. \tag{5.10}$$

Especially, this includes the Johnson–Segalman integral model, which does not seem to be known before (see [22, p. 15]). Second, the expression for $\Phi(s,t)$ in (5.8) is quite useful in the computational viewpoint. Namely, combining an approximation for $E(s,t)$ that is ubiquitous in viscoelastic models with an approximation of (5.9), we can handle various non-linear models without much extra efforts.

Now, we shall illustrate the procedure of reformulations by taking several interesting models. Some of constitutive equations that are interesting to us are originally given as follows:

$$u\tau + We\frac{\delta_E\tau}{\delta_E t} = 2\mu_{\mathrm{p}}\mathscr{D}. \tag{5.11}$$

Here the function u is defined through

$$u = \exp\left(\frac{\varepsilon We}{\mu_{\mathrm{p}}}tr(\tau)\right), \tag{5.12}$$

where ε is a parameter. This corresponds to so-called the Phan-Thien and Tanner model, [41]. If $\varepsilon = 0$ or $u = 1$, then the Jonson–Segalman model, [25] results and if further $E = F$ and $a = 1$, the Oldroyd-B model (3.4) results.

Note that the Eq. (5.11) relates the stress and the rate of strain. The reformulation shall hide this relation. Observing the relation (5.3) and simple change of variables, we obtain the following equations for τ_A:

$$We\frac{\delta_E\tau_A}{\delta_E t} = -u\tau_A + \frac{\mu_{\mathrm{p}}}{aWe}uI.$$

We then obtain the expressions listed in Table 1 except for the FENE-PM model.

Table 1
The coefficient functions α and β of some typical viscoelastic models written in the form of (5.5)

Model	$\alpha(t)$	$\beta(t)$
Oldroyd-B ($a = 1$)	$1/We$	μ_{p}/We^2
Johnson–Segalman	$1/We$	μ_{p}/aWe^2
Phan-Thien and Tanner	u/We	μ_{p}/aWe^2
FENE-PM	$\frac{g}{We_j} - \frac{D\ln g}{Dt}$	$\frac{\mu_{\mathrm{p}}}{We_j^2}g$

Let us now consider the multi-mode FENE-PM model [42]. This model is also formulated in a way that it relates the stress and the rate of strain, however, similarly to what was done before, by introducing the conformation tensor in each mode and non-dimensionalizing appropriately, we can obtain the following equations:

$$\tau = \sum_{j=1}^{N-1} \tau_j,$$
$$\frac{\mu_p}{We_j} g = \left(g - We_j \frac{D \ln g}{Dt} \right) \tau_{A,j} + We_j \frac{\delta_F \tau_{A,j}}{\delta_F t},$$

where

$$g = 1 + (3/b) \left\{ 1 + \frac{We_j}{\mu_p} \left(\frac{\mathrm{tr}(\tau)}{3(N-1)} \right) \right\}, \tag{5.13}$$

and b is the so-called FENE parameter, We_j is a positive constant and $\tau_{A,j} = \tau_j + (\mu_p / We_j)I$. Hence, in this case, α and β are given as follows:

$$\alpha = \frac{D \ln g}{Dt} - \frac{g}{We_j} \quad \text{and} \quad \beta = \frac{\mu_p}{We_j^2} g.$$

The general single variable models introduced in Hulsen [19] and Beris and Edward [3] can be given in terms of the conformation tensor τ_A as follows:

$$\frac{D\tau_A(t)}{Dt} = A(t)\tau_A(t) + \tau_A(t)A(t) + g_1(t)I + g_2(t)\tau_A + g_3(t)\tau_A^2, \tag{5.14}$$

where g_i, $(i = 1, 2, 3)$ may be functions of τ_A. As mentioned before, Hulsen [19] provided a sufficient condition that $g_1(\tau_A) > 0$ for which the conformation tensor τ_A for models of the form (5.14) remains positive definite. His arguments were based on the investigation of the rate of change of the determinant of τ_A along the trajectory, from which he showed that an initially positive tensor τ_A cannot attain non-negative eigenvalues under the assumption that $g_1(\tau_A) > 0$. Our new framework cast (5.14) into the general Riccati equation

$$\frac{D\tau_A(t)}{Dt} = \tilde{A}(t)\tau_A(t) + \tau_A(t)\tilde{A}(t)^{\mathrm{T}} - \tau_A(t)B(t)\tau_A(t) + U(t),$$

where

$$\tilde{A}(t) = A(t) + \frac{g_2(\tau_A)}{2} I, \quad B(t) = -g_3(\tau_A)I \quad \text{and} \quad U(t) = g_1(\tau_A)I.$$

or

$$\frac{\delta_\Phi \tau_A(t)}{\delta_\Phi t} = -\tau_A(t)B(t)\tau_A(t) + U(t),$$

where

$$\frac{D\Phi(s,t)}{Dt} = \tilde{A}(t)\Phi(s,t), \quad \Phi(s,s) = I.$$

Under the assumption that τ_A is symmetric positive semi-definite initially, the simple application of the proposition (4.1) immediately implies that the conformation tensor τ_A evolves in time with the property of the positivity if $g_1(\tau_A) > 0$. Hence, our general framework recovers his observation in a very transparent manner.

6. A semi-Lagrangian finite element method that preserves positivity

In this section, we shall propose numerical approximations to the following systems of viscoelastic flow equations that preserve the positivity of the conformation tensor τ_A in both time and space discrete senses regardless of the time step size and the mesh size:

$$Re\frac{D\mathbf{u}}{Dt} = -\nabla p + \operatorname{div}\tau_A + \eta_s \operatorname{div}\mathscr{D}(\mathbf{u}), \tag{6.1}$$

$$\mathbf{div}\,\mathbf{u} = 0, \tag{6.2}$$

and

$$\frac{\delta_E \tau_A}{\delta_E t} = -\alpha\tau_A + \beta I. \tag{6.3}$$

Here α and β are positive and may depend on τ_A. For simplicity, we shall assume that the velocity has no-slip boundary condition, namely $\mathbf{u} = 0$ on $\partial\Omega$.

Throughout this section, let us denote the current time $t = t^{n+1}$, the previous time t^n, the time step size $t^{n+1} - t^n = k$, $\mathbf{u}_h^{n+1} = \mathbf{u}_h(X, t^{n+1}), p_h^{n+1} = p_h(X, t^{n+1}), \tau_{A,h}^{n+1} = \tau_{A,h}(X, t^{n+1})$ and $y^n = y(X, t^{n+1}, t^n)$.

As discussed in the previous section, (6.3) represents a large class of constitutive equations. Recasting these constitutive equations in such a special form plays a crucial role in obtaining positivity preserving schemes. If a discretization is performed in their original formulations such as (3.4) and (5.11) or in the reformulation based on the identity (2.7) used in some literatures including [2,40] rather than (2.6) used in this paper, the positivity is difficult to be preserved.

Let us illustrate this using the Oldroyd-B model (3.4). Using the identity (2.7), an application of the implicit Euler method on the Lagrangian frame leads to the following discrete system:

$$\begin{aligned}\tau_A^{n+1} = {} & \frac{\mu_p(2We + k)}{We(We + k)}I + \frac{We}{We + k}F(t^n, t^{n+1})\tau_A(t^{n+1}, t^n)F^{\mathrm{T}}(t^n, t^{n+1}) \\ & - \frac{\mu_p}{We + k}\left(F(t^n, t^{n+1})F^{\mathrm{T}}(t^n, t^{n+1}) + F^{\mathrm{T}}(t^{n+1}, t^n)F(t^{n+1}, t^n)\right).\end{aligned}$$

It is immediate to see that the positivity of tensor τ_A^{n+1} may not be preserved unless k is sufficiently small and, even for sufficiently small k, the positivity property may still not be preserved after sufficiently many time steps.

In the rest of this section, we shall introduce the full numerical approximations that preserve the positivity of tensor τ_A based on the so-called Lagrange–Galerkin method. Before considering temporal discretization, let us first consider discretizations on spatial variables.

6.1. Spatial discretization

In this section, we shall take a spatial discretization based on the finite element method and introduce a property that the approximation space for the stress are required to possess in achieving the positivity. We assume that the domain $\Omega \subset \mathbb{R}^d$ has been partitioned into elements $\mathfrak{I}_h = \{K\}$ and that the partitions $\mathfrak{I}_h$ satisfies

$$\bar{\Omega} = \bigcup_{K\in\mathfrak{I}_h} \bar{K}.$$

Based on this partitions $\mathfrak{I}_h$, we shall choose appropriate approximation spaces $\mathbf{V}_h$, W_h and $\mathbf{S}_h$ for the primitive variables, $\mathbf{u}$, p and τ_A at any instant time t, respectively. Let us denote $\Pi_h^{\mathbf{V}}, \Pi_h^W$ and $\Pi_h^{\mathbf{S}}$ by the standard interpolation operators determined by $\mathbf{V}_h$, W_h and $\mathbf{S}_h$, respectively. We shall also use the standard notation that $(\cdot,\cdot)$ denotes the usual $L^2(\Omega)$ inner product between vector-valued or scalar-valued functions and $(\cdot:\cdot)$ acting on two matrix-valued functions A and B denotes

$$(A : B) = \int_\Omega \sum_{ij} A_{ij}B_{ij}\,\mathrm{d}x = \int_\Omega \mathrm{tr}(AB)\,\mathrm{d}x. \tag{6.4}$$

The semi-discrete weak formulation of the system of equations (6.1)–(6.3) based on the aforementioned finite elements shall then be formulated as follows: Find $(\mathbf{u}_h(\cdot,t), p_h(\cdot,t), \tau_{A,h}(\cdot,t)) \in \mathbf{V}_h \times W_h \times \mathbf{S}_h$ such that $\forall(\mathbf{v}_h, q_h, \sigma_h) \in \mathbf{V}_h \times W_h \times \mathbf{S}_h$

$$\begin{aligned} &Re\left(\frac{D\mathbf{u}_h}{Dt}, \mathbf{v}_h\right) + (p_h, \mathbf{div}\,\mathbf{v}_h) + \eta_s(\mathscr{D}(\mathbf{u}_h), \mathscr{D}(\mathbf{v}_h)) = (\tau_{A,h} : \mathscr{D}(\mathbf{v}_h)),\\ &(\mathbf{div}\,\mathbf{u}_h, q_h) = 0,\\ &\left(\frac{\delta_E\tau_{A,h}}{\delta_E t}, \sigma_h\right) = -(\alpha\tau_{A,h}, \sigma_h) + (\beta I, \sigma_h). \end{aligned} \tag{6.5}$$

Let $\mathbf{V}_h^*$, W_h^* and $\mathbf{S}_h^*$ denote the dual spaces for $\mathbf{V}_h$, W_h and $\mathbf{S}_h$, respectively. For ease of our presentations, we shall define the following operators $A_h : \mathbf{V}_h \mapsto \mathbf{V}_h^*$, $\nabla_h : W_h \mapsto \mathbf{V}_h^*$ and $\mathrm{div}_h : \mathbf{S}_h \mapsto \mathbf{V}_h^*$ by

$$\begin{aligned} &\langle A_h\mathbf{u}_h, \mathbf{v}_h\rangle = (\mathscr{D}(\mathbf{u}_h) : \mathscr{D}(\mathbf{v}_h)), \forall \mathbf{v}_h \in \mathbf{V}_h,\\ &\langle \nabla_h p_h, \mathbf{v}_h\rangle = -(p_h, \mathbf{div}\,\mathbf{v}_h), \forall \mathbf{v}_h \in \mathbf{V}_h,\\ &\langle \mathrm{div}_h\tau_{A,h}, \mathbf{v}_h\rangle = -(\tau_{A,h} : \mathscr{D}(\mathbf{v}_h)), \forall \mathbf{v}_h \in \mathbf{V}_h, \end{aligned}$$

where the bracket $\langle\cdot,\cdot\rangle$ denotes the duality pairing.

The weak formulation (6.5) can then be written as follows:

$$Re\frac{D\mathbf{u}_h}{Dt} + \nabla_h p_h + \eta_s A_h\mathbf{u}_h = \mathrm{div}_h\tau_{A,h} \text{ in } \mathbf{V}_h^*, \tag{6.6}$$

$$\mathbf{div}\,\mathbf{u}_h = 0 \text{ in } W_h^*, \tag{6.7}$$

$$\frac{\delta_E\tau_{A,h}}{\delta_E t} = -\alpha\tau_{A,h} + \beta I \text{ in } \mathbf{S}_h^*. \tag{6.8}$$

The actual choice of finite element spaces $\mathbf{V}_h$, W_h and $\mathbf{S}_h$ depends on many considerations including the stability and approximation property. For example, $\mathbf{V}_h$ and W_h can be chosen among the stable pairs (which satisfy certain inf–sup conditions) for the Navier–Stokes equations (see [6] or [13]). The choice of $\mathbf{S}_h$ requires special caution as it is the crucial space that leads to positivity preserving schemes.

6.2. The choice of $\mathbf{S}_h$ and positivity preserving interpolant

In this subsection, we shall address details about the choice of the approximation space $\mathbf{S}_h$. To keep the positivity of τ_A, there should exist a linear operator $\Pi_h^{\mathbf{S}}$ whose range is $\mathbf{S}_h$ and that preserves the positivity in the following sense:

$$\sigma > 0 \Rightarrow \Pi_h^{\mathbf{S}}(\sigma) > 0. \tag{6.9}$$

Here σ is any $d \times d$ symmetric tensor and $\sigma > 0$ means that the tensor σ is symmetric and positive definite. See e.g. (6.17), (6.21) and remarks that follow.

Such an operator can be in particular generated by the following linear and positive operator Π_h defined on scalar functions

$$u > 0 \Rightarrow \Pi_h(u) > 0, \tag{6.10}$$

where u is any scalar function.

Note that the inequality ">" is meant to be ">" almost everywhere since functions may not be defined pointwise. To see Π_h^{S} can be constructed by Π_h, take any $\sigma = (\sigma_{ij})_{i,j=1,\ldots,d}$, $d \times d$ symmetric tensor and consider any nonzero vector $\xi = (\xi_i)_{i=1,\ldots,d}$ and observe that

$$0 < \xi^{\mathrm{T}}\sigma\xi = \sum_{i,j=1}^{d} \xi_i \sigma_{ij} \xi_j \Rightarrow 0 < \Pi_h(\xi^{\mathrm{T}}\sigma\xi) \quad \text{by (6.10).}$$

Now, by the linearity of Π_h, we see that

$$\Pi_h(\xi^{\mathrm{T}}\sigma\xi) = \sum_{i,j=1}^{d} \xi_i \Pi_h(\sigma_{ij}) \xi_j \in S(\Omega;h).$$

Hence Π_h^{S} is defined through

$$\Pi_h^{\mathrm{S}}(\sigma) = (\Pi_h(\sigma_{ij}))_{ij=1,\ldots,d} \in S^{d\times d}(\Omega;h).$$

Here, $S(\Omega;h)$ is some finite element space for the scalar functions.

The most natural candidate for $S(\Omega;h)$ is the space of Lagrange finite elements of total polynomial degree $\leqslant k$ with $k \geqslant 0$. For $k = 0$, we have a finite element space of piecewise constant. In this case, the existence of the positivity preserving Π_h is obvious. For example, we can take, on each element K,

$$\Pi_h(u)(x) = \frac{1}{|K|} \int_K u \,\mathrm{d}x \quad \forall x \in K. \tag{6.11}$$

Of course, this choice of $S(\Omega;h)$ only leads to the first-order approximation for the conformation tensor.

For $k = 1$, there are two possibilities. The first one is to choose globally continuous piecewise linear finite element function. In this case, the standard pointwise nodal value interpolant certainly would be positivity preserving. In case u is rough, point values of u are not well-defined, we may define the nodal value of $\Pi_h(u)(x_i)$ as the local mean-value as follows:

$$\Pi_h(u)(x_i) := \frac{1}{|B_i|} \int_{B_i} u \,\mathrm{d}x, \tag{6.12}$$

where $B_i = B(x_i, r_i(x_i))$, the ball centered at x_i with radius $r_i(x_i)$ with $r_i(x_i)$ chosen small enough so that B_i is contained in the union of closed elements containing x_i. The above construction (6.12) was proposed recently by Nochetto and Wahlbin [31] and it is easy to see that such an operator Π_h preserves linear functions and has a second-order accuracy.

Another possibility for $k = 1$ is the discontinuous piecewise linear finite element space. In this case, the construction of positivity preserving operator Π_h for the above continuous piecewise linear element case can obviously be applied here.

For $k \geqslant 2$, however, it is known that it is impossible to construct a positivity preserving interpolant that has more than second-order accuracy. For details, we refer to [31].

In summary, we can choose $\mathbf{S}_h$ as either piecewise constant or piecewise linear finite element spaces. The approximation accuracy for such choices is either first-order or second-order. It is in general not possible to construct a positivity preserving scheme for the conformation tensor whose approximation accuracy is more than second-order.

6.3. Time discretizations

In this section, we shall discretize the Eqs. (6.6) and (6.8) in time. We shall use the particle following approach in order to exploit the connection between the Riccati equation and the constitutive Eq. (6.3). In doing so, the semi-Lagrangian methodology will be taken, (see [34,38,35]) rather than the Lagrangian method since in the Lagrangian framework, the mesh moves with the particle and in case of large deformation, the mesh can be severely distorted and re-meshing is inevitable introducing additional numerical errors (see e.g. [2] or [34] and the references cited therein). To implement the semi-Lagrangian method, given any material particle, X at the current time t^{n+1}, the particle path should be determined by

$$\frac{\mathrm{d}y(X,t^{n+1},s)}{\mathrm{d}s} = \mathbf{u}(y(X,t^{n+1},s),s), \quad y(X,t^{n+1},t^{n+1}) = X. \tag{6.13}$$

The Lie derivative $\frac{\delta_L \xi}{\delta_L t}$ at time t^{n+1} can then be approximated on the time interval $[t^n, t^{n+1}]$, for example, by the following first-order time discretization:

$$\frac{\delta_L \xi}{\delta_L t}(t^{n+1}) \approx \frac{\xi(t^{n+1}) - L(t^n,t^{n+1})\xi(t^{n+1},t^n)L(t^n,t^{n+1})}{k}, \tag{6.14}$$

where ξ is either a vector or a tensor and correspondingly L is either I or E and $\xi(t^{n+1},t^n) = \xi(t^n) \circ y^n$.

Throughout this section, we shall assume that $\mathbf{S}_h$ has been chosen so that it is the range of Π_h^{S}, which satisfies the property (6.9).

The main goal of this section is to develop the positivity preserving time discretization of (6.8). The following two approaches will be taken. The first approach is to discretize the material derivative. It will be first-order time accurate. The second approach is to use the analytic solution (5.6) introduced in Section 5. Most of our presentations here is based on the work by Dieci and Eirola [10].

Let us begin by recalling that

$$\frac{\delta_E \tau_A}{\delta_E t} = \frac{D\tau_A}{Dt} - R(t)\tau_A - \tau_A R(t)^{\mathrm{T}}. \tag{6.15}$$

Regarding the time derivative as the material derivative, taking an implicit Euler scheme to (6.8), we obtain

$$\alpha^{n+1}\tau_{A,h}^{n+1} + \left(\frac{\tau_{A,h}^{n+1} - \Pi_h^{\mathrm{S}}(\tau_{A,h}^n \circ y^n)}{k} - \Pi_h^{\mathrm{S}}(R_h^{n+1}\tau_{A,h}^{n+1}) - \Pi_h^{\mathrm{S}}(\tau_{A,h}^{n+1}(R_h^{n+1})^{\mathrm{T}})\right) = \beta^{n+1}I. \tag{6.16}$$

An interesting fact is that this equation can be recast into the well-known algebraic Riccati differential equation as follows:

$$\left(\frac{\alpha^{n+1}k+1}{2k} - R_h^{n+1}\right)\tau_{A,h}^{n+1} + \tau_{A,h}^{n+1}\left(\frac{\alpha^{n+1}k+1}{2k} - R_h^{n+1}\right)^{\mathrm{T}} = \frac{\tau_{A,h}^n \circ y^n}{k} + \beta^{n+1}I. \tag{6.17}$$

Note that the equivalence between two Eqs. (6.16) and (6.17) should be asserted with taking Π_h^{S} for both sides of Eq. (6.17). We simply did not write it to clarify (6.17) is an algebraic Riccati equation. We also note that it is necessary to consider the range of Π_h^{S} with the property (6.9) as the approximation space τ_A to make sure $\tau_{A,h}^n \circ y^n > 0$ and under this condition, it can be also shown that the Eq. (6.17) has a unique positive definite solution $\tau_{A,h}^{n+1}$ (see e.g. [10] or [26]).

The numerical schemes based on the analytic solution (5.6) to (6.8) require approximations of (5.9), $E(s,t)$ and the integral expression in (5.6). Approximations of the first two quantities can be made in any ways since these do not affect the positivity property. However the integral expression in (5.6) should be approximated, for example by using numerical quadrature with positive weights in order to keep the positivity.

We shall introduce three different approximations for each of them. For every cases, the first scheme is a first-order implicit scheme, the second scheme is a second-order single step implicit scheme and the third scheme is a second-order two step explicit scheme.

- Approximations of $\exp(-\int_s^t \alpha(v)\,\mathrm{d}v)$:

$$\alpha_{t^n,t^{n+1}} := 1 - \alpha^{n+1}k,$$
$$\widetilde{\alpha}_{t^n,t^{n+1}} := \exp\left(-\frac{k}{2}[\alpha(t^n) + \alpha(t^{n+1})]\right),$$
$$\widehat{\alpha}_{t^{n-1},t^{n+1}} := \exp(-k\alpha(t^n)).$$

- Approximations of $E(s,t)$:

$$E_h(t^n,t^{n+1}) := I + kR_h(t^n)\circ y^n \quad \text{or} \quad (I - kR_h(t^{n+1}))^{-1},$$
$$\widetilde{E_h}(t^n,t^{n+1}) := \left(I - \frac{k}{2}\left(R_h^{n+1} + R_h^n \circ y^n\right)\right)^{-1}\left(I + \frac{k}{2}\left(R_h^{n+1} + R_h^n\circ y^n\right)\right),$$
$$\widehat{E_h}(t^{n-1},t^{n+1}) := \left(I - kR_h^n\circ y^n\right)^{-1}(I + kR_h^n\circ y^n),$$

where

$$R_h(t) = \frac{a+1}{2}\nabla_h \mathbf{u}_h(t) + \frac{a-1}{2}\nabla_h\mathbf{u}_h(t)^{\mathrm{T}}. \tag{6.18}$$

- Approximations of $\int_s^t \beta(t)\Phi(v,t)\Phi(v,t)^{\mathrm{T}}\,\mathrm{d}v$:

$$I_{t^n,t^{n+1}} := k\beta^{n+1},$$
$$\widetilde{I}_{t^n,t^{n+1}} := \frac{k}{2}\left(\beta^n\widetilde{\Phi_h}(t^n,t^{n+1})\widetilde{\Phi_h}(t^n,t^{n+1})^{\mathrm{T}} + \beta^{n+1}\right),$$
$$\widehat{I}_{t^{n-1},t^{n+1}} := k\beta^n\left(\frac{I + \widehat{\Phi_h}(t^{n-1},t^{n+1})}{2}\right)\left(\frac{I + \widehat{\Phi_h}(t^{n-1},t^{n+1})}{2}\right)^{\mathrm{T}},$$

where

$$\widetilde{\Phi_h}(t^n,t^{n+1}) := \widetilde{\alpha}_{t^n,t^{n+1}}\widetilde{E_h}(t^n,t^{n+1}),$$
$$\widehat{\Phi_h}(t^{n-1},t^{n+1}) := \widehat{\alpha}_{t^{n-1},t^{n+1}}\widehat{E_h}(t^{n-1},t^{n+1}).$$

Based on the aforementioned various approximations, we can devise three different approximations for (6.8).

First, based on the first-order approximations $\alpha_{t^n,t^{n+1}}$ and $I_{t^n,t^{n+1}}$, we have

$$\frac{\tau_{A,h}^{n+1} - \Pi_h^{\mathrm{S}}\left(E_h(t^n,t^{n+1})(\tau_{A,h}^n\circ y^n)E_h(t^n,t^{n+1})^{\mathrm{T}}\right)}{k} = -\alpha^{n+1}\tau_{A,h}^{n+1} + \beta^{n+1}I. \tag{6.19}$$

It is interesting to note that (6.19) can also be obtained by a direct application of implicit Euler method to (6.3) based on the time discretization (6.14).

The numerical approximation based on the implicit second-order single step scheme, namely $\widetilde{I}_{t^n,t^{n+1}}$ can be given as follows:

$$\tau_{A,h}^{n+1} = \Pi_h^{\mathrm{S}}\left(\widetilde{\Phi_h}(t^n,t^{n+1})\left(\tau_{A,h}^n\circ y^n + \frac{k}{2}\beta^n\right)\widetilde{\Phi_h}(t^n,t^{n+1})^{\mathrm{T}}\right) + \frac{k}{2}\beta^{n+1}. \tag{6.20}$$

Finally, two step explicit scheme $\widehat{I}_{t^{n-1},t^{n+1}}$ produces the following formula:

$$\tau_{A,h}^{n+1} = \Pi_h^{\mathrm{S}}\left(\widehat{\Phi_h}(t^{n-1},t^{n+1})\left(\tau_{A,h}^{n-1}\circ y^{n-1}\right)\widehat{\Phi_h}(t^{n-1},t^{n+1})^{\mathrm{T}}\right)$$
$$+\frac{k}{4}\Pi_h^{\mathrm{S}}\left(\beta^n\left(I + \widehat{\Phi_h}(t^{n-1},t^{n+1})\right)\left(I + \widehat{\Phi_h}(t^{n-1},t^{n+1})\right)^{\mathrm{T}}\right). \tag{6.21}$$

Recall that the time discrete Eq. (6.8) is positivity preserving under the assumption that $\tau^n_{A,h} \circ y^n$ is positive definite and this holds for any spaces $\mathbf{S}_h$ which is the range of $\Pi^{\mathbf{S}}_h$ with the property (6.9).

6.4. Full space and time discretizations

In this section, we shall complete our numerical approximations combining discretizations of the momentum Eq. (6.6) with the aforementioned discretizations of the constitutive equations (6.8).

Taking first-order approximation implicit Euler for (6.6) together with (6.19) for the constitutive equation, we obtain:

First-order scheme

$$Re\frac{\mathbf{u}^{n+1}_h - \Pi^{\mathbf{V}}_h(\mathbf{u}^n_h \circ y^n)}{k} + \nabla_h p^{n+1}_h + \eta_s A_h \mathbf{u}^{n+1}_h = \mathrm{div}_h \tau^{n+1}_{A,h}, \tag{6.22}$$

$$\mathbf{div}\,\mathbf{u}^{n+1}_h = 0, \tag{6.23}$$

$$\frac{\tau^{n+1}_{A,h} - \Pi^{\mathbf{S}}_h\Big(E_h(t^n,t^{n+1})(\tau_{A,h}(t^n)\circ y^n)E_h(t^n,t^{n+1})^{\mathrm{T}}\Big)}{k} = -\alpha^{n+1}\tau^{n+1}_{A,h} + \beta^{n+1} I. \tag{6.24}$$

The Crank–Nicolson scheme for (6.6) combined with the implicit second-order scheme (6.20) for (6.8) results in

Second-order single step scheme

$$\begin{aligned} &Re\frac{\mathbf{u}^{n+1}_h - \Pi^{\mathbf{V}}_h(\mathbf{u}^n_h \circ y^n)}{k} + \frac{1}{2}\left(\nabla_h p^{n+1}_h + \nabla_h \Pi^W_h(p^n_h \circ y^n)\right) + \frac{\eta_s}{2}\left(A_h\mathbf{u}^{n+1}_h + A_h\Pi^{\mathbf{V}}_h(\mathbf{u}^n_h\circ y^n)\right)\\ &\quad = \frac{1}{2}\left(\mathrm{div}_h\tau^{n+1}_{A,h} + \mathrm{div}_h\Pi^{\mathbf{S}}_h\left(\tau^n_{A,h}\circ y^n\right)\right),\\ &\mathbf{div}\,\mathbf{u}^{n+1}_h = 0,\\ &\tau^{n+1}_{A,h} = \Pi^{\mathbf{S}}_h\left(\widetilde{\Phi_h}(t^n,t^{n+1})\left(\tau^n_{A,h}\circ y^n + \frac{k}{2}\beta^n\right)\widetilde{\Phi_h}(t^n,t^{n+1})^{\mathrm{T}}\right) + \frac{k}{2}\beta^{n+1}. \end{aligned} \tag{6.25}$$

Finally, the combination of the stiffly stable second-order BDF, [43] for (6.6) and second-order explicit two step scheme (6.21) for (6.8) produces another second-order schemes as follows:

Second-order two step scheme

$$\begin{aligned} &Re\frac{\frac{3}{2}\mathbf{u}^{n+1}_h - \Pi^{\mathbf{V}}_h\left(2\mathbf{u}^n_h\circ y^n + \frac{1}{2}\mathbf{u}^{n-1}_h\circ y^{n-1}\right)}{k} - \nabla_h p^{n+1}_h + \eta_s A_h\mathbf{u}^{n+1}_h = \mathrm{div}_h\tau^{n+1}_{A,h},\\ &\mathbf{div}\,\mathbf{u}^{n+1}_h = 0,\\ &\tau^{n+1}_{A,h} = \Pi^{\mathbf{S}}_h\left(\widehat{\Phi_h}(t^{n-1},t^{n+1})\left(\tau^{n-1}_{A,h}\circ y^{n-1}\right)\widehat{\Phi_h}(t^{n-1},t^{n+1})^{\mathrm{T}}\right)\\ &\qquad + \frac{k}{4}\Pi^{\mathbf{S}}_h\left(\beta^n\left(I+\widehat{\Phi_h}(t^{n-1},t^{n+1})\right)\left(I+\widehat{\Phi_h}(t^{n-1},t^{n+1})\right)^{\mathrm{T}}\right). \end{aligned} \tag{6.26}$$

We note that the stiffly stable scheme (6.26) is preferred especially for the long time computations for the Crank–Nicolson scheme (6.25) since it is known that the presence of the explicit part of the pressure in such a formulation may incur some numerical instability (see e.g. [43]). We would like to remark that for such a two step scheme, at least two previous step solutions should be available to proceed to the current step solution and so it may not be applied to obtain the first step solution. However, to get the first step solution, a single step second-order scheme can be used instead. This allows us to keep the overall temporal accuracy.

7. Stability analysis: continuous and discrete energy estimates

The purpose of this section is to show the importance of keeping the positivity in the discrete sense. We shall first derive the energy estimates of the general form of viscoelastic models (6.1)–(6.3) in the continuous level. We then take a specific algorithm (6.22)–(6.24) presented in Section 6 to show the discrete analogue of energy estimate. Namely, we shall show several a priori estimate of the numerical solutions. By this, we confirm both the stability and the robustness of the algorithm. Our analysis crucially relies on the positivity of the conformation tensor and energy estimate holds no matter how large the Weissenberg number is. The analysis indeed includes the limiting case when $We = \infty$.

For any positive definite tensor σ, the $L^1(\Omega)$ norm for σ shall be defined as follows:

$$\|\sigma\|_{L^1} := \int_\Omega \mathrm{tr}(\sigma)\,\mathrm{d}x. \tag{7.1}$$

In the following discussion, we shall further adopt the standard notation for Sobolev spaces $H_0^k(\Omega), H^k(\Omega)$ with norms denoted by $\|\cdot\|_k$.
As usual, $\|\cdot\|_0$ shall denote the L^2 norm.

7.1. Continuous energy estimates

In this section, we shall derive the energy law of models (6.1)–(6.3) and then we further show the energy estimates in the continuous level. In doing so, we shall make the following assumptions:

A_1: $\alpha(t) \in L^\infty(\Omega)$ with $\alpha \geqslant c > 0$ for all $t \geqslant 0$, for some constant c.
A_2: $\beta(t) \in L^1(\Omega)$ with $\beta \geqslant 0$ for all $t \geqslant 0$.
A_3: $\tau_A(x,0)$ is semi-positive definite.

The assumption $A1$ is related to damping. This holds for all the models in Table 1 except for the FENE-PM model for which the definiteness of α seems to be difficult to determine. $A2$ and $A3$ are necessary for the positivity of the conformation tensor in time evolutions and especially $A2$ is also for the boundedness of the energy.

Let us first state an energy law.

Lemma 7.1. *Under the assumptions A_2 and A_3, we have the following energy law for the models*, (6.1)–(6.3):

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(Re\|\mathbf{u}(\cdot,t)\|_0^2 + \frac{1}{2a}\|\tau_A(\cdot,t)\|_{L^1}\right) = -\eta_s\|\mathscr{D}(\mathbf{u}(\cdot,t))\|_0^2 - \frac{1}{2a}\int_\Omega \mathrm{tr}(\alpha\tau_A(\cdot,t))\,\mathrm{d}x + \frac{d}{2a}\int_\Omega \beta(\cdot,t)\,\mathrm{d}x. \tag{7.2}$$

Proof. We first take the trace on the Eq. (6.3) and then take the integration. Using the fact that $\mathbf{div}\,\mathbf{u} = 0$, we can obtain:

$$\int_\Omega \mathrm{tr}(\alpha\tau_A(\cdot,t))\,\mathrm{d}x + \frac{\mathrm{d}}{\mathrm{d}t}\|\tau_A(\cdot,t)\|_{L^1} - \int_\Omega \mathrm{tr}(R(t)\tau_A(\cdot,t))\,\mathrm{d}x - \int_\Omega \mathrm{tr}\left(\tau_A(\cdot,t)R(t)^\mathrm{T}\right)\mathrm{d}x = d\int_\Omega \beta(\cdot,t)\,\mathrm{d}x. \tag{7.3}$$

We notice the following simple but important relation:

$$(\tau_A(\cdot,t) : \mathscr{D}(\mathbf{u}(\cdot,t))) = \frac{1}{2a}\int_\Omega \mathrm{tr}(R(t)\tau_A)\,\mathrm{d}x = \frac{1}{2a}\int_\Omega \mathrm{tr}(\tau_A R(t)^\mathrm{T})\,\mathrm{d}x. \tag{7.4}$$

Let us now consider the momentum equation. Multiplying $\mathbf{u}$ to (6.1) and taking the integration, we obtain that

$$Re\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbf{u}(\cdot,t)\|_0^2+\eta_s\|\mathscr{D}(\mathbf{u}(\cdot,t))\|_0^2\mathrm{d}x=-(\tau_A(\cdot,t):\ \mathscr{D}(\mathbf{u}(\cdot,t))). \tag{7.5}$$

From (7.3) and (7.4), we obtain

$$Re\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbf{u}(\cdot,t)\|_0^2+\frac{1}{2a}\frac{\mathrm{d}}{\mathrm{d}t}\|\tau_A(\cdot,t)\|_{L^1}+\eta_s\|\mathscr{D}(\mathbf{u}(\cdot,t))\|_0^2=-\frac{1}{2a}\int_\Omega \mathrm{tr}(\alpha\tau_A(\cdot,t))\,\mathrm{d}x+\frac{d}{2a}\int_\Omega\beta(\cdot,t)\,\mathrm{d}x. \tag{7.6}$$

This completes the proof. □

Note that physically, the trace of the conformation tensor can be thought of as the length from the tail to the head of the macromolecule. As fluid flows, the molecules can be stretched, which means that the molecules store an energy. The more stretched, the more energy they store. One may then view $\|\tau_A\|_{L^1}$ as a total elastic energy due to the interaction between macromolecules and fluids. This is an elaborate argument on the importance of keeping the positivity of the conformation tensor in the physical terms.

Theorem 7.1. *Under the assumptions A_1, A_2 and A_3. The following estimates hold for $t\geqslant 0$.*

$$Re\|\mathbf{u}(\cdot,t)\|_0^2+\frac{1}{2a}\|\tau_A(\cdot,t)\|_{L^1}\leqslant \exp(-C_1t)\left(Re\|\mathbf{u}(\cdot,0)\|_0^2+\frac{1}{2a}\|\tau_A(\cdot,0)\|_{L^1}\right)+\frac{C_2(t)}{C_1}(1-\exp(-C_1t)) \tag{7.7}$$

and

$$\eta_s\int_0^t\|\mathscr{D}(\mathbf{u}(\cdot,v))\|_0^2\mathrm{d}v\leqslant\left(Re\|\mathbf{u}(\cdot,0)\|_0^2+\frac{1}{2a}\|\tau_A(\cdot,0)\|_{L^1}+C_2(t)t\right), \tag{7.8}$$

where

$$C_1=\min\left(\frac{c_\Omega\eta_s}{Re},c\right)\quad\textit{and}\quad C_2(t)=\frac{d}{2a}\sup_{0\leqslant s\leqslant t}\|\beta(\cdot,s)\|_{L^1}. \tag{7.9}$$

Here c_Ω is a positive constant depending only on Ω from the Korn's inequality.

Proof. To obtain the estimates (7.7) and (7.8), we shall start with the energy law (7.2) from Lemma 7.1. Using the Korn's inequality and the assumption $c=\min_\Omega\alpha>0$, we obtain the following inequality from (7.2):

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(Re\|\mathbf{u}(\cdot,t)\|_0^2+\frac{1}{2a}\|\tau_A(\cdot,t)\|_{L^1}\right)\leqslant-\eta_s c_\Omega\|\mathbf{u}(\cdot,t)\|_0^2-\frac{c}{2a}\|\tau_A(\cdot,t)\|_{L^1}+\frac{d}{2a}\int_\Omega\beta(\cdot,t)\,\mathrm{d}x, \tag{7.10}$$

where c_Ω is a generic constant depending only on Ω from the Korn's inequality. Let us denote $C_1=\min(\frac{c_\Omega\eta_s}{Re},c)$. With C_1, we then obtain the following inequality:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(Re\|\mathbf{u}(\cdot,t)\|_0^2+\frac{1}{2a}\|\tau_A(\cdot,t)\|_{L^1}\right)\leqslant-C_1\left(Re\|\mathbf{u}(\cdot,t)\|_0^2+\frac{1}{2a}\|\tau_A(\cdot,t)\|_{L^1}\right)+\frac{d}{2a}\int_\Omega\beta(\cdot,t)\,\mathrm{d}x. \tag{7.11}$$

It is easy to derive the following inequality from (7.11):

$$Re\|\mathbf{u}(\cdot,t)\|_0^2+\frac{1}{2a}\|\tau_A(\cdot,t)\|_{L^1}\leqslant e^{-C_1t}\left(Re\|\mathbf{u}(\cdot,0)\|_0^2+\frac{1}{2a}\|\tau_A(\cdot,0)\|_{L^1}\right)+\frac{C_2(t)}{C_1}(1-\exp(-C_1t)), \tag{7.12}$$

where $C_2=\frac{d}{2a}\sup_{0\leqslant s\leqslant t}\|\beta(\cdot,s)\|_{L^1}$. So the estimate (7.7) follows. To obtain the estimate (7.8), we take the integration of (7.2) to get

$$
\begin{aligned}
&Re\|\mathbf{u}(\cdot,t)\|_0^2 + \frac{1}{2a}\|\tau_A(\cdot,t)\|_{L^1} + \eta_s\int_0^t \|\mathscr{D}(\mathbf{u}(\cdot,v))\|_0^2\,\mathrm{d}v \\
&\quad \leqslant Re\|\mathbf{u}(\cdot,0)\|_0^2 + \frac{1}{2a}\|\tau_A(\cdot,0)\|_{L^1} - \int_0^t \frac{1}{2a}\|\alpha\tau_A(\cdot,v)\|_{L^1}\,\mathrm{d}v + C_2(t)t \\
&\quad \leqslant Re\|\mathbf{u}(\cdot,0)\|_0^2 + \frac{1}{2a}\|\tau_A(\cdot,0)\|_{L^1} + C_2(t)t. \qquad (7.13)
\end{aligned}
$$

This completes the proof. □

Next, we shall consider the limiting case when $We = \infty$. In this case, for most of models presented in the previous sections, $\alpha = \beta = 0$. So, we shall discuss the limiting case restricted to such cases.

Corollary 7.1. *Under the assumptions that* $We = \infty$, $\alpha = \beta = 0$ *and* A_3, *we have the following estimates*:

$$
Re\|\mathbf{u}(\cdot,t)\|_0^2 + \frac{1}{2a}\|\tau_A(\cdot,t)\|_{L^1} \leqslant Re\|\mathbf{u}(\cdot,0)\|_0^2 + \frac{1}{2a}\|\tau_A(\cdot,0)\|_{L^1}. \qquad (7.14)
$$

and

$$
\eta_s\int_0^t \|\mathscr{D}(\mathbf{u}(\cdot,v))\|_0^2 \leqslant Re\|\mathbf{u}(\cdot,0)\|_0^2 + \frac{1}{2a}\|\tau_A(\cdot,0)\|_{L^1}. \qquad (7.15)
$$

Proof. Both estimates (7.14) and (7.15) immediately follow from (7.7) and (7.8) due to the fact that $\alpha = \beta = 0$ imply $C_1 = C_2(t) = 0$. This completes the proof. □

A priori estimates like what are obtained in this section are often essential ingredients in establishing the global (in time) well-posedness of non-linear partial differential equations. It is still an open problem if any of the non-Newtonian models discussed in this paper is globally well-posed (in weak sense). This is a topic of active research, see e.g. [7,27,29,28].

7.2. Discrete energy estimates

In this section, we shall derive a discrete analogue of the energy estimate and shall demonstrate the stability and robustness of our new algorithms. We do not intend to give a general analysis but rather use a special scheme under some special assumptions to illustrate the main ideas. More general analysis under weaker assumptions is a topic of further research.

Specifically, we shall consider the scheme (6.22)–(6.24) and show how the positivity play a role in the stability analysis. Let us begin this section by the Galerkin finite element method for discretizations (6.22)–(6.24). Namely, given $(\mathbf{u}_h^n, \tau_{A,h}^n) \in \mathbf{V}_h \times \mathbf{S}_h$, find $(\mathbf{u}_h^{n+1}, \tau_{A,h}^{n+1}) \in \mathbf{V}_h \times \mathbf{S}_h$ such that for all $(\mathbf{v}_h, \sigma_h) \in \mathbf{V}_h \times \mathbf{S}_h$,

$$
Re\left(\frac{\mathbf{u}_h^{n+1} - \Pi_h^{\mathbf{V}}\left(\mathbf{u}_h^n \circ y^n\right)}{k}, \mathbf{v}_h\right) + \eta_s\left(\mathscr{D}(\mathbf{u}_h^{n+1}) : \mathscr{D}(\mathbf{v}_h)\right) = -\left(\tau_{A,h}^{n+1} : \mathscr{D}(\mathbf{v}_h)\right), \qquad (7.16)
$$

$$
\left(\frac{\tau_{A,h}^{n+1} - \Pi_h^{\mathbf{S}}\left(E_h(t^n,t^{n+1})(\tau_{A,h}^n \circ y^n)E_h(t^n,t^{n+1})^{\mathrm{T}}\right)}{k}, \sigma_h\right) = \left(-\alpha^{n+1}\tau_{A,h}^{n+1} + \beta^{n+1}I, \sigma_h\right), \qquad (7.17)
$$

where

$$
E_h(t^n,t^{n+1}) := \left(I - kR_h^{n+1}\right)^{-1}. \qquad (7.18)
$$

For simplicity, we shall assume that $\mathbf{V}_h$ and W_h are chosen in a way that

$$
\mathbf{div}\,\mathbf{u}_h \in W_h, \quad \forall \mathbf{u}_h \in \mathbf{V}_h. \qquad (7.19)
$$

Throughout this section, we shall further assume that the interpolation operator Π_h^{S} for the stress field is given by

$$\Pi_h^{\mathrm{S}}(\sigma) = \big(\Pi_h(\sigma_{ij})\big)_{ij=1,\ldots,d}, \tag{7.20}$$

where Π_h is defined through (see (6.11) in Section 6)

$$\Pi_h(u)(y) := \sum_{l=1}^{N}\left(\frac{1}{|K_l|}\int_{K_l} u\,\mathrm{d}x\right)\phi_l(y). \tag{7.21}$$

Here $\Im_h = \{K_l\}_{l=1}^N$ and $\phi_l(y)$ is a characteristic function which is one for $y \in \bar{K}_l$ and zero elsewhere. Furthermore, we apply the following approach to update $\tau_{A,h}^{n+1}$ from (7.17). More precisely, the interpolation Π_h^{S} operator shall be taken by the following procedures:

$$\Pi_h^{\mathrm{S}}\Big(E_h(t^n,t^{n+1})(\tau_{A,h}^n \circ y^n)E_h(t^n,t^{n+1})\Big) = \big(I - k(R_h^{n+1})_h\big)^{-1}(\tau_{A,h}^n \circ y^n)\big(I - k(R_h^{n+1})_h\big)^{-\mathrm{T}}, \tag{7.22}$$

where $(R_h^{n+1})_h := \Pi_h^{\mathrm{S}}(R_h^{n+1})$. We shall also assume that the volume preserving numerical approximation for the characteristic feet has been used. We would like to remark that a stable pair of spaces $\mathbf{V}_h$ and W_h satisfying the relation (7.19) can indeed be made especially with continuous piecewise polynomial of degree k and $k-1$ for $\mathbf{V}_h$ and W_h, respectively with $k \geqslant 4$ (see [5] or [39]). We note that (7.19) implies that $\mathbf{div}\,\mathbf{u}_h = 0$ on each element and so, volume preserving schemes for the characteristic feet can be devised for both two and three space dimensions (see e.g. [12]).

Finally, we shall make the following discrete analogue of the assumptions $A1$, $A2$ and $A3$:

A_1^h: $\alpha^n \in L^\infty(\Omega)$ with $\alpha^n \geqslant c > 0$ for all $n \geqslant 0$, for some constant c.
A_2^h: $\beta^n \in L^1(\Omega)$ with $\beta^n \geqslant 0$ for all $n \geqslant 0$.
A_3^h: $\tau_{A,h}^0$ is semi-positive definite.

The following simple lemma is instrumental to derive a discrete analogue of energy estimate.

Lemma 7.2. *Assume A and B are matrix-valued functions, $A_h = \Pi_h^{\mathrm{S}}(A)$ and $B_h = \Pi_h^{\mathrm{S}}(B)$. Then the following holds true*:

$$(A_h : B) = (A_h : B_h) = (A : B_h). \tag{7.23}$$

Proof. Since

$$(A : B) = \int_\Omega \mathrm{tr}(AB)\,\mathrm{d}x \tag{7.24}$$

and the trace operator is linear, it is enough to show that for any scalar functions f and g, the following holds true:

$$\int_\Omega f g_h\,\mathrm{d}x = \int_\Omega f_h g_h\,\mathrm{d}x = \int_\Omega f_h g\,\mathrm{d}x, \tag{7.25}$$

where $f_h = \Pi_h(f)$ and $g_h = \Pi_h(g)$. We observe that

$$\begin{aligned}\int_\Omega f g_h\,\mathrm{d}x &= \int_\Omega f \sum_{l=1}^N \left(\frac{1}{|K_l|}\int_{K_l} g\,\mathrm{d}x\right)\phi_l\,\mathrm{d}y \\ &= \sum_{l=1}^N\left(\int_\Omega f\phi_l\,\mathrm{d}y\right)\left(\frac{1}{|K_l|}\int_{K_l} g\,\mathrm{d}x\right)\end{aligned}$$

$$= \sum_{l=1}^{N} \int_\Omega \left(\frac{1}{|K_l|} \int_{K_l} f \, \mathrm{d}y \right) \phi_l \, \mathrm{d}z \left(\frac{1}{|K_l|} \int_{K_l} g \, \mathrm{d}x \right)$$

$$= \int_\Omega \sum_{l=1}^{N} \left(\frac{1}{|K_l|} \int_{K_l} f \, \mathrm{d}y \right) \phi_l \left(\frac{1}{|K_l|} \int_{K_l} g \, \mathrm{d}x \right) \phi_l \, \mathrm{d}z = \int_\Omega f_h g_h \, \mathrm{d}x.$$

The other equality $\int_\Omega f_h g_h \, \mathrm{d}x = \int_\Omega f_h g \, \mathrm{d}x$ follows in a straightforward manner from the similar argument. This completes the proof. □

We shall now state and prove our main theorem in this section.

Theorem 7.2. *Under the assumptions A_1^h, A_2^h and A_3^h. The Lagrange–Galerkin formulation (7.16), (7.17) together with (7.18) provide solutions $\mathbf{u}_h^n$ and $\tau_{A,h}^n$ for $n \geqslant 1$ satisfying the following estimate*:

$$Re\|\mathbf{u}_h^n\|_0^2 + \frac{1}{2a}\|\tau_{A,h}^n\|_{L^1} \leqslant c_1 \exp(-C_1 t^n) \left(Re\|\mathbf{u}_h^0\|_0^2 + \frac{1}{2a}\|\tau_{A,h}^0\|_{L^1} \right) + c_2 C_2^n \tag{7.26}$$

and

$$2\eta_s \sum_{l=1}^{n} k\|\mathscr{D}(\mathbf{u}_h^l)\|_0^2 \leqslant c_1 \left(Re\|\mathbf{u}_h^0\|_0^2 + \frac{1}{2a}\|\tau_{A,h}^0\|_{L^1} \right) + 2C_2^n t^n, \tag{7.27}$$

where $C_2^n = \frac{d}{2a}\max_{0\leqslant l\leqslant n}\|\beta^l\|_{L^1}$ with c_1 and c_2 being generic constants.

Proof. From (7.17) and (7.22), the following relation holds:

$$\left(\frac{1}{k} + \alpha^{n+1} \right) \tau_{A,h}^{n+1} = \frac{1}{k} \left(I - k(R_h^{n+1})_h \right)^{-1} (\tau_{A,h}^n \circ y^n) \left(I - k(R_h^{n+1})_h \right)^{-\mathrm{T}} + \beta^{n+1} I. \tag{7.28}$$

To obtain the discrete energy estimate, we first multiply $(I - k(R_h^{n+1})_h)$ on the left and $(I - k(R_h^{n+1})_h^{\mathrm{T}})$ on the right of the Eq. (7.28), respectively and rearrange various terms appropriately. Finally, by taking the trace operator followed by taking the integration, we obtain that

$$\begin{aligned}
&(1 + k\alpha^{n+1}) \int_\Omega \mathrm{tr}\left((R_h^{n+1})_h \tau_{A,h}^{n+1} + \tau_{A,h}^{n+1} (R_h^{n+1})_h^{\mathrm{T}} \right) \mathrm{d}x \\
&= \left(\frac{1}{k} + \alpha^{n+1} \right) \|\tau_{A,h}^{n+1}\|_{L^1} - \frac{1}{k}\|\tau_{A,h}^n \circ y^n\|_{L^1} + k(1 + k\alpha^{n+1}) \int_\Omega \mathrm{tr}\left((R_h^{n+1})_h \left(\tau_{A,h}^{n+1} - \frac{k}{1 + k\alpha^{n+1}} \beta^{n+1} I \right) (R_h^{n+1})_h^{\mathrm{T}} \right) \mathrm{d}x \\
&\quad - d \int_\Omega \beta^{n+1} \, \mathrm{d}x + k \int_\Omega \beta^{n+1} \mathrm{tr}\left((R_h^{n+1})_h + (R_h^{n+1})_h^{\mathrm{T}} \right) \mathrm{d}x.
\end{aligned} \tag{7.29}$$

We note that from (7.28), $\tau_{A,h}^{n+1}$ has the following lower bounds:

$$\tau_{A,h}^{n+1} \geqslant \frac{k}{1 + k\alpha^{n+1}} \beta^{n+1} I \quad \forall n \geqslant 1. \tag{7.30}$$

Further, by Lemma 7.2,

$$\int_\Omega \beta^{n+1} \mathrm{tr}\left((R_h^{n+1})_h + (R_h^{n+1})_h^{\mathrm{T}} \right) \mathrm{d}x = \int_\Omega \beta^{n+1} \mathrm{tr}\left(R_h^{n+1} + (R_h^{n+1})^{\mathrm{T}} \right) \mathrm{d}x = 2a \int_\Omega \beta^{n+1} \mathbf{div}\, \mathbf{u}_h^{n+1} \, \mathrm{d}x = 0 \tag{7.31}$$

and

$$\int_\Omega \mathrm{tr}\left((R_h^{n+1})_h \tau_{A,h}^{n+1} \right) \mathrm{d}x = \int_\Omega \mathrm{tr}\left(\tau_{A,h}^{n+1} (R_h^{n+1})_h^{\mathrm{T}} \right) \mathrm{d}x = a\left(\tau_{A,h}^{n+1} : (\mathscr{D}_h(\mathbf{u}_h^{n+1}))_h \right) = a\left(\tau_{A,h}^{n+1} : \mathscr{D}(\mathbf{u}_h^{n+1}) \right). \tag{7.32}$$

Finally, based on the volume preserving property of y^n, we have

$$\|\tau^n_{A,h} \circ y^n\|_{L^1} = \|\tau^n_{A,h}\|_{L^1}. \tag{7.33}$$

Taking into account (7.30)–(7.33), from (7.29), we obtain the following inequality:

$$\left(\tau^{n+1}_{A,h} : \mathscr{D}(\mathbf{u}^{n+1}_h)\right) \geqslant \gamma\left(\frac{1}{k} + c\right)\|\tau^{n+1}_{A,h}\|_{L^1} - \frac{\gamma}{k}\|\tau^n_{A,h}\|_{L^1} - \gamma d\int_\Omega \beta^{n+1}\,\mathrm{d}x, \tag{7.34}$$

where $\gamma = \frac{1}{2a(1+ck)}$ with $c = \inf_{n\geqslant 0, x\in\Omega}\alpha^n(x)$. We now consider the momentum equation (7.16) together with (7.34) to obtain that

$$\begin{aligned}\frac{Re}{k}\|\mathbf{u}^{n+1}_h\|^2_0 + \eta_s\|\mathbf{u}^{n+1}_h\|^2_1 &= \frac{Re}{k}\left(\Pi^{\mathbf{V}}_h(\mathbf{u}^n_h \circ y^n), \mathbf{u}^{n+1}_h\right) - \left(\tau^{n+1}_{A,h} : \mathscr{D}(\mathbf{u}^{n+1}_h)\right)\\ &\leqslant \frac{Re}{k}\left(\mathbf{u}^n_h \circ y^n, \mathbf{u}^{n+1}_h\right) - \gamma\left(\frac{1}{k} + c\right)\|\tau^{n+1}_{A,h}\|_{L^1} + \frac{\gamma}{k}\|\tau^n_{A,h}\|_{L^1} + \gamma d\int_\Omega \beta^{n+1}\,\mathrm{d}x.\end{aligned}$$

Applying the Cauchy–Schwarz inequality and the standard kick-back argument, we obtain the following relation:

$$\frac{Re}{2k}\|\mathbf{u}^{n+1}_h\|^2_0 + \eta_s\|\mathscr{D}(\mathbf{u}^{n+1}_h)\|^2_0 + \gamma\left(\frac{1}{k} + c\right)\|\tau^{n+1}_{A,h}\|_{L^1} \leqslant \frac{Re}{2k}\|\mathbf{u}^n_h\|^2_0 + \frac{\gamma}{k}\|\tau^n_{A,h}\|_{L^1} + \gamma d\int_\Omega \beta^{n+1}\,\mathrm{d}x. \tag{7.35}$$

We shall now show the first estimate (7.26). Multiplying k by both sides of (7.35) and using the Korn's inequality, we obtain that

$$\begin{aligned}\kappa_1\|\mathbf{u}^{n+1}_h\|^2_0 + \kappa_2\|\tau^{n+1}_{A,h}\|_{L^1} &\leqslant Re\|\mathbf{u}^n_h\|^2_0 + \gamma\|\tau^n_{A,h}\|_{L^1} + k\gamma d\int_\Omega \beta^{n+1}\,\mathrm{d}x\\ &\leqslant \exp(-C_1k)\left(\kappa_1\|\mathbf{u}^n_h\|^2_0 + \kappa_2\|\tau^n_{A,h}\|_{L^1}\right) + k\gamma d\int_\Omega \beta^{n+1}\,\mathrm{d}x,\end{aligned} \tag{7.36}$$

where $\kappa_1 = Re + k\eta_s c_\Omega$, $\kappa_2 = \gamma\,(1 + ck)$, c_Ω is a positive constant depending only on Ω and $C_1 > 0$ is a constant given by

$$\max\left(\frac{Re}{Re + k\eta_s c_\Omega}, \frac{1}{1 + ck}\right) \leqslant \exp(-C_1k), \quad 0 \leqslant k \leqslant 1. \tag{7.37}$$

Now, we use the induction argument to obtain:

$$\kappa_1\|\mathbf{u}^n_h\|^2_0 + \kappa_2\|\tau^n_{A,h}\|_{L^1} \leqslant \exp(-C_1t^n)\left(\kappa_1\|\mathbf{u}^0_h\|^2_0 + \kappa_2\|\tau^0_{A,h}\|_{L^1}\right) + k\,\mathrm{d}\gamma\int_\Omega \beta^{n+1}\,\mathrm{d}x\sum_{l=0}^{n}\exp(-C_1t^l) \tag{7.38}$$

$$\leqslant \exp(-C_1t^n)\left(\kappa_1\|\mathbf{u}^0_h\|^2_0 + \kappa_2\|\tau^0_{A,h}\|_{L^1}\right) + \tilde{C}^n_2, \tag{7.39}$$

where

$$\tilde{C}^n_2 = k\frac{d}{2a}\int_\Omega \beta^n\,\mathrm{d}x\left(\frac{1 - \exp(-C_1t^n)}{1 - \exp(-C_1k)}\right). \tag{7.40}$$

It is easy to see that we can choose generic constants c_1 and c_2 such that

$$\kappa_1\|\mathbf{u}^0_h\|^2_0 + \kappa_2\|\tau^0_{A,h}\|_{L^1} \leqslant c_1\left(Re\|\mathbf{u}^0_h\|^2_0 + \frac{1}{2a}\|\tau^0_{A,h}\|_{L^1}\right) \quad \text{and} \quad \tilde{C}^n_2 \leqslant c_2C^n_2, \tag{7.41}$$

where $C^n_2 = \frac{d}{2a}\max_{0\leqslant l\leqslant n}\|\beta(\cdot,t^l)\|_{L^1}$. We then obtain the desired result (7.26). We now derive the other estimate (7.27). First we multiply $2k$ to both sides of (7.35) and take summation from $l = 1$ to $l = n$ for both sides to obtain:

$$2\eta_s \sum_{l=1}^{n} k\|\mathscr{D}(\mathbf{u}_h^l)\|_0^2 \leqslant c_1\left(Re\|\mathbf{u}_h^0\|_0^2 + \frac{1}{2a}\|\tau_{A,h}^0\|_{L^1}\right) + \sum_{l=1}^{n} 2k\frac{d}{2a}\int_\Omega \beta^l\,\mathrm{d}x,$$
$$\leqslant c_1\left(Re\|\mathbf{u}_h^0\|_0^2 + \frac{1}{2a}\|\tau_{A,h}^0\|_{L^1}\right) + 2C_2^n t^n.$$

This completes the proof. □

We shall now consider the limiting case when $We = \infty$ especially for models $\alpha = \beta = 0$ in such a case.

Corollary 7.2. *Under the assumption that* $We = \infty$, $\alpha = \beta = 0$ *and* A_3^h, *the following estimates hold true*:

$$Re\|\mathbf{u}_h^n\|_0^2 + \|\tau_h^n\|_{L^1} \leqslant c\Big(Re\|\mathbf{u}_h^0\|_0^2 + \|\tau_h^0\|_{L^1}\Big) \quad \forall n \geqslant 1.$$

and

$$\eta_s \sum_{l=1}^{n} k\|\nabla \mathbf{u}_h^l\|_0^2 \leqslant c\Big(Re\|\mathbf{u}_h^0\|_0^2 + \|\tau_h^0\|_{L^1}\Big), \tag{7.42}$$

where c is a generic constant.

Proof. Note that in the limiting case, $\alpha = \beta = 0$ and τ_h^n is itself a conformation tensor for $n \geqslant 0$. The result then immediately follows from two estimate (7.26) and (7.27) since $C_1 = 0$ and $C_2^n = 0$ for all $n \geqslant 0$. This completes the proof. □

In summary, apparently, the stability analysis indicates that keeping the positivity of the conformation tensor in the discrete level is crucial in the numerical stability and that the so-called "the high Weissenberg number problem" will not be presented in our scheme as is the case for currently available schemes in the literatures. Based on the new frameworks in this paper, we then confirmed the common belief affirmatively that the positivity preserving scheme shall allow to overcome the difficulty arising in simulating the time dependent non-Newtonian fluid flows. Furthermore, we have also extended such a confirmation to other models.

8. Concluding remarks

This paper presents a unified approach to discretize a large class of rate-type constitutive models having a property of the positive-definiteness of the conformation tensor in a way that such an important physical quantity is preserved, namely the conformation tensor evolves in time with the property of positive-definiteness in the discrete sense. The proposed discretization schemes are introduced based upon the important observation that the rate-type constitutive equations can be cast into the formulation of the Riccati Differential Equations and demonstrated that some second-order accurate schemes for both time and space can be devised. This approach is unique in its simplicity as well as its generality and also shown to lead to robust and stable schemes.

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