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Stability Analysis of the One-dimensional GLD-Lagrangian Scheme

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Abstract. Given the ongoing study of formulations and stabilizing methods for constitutive models, this work discusses the stability analysis of a particular case of a new discretization scheme. The proposed scheme is based on a reformulation of the upper-convected time derivative. This reformulation is over a Lagrangian framework and uses the generalized Lie derivative. The stability analysis is carried out for the first-order scheme and shows that the scheme supports the CFL type restriction, proving to be viable for numerical simulations.

Keywords. Generalized Lie Derivative, Lagrangian Scheme, Finite Difference Method, Numerical Stability

1 Introduction

A variety of viscoelastic fluids are modeled by constitutive equations that have the upper-convected time derivative term, such as Oldroyd-B [12] or Geisekus [5]. There exists a constant search in the area of simulation of viscoelastic fluid flows, to improve the numerical stability related to models and their dimensionless parameters [1, 7]. Furthermore, there are still discussions about the mathematical construction of viscoelastic models [6].

Based on the works [8, 9], a reformulation of the upper-convected time derivative term was proposed by [10, 11] to allow the study of the numerical instabilities that plague the area. The studies involve the generalized Lie derivative (GLD) [9], and use the concept of a transition matrix based upon particle paths, to reformulate the upper-convected time derivative along its characteristics.

Considering the good results for the truncation error analysis [11], and the ease of extending the method to compute High Weissenberg Number Problems (HWNP), this work performs the stability analysis for a particular one-dimensional case of the scheme proposed by [10, 11]. However, when solving differential equations numerically, it is necessary to discretize the continuous domain and continuous functions by a finite set of discrete values [2, 4].

This discretization introduces errors into the solution, and it is important to understand how these errors propagate over time and how they affect the accuracy of the numerical solution. Numerical stability studies aim to prevent small errors from causing incorrect or meaningless results in numerical approximations. A stable numerical method produces solutions that remain bounded and do not exhibit significant amplification of errors as the computation progresses.

The present work is organized with the presentation of the GLD for the one-dimensional case, the development of the first-order finite difference scheme based on [11], and the results obtained by the stability analysis of the proposed numerical scheme.

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2 Equations

Let $\Omega \subset \mathbb{R}$ be a bounded domain and T a positive constant. Let $\mathbf{T} : \Omega \times [0,T] \to \mathbb{R}$ be a scalar function and $u : \Omega \times [0,T] \to \mathbb{R}$ a given smooth function for velocity. We consider the following one-dimensional problem:

$$\overset{\triangledown}{\mathbf{T}}(x,t) = F(x,t), \qquad \text{in } \Omega \times [0,T], \tag{1a}$$

$$\mathbf{T}(x,t) = \mathbf{T}^0(x), \qquad \text{in } \Omega, \text{ at } t = 0, \tag{1b}$$

$$\mathbf{T}(x,t) = \mathbf{T}_{in}(x,t), \qquad \text{in } \partial\Omega \times [0,T], \tag{1c}$$

where $\overset{\triangledown}{\mathbf{T}}$ is the one-dimensional representation of the upper-convected time derivative, given by:

$$\overset{\triangledown}{\mathbf{T}}(x,t) = \frac{\partial \mathbf{T}(x,t)}{\partial t} + u(x,t)\frac{\partial \mathbf{T}(x,t)}{\partial x} - 2\frac{\partial u(x,t)}{\partial x}\mathbf{T}(x,t). \tag{2}$$

The function $F(x,t)$ is the source term, $\mathbf{T}^0(x)$ is the initial condition, and $\mathbf{T}_{in}(x,t)$ the boundary condition. In this notation, $\mathbf{T}(x,t)$ is defined in an Eulerian framework.

To introduce the Lagrangian framework and the GLD, we will assume that the flow map $X(x,t;s) \in \mathbb{R}$, for time instants $t,\ s \in (0,T)$, satisfies the ordinary differential equation (ODE) and the initial condition stated below:

$$\frac{\partial X(x,t;s)}{\partial s} = u(X(x,t;s),s), \quad s \in (0,T), \tag{3a}$$

$$X(x,t;t) = x, \quad (x,t) \in \Omega \times (0,T). \tag{3b}$$

Related to the problem (3a-3b), we shall also consider the transition matrix $L(x,t;\cdot) : \Omega \times (0,T) \times (0,T) \to \mathbb{R}$, defined in [9–11].

The $L(x,t,s)$ is the transition matrix between two-time instants t and s, a particular case of the gradient deformation of flow maps, and has the following properties, one-dimensional case: for all $t_1, t_2 \in [0,T]$

$$L(x,t_1,t_2)L(x,t_2,t_1) = L(x,t_1,t_1) = 1, \tag{4a}$$

$$\frac{\partial L(x,t_1,s)}{\partial s} = \frac{\partial u\left(X(x,t_1;s),s\right)}{\partial x}L(x,t_1,s), \tag{4b}$$

$$\frac{\partial L(x,s,t_1)}{\partial s} = -L(x,s,t_1)\frac{\partial u\left(X(x,t;s),s\right)}{\partial x}. \tag{4c}$$

The generalized Lie derivative on a Lagrangian framework can now be defined as follows.

Definition 2.1. *The generalized Lie derivative of a scalar function* $\boldsymbol{T}$ *with respect to some function* u*, in a Lagrangian framework, is*

$$\mathcal{L}_u \boldsymbol{T}\big(X(x,t;s),s\big) \coloneqq L(x,t,s)\frac{\partial}{\partial s}\Big[L(x,s,t)\,\boldsymbol{T}\big(X(x,t;s),s\big)L(x,s,t)\Big]L(x,t,s). \tag{5}$$

Note that the GLD can be interpreted from an Eulerian point of view. To do this, we just take the derivative of the product of functions in Definition 2.1, apply the properties of the transition matrices, and finally set $s = t$. Then, the GLD equation (5) in the Eulerian framework can be rewritten as: $\mathcal{L}_u\mathbf{T}\big(X(x,t;s),s\big)\Big|_{s=t} = \overset{\triangledown}{\mathbf{T}}(x,t)$ (for more details, cf. [9, 10]). Therefore, equation (1a) may be rewritten as:

$$\mathcal{L}_u\mathbf{T}\big(X(x,t;s),s\big) = F(x,t), \quad \text{in } \Omega \times [0,T]. \tag{6}$$

Thus, we are able to solve an equivalent problem to (1), given by equations (6), (1b) and (1c).

3 Numerical Scheme

In this section, we discuss first-order implicit numerical approximations for our problem. Let the integer N_T be the number of time discretization points and Δt be the time step, related to N_T by $N_T := \lfloor T/\Delta t \rfloor$. For convenience of notation, we write $t^n := n\Delta t$ and $f^n := f(\cdot, t^n)$ $(n \in \mathbb{N})$ for some function $f : \Omega \times (0, T)$.

The term $\mathcal{L}_u \mathbf{T}(x, t; s)$ in Definition 2.1, can be approximated by a first-order implicit Euler method in time:

$$\begin{aligned}\mathcal{L}_u \mathbf{T}\big(X(x,t;s),s\big) \quad &\approx \quad L(x,t,s)\frac{1}{\Delta t}\left[L(x,s,t)\mathbf{T}\big(X(x,t;s),s\big)L(x,s,t) - \right.\\ &\left. L(x,s-\Delta t,t)\mathbf{T}\big(X(x,t;s-\Delta t),s-\Delta t\big)L(x,s-\Delta t,t)\right]L(x,t,s). \quad (7)\end{aligned}$$

Assuming $s = t = n\Delta t$, then:

$$\begin{aligned}\mathcal{L}_u \mathbf{T}\big(X(x,t^n;t^n),t^n\big) \quad &\approx \quad L(x,t^n,t^n)\frac{1}{\Delta t}\left[L(x,t^n,t^n)\mathbf{T}\big(X(x,t^n;t^n),t^n\big)L(x,t^n,t^n) - \right.\\ &\left. L(x,t^{n-1},t^n)\mathbf{T}\big(X(x,t^n;t^{n-1}),t^{n-1}\big)L(x,t^{n-1},t^n)\right]L(x,t^n,t^n), \quad (8)\end{aligned}$$

from the first property of the transition matrices and from the ODE initial condition (3b):

$$\begin{aligned}\mathcal{L}_u \mathbf{T}\left(x,t^n\right) \quad &\approx \quad \frac{1}{\Delta t}\left[\mathbf{T}\big(x,t^n\big) - \right.\\ &\left. L(x,t^{n-1},t^n)\mathbf{T}\big(X(x,t^n;t^{n-1}),t^{n-1}\big)L(x,t^{n-1},t^n)\right]. \quad (9)\end{aligned}$$

For convenience, let's consider the third property of transition matrices (4c) and apply a first-order implicit Euler method to approximate the term $L(x, t^{n-1}, t^n)$. That is,

$$\begin{aligned}\left.\frac{\partial L(x,s,t^n)}{\partial s}\right|_{s=t^n} \quad &= \quad -L(x,s,t^n)\left.\frac{\partial u\left(X(x,t^n;s),s\right)}{\partial x}\right|_{s=t^n}\\ \frac{L(x,t^n,t^n)-L(x,t^{n-1},t^n)}{\Delta t} \quad &\approx \quad -L(x,t^n,t^n)\frac{\partial u\left(X(x,t^n;t^n),t^n\right)}{\partial x}.\\ L(x,t^{n-1},t^n) \quad &\approx \quad L(x,t^n,t^n)+L(x,t^n,t^n)\Delta t\frac{\partial u\left(x,t^n\right)}{\partial x}\\ L(x,t^{n-1},t^n) \quad &\approx \quad 1+\Delta t\frac{\partial u\left(x,t^n\right)}{\partial x}. \quad (10)\end{aligned}$$

Thus, substituting the approximation of $L(x, t^{n-1}, t^n)$ given by (10), in the proposed scheme (9), we obtain:

$$\begin{aligned}\mathcal{L}_u \mathbf{T}\left(x,t^n\right) \quad &\approx \quad \frac{1}{\Delta t}\left[\mathbf{T}\big(x,t^n\big) - \right.\\ &\left. -\left[1+\Delta t\frac{\partial u\left(x,t^n\right)}{\partial x}\right]\mathbf{T}\big(X(x,t^n;t^{n-1}),t^{n-1}\big)\left[1+\Delta t\frac{\partial u\left(x,t^n\right)}{\partial x}\right]\right] \quad (11)\end{aligned}$$

Finally, the temporal approximation for the problem given by (6), becomes:

$$\begin{aligned}\mathbf{T}\big(x,t^n\big) \quad &\approx \quad \left[1+\Delta t\frac{\partial u\left(x,t^n\right)}{\partial x}\right]\cdot\left[\mathbf{T}\big(X(x,t^{n-1}),t^{n-1}\big)\right]\cdot\left[1+\Delta t\frac{\partial u\left(x,t^n\right)}{\partial x}\right]\\ &+\Delta t F\left(x,t^n\right). \quad (12)\end{aligned}$$

The domain $\Omega = [a, b]$ is discretized by a spatial Eulerian mesh, where the nodes are $x_i = a + i\Delta x$, for $i = 0, 1, 2, \ldots, N_x$, and $\Delta x = (b - a)/N_x$. The notation $f_i^n := f(x_i, t^n)$ is going to be used for a function $f : \Omega \times (0, T)$.

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Let's assume that the map value $X(x_i, t^n; t^{n-1})$ belongs to one of the sub-intervals of the mesh, that is, $X(x_i, t^n; t^{n-1}) \in [x_l, x_{l+1}]$, for some $l = 0, 1, 2, \ldots, N_x-1$. For the term $\mathbf{T}\big(X(x_i, t^n; t^{n-1}), t^{n-1}\big)$ in the approximation, we choose the linear interpolation of the tensor $\mathbf{T}$ at time t^{n-1}, in some sub-interval mesh.

Thus, we approximate the term $\mathbf{T}\big(X(x_i, t^n; t^{n-1}), t^{n-1}\big)$ by:

$$\mathbf{T}\big(X(x_i, t^n; t^{n-1}), t^{n-1}\big) = \mathbf{T}_l^{n-1}\phi_l(X(x_i, t^n; t^{n-1})) + \mathbf{T}_{l+1}^{n-1}\phi_{l+1}(X(x_i, t^n; t^{n-1})), \tag{13}$$

where the functions ϕ_l and ϕ_{l+1} are hat functions, cf. [11]. Therefore, the complete discretization given by equations (12) and (13) provides the following numerical scheme:

$$\begin{aligned}\mathbf{T}_i^n \quad \approx \quad & \left[1 + \Delta t \frac{\partial u}{\partial x}\bigg|_i^n\right]^2 \cdot \left[\mathbf{T}_l^{n-1}\phi_l(X(x_i, t^n; t^{n-1})) + \mathbf{T}_{l+1}^{n-1}\phi_{l+1}(X(x_i, t^n; t^{n-1}))\right] \\ & + \Delta t F_i^n.\end{aligned} \tag{14}$$

Furthermore, we will take $X(x_i, t^n; t^{n-1})$ given by the ODE (3), and it's numerical approximation:

$$X(x_i, t^n; t^{n-1}) = x_i - \Delta t u_i^n. \tag{15}$$

4 Stability Analysis

To study the stability of the numerical scheme given by (14), we use the matrix criterion. So, we evaluate the iteration matrix $\mathbf{A}$ associated with the scheme, considering the homogeneous problem $(F(x, t) = 0)$.

To determine the iteration matrix we apply the proposed method to the entire domain, for some mesh with space size $h = \Delta x$, and write the full scheme as:

$$\mathbf{T}_h^n = \mathbf{A}\mathbf{T}_h^{n-1}, \tag{16}$$

where $\mathbf{T}_h^n = (T_0^n, T_1^n, \ldots, T_{N_x}^n)^\top$ represents the approximate solution vector in the nodes of the spatial mesh and each coefficient a_{ij} of matrix A can be written as:

$$a_{ij} = \begin{cases} \left[1 + \Delta t \frac{\partial u}{\partial x}\Big|_i^n\right]^2 \phi_j(X(x_i, t^n; t^{n-1})), & \text{if } X(x_i, t^n; t^{n-1}) \in [x_{j-1}, x_{j+1}], \\ 0, & \text{otherwise}, \end{cases} \tag{17}$$

for $i = 0, 1, \ldots, N_x$. Note that from (14), for each row i we have only columns l and $l+1$ with non-zero values. If we have a boundary value problem then $a_{11} = a_{N_x N_x} = 1$ and the remaining terms in lines 1 and N_x are zero.

When we rewrite this same method using a known exact solution $\mathbf{T}$, we have:

$$\mathbf{T}^n = \mathbf{A}\mathbf{T}^{n-1} + \boldsymbol{\tau}_h, \tag{18}$$

where $\mathbf{T}^n = (\mathbf{T}(x_0, t^n), \mathbf{T}(x_1, t^n), \ldots, \mathbf{T}(x_{N_x}, t^n))^\top$ is the exact solution in the nodes of the spatial mesh at time t^n, and $\boldsymbol{\tau}_h$ is the local truncation error. To obtain a relation between the local truncation error and the global error ($\mathbf{E}_h^n = \mathbf{T}_h^n - \mathbf{T}^n$), we subtract equation (18) from (16) and we get:

$$\mathbf{E}_h^n = \mathbf{A}\mathbf{E}_h^{n-1} - \boldsymbol{\tau}_h. \tag{19}$$

Note that, for known values of the boundary and initial conditions we have that $\mathbf{E}(\mathbf{x}, t)|_{\partial\Omega} = 0$ and $\mathbf{E}(\mathbf{x}, 0) = \mathbf{E}^0 = 0$, respectively. Furthermore, each coefficient a_{ij} of matrix A related to some variable E_j^{n-1} remains defined by (17).

If the proposed scheme is stable, then the magnitude of the error $\mathbf{E}_h^n$ on (19) are not amplified during the evolution of the simulation, on the contrary, the rounding and truncation errors are attenuated during the simulation process.

Note that, the iteration matrix $\mathbf{A}$ is sparse by construction. Depending on the velocity function u and the time step Δt taken, the matrix $\mathbf{A}$ can have only 2 neighboring non-zero entries (from (14) and (17)). Hence, the matrix $\mathbf{A}$ can be constructed having at its main diagonal the values 0, 1, or $\left[1 + \Delta t \frac{\partial u}{\partial x}\Big|_i^n\right]^2 \phi_j(X(x_i, t^n; t^{n-1}))$, and then its eigenvalues are the main diagonal elements.

We know that the numerical method is stable if the eigenvalues λ_i, for $i = 0, 1, \ldots, N_x$, are such that $|\lambda_i| \leq 1$, for all i. The following Theorem presents a result for the stability analysis by the matrix criterion based on [2], for the $1D$ specific case of this work with the iteration matrix given by (17).

Theorem 4.1. *Let be $\Omega = [a, b] \subset \mathbb{R}$, $t, s, t^n, t^{n-1} \in [0, T]$, $u = u(x, t)$ a smooth non-constant function, and assume that the flow map $X(x, t; s) \in [a, b]$ satisfies the ODE* (3)*. Then, the first-order scheme given by* (14)*, is stable if, and only if*

$$\left|1 + \Delta t \frac{\partial u}{\partial x}\Big|_i^n\right|^2 \phi_j\Big(X(x_i, t^n; t^{n-1})\Big) \leq 1, \quad \forall x_i \in [a, b],$$

where $i = 0, 1, \ldots, N_x$, $j = 0, 1, \ldots, N_x - 1$ and $n = 1, \ldots, N_T$.

To prove the Theorem 4.1, it is enough to verify that $|\lambda_i| = \left|1 + \Delta t \frac{\partial u}{\partial x}\Big|_i^n\right|^2 \phi_j\Big(X(x_i, t^n; t^{n-1})\Big)$, or $\lambda_i = 1$, where λ_i is an eigenvalue of the method's iteration matrix. Then, the definition of stability by the matrix criterion (cf. Definition 3.1, [2]), completes the proof.

Note that the base function $0 \leq \phi_j(x_i) \leq 1$, $i = 0, 1, \ldots, N_x$, then Theorem 4.1 can be rewritten, without loss of generality, as:

Theorem 4.2. *Let be $\Omega = [a, b] \subset \mathbb{R}$, $t, s, t^n, t^{n-1} \in [0, T]$, $u = u(x, t)$ a smooth non-constant function, and assume that the flow map $X(x, t; s) \in [a, b]$ satisfies the ODE* (3)*. Then, the first-order scheme given by* (14)*, is stable if, and only if*

$$\frac{-2}{\Delta t} < \frac{\partial u_i^n}{\partial x} < 0, \qquad \text{or} \qquad \frac{\Delta t\, u_i^n}{\Delta x} < 1,$$

where $X(x_i, t^n; t^{n-1}) \approx x_i - \Delta t u(x_i, t^n)$, and $u(x_i, t^n) = u_i^n$, for all $i = 0, 1, \ldots, N_x$, and $n = 1, \ldots, N_T$.

Proof. (idea)

Let's suppose that the scheme (12) and (13) is applied to a homogeneous problem.

Note that $0 \leq \phi_j(x) \leq 1$, $\forall x \in [a, b]$, and then from Theorem 4.1, we have:

$$\left|1 + \Delta t \frac{\partial u_i^n}{\partial x}\right|^2 \phi_j\Big(X(x_i, t^n; t^{n-1})\Big) \leq 1.$$

Supposing that $\phi_j(x) = 0, \forall x \in [a, b]$, then we have a stable scheme.

If $\phi_j(x_i) = 1$, for some $x_i \in [a, b]$, for a stable scheme we should have

$$\frac{-2}{\Delta t} < \frac{\partial u_i^n}{\partial x} < 0.$$

In the other hand, let's suppose that the hat function $\phi_j(x_i) \in (0, 1)$, and $x_i \in [a, b]$. Checking this statement, let's consider $u(x_i, t^n)$ a positive velocity field and $X(x_i, t^n; t^{n-1}) \approx x_i - \Delta t u(x_i, t^n)$,

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such that

$$\begin{aligned} & x_i - \Delta x < x_i - \Delta t u(x_i, t^n) < x_i \\ \Leftrightarrow \quad & -\Delta x < -\Delta t u(x_i, t^n) < 0 \\ \Leftrightarrow \quad & \Delta x > \Delta t u(x_i, t^n) > 0, \end{aligned}$$

as Δt, $\Delta x > 0$, then:

$$1 > \frac{\Delta t u(x_i, t^n)}{\Delta x},$$

that is,

$$C = \frac{\Delta t u_i^n}{\Delta x} < 1, \tag{20}$$

where the dimensionless number C is called the Courant number [2, 4]. If the relation (20) holds for all $i = 0, \ldots, N_x$, then there exists a velocity u such that our constraint coincides with the CFL condition:

$$\frac{\Delta t\, u}{\Delta x} < 1.$$

□

Note that, if the velocity derivative is negative but too large in absolute value, i.e., if $\left|\Delta t \frac{\partial u}{\partial x}\right| > 2$, it may result in eigenvalues > 1, which makes the numerical scheme unstable.

In particular, if the velocity field is constant we can have a simpler case of numerical stability analysis, as presented in the corollary below.

Corollary 4.1. *In the same conditions of the Theorem 4.2, where $u = u(x, t) = f(t) \in \mathbb{R}$, i.e., for a constant velocity field for the $x-$variable, we have that the first-order scheme* (14) *is absolute stable.*

Corollary 4.1 is easily checked. If the velocity field in $1D$ is a constant function for the $x-$variable, we have its first derivative equal to zero ($\frac{\partial u}{\partial x} = 0$, $\forall x \in [a, b]$), and the hat functions are defined such that $0 \leq \phi_j(x) \leq 1$, for all $x \in \Omega$, then the numerical scheme will be stable for any $x \in \Omega$.

5 Conclusion

The stability analysis carried out allows us to observe which conditions of the problem provide us a stable method. Thus, our method is said to be conditionally stable, depending on the velocity field u or the choice of time step.

It is interesting to note that, for a more general case, when the flow map does not fall at a point of the mesh, and we have a positive velocity field, we verify that the proposed method is restricted to the CFL condition, the same condition observed for methods for hyperbolic equations[3, 4]. Therefore, the proposed method does not add more severe temporal constraints than other methods.

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