

An optimization based numerical approach for free boundary problems modeled by variational inequalities of the second kind

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Free Boundary Problems, June 2012

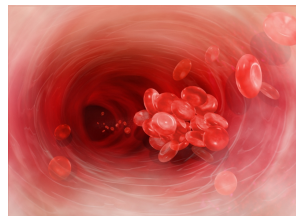
- 1 Motivation and problem statement
- 2 Dual based approach I (joint with S. González)
- 3 Dual based approach II (joint with M. Hintermüller)
- 4 Concluding remarks

What is a viscoplastic (Bingham) flow?

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Mathematical model

Boundary value problem

$$\begin{aligned} -\operatorname{Div} \sigma + (\mathbf{y} \cdot \nabla) \mathbf{y} + \nabla \phi &= \mathbf{f} && \text{in } \Omega \\ \operatorname{div} \mathbf{y} &= 0, && \text{in } \Omega \\ \mathbf{y} &= 0, && \text{on } \Gamma, \\ \sigma &= 2\mu \mathcal{E} \mathbf{y} \end{aligned}$$

\mathbf{y} : velocity vector field
 \mathcal{E} : rate of strain tensor

ϕ : pressure
 \mathbf{f} : volume force
 μ : viscosity coefficient

Mathematical model

Boundary value problem

$$\begin{aligned}
 -\operatorname{Div} \sigma + (y \cdot \nabla) y + \nabla \phi &= f && \text{in } \Omega \\
 \operatorname{div} y &= 0, && \text{in } \Omega \\
 y &= 0, && \text{on } \Gamma, \\
 \sigma &= 2\mu \mathcal{E} y + g \frac{\mathcal{E} y}{|\mathcal{E} y|}, && \text{if } \mathcal{E} y \neq 0, \\
 |\sigma| &\leq g, && \text{if } \mathcal{E} y = 0,
 \end{aligned}$$

y : velocity vector field

\mathcal{E} : rate of strain tensor

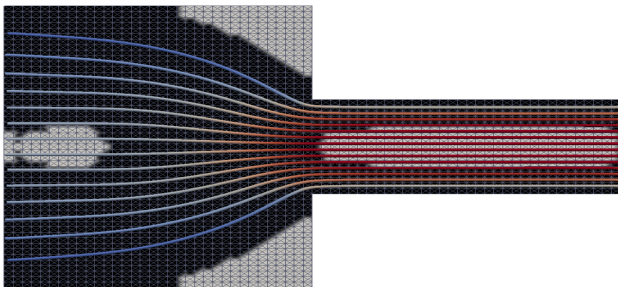
g : plasticity threshold

ϕ : pressure

f : volume force

μ : viscosity coefficient

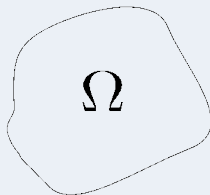
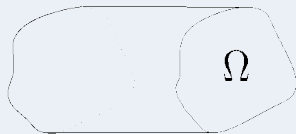
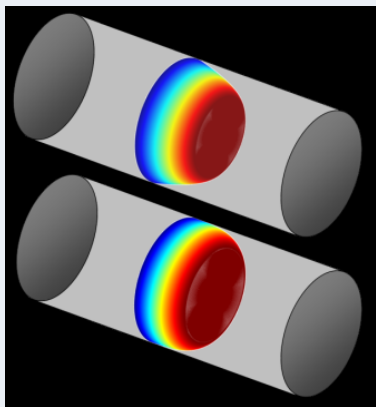
Challenges in the numerical simulation



Identification of fluid zones, rigid solid motion zones and stagnation zones.

Simplified case

Pipe of cross section Ω



Simplified mathematical model

Energy minimization (Mosolov-Miasnikov (1965))

$$\min_{y(x) \in H_0^1(\Omega)} \int_{\Omega} |\nabla y|^2 dx + g \int_{\Omega} |\nabla y| dx - \int_{\Omega} f \cdot y dx$$

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Convex nondifferentiable term!

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Variational inequality (necessary and sufficient condition)

$$a(y, v-y) + g \int_{\Omega} |\nabla v| dx - g \int_{\Omega} |\nabla y| dx \geq \int_{\Omega} f(v-y) dx, \forall v \in H_0^1(\Omega)$$

where $a(y, w) := \int_{\Omega} \nabla y^T \nabla w dx$.

Duality

Primal problem

$$\inf_{y \in H_0^1(\Omega)} J(y) = \frac{1}{2} a(y, y) + g \int_{\Omega} |\nabla y| \, dx - \int_{\Omega} f \cdot y \, dx.$$

Duality

Primal problem

$$\inf_{y \in H_0^1(\Omega)} J(y) = \frac{1}{2} a(y, y) + g \int_{\Omega} |\nabla y| \, dx - \int_{\Omega} f \cdot y \, dx.$$



Dual Problem

$$\sup_{|q(x)| \leq g} -\frac{1}{2} a(y, y)$$

subject to:

$$a(y, v) + (q, \nabla v) = (f, v), \text{ for all } v \in H_0^1(\Omega)$$

Some references

Primal approach: direct global regularization

Glowinski-Lions-Tremolieres (1976), Glowinski (1984),
Frigaard-Nouar (2005), Dean-Glowinski-Guidoboni (2007),...

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Multiplier approach: use of dual information

Glowinski (1984), Glowinski-Le Tallec (1989), Sánchez (1998), Roquet-Saramito (2003,2008), Huilgol-You (2005), Dean et al. (2007), Muravleva-Muravleva (2009), Olshanskii (2009)

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Drawback: use of rather slow methods.

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Guiding Idea: design Newton type algorithms in combination with multiplier approach

Tikhonov's Regularization

Dual Problem

$$\left\{ \begin{array}{l} \min_{|q(x)| \leq g} \frac{1}{2} a(y, y) \\ \text{subject to:} \\ a(y, v) + (q, \nabla v) = (f, v), \text{ for all } v \in H_0^1(\Omega) \end{array} \right.$$

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No unique solution!

Tikhonov's Regularization

Penalized Dual Problem

$$\left\{ \begin{array}{l} \min_{|q(x)| \leq g} \frac{1}{2} a(y, y) + \frac{1}{2\gamma} \|q\|_{\mathbb{L}^2}^2 \\ \text{subject to:} \\ a(y, v) + (q, \nabla v) = (f, v), \text{ for all } v \in H_0^1(\Omega) \end{array} \right.$$

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Theorem

There exists a unique solution $(q_\gamma, y_\gamma) \in \mathbb{L}^2(\Omega) \times H_0^1(\Omega)$ to the penalized dual problem.

Theorem

The regularized dual solutions q_γ converge to a solution \bar{q} weakly in $\mathbb{L}^2(\Omega)$ as $\gamma \rightarrow \infty$. Moreover, the correspondent primal solutions y_γ converge to the original solution \bar{y} strongly in $H_0^1(\Omega)$ as $\gamma \rightarrow \infty$.

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Regularized optimality system

$$a(y_\gamma, v) + (q_\gamma, \nabla v) = (f, v), \text{ for all } v \in H_0^1(\Omega)$$

$$\max(g, \gamma |\nabla(y_\gamma)|) q_\gamma = g \gamma \nabla(y_\gamma), \text{ for } \gamma > 0.$$

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$$\max(g, \gamma |\nabla(y_\gamma)|) q_\gamma = g \gamma \nabla(y_\gamma), \text{ for } \gamma > 0.$$

Difficulty for Newton type algorithm: *max* function is not differentiable!

Semismooth Newton method

Definition (Newton differentiability)

If there exists a neighborhood $N(x^*) \subset S$ and a family of mappings $G : N(x^*) \rightarrow \mathcal{L}(X, Y)$ such that

$$\lim_{\|h\|_X \rightarrow 0} \frac{\|\mathcal{F}(x^* + h) - \mathcal{F}(x^*) - G(x^* + h)(h)\|_Y}{\|h\|_X} = 0,$$

then \mathcal{F} is called Newton differentiable at x^* .

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Semi-smooth Newton step

$$x^{k+1} = x^k - G(x^k)^{-1} \mathcal{F}(x^k).$$

References: Hintermüller-Ito-Kunisch (2003), M. Ulbrich (2003).

Differentiability of the *max* function

The mapping $y \mapsto \max(0, y)$ from $\mathbb{R}^n \rightarrow \mathbb{R}^n$ with

$$g(y) = \begin{cases} 1 & \text{if } y \geq 0 \\ 0 & \text{if } y < 0 \end{cases}$$

as generalized derivative, is Newton differentiable.

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In function space

The mapping $\max(0, \cdot)$ from $L^q(\Omega) \rightarrow L^p(\Omega)$, with $1 \leq p < q \leq \infty$ and

$$g(v)(x) = \begin{cases} 1 & \text{if } v(x) \geq 0 \\ 0 & \text{if } v(x) < 0 \end{cases}$$

as generalized derivative, is Newton differentiable.

Algorithm for discretized problem

No regularity gain \Rightarrow finite dimensional analysis

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Convergence

If (y_h^0, q_h^0) is sufficiently close to (y_h, q_h) then the iterates (y_h^k, q_h^k) converge superlinearly to (y_h, q_h) .

Globalization based on modified Jacobian:

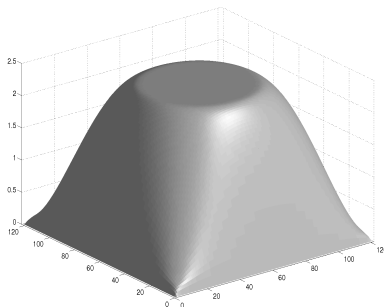


[M. Hintermüller and G. Stadler.](#)

An infeasible primal-dual algorithm for TV-based inf-convolution-type image restoration. *SIAM Journal on Scientific Computing*, 28 (1), pp. 1-23, 2006.

Numerics

- Data: $\Omega = (0, 1)^2$, $g = 1$, $\mu = 0.1$, $\gamma = 10^3$ and $f = 10$.
- Finite differences, centered differences for the gradient



- Superlinear convergence
- Very accurate determination of solid-fluid zones.

Extension to 2d Bingham flow model

Stationary model

$$\min_{y \in V} \mu \int_{\Omega} |\mathcal{E}(y)|^2 dx + g \int_{\Omega} |\mathcal{E}(v)| dx - \int_{\Omega} f \cdot y dx$$

where $V := \{v \in \mathbb{H}_0^1 : \operatorname{div} v = 0\}$, $\mathcal{E}(v) = \frac{1}{2} (\nabla v + (\nabla v)^T)$

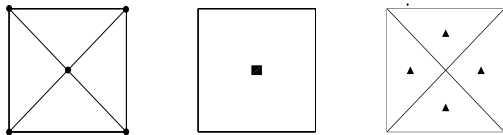
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Discretization (cross-grid \mathbb{P}_1)- \mathbb{Q}_0 elements

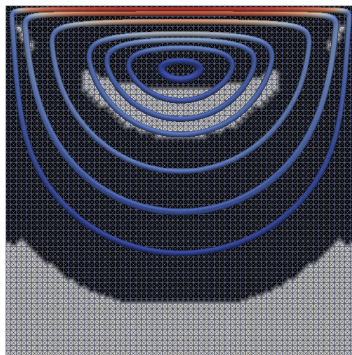
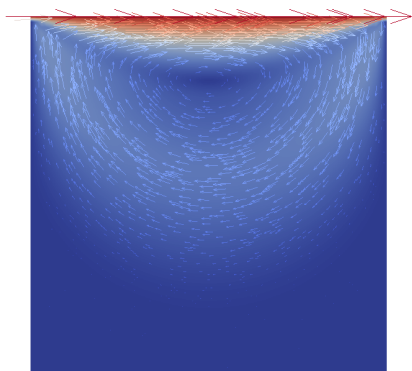


De Los R. and S. González.

Numerical simulation of two-dimensional Bingham fluid flow by semismooth Newton methods. *Journal of Computational and Applied Mathematics*, 2010.

Driven cavity flow

Data: $\Omega =]0, 1[^2$, $g = 2.5$, $\mu = 1$, $\gamma = 10^3$ and $f = 0$.



Time-dependent convective problem

Regularized system

$$\partial_t \mathbf{y}_\gamma(t) - \operatorname{Div} \Delta \mathbf{y}_\gamma(t) - \operatorname{Div} \mathbf{q}_\gamma(t) + (\mathbf{y}(t) \cdot \nabla) \mathbf{y}(t) + \nabla p(t) = \mathbf{f}(t)$$

$$\operatorname{div} \mathbf{y}_\gamma(t) = 0,$$

$$\max \left(\frac{g}{\gamma}, \|\mathcal{E} \mathbf{y}_\gamma(x, t)\| \right) \mathbf{q}_\gamma(x, t) = g \mathcal{E} \mathbf{y}_\gamma(x, t), \text{ a.e. in } Q, \gamma > 0,$$

+ I.C. and B.C..

Property: $\|\mathbf{q}_\gamma(x, t)\| \leq g$ a.e. in Q .

Suitability of the Regularized-Multiplier Approach

Theorem

There exists a unique solution $\mathbf{y}_\gamma \in L^2(0, T; V)$ for the proposed regularized system of equations, for an appropriate initial condition \mathbf{y}_0 .

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Theorem

The regularized solutions $(\mathbf{y}_\gamma, \mathbf{q}_\gamma)$ converge to the original solution $(\mathbf{y}, \bar{\mathbf{q}})$, as $\gamma \rightarrow \infty$, in the sense that

$$\int_Q |\mathbf{y}_\gamma - \mathbf{y}|^2 + \int_Q \|\nabla(\mathbf{y}_\gamma - \mathbf{y})\|^2 \rightarrow 0, \text{ and}$$

$$\mathbf{q}_\gamma \rightharpoonup \bar{\mathbf{q}} \text{ weakly in } L^2(\mathbb{L}^{2 \times 2}).$$

Semi-Discretized Regularized-Multiplier System

$$\mathbf{M}^h \frac{\partial}{\partial t} \vec{\mathbf{y}}(t) + \mathbf{A}_{\mu}^h \vec{\mathbf{y}}(t) + \mathbf{Q}^h \vec{\mathbf{q}}(t) + \mathbf{C}^h(\vec{\mathbf{y}}(t)) \vec{\mathbf{y}}(t) + B^h \vec{\mathbf{p}}(t) = \vec{\mathbf{f}}(t)$$

$$-(B^h)^{\top} \vec{\mathbf{y}}(t) = 0$$

$$\max \left(\frac{g}{\gamma}, N(\mathcal{E}^h \vec{\mathbf{y}}(t)) \right) \star \vec{\mathbf{q}}(t) = g \mathcal{E}^h \vec{\mathbf{y}}(t),$$

+ I.C.

where $\mathbf{C}^h(\vec{\mathbf{w}})$ is the F.E.M. matrix associated with the nonlinear form $(\mathbf{y}(t) \cdot \nabla) \mathbf{y}(t)$.

Time-Discretization

Backward differentiation formulae

When applied to $y' = \Psi(y)$, the BDF2 scheme reads as:

$$y^{k+2} - \frac{4}{3}y^{k+1} + \frac{1}{3}y^k = \frac{2}{3}k\Psi^{k+2}, \text{ for } k \leq \mathcal{N} - 2$$

where y^k : approximation of y at each time step k .

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Property: Second order in time

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where y^k : approximation of y at each time step k .

Property: Second order in time

BDF2: multistep method \Rightarrow requires initialization for y^0 and y^1 .

Fully-Discretized Regularized-Multiplier System

BDF2 discretization: at $t_{k+1} = (k + 1)\delta t$, for $k = 0, \dots, \mathcal{N} - 1$:

$$\left(\frac{3}{2\delta t}\mathbf{M}^h + \mathbf{A}_{\mu}^h\right) \vec{\mathbf{y}}^{k+2} + \mathbf{Q}^h \vec{\mathbf{q}}^{k+2} + B^h \vec{\mathbf{p}}^{k+2} = \vec{\mathbf{F}}^{k+2}$$

$$-(B^h)^{\top} \vec{\mathbf{y}}^{k+2} = 0$$

$$\max\left(\frac{g}{\gamma}, N(\mathcal{E}^h \mathbf{y}^{k+2})\right) \star \mathbf{q}^{\vec{k}+2} = g \mathcal{E}^h \mathbf{y}^{\vec{k}+2}.$$

$$\vec{\mathbf{F}}^{k+2} := \vec{\mathbf{f}}^{k+2} - \mathbf{C}^h(\vec{\mathbf{y}}^k) \vec{\mathbf{y}}^k + \mathbf{M}^h \left(\frac{2}{\delta t} \vec{\mathbf{y}}^{k+1} - \frac{1}{2\delta t} \vec{\mathbf{y}}^k\right) \text{ and}$$

$$\vec{\mathbf{y}} := 2\vec{\mathbf{y}}^{k+1} - \vec{\mathbf{y}}^k$$

Here $\vec{\mathbf{y}}^0 \Rightarrow$ I.C. and $\vec{\mathbf{y}}^1 \Rightarrow$ implicit Euler.



G.A. Baker, V.A. Dougalis and O.A. Karakashian

On a Higher Order Accuracy Fully Discrete Galerkin Approximation to the Navier-Stokes Equations.
Mathematics of Computation., 1982.

Flow driven cavity.

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Flow driven cavity.

$\Omega := (0, 1)^2$, plasticity threshold $g = 2.5$ and viscosity $\mu = 1$.
Mesh information: $h = \frac{1}{300}$ and $\delta t = 0.001 (\approx 0.2 * (h^{4/5}))$

Figure: Vector velocity field (left) and Rigid-Plastic zones (right)

What about mesh independence?

Regularization

Regularized dual

$$\left\{ \begin{array}{l} \min_{|q(x)| \leq g} \frac{1}{2} a(y, y) \\ \text{subject to:} \\ a(y, v) + (q, \nabla v) = (f, v), \text{ for all } v \in H_0^1(\Omega) \end{array} \right.$$

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Regularized dual

$$\left\{ \begin{array}{l} \min \quad \frac{1}{2}a(y, y) + \frac{\gamma}{2} \|(|q| - g)^+\|_{L^2(\Omega)}^2 \\ \text{subject to:} \\ a(y, v) + (q, \nabla v) = (f, v), \text{ for all } v \in H_0^1(\Omega) \end{array} \right.$$

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where $\gamma > 0$, $(\cdot)^+ = \max(0, \cdot)$.

Theorem (Convergence as $\gamma \rightarrow \infty$)

The solutions $\{q_\gamma\}$ to the regularized dual problem converge to the original solution q weakly in $\mathbb{L}^2(\Omega)$ as $\gamma \rightarrow \infty$ and

$$\operatorname{div} q_\gamma \rightarrow \operatorname{div} q \text{ strongly in } \mathbb{H}^{-1}(\Omega) \text{ as } \gamma \rightarrow \infty.$$

Moreover, the correspondent primal solutions y_γ converge to the original solution \bar{y} strongly in $H_0^1(\Omega)$ as $\gamma \rightarrow \infty$.

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Moreover, the correspondent primal solutions y_γ converge to the original solution \bar{y} strongly in $H_0^1(\Omega)$ as $\gamma \rightarrow \infty$.

Optimality system

$$\begin{aligned} -\mu \Delta y_\gamma - \text{div } q_\gamma &= f \\ \nabla y_\gamma - \frac{1}{\gamma} \overrightarrow{\Delta} q_\gamma + \max(0, \gamma(|q_\gamma| - g)) \frac{q_\gamma}{|q_\gamma|} &= 0 \end{aligned}$$

Nonsmooth system

Reformulation as operator equation

$$W(\mathbf{q}_\gamma, \mathbf{y}_\gamma) = \begin{pmatrix} -\mu \Delta \mathbf{y}_\gamma - \operatorname{div} \mathbf{q}_\gamma - \mathbf{f} \\ \nabla \mathbf{y}_\gamma - \frac{1}{\gamma} \vec{\Delta} \mathbf{q}_\gamma + \gamma \max(0, |\mathbf{q}_\gamma| - g) \frac{\mathbf{q}_\gamma}{|\mathbf{q}_\gamma|} \end{pmatrix} = \mathbf{0}.$$

Nonsmooth system

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max function is not differentiable
 \implies semismooth Newton method

Semismoothness

The mapping

$$q \mapsto (|q| - g)^+ \frac{q}{|q|}$$

is Newton differentiable from $\mathbb{L}^q(\Omega) \rightarrow \mathbb{L}^p(\Omega)$, $q > p$ with derivative

$$\mathcal{M}(q) = \chi_A(q) \frac{qq^T}{|q|} + (|q| - g)^+ \frac{1}{|q|} (id + \frac{qq^T}{|q|^2}).$$

Here $\chi_A(q)$ denotes the characteristic function of

$$\mathcal{A}(q) = \{x \in S : |q(x)| > \bar{g}\}.$$

SSN Algorithm

- (i) Choose a $q^0 \in H$; set $k := 0$
- (ii) Solve

$$\begin{aligned} & \begin{pmatrix} -\mu\Delta & -\text{div} \\ \nabla & -\frac{1}{\gamma}\vec{\Delta} + \gamma\mathcal{M}(q_k) \end{pmatrix} \begin{pmatrix} \delta_y \\ \delta_q \end{pmatrix} \\ &= \begin{pmatrix} \mu\Delta y_k + \text{div } q_k + f \\ -\nabla y_k + \frac{1}{\gamma}\vec{\Delta} q_k + \gamma \max(0, |q_k| - g) \frac{q_k}{|q_k|} \end{pmatrix} \end{aligned}$$

- (iii) Set $q^{k+1} = q^k + \delta_q$, $y^{k+1} = y^k + \delta_y^k$ and $k = k + 1$. Return to (ii).

Convergence

Theorem (Local superlinear convergence)

The Newton derivative operator is uniformly invertible. If q^0 is sufficiently close to q_γ , then the generalized Newton iteration is well-defined and satisfies

$$\|q^{k+1} - q_\gamma\|_{\mathbb{L}^2(\Omega)} = o(\|q^k - q_\gamma\|_{\mathbb{L}^2(\Omega)}) \text{ as } k \rightarrow \infty.$$

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Theorem (Global convergence)

The Newton direction is a descent direction and (with a suitable line search rule) the method converges globally.

Convergence behavior

Superlinear convergence

| Iteration | $ \mathcal{A}_k $ | increment | rate |
|-----------|-------------------|-----------|----------|
| 1 | 12800 | 0.3551 | - |
| 2 | 6518 | 1.3968 | 3.934147 |
| 3 | 11456 | 0.4949 | 0.354309 |
| \vdots | \vdots | \vdots | \vdots |
| 11 | 9932 | 0.001176 | 0.088149 |
| 12 | 9928 | 2.2032e-5 | 0.018734 |
| 13 | 9928 | 1.8242e-9 | 0.000083 |

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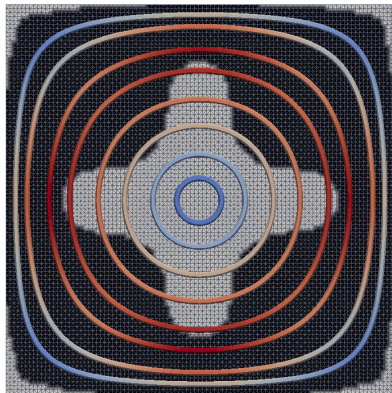
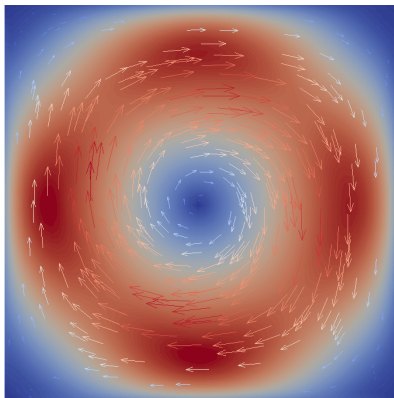
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Mesh independence:

| | | | | | | |
|-------|----|----|----|----|----|----|
| $1/h$ | 10 | 20 | 30 | 40 | 50 | 80 |
| # it. | 15 | 14 | 13 | 15 | 14 | 15 |

Reservoir flow

$$\Omega =]0, 1[^2, g = 10, \mu = 1, \gamma = 10^4, f = 300(x_2 - 0.5, 0.5 - x_1)^T.$$



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- Extension to other phenomena modeled by variational inequalities of the second kind.

Thank you!