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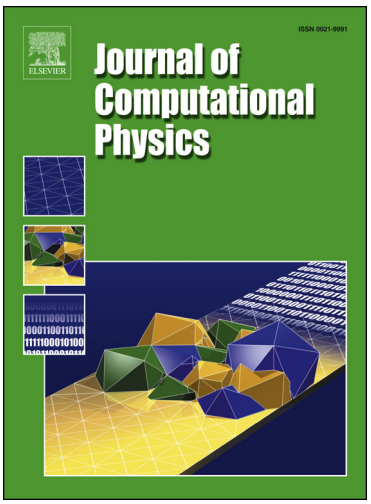

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Reduced order modeling for parametrized generalized Newtonian fluid flows

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Abstract

Non-Newtonian fluids are present in most manufacturing industry processes. Computational models used to describe the rheological behavior of such materials can be costly due to the non-linear behavior of the viscosity. This work presents a parametrized projection-based model reduction approach to address time-dependent generalized Newtonian fluids in a computational framework. We develop our discrete formulation using three ingredients: an offline-online setting for the model reduction based on a proper orthogonal and Tucker decompositions, the finite element method for the discretization of the spatial domain and finite differences for the temporal integration, and the variational multiscale approach as a stabilization technique for both the full and reduced order models. We also evaluate the reduced method with some numerical tests, where the first part involves testing the accuracy of the model reduction method for time as a single parameter of the dynamic reduced problem. The second part involves the solution of parametrized time-dependent reduced problems with the Reynolds number and the power-law index of the fluid as the varying parameters.

Keywords: Reduced Order Models, Generalized Newtonian fluids, Stabilized Finite Element Methods, Variational Multiscale Method

1. Introduction

Generalized Newtonian behavior is found in different natural and industrial problems, including petroleum sub-products [1; 2], liquid food [3; 4], liquid-solid phase change processes [5; 6], nanofluids [7; 8], and biological fluids [9; 10] (among others). The dependence of the viscosity on the velocity gradient increases the non-linearity of the problem, making it necessary to use finer meshes than Newtonian fluids, increasing the computational costs of converged solutions [11–13].

Regardless of the method, the numerical approximation of generalized Newtonian fluid flows requires an additional treatment to deal with the viscosity thinning. One consequence is the increase of the local Reynolds number and therefore, of convective instabilities. Another is the high-velocity gradient at boundary layer regions. The incompressible nature of the flow is also a classical and well-known concern regarding accurate numerical approximations. In this work, we adopt the finite element method, for which the Galerkin Least-Squares (GLS) [14; 15] and Variational MultiScale (VMS) [16; 17] stabilization methods have been successfully used in convective-dominant cases of generalized Newtonian flows. In this article, we choose the VMS formulation proposed in [18] and verified numerically in [19; 20] (see the survey in [21] for a more detailed description of the method). Additionally, we consider the issues

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discussed in [22; 23] concerning the residual-based approach lack of accuracy and the local instabilities arising from the inclusion of cross–local inner products terms.

The main issues concerning the application of fluid flow models in real-life problems are the large storage units involved in the solution and output processes, and the computational and time cost, specially in time-dependent flows. That is particularly noticeable in simulations that require solving a big set of related problems or repeatedly solving the same problem (e.g., optimization, design, etc.). Hence, the use of data-based Reduced Order Models (ROMs) has been used in different contexts [24–27] to obtain a more cost-effective numerical approximation. Any reduced modeling technique has some intrinsic drawbacks in the accuracy and stability of the solution, and some additional issues that are related to the 'high fidelity' discretization, e.g. the finite element method. Hence, extra attention should be given to stability and compatibility issues that appear in the particular case of the discrete Navier-Stokes equations. These issues are traditionally addressed with closure models that are inspired in Full Order Models (FOMs) stabilization techniques. Some of these closure models include Stream-Upward Petrov-Galerkin (SUPG) approaches in [28–30], VMS approaches in [28; 31; 32], Mori-Zwanzig approaches in [33–35] and neural network models in [35; 36]. See [37; 38] for a more extensive description and comparison of different closure models for model reduction problems.

Reduced-order modeling for non-Newtonian fluids is scarce, with a broad potential for engineering applications. In [39], a ROM based on residual minimization predicts the behavior of a power-law fluid as a function of the Reynolds number and power-law index for the steady 4:1 expansion problem. In [40], a parametrized reduced-order model for the energy equation has been formulated for steady generalized Newtonian fluids including thermal-dependency of the viscosity parameters.

In the parametrized numerical modeling of non-Newtonian fluid flows (purely viscous, viscoplastic, or viscoelastic), the rheological behavior of the fluid has to be accounted for in addition to time and global Reynolds number. This dependence on the fluid parameters can lead to abrupt changes in the apparent viscosity and hence in the local Reynolds numbers, which determine the physical response of the problem [41; 42]. The parametric calculation requires unfolding techniques to manage the third-order tensor coming from the data collection of time-dependent solutions with variable flow and fluid parameters. The essence of the parametric calculation is the same regardless of the parameter analyzed; however, the non-linearity induced by the rheological nature of the fluid poses a numerical challenge which requires the use of accurate and robust full and reduced order solvers. The parametric model reduction in the time-dependent context has been addressed in the literature with traditional projection model reduction techniques in different contexts in [43–46]. Alternatively, other methods such as Gaussian processes, Laplace transforms, and deep learning techniques have been adopted (see [47–51]). An extensive review of time-dependent model reduction methods can be found in [52].

In this work, we propose a parametrized model reduction approach for power-law non-Newtonian fluids, based in the model reduction technique first described in [53] for incompressible Navier-Stokes problems and thereafter extended to thermally coupled flows and fluid–structure interaction problems in [54; 55]. The method is an offline-online model reduction technique that involves the combination of a Proper Orthogonal Decomposition (POD), a dynamic fully residual VMS stabilization, and a Petrov-Galerkin projection for the ROM linear system solver. By considering this design, we can easily implement stabilization techniques originated in the VMS framework. Thus, the novelty of this work lies in extending the original VMS-ROM approach in two ways: a specific stabilization technique aimed at the generalized Newtonian fluids and a parametric approach of the time-dependent ROM that allows us to deal with parametrization of the fluid physical properties in an efficient way.

In the case of the VMS stabilization, we explore the term-by-term approach, which has been shown to offer better numerical performance and accuracy for non-Newtonian fluids [56–60]. This approach is advantageous in the VMS-ROM technique, since the subscales belong to a complementary space to the reduced space, rather than to the truncated POD basis alone. To address the parametric part of the ROM, we construct the reduced basis by unfolding the high-rank sampled data set onto a matrix, and then applying the Singular Value Decomposition (SVD) over such matrix. We test the proposed

approach for different problem settings using the power-law index of the fluid viscosity and the Reynolds number as parameters.

This paper is organized as follows: in section 2 we set the fundamental equations and definitions for the generalized Newtonian fluid flow problem. In section 3 we summarize the stabilized finite element formulation. In section 4 we summarize the model reduction approach: the standard POD and the POD-like algorithm for the parametric basis; and we also explain the stabilized ROM method. In section 5 we validate and test the stabilized ROM method for shear-thinning and shear-thickening fluids. Specially addressing the accuracy of the method for different power-law indices and Reynolds numbers. And lastly, in section 6 we close the paper with some conclusions and remarks.

2. Problem statement

2.1. Governing equations

Let $\Omega \subset \mathbb{R}^d$ ($d = 2, 3$) a bounded domain with boundaries defined by $\partial\Omega$, and $(0, T)$ the time interval. The strong form of the incompressible Navier-Stokes equations of a generalized Newtonian fluid consists in finding the velocity field ($\boldsymbol{u}$) and the pressure field (p), such that

$$\rho\frac{\partial \boldsymbol{u}}{\partial t} + \rho\boldsymbol{u}\cdot\nabla\boldsymbol{u} + \nabla p - \nabla\cdot 2\eta(\boldsymbol{u})\nabla^s\boldsymbol{u} = \boldsymbol{f} \quad \text{in } \Omega,\ t\in(0,T), \tag{1a}$$

$$\nabla\cdot\boldsymbol{u} = 0 \quad \text{in } \Omega,\ t\in(0,T), \tag{1b}$$

where $\boldsymbol{f}$ represents the vector of external forces, ρ is the density of the fluid, and $\eta(\boldsymbol{u})$ is the kinematic viscosity of the fluid, which for a generalized Newtonian fluid, depends on the velocity gradient and is called apparent viscosity. Take into account that bold characters are associated with vectors and tensors as notation. Equations (1a) and (1b) have to be supplied with appropriate initial and boundary condition

In this work, we describe the non-Newtonian behavior of the fluid using the power-law model, which defines the apparent viscosity as

$$\eta(\boldsymbol{u}) = m\dot{\gamma}^{n-1}, \tag{2}$$

where $\dot{\gamma} = \sqrt{\frac{1}{2}\left(\dot{\boldsymbol{\gamma}} : \dot{\boldsymbol{\gamma}}\right)}$ represents the magnitude of the rate of deformation tensor $\dot{\boldsymbol{\gamma}} = \nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T$. As constitutive parameters, m represents the consistency index and n the power-law index of the fluid. It is well known that if $n > 1$, the fluid is called shear-thickening, and if $n < 1$, the fluid is called shear-thinning. A typical issue when using this model is the possibilities of zero and infinity viscosities, this is addressed by setting a parameter that depends on the consistency index that does not allow viscosity to go above $\eta = 10,000m$ or below $\eta = m/10,000$.

Other purely-viscous constitutive laws used in numerical modeling and engineering are the Carreau or Carreau-Yasuda, the Cross, and the Ellis models. These models, under the inclusion of other constitutive parameters, allow adjusting the transition from the Newtonian plateau into the power-law region, and includes cut-off limits for the apparent viscosity [10; 13; 61]. We choose to use the the power-law model in this work because it is the simplest of all non-Newtonian alternatives, most of the generalized Newtonian models include it among their constitutive parameters, and it can be used as a proof of concept for the method.

2.2. Variational formulation and Galerkin problem

In order to write the weak form of the problem, let us introduce some standard notation. As usual, the space of square integrable functions in a domain Ω is denoted by $L^2(\Omega)$, while the space of functions whose first derivative is square integrable, is denoted by $H^1(\Omega)$. The space $H^1_0(\Omega)$ consist of functions in $H^1(\Omega)$ vanishing on $\partial\Omega$. Additionally, the parenthesis $\langle\cdot,\cdot\rangle$ are used to denote the product of two functions. If $f, g \in L^2(\Omega)$, we write the inner product as $\langle\cdot,\cdot\rangle = (\cdot,\cdot)$.

Let $\mathcal{V} = H_0^1(\Omega)^d$ be the velocity space and $\mathcal{Q} = L^2(\Omega)/\mathbb{R}$ the pressure space. If we denote $\mathcal{Y} := \mathcal{V} \times \mathcal{Q}$ as the space of the unknowns, the weak form of the equation (1) consists in finding $\boldsymbol{y} = [\boldsymbol{u}, p] : (0, T) \to \mathcal{Y}$ and satisfying the initial condition, such that

$$\left(\rho \frac{\partial \boldsymbol{u}}{\partial t}, \boldsymbol{v}\right) + B(\boldsymbol{u}; \boldsymbol{y}, \boldsymbol{\psi}) = \langle \boldsymbol{f}, \boldsymbol{v} \rangle, \quad \forall \boldsymbol{\psi} = [\boldsymbol{v}, q] \in \mathcal{Y}, \tag{3}$$

where $\boldsymbol{f}$ belongs to $(H^{-1}(\Omega))^d$, which represents the topological dual of $H_0^1(\Omega)$. Here, the bilinear form is defined as

$$B(\hat{\boldsymbol{u}}; \boldsymbol{y}, \boldsymbol{\psi}) := 2\eta(\boldsymbol{u})(\nabla^s \boldsymbol{u}, \nabla^s \boldsymbol{v}) + \langle \rho \hat{\boldsymbol{u}} \cdot \nabla \boldsymbol{u}, \boldsymbol{v} \rangle - (p, \nabla \cdot \boldsymbol{v}) + (q, \nabla \cdot \boldsymbol{u}),$$

with $\hat{\boldsymbol{u}}$ used to highlight the non-linearity of the problem, which will also be used in the discrete problem as the fixed point velocity by adding the sub-index h.

The Galerkin approximation is obtained using conforming finite element spaces $\mathcal{V}_h \subset \mathcal{V}$ and $\mathcal{Q}_h \subset \mathcal{Q}$ in the usual manner. If $\mathcal{Y}_h := \mathcal{V}_h \times \mathcal{Q}_h$ and $\boldsymbol{y}_h = [\boldsymbol{u}_h, p_h]$, the Galerkin problem consist in finding $\boldsymbol{y}_h : (0, T) \to \mathcal{Y}_h$, such that

$$\left(\rho \frac{\partial \boldsymbol{u}_h}{\partial t}, \boldsymbol{v}_h\right) + B(\boldsymbol{u}_h; \boldsymbol{y}_h, \boldsymbol{\psi}_h) = \langle \boldsymbol{f}, \boldsymbol{v}_h \rangle, \tag{4}$$

for all $\boldsymbol{\psi}_h = [\boldsymbol{v}_h, q_h] \in \mathcal{Y}_h$, and satisfying the initial condition in a weak sense.

For the time derivative of the momentum equation, the second-order backward difference scheme is used, which reads as

$$\frac{\partial \boldsymbol{u}_h}{\partial t} = \frac{3\boldsymbol{u}_h^{j+1} - 4\boldsymbol{u}_h^j + \boldsymbol{u}_h^{j-1}}{2\delta t} + \mathcal{O}(\delta t^2), \tag{5}$$

where δt corresponds to the size of a uniform partition of the time interval $(0, T)$, while, $\mathcal{O}(\cdot)$ represents the approximation order of the scheme. The superscript indicates the time step where the variable is being approximated, so that $\boldsymbol{u}_h^j$ is an approximation to $\boldsymbol{u}_h$ at time $t^j = j\delta t$.

3. Stabilized finite element formulation

The idea of the VMS framework is to decompose the space of the unknown into the finite-dimensional space $\mathcal{Y}_h$, and an infinite-dimensional one, $\breve{\mathcal{Y}}$, so that $\mathcal{Y} = \mathcal{Y}_h \oplus \breve{\mathcal{Y}}$. The unknown and the test functions are accordingly split as $\boldsymbol{y} = \boldsymbol{y}_h + \breve{\boldsymbol{y}}$ and $\boldsymbol{v} = \boldsymbol{v}_h + \breve{\boldsymbol{v}}$, respectively. Among other benefits, the VMS improves the stability of the Galerkin finite element method. The main task behind the method is to model the infinite scale or *subscales* in terms of the resolved finite element scales, thus maintaining the number of unknowns of the original problem.

3.1. Non-residual term-by-term VMS formulation

We follow the non-residual VMS formulation proposed and tested numerically in [18; 19], which we denote as term-by-term VMS stabilization. To avoid repeating information from the original paper, we summarize the key points.

The stabilized methods modify the discrete Galerkin formulation by adding terms designed to enhance stability without upsetting accuracy. The distinctive feature of this stabilization technique is its non-residual structure, which guarantees that the number of stabilization terms is the minimum. That is achieved by using the Helmholtz decomposition and by neglecting all cross inner product terms