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Non-Newtonian Fluids and Finite Elements

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Definitions

Fluid: a substance that continually deforms (flows) under an applied shear stress



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Definitions

Viscosity: a measure of the resistance of a fluid to deform under shear stress. It is commonly perceived as "thickness", or resistance to pouring.



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Definitions



Sir Isaac Newton

Newtonian Fluid: The concept was first deduced by Isaac Newton and is directly analogous to Hooke's law for a solid. A fluid that flows like water and whose stress at each point is proportional to its strain rate at that point.

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Definitions

Non-Newtonian A fluid that is not Newtonian! That is, the stress and the strain are no longer linearly related.

Shear-Thinning Viscosity decreases with increasing applied stress







Shear-Thickening Viscosity increases with increasing applied stress.

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The Physical Problem

Tightly confined flow of a non-Newtonian fluid.



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Cauchy's Equation of Motion

Equates the rate of change of momentum of a selected fluid element and the sum of all forces acting on that fluid element.

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = \nabla \cdot \mathbf{T} + \rho \mathbf{f}$$
$$\nabla \cdot \mathbf{u} = \mathbf{0}$$

- **u** velocity of fluid,
- **T** stress tensor (internal forces),
- **f** forcing function (external forces),
- ρ density.

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A Viscous Fluid



Figure: Two elemental volumes.

The stress tensor for a viscous fluid is

$$\mathbf{T} = -\mathbf{p}\mathbf{I} + \tau = \begin{bmatrix} -p & 0 & 0\\ 0 & -p & 0\\ 0 & 0 & -p \end{bmatrix} + \begin{bmatrix} \tau_{11} & \tau_{12} & \tau_{13}\\ \tau_{21} & \tau_{22} & \tau_{23}\\ \tau_{31} & \tau_{32} & \tau_{33} \end{bmatrix}$$

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A Viscous Fluid



Figure: Two elemental volumes.

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- $\tau = \mu \mathbf{e}(\mathbf{u})$ Deviatoric stress tensor.
- μ is the apparent viscosity.
- $\mathbf{e}(\mathbf{u}) = \frac{1}{2} \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^{\top} \right)$ is the rate of strain tensor.

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Navier-Stokes Equations

The stress tensor is $\mathbf{T} = -\mathbf{p}\mathbf{I} + \frac{\mu}{2} \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^{\top} \right)$

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Navier-Stokes Equations

The stress tensor is
$$\mathbf{T} = -\mathbf{p}\mathbf{I} + rac{\mu}{2}\left(
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ight)$$

Navier-Stokes Equations

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\frac{1}{\rho} \nabla \rho + \nu \nabla^2 \mathbf{u} + \mathbf{f}$$
$$\nabla \cdot \mathbf{u} = 0$$

• $\nu = \frac{\mu}{\rho}$ Kinematic viscosity.

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Newtonian Fluids

The Newtonian property is encoded in the stress tensor

$\mathbf{T}=-\mathbf{p}\mathbf{I}+\tau$

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Newtonian Fluids

The Newtonian property is encoded in the stress tensor

 $\mathbf{T} = -\mathbf{p}\mathbf{I} + \tau$

with

$$\tau = \mu \mathbf{e}(\mathbf{u}).$$

The apparent viscosity, μ , is a constant and so the stress and rate of strain are proportional – linearly related. This models a Newtonian fluid.

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Non-Newtonian Fluids

Non-linear stress tensor

$$\mathbf{T} = -\mathbf{p}\mathbf{I} + \mu\mathbf{k}\left(\mathbf{x}, |\mathbf{e}(\mathbf{u})|\right)\mathbf{e}(\mathbf{u})$$

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Non-Newtonian Fluids

Non-linear stress tensor

$$\mathbf{T} = -\mathbf{p}\mathbf{I} + \mu\mathbf{k}\left(\mathbf{x}, |\mathbf{e}(\mathbf{u})|\right)\mathbf{e}(\mathbf{u})$$

- $\mu k \left(\mathbf{x}, |\mathbf{e}(\mathbf{u})| \right)$ is the apparent viscosity,
- $|\cdot|$ is the Frobenius norm.

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Non-Newtonian Fluids

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• $\mu k \left(\mathbf{x}, |\mathbf{e}(\mathbf{u})| \right)$ is the apparent viscosity,

• $|\cdot|$ is the Frobenius norm.

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\frac{1}{\rho} \nabla \rho + 2\nu \nabla \cdot (k (\mathbf{x}, |\mathbf{e}(\mathbf{u})|) \mathbf{e}(\mathbf{u})) + \mathbf{f}$$
$$\nabla \cdot \mathbf{u} = 0$$

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Simplifying the System

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\frac{1}{\rho} \nabla \rho + 2\nu \nabla \cdot (k (\mathbf{x}, |\mathbf{e}(\mathbf{u})|) \mathbf{e}(\mathbf{u})) + \mathbf{f}$$

$$\nabla \cdot \mathbf{u} = 0$$

Assuming that the flow is tightly confined and slow, we can drop the non-linear term and neglect inertial effects. Also we assume steady flow.

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$$rac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot
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Under such restrictions, the governing equations are

$$-\mu
abla \cdot (k\left(\mathbf{x}, |\mathbf{e}(\mathbf{u})|
ight) \mathbf{e}(\mathbf{u})) + rac{1}{
ho}
abla p ~=~ \mathbf{f}$$

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The Power-Law

Observation: For typical shear-thinning fluids, μ falls with increasing shear rate

Experimental Data: The log-log plot of shear stress to rate of shear is often found to be linear with a slope between zero and one:

$$\log k (|\mathbf{e}(\mathbf{u})|) = (r-2) \log |\mathbf{e}(\mathbf{u})| + \log 2\mu$$

$$\Rightarrow k (|\mathbf{e}(\mathbf{u})|) = 2\mu |\mathbf{e}(\mathbf{u})|^{r-2}$$

Power-Law

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Choice of Constitutive Relation

Possible choices are:

- Stokes flow: $k(|\mathbf{e}(\mathbf{u})|) \equiv 1$
- Power-law model: $k(|\mathbf{e}(\mathbf{u})|) = |\mathbf{e}(\mathbf{u})|^{r-2}, \quad 1 < r < \infty$
- Ladyzhenskaya model: $k(|\mathbf{e}(\mathbf{u})|) = \mu_0 + \mu_1 |\mathbf{e}(\mathbf{u})|^{r-2}, \quad \mu_0, \mu_1 > 0$

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Of greater generality and of more practical significance is the

• Carreau model:

$$\begin{aligned} &k(|\mathbf{e}(\mathbf{u})|) = \mu_{\infty} + (\mu_0 - \mu_{\infty})(1 + \lambda |\mathbf{e}(\mathbf{u})|^2)^{(\theta - 2)/2}, \\ &\mu_0 > \mu_{\infty} \ge 0, \ \lambda > 0, \ \theta \in (0, \infty) \end{aligned}$$

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What do we Want?

• Numerical simulation of incompressible, viscous extrusion flows for shear-thinning power-law fluids.

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What do we Want?

- Numerical simulation of incompressible, viscous extrusion flows for shear-thinning power-law fluids.
- Accurate capturing of the thin boundary layers in the flow.

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What do we Want?

- Numerical simulation of incompressible, viscous extrusion flows for shear-thinning power-law fluids.
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- The accurate prediction of the free surface between two pastes with different rheological properties flowing in channels or extruders.

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Adaptive Finite Element Methods!!

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Adaptive Finite Element Methods!!

 $\mathsf{SOLVE} \to \mathsf{ESTIMATE} \to \mathsf{MARK} \to \mathsf{REFINE}$

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Adaptivity in a Channel



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Weak Formulation

Find
$$\mathbf{u} \in V = [W_0^{1,r}(\Omega)]^d$$
 and $p \in Q = L_0^{r'}(\Omega) = L^{r'}(\Omega)/\mathbb{R}$
$$a(\mathbf{u}, \mathbf{v}) + b(p, \mathbf{v}) = (\mathbf{f}, \mathbf{v}) \quad \forall \mathbf{v} \in V$$
$$b(q, \mathbf{u}) = 0 \quad \forall q \in Q.$$

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Weak Formulation

Find
$$\mathbf{u} \in V = [W_0^{1,r}(\Omega)]^d$$
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Here

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Weak Formulation

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$$a(\mathbf{u}, \mathbf{v}) + b(p, \mathbf{v}) = (\mathbf{f}, \mathbf{v}) \quad \forall \mathbf{v} \in V$$
$$b(q, \mathbf{u}) = 0 \quad \forall q \in Q.$$

Here

Inf-sup condition [Amrouche & Girault (1990)]: $\exists c_0 > 0 \text{ s.t.}$

$$\inf_{q\in \mathcal{Q}}\sup_{\mathbf{v}\in V}\frac{b(q,\mathbf{v})}{\|q\|_{\mathcal{Q}}\|\mathbf{v}\|_{V}}\geq c_{0}\qquad\forall q\in Q.$$

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Finite Element Approximation

Let $V_h \subset V$ and $Q_h \subset Q$ be finite-dimensional spaces consisting of p.w. polynomial functions, defined on a triangulation $\mathcal{T}_h = \{T\}$ of the computational domain Ω .

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Finite Element Approximation

Let $V_h \subset V$ and $Q_h \subset Q$ be finite-dimensional spaces consisting of p.w. polynomial functions, defined on a triangulation $\mathcal{T}_h = \{T\}$ of the computational domain Ω . Find $\mathbf{u}_h \in V_h$ and $p_h \in Q_h$ such that

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Finite Element Approximation

Let $V_h \subset V$ and $Q_h \subset Q$ be finite-dimensional spaces consisting of p.w. polynomial functions, defined on a triangulation $\mathcal{T}_h = \{T\}$ of the computational domain Ω . Find $\mathbf{u}_h \in V_h$ and $p_h \in Q_h$ such that

$$\begin{array}{rcl} a(\mathbf{u}_h,\mathbf{v}_h)+b(p_h,\mathbf{v}_h) &=& (\mathbf{f},\mathbf{v}_h) & \forall \mathbf{v}_h \in V_h \\ b(q_h,\mathbf{u}_h) &=& 0 & \forall q_h \in Q_h. \end{array}$$

Discrete inf-sup condition: there exists $c_0 > 0$, s.t.

$$\inf_{q_h\in Q_h}\sup_{\mathbf{v}_h\in V_h}\frac{b(q_h,\mathbf{v}_h)}{\|q_h\|_Q\|\mathbf{v}_h\|_V}\geq c_0\qquad\forall q_h\in Q_h.$$

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A Posteriori Error Analysis

How to quantify the size of the error

$$\mathbf{u}-\mathbf{u}_h, \qquad p-p_h$$

in terms of a computable bound?

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A Posteriori Error Analysis

How to quantify the size of the error

$$\mathbf{u} - \mathbf{u}_h, \qquad p - p_h$$

in terms of a computable bound?

We define the residual functionals $\mathbf{S}_1 \in V'$ and $S_2 \in Q'$ by

$$egin{array}{rcl} \langle {f S}_1,{f w}
angle &=& ({f f},{f w})-a({f u}_h,{f w})-b(p_h,{f w}) & & orall w\in V \ \langle S_2,q
angle &=& -b(q,{f u}_h) & & orall q\in Q. \end{array}$$

Our aim is to bound $\mathbf{u} - \mathbf{u}_h$ and $p - p_h$ in terms of norms of \mathbf{S}_1 and S_2 .

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Residual functionals

Here $\mathbf{S}_1 \in V'$ and $S_2 \in Q'$ are defined by:

$$egin{array}{rcl} \langle {f S}_1,{f w}
angle &=& ({f f},{f w})-a({f u}_h,{f w})-b(p_h,{f w}) & & orall w\in V \ \langle S_2,q
angle &=& -b(q,{f u}_h) & & orall q\in Q. \end{array}$$

Note the error representation formula:

$$\begin{array}{lll} a(\mathbf{u},\mathbf{w})-a(\mathbf{u}_h,\mathbf{w})+b(p-p_h,\mathbf{w}) &=& \langle \mathbf{S}_1,\mathbf{w}\rangle\\ && b(q,\mathbf{u}-\mathbf{u}_h) &=& \langle S_2,q\rangle \end{array}$$

for all $\mathbf{w} \in V$ and all $q \in Q$.

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Bounding the residual functionals

We have that

$$\langle \mathbf{S}_{1}, \mathbf{w} \rangle = \sum_{T \in \mathcal{T}_{h}} \int_{T} (\mathbf{f} + \nabla \cdot (k(|e(\mathbf{u}_{h})|)e(\mathbf{u}_{h})) - \nabla p_{h}) \cdot (\mathbf{w} - I_{h}\mathbf{w}) \, \mathrm{d}T$$
$$- \sum_{T \in \mathcal{T}_{h}} \int_{\partial T} [k(|e(\mathbf{u}_{h})|)e(\mathbf{u}_{h})\mathbf{n}_{T} - p_{h}\mathbf{n}_{T}] \cdot (\mathbf{w} - I_{h}\mathbf{w}) \, \mathrm{d}s$$

and

$$\langle S_2, q \rangle = \sum_{T \in \mathcal{T}_h} \int_T (\nabla \cdot \mathbf{u}_h) q \, \mathrm{d} T$$

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Bounding the residual functionals

$$\|\mathbf{S}_{1}\|_{V'} \leq C \left[\left(\sum_{T \in \mathcal{T}_{h}} h_{T}^{r'} \|\mathbf{R}_{1}\|_{\mathrm{L}^{r'}(T)}^{r'} \right)^{1/r'} + \left(\sum_{T \in \mathcal{T}_{h}} \sum_{e \subset \partial T \cap \Omega} h_{T} \|\mathbf{R}_{2}\|_{\mathrm{L}^{r'}(e)}^{r'} \right)^{1/r'} \right].$$

and

$$\|\mathbf{S}_2\|_{\mathcal{Q}'} \le \left(\sum_{\mathcal{T}\in\mathcal{T}_h} \|\mathbf{R}_3\|_{\mathbf{L}'(\mathcal{T})}^{r}\right)^{1/r}$$

 $\mathbf{R}_1 = \mathbf{f} + \nabla \cdot (k(|e(\mathbf{u}_h)|)e(\mathbf{u}_h)) - \nabla p_h, \qquad \mathbf{R}_3 = \nabla \cdot \mathbf{u}_h$

 $\mathbf{R}_2 = \frac{1}{2} \left[\!\!\left[\sigma_h \mathbf{n} \right]\!\!\right], \qquad \sigma_h = -\left(k(|e(\mathbf{u}_h)|)e(\mathbf{u}_h) - p_h I\right).$

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A posteriori error bound

Theorem. Let $(\mathbf{u}, p) \in V \times Q$ denote the solution to b.v.p., and let $(\mathbf{u}_h, p_h) \in V_h \times Q_h$ denote its finite element approximation. Then, there is a positive constant $C = C(K_1, K_2, c_0, c'_0, r, \|\mathbf{f}\|_{V'})$ s.t.

$$\|\mathbf{u}-\mathbf{u}_{h}\|_{V}^{\mathsf{R}}+\|\boldsymbol{p}-\boldsymbol{p}_{h}\|_{Q}^{\hat{\mathsf{R}}} \leq C\left(\|\mathbf{S}_{1}\|_{V'}^{\mathsf{R}'}+\|\mathbf{S}_{2}\|_{Q'}^{\hat{\mathsf{R}}'}\right),$$

where

$$R = \max\{r, 2\}, \ \hat{R} = \max\{r', 2\}, \ 1/R + 1/R' = 1, \ 1/\hat{R} + 1/\hat{R}' = 1,$$

and S_1 and S_2 residual functionals which are computably bounded.

[Barrett, Robson, Süli (2004)]

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r = 1.3

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Conclusions, ongoing and future research

- We developed the a posteriori error analysis of finite element approximations to a class on non-Newtonian flows.
- Ongoing research: implementation into an adaptive finite element method in 2D.
- Future work: application to multiple fluids, time-dependent problems in time-dependent geometries.