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Abstract: *Developing a numerical and algorithmic tool which correctly identifies unyielded regions in yield stress fluid flow is a challenging task. Two approaches are commonly used to handle the singular behaviour at the yield surface, i.e. the Augmented Lagrangian approach and the regularization approach, respectively. Generally in the regularization approach, solvers do not perform efficiently when the regularization parameter gets very small. In this work, we use a formulation introducing a new auxiliary stress. The three field formulation of the yield stress fluid corresponds to a regularization-free Bingham formulation. The resulting set of equations arising from the three field formulation is solved efficiently and accurately by a monolithic finite element method. The velocity and pressure are discretized by the higher order stable FEM pair* Q_2/P_1^{disc} *and the auxiliary stress is discretized by the* Q_2 *element.*

Furthermore, this problem is highly nonlinear and presents a big challenge to any nonlinear solver. Therefore, we developed a new adaptive discrete Newton method, which evaluates the Jacobian with the divided difference approach. We relate the step length to the rate of the actual nonlinear reduction for achieving a robust adaptive Newton method. We analyse the solvability of the problem along with the adaptive Newton method for Bingham fluids by doing numerical studies for a prototypical configuration "viscoplastic fluid flow in a channel".

1 INTRODUCTION

A viscoplastic fluid is a viscous fluid with yield stress: A fluid that requires the applied stress above a certain non-zero limit of the yield stress to deform and to start flowing like a fluid. Below this non-zero limit of the yield stress the fluid behaves like a solid. The difference of this behaviour can be seen from the constitutive law of Bingham viscoplastic fluids.

$$\boldsymbol{\tau} = \begin{cases} 2\eta \mathbf{D}(\boldsymbol{u}) + \tau_s \dfrac{\mathbf{D}(\boldsymbol{u})}{\|\mathbf{D}(\boldsymbol{u})\|} & \text{if } \|\mathbf{D}(\boldsymbol{u})\| \neq 0 \\ \|\boldsymbol{\tau}\| \leq \tau_s & \text{if } \|\mathbf{D}(\boldsymbol{u})\| = 0 \end{cases} \tag{1}$$

where $\mathbf{D}(\boldsymbol{u}) = \frac{1}{2}(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T)$ denotes the strain rate tensor, and τ_s denotes the yield stress. The Bingham model describes the nature of the viscoplastic fluids. These fluids are found in many practical applications, for example health/cosmetics (gels, creams, etc.), foods (yoghurt, butter, etc.), industrial (cement slurries, drilling mud, co-extrusion operations, etc.). One direct application is viscoplastic lubrication (hydraulic fracturing) and macro encapsulation [1]: Heavy crude oil transportation along pipelines, coal-water slurry transportation and co-extrusion operations are examples of such lubrication. In this process, the stabilization of the interfaces in multi-layer shear flows [2] by means of viscoplastic fluids is the main interest. However, the accurate determination of yield surfaces is required. Developing a numerical and algorithmic tool which correctly identifies unyielded regions in the flow is a challenging task. Indeed, to handle the singular behaviour at the yield surface leads researchers in the viscoplastic community to adopt two approaches. Firstly, the regularization approach [3, 4, 5] where the potentially "infinite" viscosity is replaced by a large finite effective viscosity making the yield surfaces dependent on the regularization. Secondly, the Augmented Lagrangian approach [6, 7] which is based on the exact yield stress model via a non-differential functional which is augmented with stabilization terms and typically solved iteratively using an Uzawa-type algorithm [8].

Generally in the regularization approach, solvers do not perform efficiently when the regularization parameter gets very small. In this work, we use a formulation introducing a new auxiliary stress [9]. The corresponding three-field formulation of yield stress fluids corresponds to a regularization-free Bingham model. The resulting saddle-point problem is solved efficiently and accurately by a monolithic finite element method.

2 GOVERNING EQUATIONS

It is difficult to model mathematically the Bingham constitutive law for viscoplastic fluids. The problem arises due to the non-differentiability of the viscosity in the constitutive law and needs to be treated in a special way. The Bingham constitutive law is given as follows

$$\boldsymbol{\tau} = \begin{cases} \left(2\eta + \dfrac{\tau_s}{\|\mathbf{D}(\boldsymbol{u})\|}\right)\mathbf{D}(\boldsymbol{u}) & \text{if } \|\mathbf{D}(\boldsymbol{u})\| \neq 0 \\ \|\boldsymbol{\tau}\| \leq \tau_s & \text{if } \|\mathbf{D}(\boldsymbol{u})\| = 0 \end{cases} \tag{2}$$

with non-linear viscosity:

$$\eta(\|\mathbf{D}(\boldsymbol{u})\|) = 2\eta + \frac{\tau_s}{\|\mathbf{D}(\boldsymbol{u})\|} \tag{3}$$

The problem of differentiability arises when the viscosity becomes infinite in the rigid zone, i.e. $\|\mathbf{D}(\boldsymbol{u})\| = 0$. Therefore, one approach is to use regularization to overcome this problem. The purpose is to make the viscosity smooth and differentiable over the whole domain. There are various regularization models in the literature. Allouche et al. [10] introduced a regularization parameter simply added in the denominator. Bercovier and Engelman [11] and Tanner et al. [12] proposed different regularization functions. Papanastasiou [13] introduced an exponential expression in the regularization model to hold for any shear rate by adding a small parameter. The corresponding Navier-Stokes equations for the steady incompressible flow reads

$$\begin{cases} -\nabla \cdot \boldsymbol{\tau} + \nabla p = 0 & \text{in } \Omega \\ \nabla \cdot \boldsymbol{u} = 0 & \text{in } \Omega \\ \boldsymbol{u} = \boldsymbol{g}_D & \text{on } \Gamma_D \end{cases} \tag{4}$$

where $\boldsymbol{\tau}$ is stress tensor from (2) with regularized viscosity. We have already discussed above that the rigid zone produces a singularity and to overcome this problem, we use the Bercovier and Engelman regularization in this work. The real viscoplastic solution can only be achieved when the regularization parameter is very small ($\epsilon \to 0$) but this situation is difficult for the numerical solver. We proceed within the framework of a three-field Stokes problem, by introducing a new auxiliary stress [9] as follows:

$$\boldsymbol{\sigma} = \frac{\mathbf{D}(\boldsymbol{u})}{\|\mathbf{D}(\boldsymbol{u})\|_\epsilon} \tag{5}$$

Then, the three-field $(\boldsymbol{u}, \boldsymbol{\sigma}, p)$ system of Bingham fluid flow equations is given as follows:

$$\begin{cases} \|\mathbf{D}(\boldsymbol{u})\|_\epsilon \boldsymbol{\sigma} - \mathbf{D}(\boldsymbol{u}) = 0 & \text{in } \Omega \\ -\nabla \cdot (2\eta \mathbf{D}(\boldsymbol{u}) + \tau_s \boldsymbol{\sigma}) + \nabla p = 0 & \text{in } \Omega \\ \nabla \cdot \boldsymbol{u} = 0 & \text{in } \Omega \\ \boldsymbol{u} = \boldsymbol{g}_D & \text{on } \Gamma_D \end{cases} \tag{6}$$

System (6) represents the mixed formulation, which solves the regularized as well as the regularization-free Bingham problem, i.e. for $\epsilon = 0$. The numerical studies shown in the next sections describe the advantages of the formulation, particularly that we can achieve a true viscoplastic solution by solving a regularization-free Bingham model.

3 FINITE ELEMENT METHOD

The finite element method is chosen for the discretization in space. The strong form of the system of equations in (6) is converted into the weak formulation by multiplying it with the test functions and integrated over the whole domain. We consider three test functions $\boldsymbol{v}, q$ and $\boldsymbol{\tau}$, and multiply then with the system of equations (6). The resulting weak forms reads after partial integration:

$$\begin{aligned} \int_\Omega \Big(\|\mathbf{D}(\boldsymbol{u})\|_\epsilon \boldsymbol{\sigma} : \boldsymbol{\tau} \Big)\, dx - \int_\Omega \Big(\mathbf{D}(\boldsymbol{u}) : \boldsymbol{\tau} \Big)\, dx = 0 \quad \text{in } \Omega \\ \int_\Omega \Big(2\eta \mathbf{D}(\boldsymbol{u}) : \mathbf{D}(\boldsymbol{v}) \Big)\, dx + \int_\Omega \tau_s \Big(\boldsymbol{\sigma} : \mathbf{D}(\boldsymbol{v}) \Big)\, dx - \int_\Omega p\ \nabla \cdot \boldsymbol{v}\, dx = 0 \quad \text{in } \Omega \\ \int_\Omega q\ \nabla \cdot \boldsymbol{u}\, dx = 0 \quad \text{in } \Omega \end{aligned} \tag{7}$$

Let $\mathbb{V} = \boldsymbol{H}_0^1(\Omega) := (H_0^1(\Omega))^2$, $\mathbb{Q} = L_0^2(\Omega)$, and $\mathbb{M} = (L^2(\Omega))^{2\times 2}_{\text{sym}}$ be the spaces for the velocity, pressure and stress, respectively, associated with $\|.\|_{1,\Omega}$ and $\|.\|_{0,\Omega}$. Let $\mathbb{V}'$, $\mathbb{Q}'$, and $\mathbb{M}'$ be their corresponding dual spaces: We introduce the approximation spaces:

$$\begin{aligned} \mathbb{V}^h &= \left\{ \boldsymbol{v}_h \in \mathbb{V}, \boldsymbol{v}_{h|K} \in (Q_2(K))^2 \right\} \\ \mathbb{M}^h &= \left\{ \boldsymbol{\tau}_h \in \mathbb{M}, \boldsymbol{\sigma}_{h|K} \in (Q_2(K))^{2\times 2} \right\} \\ \mathbb{Q}^h &= \left\{ q_h \in \mathbb{Q}, q_{h|K} \in P_1^{\text{disc}}(K) \right\} \end{aligned} \tag{8}$$

Velocity, stress and pressure are discretized using $Q_2, Q_2, P_1^{\text{disc}}$ finite elements, respectively, as shown in Figure 1.

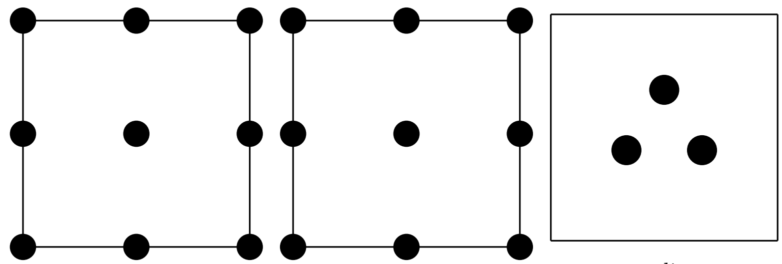


Figure 1: Finite elements Q_2, Q_2, P_1^{disc} for velocity, stress and pressure, respectively, on each quadrilateral

However, in the rigid zone $\|D\| = 0$, the finite element space $\mathbb{V}^h$ and $\mathbb{M}^h$ do not satisfy the LBB condition, the remedy is an apropriate stabilization technique. The following jump term might be added [14, 15]

$$j_{\boldsymbol{u}}(\boldsymbol{u}_h, \boldsymbol{v}_h) = \sum_{E\in\mathcal{E}_i} \gamma_u h \int_E [\nabla \boldsymbol{u}_h] : [\nabla \boldsymbol{v}_h] \; d\Omega \tag{9}$$

where γ_u is a constant parameter and h is the mesh size.

4 ADAPTIVE DISCRETE NEWTON

The problem (6) is highly nonlinear and presents a big challenge to any nonlinear solver. Iterative solvers, e.g. Newton and the fixed point iteration method, are used to solve such nonlinear problems in fluid dynamics. Since the Newton method usually has a faster convergence rate than the fixed point method, it is preferred in most of the cases but it is also very sensitive regarding the initial guess of the solution and depends strongly on the properties of the Jacobian matrices during the iterations. The Newton method solves the nonlinear steady system from (6) by the following steps:

Algorithm 1: Newton method solver

- Provide the input parameters, e.g. tolerance, parameters of the non linear solver, initial guess and the iteration number n
- Repeat until the tolerance is achieved
- Calculate the residual $\mathcal{R}(\mathcal{U}^n) = A\,\mathcal{U}^n - b$
- Build the Jacobian $J(\mathcal{U}^n) = \frac{\partial \mathcal{R}(\mathcal{U}^n)}{\partial \mathcal{U}^n}$
- Solve $J(\mathcal{U}^n)\; \delta\mathcal{U}^n = \mathcal{R}(\mathcal{U}^n)$
- Find the optimal value of the damping factor $\omega^n \in (-1, 0]$
- Approximate $\mathcal{U}^{n+1} = \mathcal{U}^n - \omega^n\; \delta\mathcal{U}^n$

The initial guess should be close to the final solution for achieving faster convergence. There are also some other factors in the Newton method which should be taken into account for the numerical stability, e.g. a damping factor when the solution is non-smooth. In our work, this factor is calculated by a root finding technique called line search method [16, 17]. First, the system of nonlinear equations is linearised using the Newton method, where $\mathcal{U} = (\boldsymbol{u}, \boldsymbol{\sigma}, p)$ and $\mathcal{R}_{\mathcal{U}}$ denote the discrete residuals. One Newton iteration reads:

$$\begin{bmatrix} \boldsymbol{u}^{n+1} \\ \boldsymbol{\sigma}^{n+1} \\ p^{n+1} \end{bmatrix} = \begin{bmatrix} \boldsymbol{u}^{n} \\ \boldsymbol{\sigma}^{n} \\ p^{n} \end{bmatrix} - \omega_n \begin{bmatrix} \frac{\partial R_{\boldsymbol{u}}(\mathcal{U}^n)}{\partial \boldsymbol{u}} & \frac{\partial R_{\boldsymbol{u}}(\mathcal{U}^n)}{\partial \boldsymbol{\sigma}} & \frac{\partial R_{\boldsymbol{u}}(\mathcal{U}^n)}{\partial p} \\ \frac{\partial R_{\boldsymbol{\sigma}}(\mathcal{U}^n)}{\partial \boldsymbol{u}} & \frac{\partial R_{\boldsymbol{\sigma}}(\mathcal{U}^n)}{\partial \boldsymbol{\sigma}} & \frac{\partial R_{\boldsymbol{\sigma}}(\mathcal{U}^n)}{\partial p} \\ \frac{\partial R_{p}(\mathcal{U}^n)}{\partial \boldsymbol{u}} & \frac{\partial R_{p}(\mathcal{U}^n)}{\partial \boldsymbol{\sigma}} & \frac{\partial R_{p}(\mathcal{U}^n)}{\partial p} \end{bmatrix}^{-1} \begin{bmatrix} \mathcal{R}_{\boldsymbol{u}}(\mathcal{U}^n) \\ \mathcal{R}_{\boldsymbol{\sigma}}(\mathcal{U}^n) \\ \mathcal{R}_{p}(\mathcal{U}^n) \end{bmatrix} \tag{10}$$

In the Newton method, first derivatives of the residual are needed in every nonlinear iteration called Jacobian matrix. The Jacobian is either calculated analytically or approximated by the divided difference method. The advantage of the approximation of the Jacobian is that this method acts in a black box manner so that it allows any nonlinear equations to be handled automatically without having to derive the corresponding calculations [18, 19]. In this work the Jacobian matrix is not computed exactly, instead its approximation is computed using divided differences and the corresponding j-th column is given as follows

$$\left[\frac{\partial \mathcal{R}(\mathcal{U}^n)}{\partial \mathcal{U}^n}\right]_j \approx \frac{\mathcal{R}(\mathcal{U}^n + \chi\delta_j) - \mathcal{R}(\mathcal{U}^n - \chi\delta_j)}{2\chi} \tag{11}$$

where δ_j is the vector with unit j-th component and zero otherwise. The parameter χ can be fixed or can be modified according to some norm of the solution $\|\mathcal{U}^n\|$ or the norm of the update in the previous step, i.e., $\|\delta\mathcal{U}^{n-1}\|$. The advantage of this approximation is that we don't need any knowledge of the Jacobian a priori. However, in this method, the step-length χ is a "free" parameter and the right choice might be a delicate task. Based on the perturbation analysis for the residum, it is often chosen according to the machine precision [20]. On the other hand, the sensitivity study of the nonlinear behavior of power law models w.r.t. the step-length parameter χ, the mesh width h and the strength of the nonlinearity suggest an adaptive choice [21, 22]. Indeed, choosing χ too big leads to the loss of the advantageous quasi-quadratic convergence behaviour, while very small parameter values for χ can lead to divergence, due to numerical instabilities. So, a process allowing for bigger step-length parameter χ is worthy for removing numerical instability. Loosely speaking, bigger step-length parameter χ increases the set of admissible Jacobian for nonregular solutions. As a result, there are thresholds of the residuum's norm which can be used for the choice of the step-length parameter χ as a step function. In order to relate continuously these thresholds of the residuum's norm to the successive nonlinear reduction

$$r_n = \frac{\|\mathcal{R}(\mathcal{U}^n)\|}{\|\mathcal{R}(\mathcal{U}^{n-1})\|} \tag{12}$$

we use the characteristic function introduced in [23]

$$f(r_n) = 0.2 + \frac{0.4}{0.7 + \exp(1.5 r_n)} \tag{13}$$

or the slightly modified ones introduced in [24]. A new adaptive step-length strategy is considered as follows

$$\chi_{n+1} = f^{-1}(r_n)\chi_n \tag{14}$$

5 NUMERICAL RESULTS

We analyse the solvability of the problem along with the adaptive Newton method for Bingham fluids by doing numerical studies for a prototypical configuration, i.e. "viscoplastic fluid flow in a channel".

5.1 Bingham viscoplastic fluid flow in channel

The two dimensional channel domain is considered as a domain between two parallel plates with h length apart and long. The problem is solved under the assumption of Dirichlet boundary conditions on the domain $\overline{\Omega} = [0, h]^2$ according to following analytical solution:

$$u_1 = \begin{cases} \frac{1}{8}\left[(h-2\tau_s)^2 - (h-2\tau_s-2y)^2\right] & 0 \le y < \frac{h}{2} - \tau_s \\ \frac{1}{8}(h-2\tau_s)^2 & \frac{h}{2} - \tau_s \le y \le \frac{h}{2} + \tau_s \\ \frac{1}{8}\left[(h-2\tau_s)^2 - (2y-2\tau_s-h)^2\right] & \frac{h}{2} + \tau_s < y \le h \end{cases} \tag{15}$$

$u_2 = 0$ and $p = -x + c$ [25]. The viscosity is set to be $\eta = 1$, the body force is $\boldsymbol{f} = 0$ and $h = 1$ is considered. The rigid zone is the region of constant velocity, i.e.

$$\frac{h}{2} - \tau_s \le y \le \frac{h}{2} + \tau_s \tag{16}$$

A comparison study is carried out between the new discrete adaptive Newton strategy and the classical Newton for the primitive variable formulation of a Bingham fluid in a channel flow. Applying both method the number of nonlinear iterations is presented in Table [1]. For the coarse refinement level (L=2 in the present case), starting with the zero solution as an initial guess, we perform Newton iterations until the tolerance is achieved. However, the next refinement level takes the solution from the previous refinement level as an initial solution. For the first test, we choose the yield stress value to be $\tau_s = 0.23$ because this value is aligned with the coarse mesh. It is observed that the primitive variable formulation along with the classical Newton method faces difficulties in convergence when the regularization parameter $\epsilon \to 0$. On the other hand, the adaptive Newton solver is able to converge even for very small values of ϵ, exhibiting the advantages of our newly developed solver. Moreover, it shows a good speed of convergence for all cases of regularized Bingham fluid.

Table 1: **Regularized viscosity approach in primitive variable $(\boldsymbol{u}, p)$:** Number of iterations of the nonlinear solver in a channel flow at yield stress $\tau_s = 0.23$ for the adaptive Newton and the classical Newton at different mesh refinement level L, the stopping criterion is 10^{-6}.

$\downarrow$ L/ϵ $\rightarrow$	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}	0	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}	0
	Newton						**Adaptive Newton**					
3	2	3	-	-	-	-	4	4	5	5	9	-
4	2	3	-	-	-	-	4	4	5	5	9	-
5	2	3	-	-	-	-	4	4	6	5	9	-

Table 2: **Regularization-free three-field formulation:** Number of iterations of the non-linear solver in a channel flow at yield stress $\tau_s = 0.23$ for the adaptive Newton and the classical Newton at different mesh refinement level L, the stopping criterion is 10^{-6}.

$\downarrow$ L/ϵ $\rightarrow$	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}	0	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}	0
	Newton						**Adaptive Newton**					
3	2	3	4	6	9	1	2	2	2	5	1	2
4	2	3	4	8	9	1	1	2	2	4	2	2
5	1	2	3	9	5	2	1	1	1	1	3	1

Testing the efficiency of the three-field formulation for the unregularized Bingham problem, a numerical study is carried out for both of the Newton strategies shown in Table 2. The efficiency of the three-field formulation and the robustness of the adaptive strategy for the discrete Newton is showcased successfully. The yield stress value is kept similar, i.e. $\tau_s = 0.23$ as in Table 1. Simulations are performed for different values of regularization parameter ϵ starting from 10^{-1} to 10^{-5} and then also for regularization-free Bingham $\epsilon = 0$. Figure 2 shows the velocity, pressure and norm of the strain rate tensor $\|\mathbf{D}(\boldsymbol{u})\|$ contours at refinement level L=5 ($h_x = 1/32, h_y = 1/96$) for regularization-free Bingham. The pressure distribution is different inside and outside of the rigid zone. It shows a discontinuity near the interface and the distribution mainly depends on the yield stress value τ_s [25].

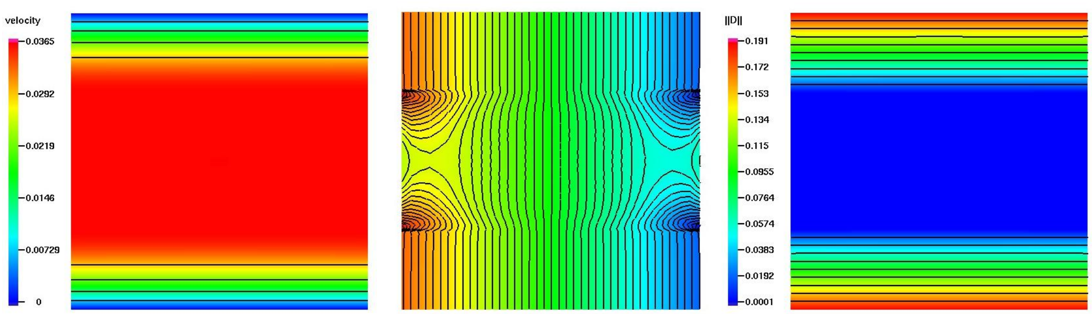
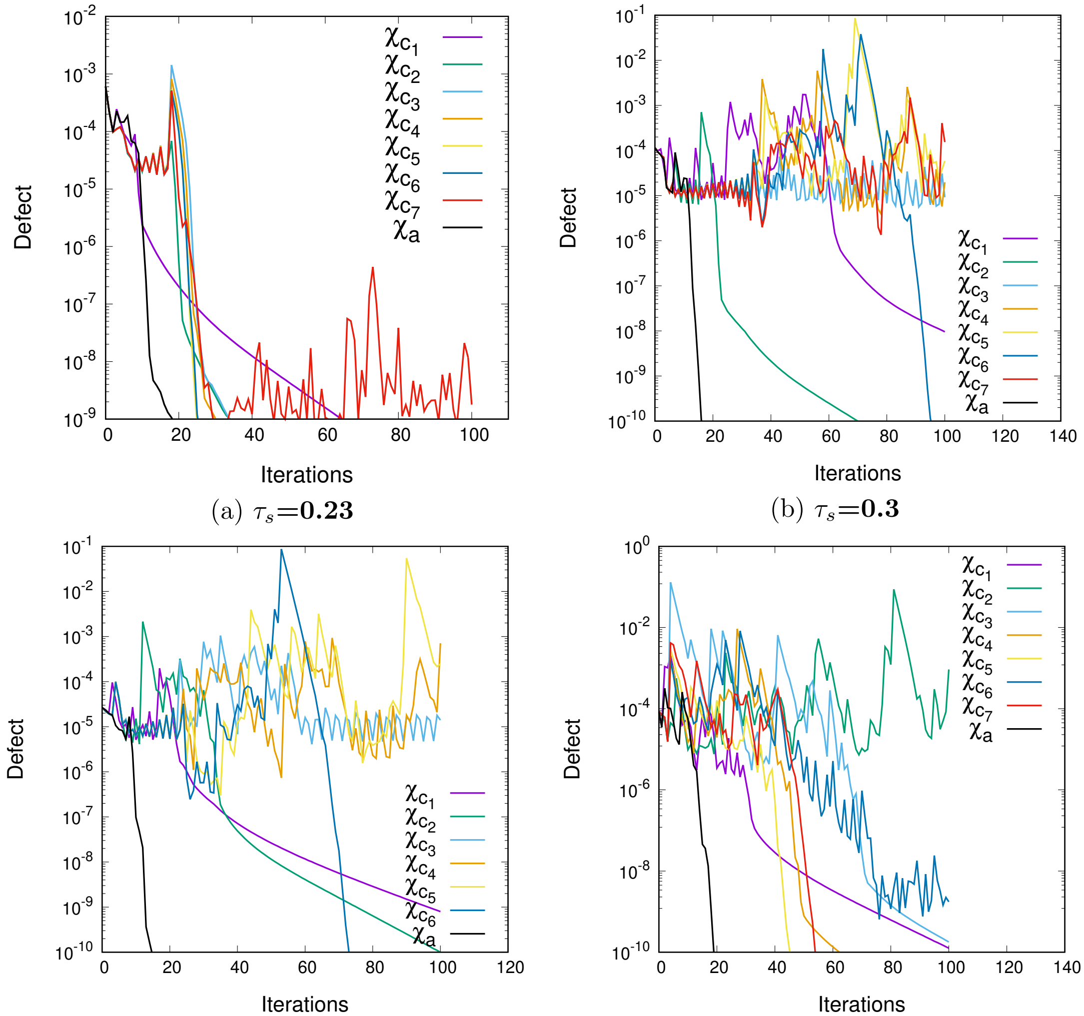


Figure 2: Visualization of the velocity contours, pressure and $\|\mathbf{D}(\boldsymbol{u})\|$ for the non-regularized Bingham fluid flow in a channel with $\tau_s = 0.23$ at refinement level L=5 ($h_x = 1/32, h_y = 1/96$).

It can be seen from the figure that the three-field formulation accurately predicts the division of the rigid and fluid zone and provides the true solutions of the problem. Moreover, the formulation can be solved exactly irrespective of the Newton solver type (classical or adaptive). Figure 3 plots the comparison of the presented discrete adaptive Newton with the classical approach. When the length χ of the Jacobian approximation in the Newton method is chosen as constant the solver either converges very slowly or it starts to oscillate. In our adaptive Newton, χ changes dynamically between the iterations. Initially it is relaxed and once the solution enters the radius of convergence then χ gets smaller to achieve the accuracy of the solution. To highlight the efficiency and robustness of our newly developed solver, the yield stress value is increased from $\tau_s = 0.23$ to $0.3, 0.35$ and $\tau_s = 0.4$. All of these tests are carried out for the regularization-free Bingham case and the solver shows fast convergence by dynamically adapting the step-length during the iterations.



(a) τ_s=**0.23** (b) τ_s=**0.3**

(c) τ_s=**0.35** (d) τ_s=**0.4**

Figure 3: **Nonlinear convergence w.r.t χ for adaptive-Newton method**: The norm of the residual versus number of iterations w.r.t two strategies (constant and adaptive) at refinement level L=2 ($h_x = 1/4, h_y = 1/12$) with the constant χ strategy (set as $\chi_{c_1} = 10^{-1}, \chi_{c_2} = 10^{-2}$,..., $\chi_{c_7} = 10^{-7}$) and the adaptive strategy (χ_a changing w.r.t non linear residuum reduction).

6 CONCLUSIONS

A new adaptive Newton and regularization-free solver for yield stress fluids is developed. Firstly, by introducing a new auxiliary stress in a three-field formulation. The resulting saddle-point problem is solved with a monolithic finite element method to simulate viscoplastic flows for the correct prediction of the yielded surfaces. The advantage of this formulation is achieving a true non-regularized viscoplastic solution, i.e. $\epsilon = 0$, efficiently and accurately. The method does not effect the shape of the yield surfaces. Secondly, a robust and accurate new adaptive discrete Newton method is developed, which evaluates the Jacobian matrix with the divided difference approach and converges faster as compared to classical Newton. We have carried out several numerical experiments for a benchmark problem. This experiment shows that the number of nonlinear iterations is significantly reduced for the three-field formulation with the combination of our newly developed adaptive discrete Newton method.

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