Least-squares formulation to solve non-Newtonian fluid flow and application of data assimilation in 2D

Solveigh Averweg1,*, Alexander Schwarz1, Carina Schwarz1, and Jörg Schröder1

1 University of Duisburg-Essen, Institute of Mechanics, Universitätsstraße 15, 45141 Essen, Germany

In this contribution, we present an approach to model steady flow of incompressible non-Newtonian fluids with data assimilation into the numerical solution based on the least-squares finite element method (LSFEM). The assimilation of data (e.g. experimental or analytical) into numerical simulations offers promising possibilities when examining complex problems. Potential applications include the enhancement of numerical models using measured data or the completion of experimental data using numerical methods, e.g. the determination of non-measured quantities such as pressure. In particular for the field of fluid mechanics, the implemented LSFEM has some theoretical advantages compared to the well-known (mixed) Galerkin finite element method, since it is not restricted to the LBB-condition. Additionally, it results in a minimization problem with symmetric positive (semi-)definite equation systems also for differential equations with non-self-adjoint operators. A further advantage in this context is that the assimilation of data can easily be performed by adding a term to the least-squares (LS) functional such that it does not significantly increase the computational cost. The approach of data assimilation is shown by solving steady flow of a non-Newtonian fluid through a channel with a smooth contraction.

1 Introduction

The material response of non-Newtonian fluids is characterized by a non-constant viscosity, which can change depending on e.g. the stress state, the flow geometry or even the flow history. In this contribution we consider generalized Newtonian fluids, whose properties are shear-thinning or shear-thickening behavior depending on the shear rate. We apply a LS stress-velocity formulation that has been extensively studied for solving steady as well as unsteady flow problems of incompressible Newtonian fluids, and in [1] it has also been applied to non-Newtonian fluids. Here, the chosen viscosity model is the Carreau-Yasuda model, which may be used e.g. for polymer melts or blood. In order to show the straightforward implementation of data assimilation to the modeling of a non-Newtonian fluid flow using the LSFEM, we apply a numerical reference solution. This is obtained by using a mixed Taylor-Hood Galerkin triangle element on a fine grid. The flow through a channel with a smooth 4:1 contraction is considered to show the application and effect of data assimilation to the numerical flow simulation.

2 The theoretical framework

The key component of the LSFEM is a functional constructed based on governing equations of continuum mechanics.

For the theoretical basis and a detailed description of the construction of the functional, we refer to [3], for instance. When applying the LSFEM to model steady flow of incompressible non-Newtonian fluids the general setup is based on the Navier-Stokes equations, consisting of the mass continuity equation and the balance of momentum equations. These are transformed into a first-order system, e.g., in terms of stresses and velocities as presented in [5]. Using the quadratic $L^2$-norm of the weighted equations leads to the least-squares functional.

For the assimilation of data, a further term is added to the functional. This contains the given data $d \in \mathbb{R}^M$, which are approximated by $d \approx H \nu$. The observation operator $H : \nu \rightarrow \mathbb{R}^M$ is used to extract the quantities located at the positions of the given data from the solution field. Also, the difference between the given data and the solution is weighted by $\zeta_i$. For more details on this approach see e.g. [6]. Considering additionally the dependence of the dynamic viscosity $\eta$ on the shear rate $\dot{\gamma} = \sqrt{2(\nabla \nu : \nabla \nu)}$, the resulting functional reads

$$F(\sigma, \nu) = \frac{1}{2} \left( ||\omega_1 (\text{div} \sigma - \rho \nabla \nu \cdot \nabla \nu)||_{L^2(\Omega)}^2 + ||\omega_2 (\text{dev} \sigma - 2 \gamma \dot{\gamma} \nabla \nu)||_{L^2(\Omega)}^2 + |||\nu|||_{L^2(\Omega)}^2 + \sum_{i=1}^{M} \zeta_i (d_i - H_i \nu)^2 \right),$$

with the Cauchy stresses $\sigma$, the velocities $\nu$, the symmetric velocity gradient defined as $\nabla \nu = 1/2 (\nabla \nu + (\nabla \nu)^T)$, the density $\rho$ and the physical weightings $\omega_1 = 1/\sqrt{\rho}$ and $\omega_2 = 1/\eta_{ch}$. The characteristic viscosity $\eta_{ch}$ is obtained by substituting $\dot{\gamma} = v_{ch}/L$, with the bulk velocity $v_{ch}$ and the characteristic length $L$, into the viscosity model. In the following, we apply the Carreau-Yasuda model presented by [2]. With the upper and lower viscosity bounds $\eta_0$ and $\eta_\infty$ and further model parameters $n$, $\lambda$ and $a$ this reads $\eta(\dot{\gamma}) = \eta_\infty + (\eta_0 - \eta_\infty) (1 + (\lambda \dot{\gamma})^a)^{n-1}$. 

* Corresponding author: e-mail solveigh averweg@uni-due.de, phone +00 49 201 183 2683, fax +00 49 201 183 2680

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The velocities and stresses are discretized using conforming approximation functions specified by

\[ V^h = \{ v \in H^1(\Omega)^2 : v|_{\Omega_e} \in P_k(\Omega_e)^2 \ \forall \ \Omega_e \} , \quad W^h = \{ \sigma \in H(\text{div},\Omega)^2 : \sigma|_{\Omega_e} \in RT_m(\Omega_e)^2 \ \forall \ \Omega_e \} , \]

with Lagrangian polynomials \( P_k(\Omega_e)^2 \) of order \( k \) and vector-valued Raviart-Thomas functions \( RT_m(\Omega_e)^2 \) of order \( m \).

### 3 Numerical example

Data assimilation into the solution of a non-Newtonian fluid flow by means of the LSFEM using the presented stress-velocity formulation is demonstrated by modeling the flow through a channel with smooth contraction as depicted in Fig. 1(left), with \( \bar{v}_1(x_2) = 0.15 - 0.6/0.008x_2^2 \) m/s. The model parameters are chosen as \( \eta_0 = 22 \times 10^{-3} \) Pa s, \( \eta_{sc} = 2.2 \times 10^{-3} \) Pa s, \( n = 0.392, \lambda = 0.11 \) s, \( \alpha = 0.644 \) and \( \rho = 1410 \) kg/m\(^3\). This choice results in a shear-thinning fluid and, according to [4], is suitable for modeling blood flow. The resulting velocity distribution is shown in Fig. 1(right).

![Fig. 1: Boundary value problem (left) and total velocity field (in m/s) for a mesh size of 3584 triangles using element RT2P3 (right)](image)

First, a grid convergence without data assimilation is performed for the element \( RT_2P_3 \) and regular refined meshes, see Tab.1. The mass loss and the absolute velocity error \( \varepsilon_{\text{abs}} \) in the cuts \( C_1 \), \( C_2 \) and \( C_4 \), see Fig. 1(left), are evaluated with respect to a fine-grid solution with a mixed Taylor-Hood Galerkin element and listed in Tab.1.

| mesh level | M1   | M2   | M3   | M4   | M2 + data assimilation |
|------------|------|------|------|------|------------------------|
| \( n_{\text{ele}} \) | 224  | 896  | 3584 | 14336 | 896                    |
| \( n_{\text{dof}} \) | 6732 | 26904| 107568 | 430176 | 26904                 |
| mass loss  | 68.8 | 45.4 | 15.4 | 1.4  | 1.04                   |
| error \( \varepsilon_{\text{abs}} \) | 3.80 \times 10^{-1} | 2.62 \times 10^{-1} | 9.07 \times 10^{-2} | 8.60 \times 10^{-3} | 1.21 \times 10^{-2} |

**Table 1**: Mesh level, number of elements (\( n_{\text{ele}} \)), number of degrees of freedom (\( n_{\text{dof}} \)) and results for mass loss (difference of inflow and outflow in %) and absolute velocity error (in cuts \( C_1 \), \( C_2 \), \( C_4 \)) compared to numerical reference solution

Then, the effect of data assimilation is evaluated by including the fine-grid reference data at cut \( C_3 \) into the numerical LSFEM solution using mesh level M2. The calculated mass loss and velocity error given in Tab.1 show the improvement of the numerical solution. This is also clearly visible in Fig. 2, which shows the velocity profiles in \( x_1 \)-direction at cuts \( C_1 \), \( C_2 \) and \( C_4 \). A comparison of the solutions obtained with different mesh levels without data assimilation to the solution with a coarse mesh including data, reveals a significant enhancement. In conclusion, the numerical accuracy can be greatly improved by data integration, such that even coarse meshes with low computational cost lead to accurate solutions.

![Fig. 2: Velocity profiles (in m/s) without data assimilation (mesh levels M2,M3,M4) and with data integrated into cut C3 (mesh M2)](image)
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