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SEMISMOOTH NEWTON METHOD FOR VISCOPLASTIC FLOW

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1. Bingham fluids

Consider the following system describing the steady state of an (homogeneous) incompressible fluid:

$$\begin{aligned} \alpha \boldsymbol{u} - \operatorname{div}(\mathbf{S} - \boldsymbol{u}\otimes\boldsymbol{u}) + \nabla p &= \boldsymbol{f} && \text{in } \Omega, \\ \operatorname{div} \boldsymbol{u} &= 0 && \text{in } \Omega, \\ \boldsymbol{u} &= 0 && \text{on } \partial\Omega, \end{aligned} \tag{1}$$

where $\boldsymbol{u}\colon \overline{\Omega} \to \mathbb{R}^d$ represents the velocity field, $p\colon \Omega \to \mathbb{R}$ is the pressure, $\mathbf{S}\colon \Omega \to \mathbb{R}^{d\times d}_{\mathrm{sym}}$ is the shear stress; $\boldsymbol{f}\colon \Omega \to \mathbb{R}^d$ is a given body force and $\alpha \geq 0$ is a parameter that arises from an implicit time discretisation. To close the system we need additionally a constitutive law that relates the shear stress $\mathbf{S}$ to the symmetric velocity gradient $\mathbf{D} := \mathbf{D}(\boldsymbol{u}) = \frac{1}{2}(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^\top)$. The motivation here is to study the Herschel–Bulkley constitutive relation for viscoplastic fluids:

$$\begin{cases} |\mathbf{S}| \leq \tau_* \iff & \mathbf{D}(\boldsymbol{u}) = \mathbf{0}, \\ |\mathbf{S}| > \tau_* \iff & \mathbf{S} = 2\nu_* |\mathbf{D}(\boldsymbol{u})|^{r-2}\mathbf{D}(\boldsymbol{u}) + \tau_* \dfrac{\mathbf{D}(\boldsymbol{u})}{|\mathbf{D}(\boldsymbol{u})|}, \end{cases} \tag{2}$$

where $r > 1$, $\nu_* > 0$, and $\tau_* \geq 0$ is the yield stress; this relation describes many fluids that appear in nature and industry, such as drilling muds, waxy crude oil, mango jam, etc. Note that (2) cannot be written in terms of a single-valued function $\mathbf{S} = \mathcal{S}(\mathbf{D})$, but it can be very naturally written implicitly, e.g. as:

$$\mathbf{G}(\mathbf{S},\mathbf{D}) := (|\mathbf{S}| - \tau_*)^+\mathbf{S} - 2\nu_*|\mathbf{D}|^{r-2}(\tau_* + (|\mathbf{S}| - \tau_*)^+)\mathbf{D} = \mathbf{0}. \tag{3}$$

The framework of implicitly constituted fluids allows for a clean proof of existence of solutions, and avoids the use of tools such as variational inequalities.

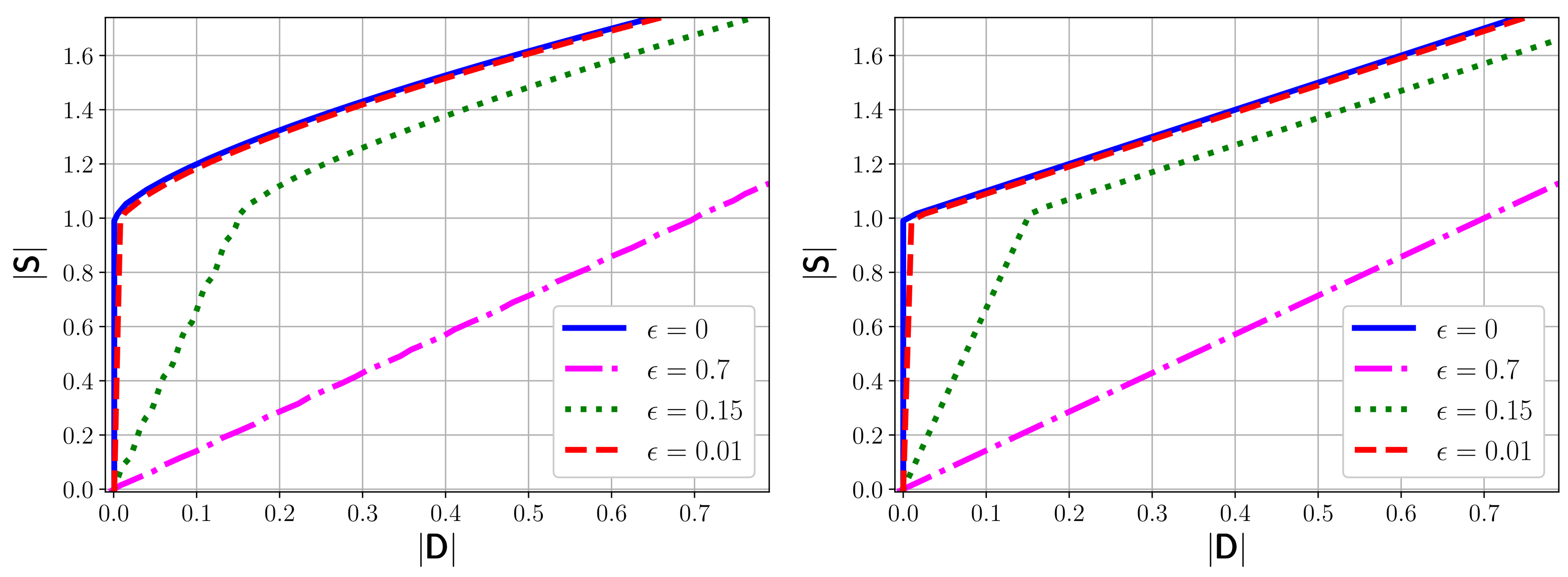
2. Regularisation

The constitutive relation (3) is not differentiable, which leads to some difficulties when performing numerical approximations. In practice, it is common to circumvent this by using regularisations such as

$$\mathbf{S}_\varepsilon = \mathcal{S}_\varepsilon(\mathbf{D}) := 2\nu_*|\mathbf{D}|^{r-2}\mathbf{D} + \tau_* \frac{\mathbf{D}}{\sqrt{|\mathbf{D}|^2 + \varepsilon^2}} \quad \varepsilon > 0,$$

but a major drawback of this is that some unphysical behaviour is introduced, and e.g. it is not clear whether $\mathbf{S}_\varepsilon \to \mathbf{S}$ as $\varepsilon \to 0$. Here we advocate the use of an alternative regularisation, introduced in [BMM2020], for which the (weak) convergence $\mathbf{S}_\varepsilon \rightharpoonup \mathbf{S}$ in $L^{r'}(\Omega)^{d\times d}$ can in fact be established. It takes the very simple form

$$\mathbf{G}_\varepsilon(\mathbf{S},\mathbf{D}) := \mathbf{G}(\mathbf{S} - \varepsilon\mathbf{D}, \mathbf{D} - \varepsilon\mathbf{S}) \quad \varepsilon > 0. \tag{4}$$



(a) Herschel–Bulkley relation ($r = 1.7$). (b) Bingham relation ($r = 2.0$).

FIGURE 1. Regularisation (4) for the relation (3) with $\tau_* = 1$.

It is known that weak solutions to the system (1)-(3) exist [BMM2020], and that finite element solutions of the nonlinear system converge [FGS2020], but the solution of such discrete nonlinear systems has not been studied in detail. Although the regularisation (4) brings several advantages (e.g. the resulting graph is strictly monotone and 2-coercive, even if the original graph does not have quadratic growth), it is not Fréchet-differentiable and so a semismooth version of Newton's method must be applied to solve the nonlinear system. The development of such a method is the purpose of this work (see [Gaz21]).

3. Semismooth Newton Method

Let $F\colon Z \to X$ be a function between two Banach spaces, U a neighborhood of $z \in Z$, and $\partial F \rightrightarrows \mathcal{L}(Z;X)$ a set-valued function with $\partial F(\hat{z}) \neq \emptyset$ for all $\hat{z} \in U$. We say that F is ∂F-semismooth (in the sense of Ulbrich [Ulb03]) if

$$\sup_{M\in\partial F(z+h)} \|F(z+h) - F(z) - Mh\|_X = o(\|h\|_Z) \quad \text{as } h \to 0. \tag{5}$$

Assuming that $\mathbf{G}\colon \mathbb{R}^{d\times d}_{\mathrm{sym}} \times \mathbb{R}^{d\times d}_{\mathrm{sym}} \to \mathbb{R}^{d\times d}_{\mathrm{sym}}$ and its local Lipschitz constant satisfy appropriate growth conditions at infinity, we can prove that its associated Nemytskii operator $\overline{\mathbf{G}}\colon L^{r'}(\Omega)^{d\times d} \times L^r(\Omega)^{d\times d} \to L^q(\Omega)^{d\times d}$ is $\partial\overline{\mathbf{G}}$-semismooth, where the elements $[\boldsymbol{d}_1, \boldsymbol{d}_2] \in \partial\overline{\mathbf{G}}$ are taken to be measurable selections of $\overline{\nabla}\mathbf{G}(\mathbf{S}(\cdot), \mathbf{D}(\boldsymbol{u}(\cdot)))$, where $\overline{\nabla}\mathbf{G}$ is the Clarke's generalised gradient of $\mathbf{G}$ (which is defined for functions between finite-dimensional spaces); note also that $\mathbf{G}_\varepsilon$ inherits these properties. Usually $q < \min\{r, r'\}$, which is an example of a norm-gap phenomenon that can result in some technical difficulties.

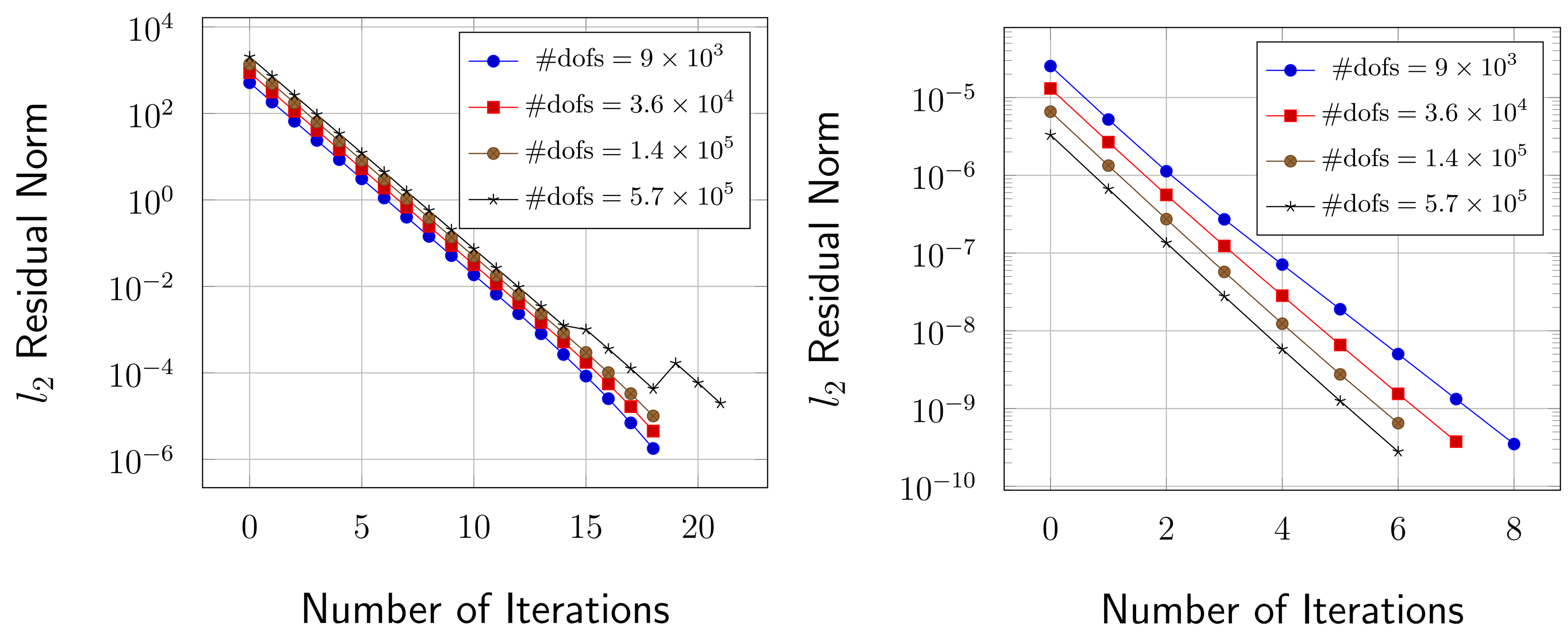
In addition, as with Newton's method, one needs to guarantee the invertibility of the derivative. In the present case, the uniform monotonicity of $\mathbf{G}_\varepsilon$ implies that the following linear system can be solved with a uniform bound (with respect to the mesh size):

$$\begin{aligned} \boldsymbol{d}_1\mathbf{T} + \boldsymbol{d}_2\mathbf{D}(\boldsymbol{v}) &= \mathbf{H}, \\ \alpha\boldsymbol{v} - \operatorname{div}\mathbf{T} + \nabla q &= \boldsymbol{h}, \\ \operatorname{div}\boldsymbol{v} &= h, \end{aligned}$$

where inertia was neglected for simplicity. Hence, if $F(z) = 0$ (with $z = (\mathbf{S}, \boldsymbol{u}, p)$) represents the system (1) with the regularised constitutive relation (4), by [Ulb03] we get that the semismooth Newton iteration $z^{k+1} \leftarrow z^k - M_k^{-1}F(z^k)$, where $M_k \in \partial F$ is arbitrary, will converge (in an appropriate function space) locally superlinearly to the solution.

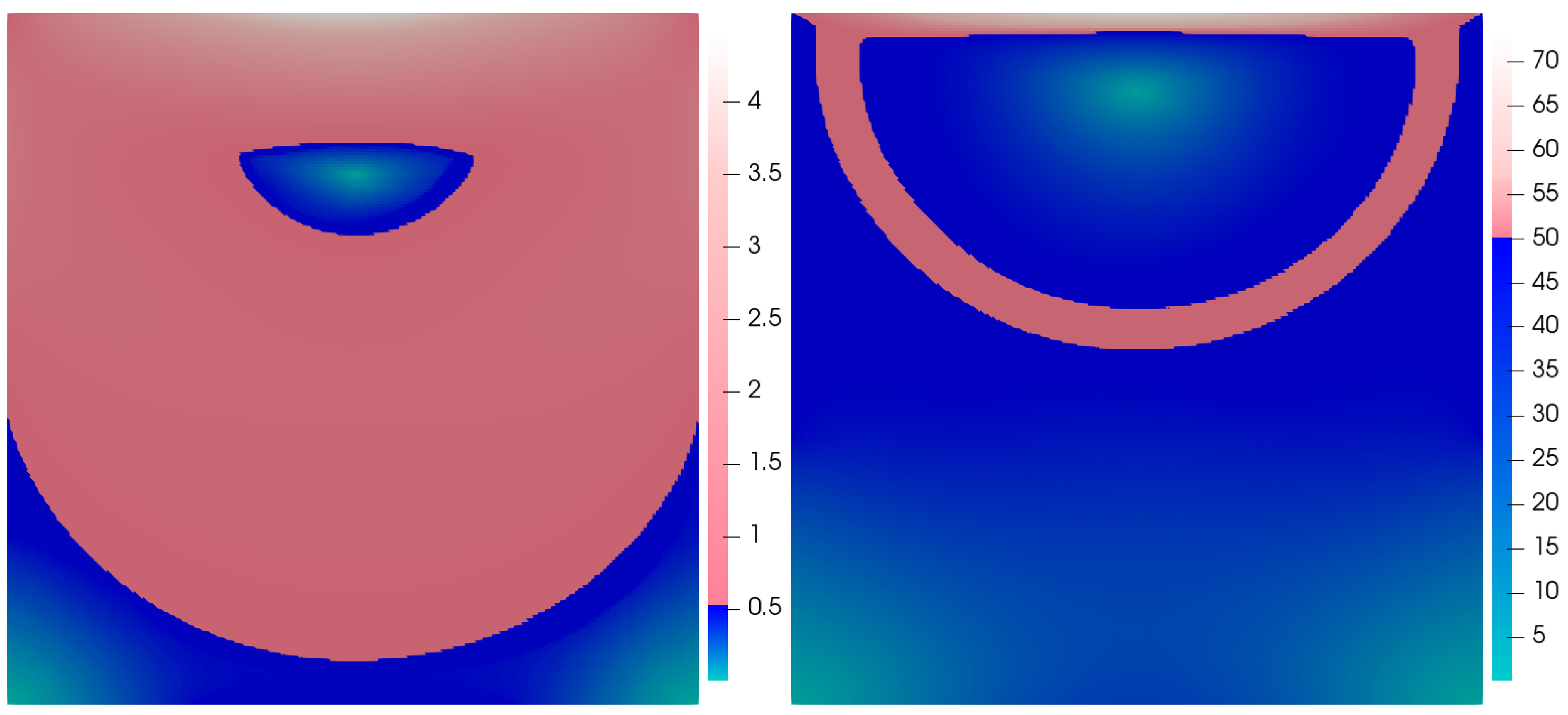
4. Numerical experiments

The semismooth Newton method was analysed at the function space level in order to avoid mesh-dependent behaviour of the iterations. This can be seen in Figure 2, where a problem of flow between two plates was solved using a stabilised $\mathbb{P}_0^{d\times d}$–$\mathbb{P}_1^d$–$\mathbb{P}_1$ element. The method also works well for a lid-driven cavity problem with moderately high values of τ_* (see Figure 3).



(c) $\varepsilon = 0.5$. (d) $\varepsilon = 0.0001$.

FIGURE 2. Mesh-independent behaviour



(e) $\tau_* = 0.5$. (f) $\tau_* = 50$.

FIGURE 3. Magnitude of $\mathbf{S}$ for the steady-state of a lid-driven cavity problem ($r = 2$, $\varepsilon = 10^{-5}$).

Selected publications

[BMM2020] Bulíček, M., Málek, J., & Maringová, E. (2020). On nonlinear problems of parabolic type with implicit constitutive relations involving flux. *ArXiv preprint: 2009.06917*

[FGS2020] Farrell, P. E., Gazca-Orozco, P. A. & Süli, E. (2020). Numerical analysis of unsteady implicitly constituted incompressible fluids: 3-field formulation. *SIAM J. Numer. Anal.*, 58(1):757–787.

[Gaz21] Gazca-Orozco, P. A. (2021). A semismooth Newton method for implicitly constituted non-Newtonian fluids and its application to the numerical approximation of Bingham flow. *ArXiv preprint: 2103.00263*

[Ulb03] Ulbrich, M. (2003). Semismooth Newton methods for operator equations in function spaces. *SIAM J. Optim.*, 13(3:805–841)

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