

Generalized quasi-Newtonian approach for modeling and simulating complex flows

A. Ouazzi, A. Afaq, N. Begum, H. Damanik, A. Fatima, S. Turek Institute of Applied Mathematics, LS III, TU Dortmund University, Dortmund, Germany

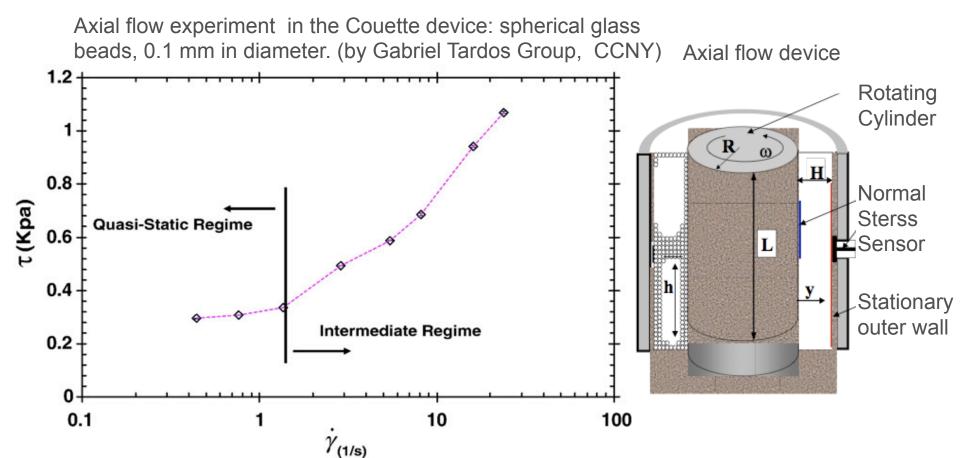
4th Indo-German Workshop on Advances in Materials, Reactions and Separation Processes February 23-26, 2020

Harnack-Haus,
Conference Venue of the Max Planck Society, Berlin, Germany.

Max Planck Institute for Dynamics of Complex Technical System Magdeburg

Behavior of dense granular material



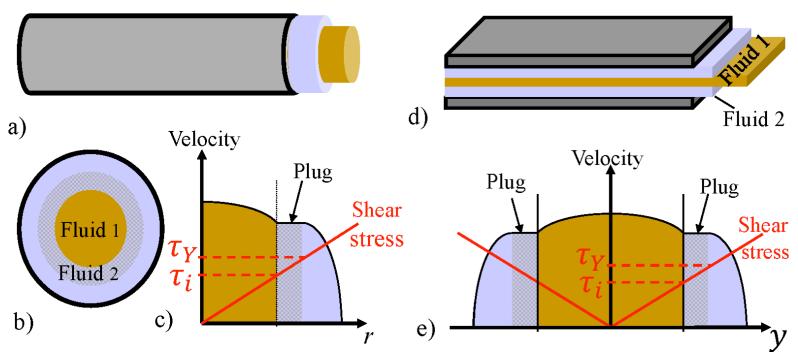


 The powder can transit from the quasi-static to the intermediate regime as the shearing rate is increased

Shear and pressure dependent viscosity

Viscoplastic flow





Viscoplastic Lubricate Flow (Yield stress fluids)

- Dependent on the stress field
- Constitutive model is dependent on different flow regimes
- Non-smooth change in the constitutive relations

Model preserving the sharp changes of the constitutive equations w.r.t. flow regimes





Thixotropy concept

- Based on viscosity
- Flow induced by time-dependent decrease of viscosity
- > The phenomena is reversible
- Aging / Build-up
 - ➤ At rest or under slow flow: fluid ages Increases of the viscosity in time
- Rejuvenation / Breakdown
 - "Faster" flow: fluid rejuvenates
 Decreases of viscosity with acceleration of the flow

Investigation of solid/liquid and liquid/solid transitions with non constant yield stress

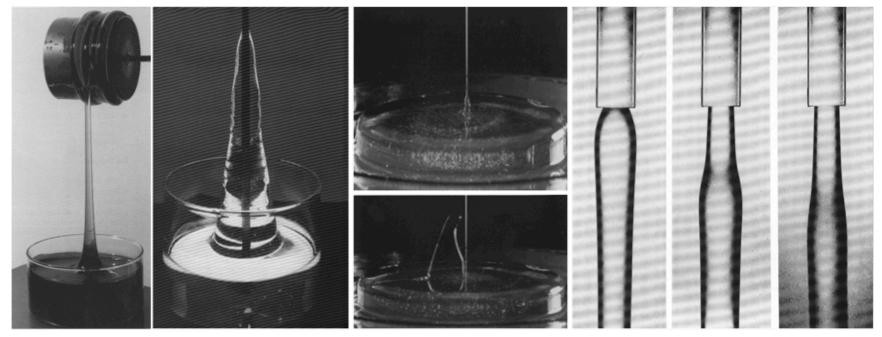




Non-Newtonian phenomena



- Effects due to normal stresses
- Effects due to elongational viscosity
- The drag reduction phenomenon



Differential models



Realization in FeatFlow



HPC features:

- Moderately parallel
- GPU computing
- Open source





Hardware -oriented Numerics

Numerical features:

- Higher order FEM in space & (semi-) Implicit FD/FEM in time
- Semi-(un)structured meshes with dynamic adaptive grid deformation
- Fictitious Boundary (FBM) methods
- Newton-Multigrid-type solvers

Non-Newtonian flow module:

- generalized Newtonian model (Power-law, Carreau,...)
- viscoelastic differential model (Giesekus, FENE, Oldroyd,...)

Multiphase flow module (resolved interfaces):

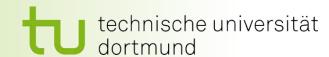
- I/I interface capturing (Level Set)
- s/l interface tracking (FBM)
- s/l/l combination of l/l and s/l

Engineering aspects:

- Geometrical design
- Modulation strategy
- Optimization

Here: FEM-based tools for the accurate simulation of (multiphase) flow problems, particularly with complex rheology

Governing equations



Generalized Navier-Stokes equations

$$\rho \left(\frac{\partial}{\partial t} + u \cdot \nabla \right) u - \nabla \cdot \sigma + \nabla p = \rho f,$$

$$\nabla \cdot u = 0,$$

$$\sigma = \sigma_s + \sigma_p,$$

Viscous stress

$$\sigma_s = 2\eta_s(D_{\mathbb{I}}, p)D(u), \quad D_{\mathbb{I}} = \operatorname{tr}\left(D(u)^2\right).$$

Elastic stress

$$\sigma_p + We \frac{\delta_a \sigma_p}{\delta t} = 2\eta_p D(u).$$



Quasi-Newtonian models



Viscous stress

$$\sigma_s = 2\eta_s(D_{\mathbb{I}}, p)D(u), \quad D_{\mathbb{I}} = \operatorname{tr}\left(D(u)^2\right)$$

Power law model

$$\eta_s(z) = \eta_0 z^{r - \frac{1}{2}} \quad (\eta_0 > 0, r > 1)$$

> Powder flow in the quasi-static and intermediate regimes

$$\begin{cases} \eta_s(z,p) = \sqrt{2}p\left(\sin\phi z^{-\frac{1}{2}} + \cos\phi z^{r-\frac{1}{2}}\right) & \text{if } z \neq 0, r > 1\\ \|\sigma_s\| \leq \sqrt{2}p\sin\phi & \text{else} \end{cases}$$

 $(\phi : \text{the angle of internal friction})$



Quasi-Newtonian models



Yield stress flow (Bingham Model)

$$\begin{cases} \eta_s(z,\lambda) = \eta_0 + \tau_0 z^{-\frac{1}{2}} & \text{if } z \neq 0 \\ \|\sigma_s\| \leq \tau_0 & \text{else} \end{cases}$$
$$(\tau_0: \text{ yield stress})$$

> Thixotropic model

$$\begin{cases} \eta_s(z,\lambda) = \eta(\lambda) + \tau(\lambda)z^{-\frac{1}{2}} & \text{if } z \neq 0 \\ \|\sigma_s\| \leq \tau(\lambda) & \text{else} \end{cases}$$

$$(\lambda : \text{structure parameter})$$

> Structure parameter equation

$$\frac{\partial \lambda}{\partial t} + u \cdot \nabla \lambda = a(1 - \lambda) - b\lambda z^{\frac{1}{2}}$$
(a, b are structure parameters)



Constitutive models



Elastic stress

$$\sigma_p + We \frac{\delta_a \sigma_p}{\delta t} = 2\eta_p D(u).$$

Upper/Lower convective derivative

$$\frac{\delta_a \sigma}{\delta t} = \left(\frac{\partial}{\partial t} + u \cdot \nabla\right) \sigma + g_a(\sigma, \nabla u)$$

$$g_a(\sigma, \nabla u) = \frac{1-a}{2} \left(\sigma \nabla u + (\nabla u)^{\mathrm{T}} \sigma \right)$$
$$-\frac{1+a}{2} \left(\nabla u \sigma + \sigma (\nabla u)^{\mathrm{T}} \right) \quad (a = \pm 1)$$



Constitutive models



Generalized differential constitutive model

$$\sigma + We \frac{\delta_a \sigma}{\delta t} + \mathbf{G}(\sigma, D) + \mathbf{H}(\sigma) = 2\eta_p D(u)$$

Oldroyd

$$\mathbf{G} = 0, \quad \mathbf{H} = 0$$

Giesekus

$$\mathbf{G} = 0, \quad \mathbf{H} = \alpha \operatorname{tr}(\sigma^2)$$

Phan-Thien and Tanner

$$\mathbf{H} = \left[\exp\left(\alpha \operatorname{tr}(\sigma)\right) - 1 \right] \sigma$$

White and Metzner

$$\mathbf{G} = \alpha \left(2 D : D\right)^{1/2}, \quad \mathbf{H} = 0$$





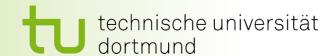
• Two-field formulation (u,p)

$$\begin{cases} -\nabla \cdot \left(2\eta D(u)\right) + \nabla p = 0 & \text{in } \Omega \\ \\ \nabla \cdot u = 0 & \text{in } \Omega \\ \\ u = g_{\scriptscriptstyle D} & \text{on } \Gamma_{\scriptscriptstyle D} \end{cases}$$

• Three-field formulation (σ, u, p)

$$\begin{cases} \sigma - 2\eta D(u) = 0 & \text{in } \Omega \\ -\nabla \cdot \left(2\eta(1-\alpha)D(u) + \alpha\sigma\right) + \nabla p = 0 & \text{in } \Omega \\ \nabla \cdot u = 0 & \text{in } \Omega \\ u = g_D & \text{on } \Gamma_D \end{cases}$$





• Two-field formulation (u,p)

$$ightharpoonup$$
 Set $\mathbb{V}:=\left[H_0^1(\Omega)
ight]^2, \mathbb{Q}:=L_0^2(\Omega)$

ightharpoonup Find $(u,p)\in\mathbb{V} imes\mathbb{Q}$ s.t.

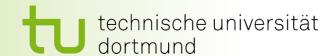
$$\langle \mathcal{K}(u,p), (v,q) \rangle = \langle \mathcal{L}, (v,q) \rangle, \quad \forall (v,q) \in \mathbb{V} \times \mathbb{Q}$$

$$\mathcal{K} = \begin{pmatrix} \mathcal{A}_u & \mathcal{B}^{\mathrm{T}} \\ \mathcal{B} & 0 \end{pmatrix}$$

Compatibily constraints

$$\sup_{v \in \mathbb{V}} \frac{\langle \mathcal{B}v, q \rangle}{\|v\|_{\mathbb{V}}} \ge \beta \|q\|_{\mathbb{Q}/Ker\mathcal{B}^{T}}, \quad \forall q \in \mathbb{Q}$$





• Three-field formulation (σ, u, p)

$$> \mathbf{Set} \ \mathbb{T} := \left(L^2(\Omega)\right)^4_{\mathrm{sym}}, \mathbb{V} := \left[H^1_0(\Omega)\right]^2, \mathbb{Q} := L^2_0(\Omega)$$

ightarrow Find $(\sigma,u,p)\in\mathbb{T}\times\mathbb{V}\times\mathbb{Q}$ s.t.

$$\langle \mathcal{K}(\sigma, u, p), (\tau, v, q) \rangle = \langle \mathcal{L}, (\tau, v, q) \rangle, \quad \forall (\tau, v, q) \in \mathbb{T} \times \mathbb{V} \times \mathbb{Q}$$

$$\mathcal{K} = \begin{pmatrix} \mathcal{A}_{\sigma} & \mathcal{C} & 0 \\ \mathcal{C}^{\mathrm{T}} & \mathcal{A}_{u} & \mathcal{B}^{\mathrm{T}} \\ 0 & \mathcal{B} & 0 \end{pmatrix}$$

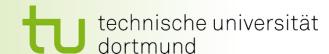
Compatibily constraints

$$\sup_{v \in \mathbb{V}} \frac{\langle \mathcal{B}v, q \rangle}{\|v\|_{\mathbb{V}}} \ge \beta \|q\|_{\mathbb{Q}/Ker\mathcal{B}^{\mathrm{T}}}, \quad \forall q \in \mathbb{Q}$$

$$\sup_{v \in \mathbb{V}} \frac{\langle \mathcal{C}v, \tau \rangle}{\|v\|_{\mathbb{V}}} \ge \gamma \|\tau\|_{\mathbb{T}/Ker\mathcal{C}^{\mathrm{T}}}, \quad \forall \tau \in \mathbb{T}$$



Approximated Stokes problem



Conforming approximations

$$\mathbb{T}_h \subset \mathbb{T}, \quad \mathbb{V}_h \subset \mathbb{V} = \tilde{\mathbb{V}}, \quad \mathbb{Q}_h \subset \mathbb{Q}$$

 $\mathcal{A}_{\sigma h} = \mathcal{A}_{\sigma}, \, \mathcal{A}_{uh} = \mathcal{A}_u, \, \mathcal{B}_h = \mathcal{B}, \, \mathcal{C}_h = \mathcal{C}$

Non-conforming approximation

$$\mathbb{T}_h \subset \mathbb{T}, \quad \mathbb{V}_h \not\subset \mathbb{V} \& \mathbb{V}_h \subset \widetilde{\mathbb{V}}, \quad \mathbb{Q}_h \subset \mathbb{Q}$$
$$\mathcal{A}_{\sigma h} = \mathcal{A}_{\sigma}, \, \mathcal{A}_{uh} \neq \mathcal{A}_u, \, \mathcal{B}_h \neq \mathcal{B}, \, \mathcal{C}_h \neq \mathcal{C}$$

Discrete inf-sup condition

$$\sup_{v_h \in \mathbb{V}_h} \frac{\left\langle \mathcal{B}_h v_h, q_h \right\rangle}{\left\| v_h \right\|_{\tilde{\mathbb{V}}}} \ge \beta_h \left\| q_h \right\|_{\mathbb{Q}/Ker\mathcal{B}_h^{\mathrm{T}}}, \quad \forall q_h \in \mathbb{Q}_h$$

$$\sup_{v_h \in \mathbb{V}_h} \frac{\left\langle \mathcal{C}_h v_h, \tau_h \right\rangle}{\left\| v_h \right\|_{\tilde{\mathbb{V}}}} \ge \gamma_h \left\| \tau_h \right\|_{\mathbb{T}/Ker\mathcal{C}_h^{\mathrm{T}}}, \quad \forall \tau_h \in \mathbb{T}_h$$



Robust non-/conforming FEM



The family of non-/conforming FEM $Q_r/P_{r-1}^{\mathrm{disc}},\,r\geq 2$ and the family of nonconforming FEM $\tilde{Q}_r/P_{r-1}^{\mathrm{disc}},\,r\geq 2$ for (u,p)

- > Inf-sup stable
- > Arbitrary order with optimal convergence order
- > Discontinuous pressure
 - Good for the solver
 - Element-wise mass conservation

The family of conforming FEM
$$Q_r/Q_r/P_{r-1}^{\mathrm{disc}}, \, r \geq 2$$
 for (σ, u, p) with stabilization $J_u(u_h, v_h) = \gamma_u \sum_{e \in \mathcal{E}_h} 2\eta \alpha h \int_e^{\mathrm{close}} [\nabla u_h] : [\nabla v_h] \, d\Omega$

- > Both Inf-sup conditions are satisfied
- ➤ Highly consistent and symmetric stabilization, penelazing any spurious current, enhancing the preconditioner, which improve accuracy and efficiency
- None tensorial FEM approximation for the tensorial field
 - > Robust solver w.r.t. the monolitic approach
 - > Efficient solver w.r.t. multigird solver



Monolitic-multigrid linear solver



- Standard geometric multigrid solver
- Full Q_r and $P_{r-1}^{
 m disc}$ restriction and prolongation
- Local Multilevel Pressure Schur Complement via Vanka-like smoother

$$\begin{pmatrix} \sigma^{l+1} \\ u^{l+1} \\ p^{l+1} \end{pmatrix} = \begin{pmatrix} \sigma^{l} \\ u^{l} \\ p^{l} \end{pmatrix} + \omega^{l} \sum_{T \in \mathcal{T}_{h}} \left(\left(\mathcal{K}_{h} + \mathcal{J}_{u} \right)_{|T} \right)^{-1} \begin{pmatrix} \mathcal{R}_{\sigma^{l}} \\ \mathcal{R}_{u^{l}} \\ \mathcal{R}_{p^{l}} \end{pmatrix}_{|T}$$

Coupled Monolithic Multigrid Solver!



Monolitic-multigrid linear solver



Flow around cylinder Benchmark tests (by Aaqib Afaq)

Two field formulation versus three field formulation

	Three-field			Two-field ¹		
Level	Lift	Drag	NL/LL	Lift	Drag	NL/LL
1	0.009498	5.5550	7/2	0.009498	5.5550	9/2
2	0.010601	5.5722	7/2	0.010601	5.5722	9/2
3	0.010616	5.5776	7/2	0.010616	5.5776	9/1
4	0.010618	5.5791	7/1	0.010618	5.5791	8/1

¹Damanik. H "FEM Simulation of Non-isothermal Viscoelastic fluids", PhD Thesis

Consistency of the stabilization for three field formulation

		No stabilization			With stabilization		
Level	$\mid \alpha \mid$	Lift	Drag	NL/LL	Lift	Drag	NL/LL
2	0	0.010601	5.5722	7/2	0.010702	5.5674	7/2
3	0	0.010616	5.5776	7/2	0.010619	5.5757	7/2
4	0	0.010618	5.5791	7/1	0.010617	5.5782	7/2
5	0	0.010619	5.5794	6/2	0.010618	5.5790	6/3



Monolitic-multigrid linear solver

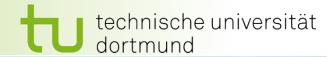


Flow around cylinder Benchmark tests (by Aaqib Afaq)

Robustness and efficiency of the stabilization for three field formulation without any viscous contribution

		No stabilization			With stabilization		
Level	$\mid \alpha \mid$	Lift	Drag	NL/LL	Lift	Drag	NL/LL
2	0	0.010601	5.5722	7/2	0.010702	5.5674	7/2
3	0	0.010616	5.5776	7/2	0.010619	5.5757	7/2
4	0	0.010618	5.5791	7/1	0.010617	5.5782	7/2
5	0	0.010619	5.5794	6/2	0.010618	5.5790	6/3
2	1			_	0.010588	5.5520	7/2
3	1				0.010600	5.5698	7/2
4	1				0.010612	5.5756	7/2
5	1				0.010617	5.5778	7/3

Accurate, robust and efficient monolitic-multigrid Stokes solver in two-field and three-field formulations



Incompressible N-S Equation)

$$\rho(\Gamma) \left(\frac{\partial}{\partial u} + u \cdot \nabla \right) u - \nabla \cdot \sigma_s + \nabla p = 0$$

Viscous stress

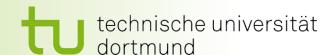
$$\sigma_s = 2\eta_s(\Gamma)D(u)$$

Interface boundary conditions

$$[u]_{|\Gamma} = 0$$

$$-[pI + \sigma_s]_{|\Gamma} \cdot n = \sigma \kappa n$$

Multiphase flow problem



New extra stress for multiphase flow

$$\sigma_m = -\sigma \left(\frac{\nabla \psi \otimes \nabla \psi}{|\nabla \psi|} \right)$$

Full set of equations for multiphase flow

$$\begin{cases}
\rho(\psi) \left(\frac{\partial u}{\partial t} + u \cdot \nabla u \right) - \nabla \cdot \tau + \nabla p = 0 \\
\nabla \cdot u = 0
\end{cases}$$

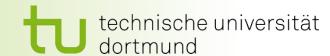
$$\tau - 2\eta_s(\psi)D(u) + \sigma \left(\frac{\nabla \psi \otimes \nabla \psi}{|\nabla \psi|} \right) = 0$$

$$\frac{\partial \psi}{\partial t} + u \cdot \nabla \psi + \nabla \cdot \left(\gamma_{nc}\psi(1 - \psi) \frac{\nabla \psi}{|\nabla \psi|} \right)$$

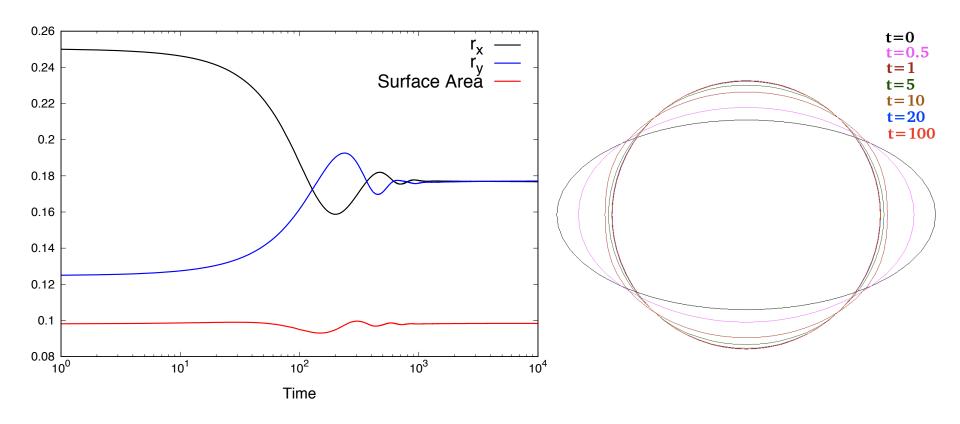
$$-\nabla \cdot \left(\gamma_{nd} \left(\nabla \psi \cdot \frac{\nabla \psi}{|\nabla \psi|} \right) \frac{\nabla \psi}{|\nabla \psi|} \right) = 0$$



Monolitic approach

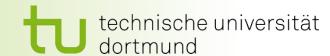


Oscillating bubble (by Aaqib Afaq)





Generalized Newton's method



Robust nonlinear solver based on Newton's method following a specefic path of convergence using the residual's convergence

- Robust w.r.t. starting guesses
- Dealing with Jacobian's singularities using generalized deriviatives or approximated one
- Full benefit from the quadratic convergence's region of classical Newton's method





Let $\mathcal{U}=(u,p)$, (σ,u,p) , or (σ,u,p,φ) and $\mathcal{R}_{\mathcal{U}}(\mathcal{U})$ be the continuous or the discrete corresponding system's residum.

 \triangleright Update of the nonlinear iteration with the correction $\delta\mathcal{U}$ i.e.

$$\mathcal{U}^N = \mathcal{U} + \delta \mathcal{U}$$

> The linearization of the residual provides

$$\mathcal{R}_{\mathcal{U}}\left(\mathcal{U}^{N}\right) = \mathcal{R}_{\mathcal{U}}\left(\mathcal{U} + \delta\mathcal{U}\right)$$
$$= \mathcal{R}_{\mathcal{U}}\left(\mathcal{U}\right) + \mathcal{J}\left(\mathcal{U}\right) \cdot \delta\mathcal{U}$$

> The Newton's method assuming invertible Jacobian

$$\mathcal{U}^{N} = \mathcal{U} - \mathcal{J}^{-1} \left(\mathcal{U} \right) \cdot \mathcal{R}_{\mathcal{U}} \left(\mathcal{U} \right)$$



Generalized Newton's method



Jacobian calculations

$$\mathcal{J}\left(\mathcal{U}\right) = \left(\frac{\partial \mathcal{R}_{\mathcal{U}}\left(\mathcal{U}\right)}{\partial \mathcal{U}}\right)$$

Exact G-Newton based on a priori study of Jacobian's properties and decompositions

$$\mathcal{J}\left(\mathcal{U}\right) = \left(\frac{\partial \hat{\mathcal{R}}_{\mathcal{U}}\left(\mathcal{U}\right)}{\partial \mathcal{U}}\right) + \delta\left(\frac{\partial \tilde{\mathcal{R}}_{\mathcal{U}}\left(\mathcal{U}\right)}{\partial \mathcal{U}}\right)$$

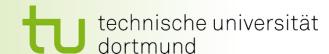
Inexact G-Newton based on the residum's convergence

$$\left(\frac{\partial \bar{\mathcal{R}}_{\mathcal{U}}\left(\mathcal{U}\right)}{\partial \mathcal{U}}\right)_{ij} \approx \left(\frac{\bar{\mathcal{R}}_{\mathcal{U}}\left(\mathcal{U} + \epsilon^{+}e_{j}\right) - \bar{\mathcal{R}}_{\mathcal{U}}\left(\mathcal{U} - \epsilon^{-}e_{i}\right)}{\left(\epsilon^{+} + \epsilon^{-}\right)}\right),\,$$

$$\bar{\mathcal{R}} = \mathcal{R}, \, \hat{\mathcal{R}}, \, \, \text{or} \, \, \tilde{\mathcal{R}} \, \, .$$



Three-field viscoplastic application



- Viscoplatic constitutive law
 - Bingham constitutive law

$$\begin{cases} \sigma = 2\eta D(u) + \tau_0 \frac{D(u)}{\|D(u)\|} & \text{if } \|D(u)\| \neq 0 \\ \|\sigma\| \leq \tau_0 & \text{if } \|D(u)\| = 0 \end{cases}$$

ightharpoonup New extra stress σ_{Y_0} for viscoplastic flow s.t.

$$||D(u)||\sigma_{Y_0} = D(u)$$

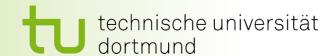
Three-field viscoplastic set of equations

$$\begin{cases} ||D(u)||\sigma_{Y_0} - D(u) = 0 & \text{in } \Omega \\ -\nabla \cdot \left(2\eta D(u) + \tau_0 \sigma_{Y_0}\right) + \nabla p = 0 & \text{in } \Omega \end{cases}$$

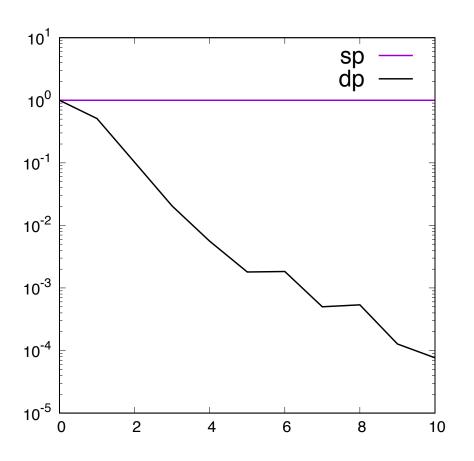
$$\nabla \cdot u = 0 & \text{in } \Omega$$

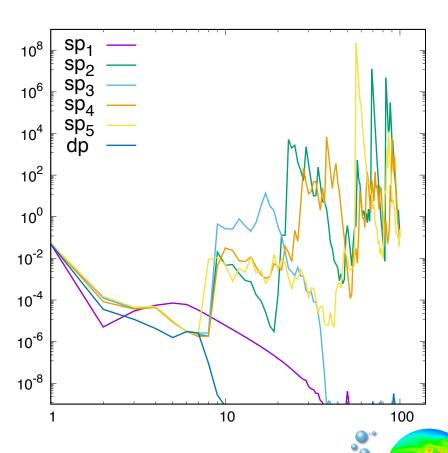


Generalized Newton's method



Dynamic path versus static one w.r.t. number of iterations, and the corresponding convergence of the residium (by Arooj Fatima)

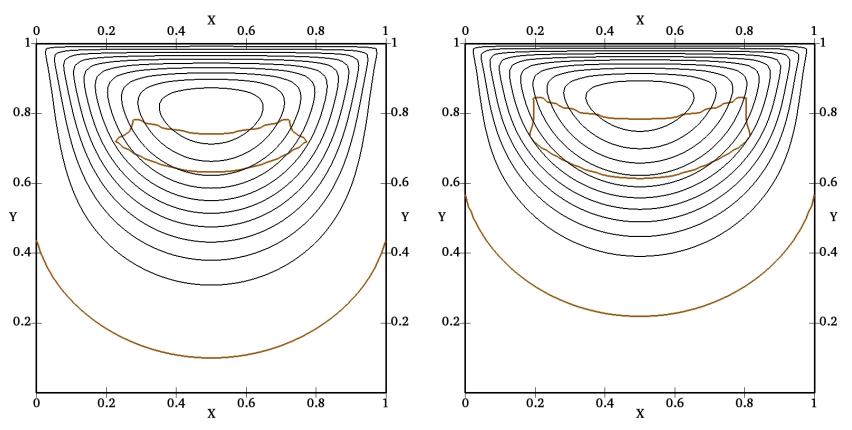




Lid driven cavity benchmark



Unyielded zone for two different yield stresses, $\tau_0=2$, and $\tau_0=5$ (by Arooj Fatima)





Constitutive models



Generalized differential constitutive model

$$\sigma + We \frac{\delta_a \sigma}{\delta t} + \mathbf{G}(\sigma, D) + \mathbf{H}(\sigma) = 2\eta_p D(u)$$

Oldroyd

$$\mathbf{G} = 0, \quad \mathbf{H} = 0$$

Giesekus

$$\mathbf{G} = 0, \quad \mathbf{H} = \alpha \operatorname{tr}(\sigma^2)$$

Phan-Thien and Tanner

$$\mathbf{H} = \left[\exp\left(\alpha \operatorname{tr}(\sigma)\right) - 1 \right] \sigma$$

White and Metzner

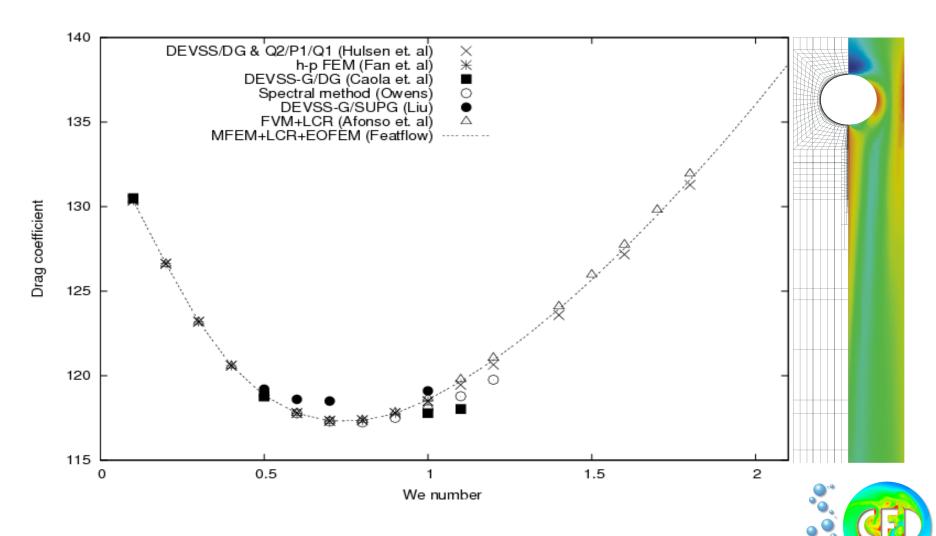
$$\mathbf{G} = \alpha \left(2 D : D\right)^{1/2}, \quad \mathbf{H} = 0$$



Viscoelastic benchmark



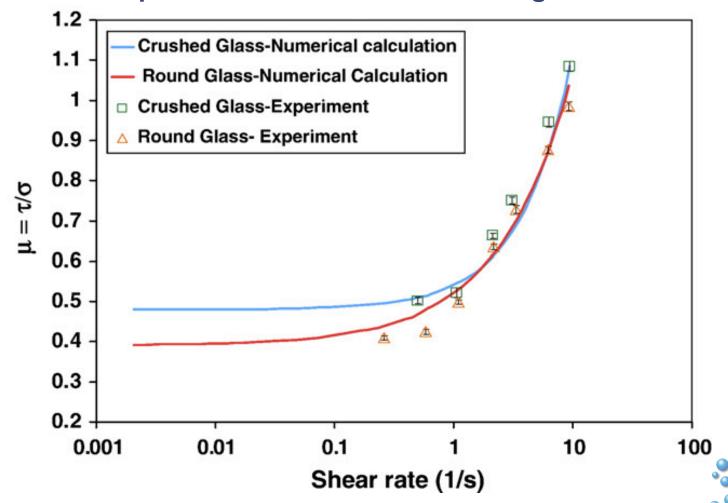
Planar flow around cylinder Oldroyd-B (by Hogenrich Damanik)



Quasi-Newtonian model for powder flow



 Experimental and numerical results for dry, frictional powder flows in the quasi-static and intermediate regimes



The numerical method do not introduce errors!

Quasi-Newtonian thixotropic model



Viscosity model for thixotropic flow i.e. extended viscosity defined on all domaine s.t.

$$\begin{cases} \eta_s(\|D(u)\|, \lambda) = \eta(\lambda) + \tau(\lambda)\|D(u)\|^{-\frac{1}{2}} & \text{if } \|D(u)\| \neq 0 \\ \|\sigma_s\| \leq \tau(\lambda) & \text{else} \end{cases}$$

 $(\lambda : structure parameter)$

Structure equation

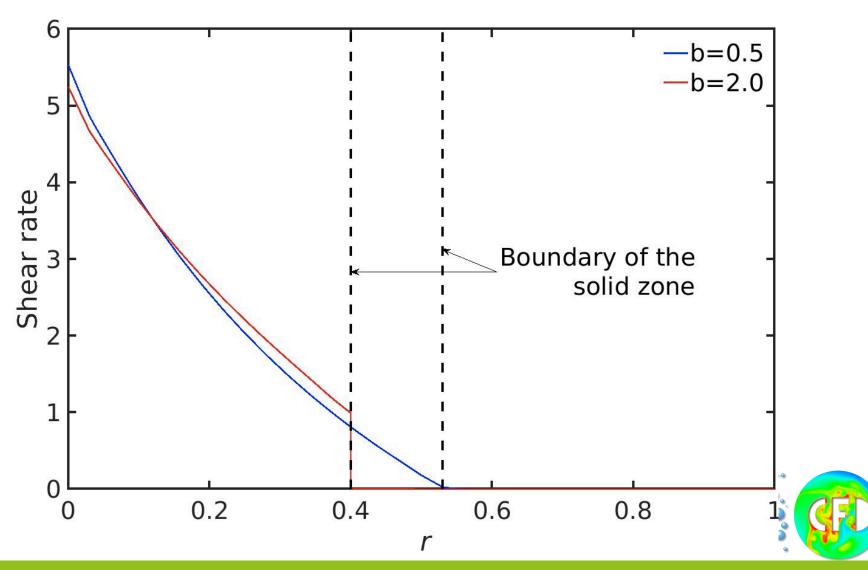
$$\frac{\partial \lambda}{\partial t} + u \cdot \nabla \lambda = a(1 - \lambda) - b\lambda z^{\frac{1}{2}}$$
(a, b are structure parameters)

Full set of equations

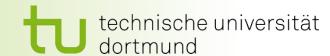
$$\begin{cases} \left(\frac{\partial}{\partial t} + u \cdot \nabla\right) u - \nabla \cdot \left(2\eta_s(\|D(u)\|, \lambda)D(u)\right) + \nabla p = 0 & \text{in } \Omega \\ \nabla \cdot u = 0 & \text{in } \Omega \\ \frac{\partial \lambda}{\partial t} + u \cdot \nabla \lambda - a(1 - \lambda) + b\lambda \|D(u)\| = 0 & \text{in } \Omega \end{cases}$$



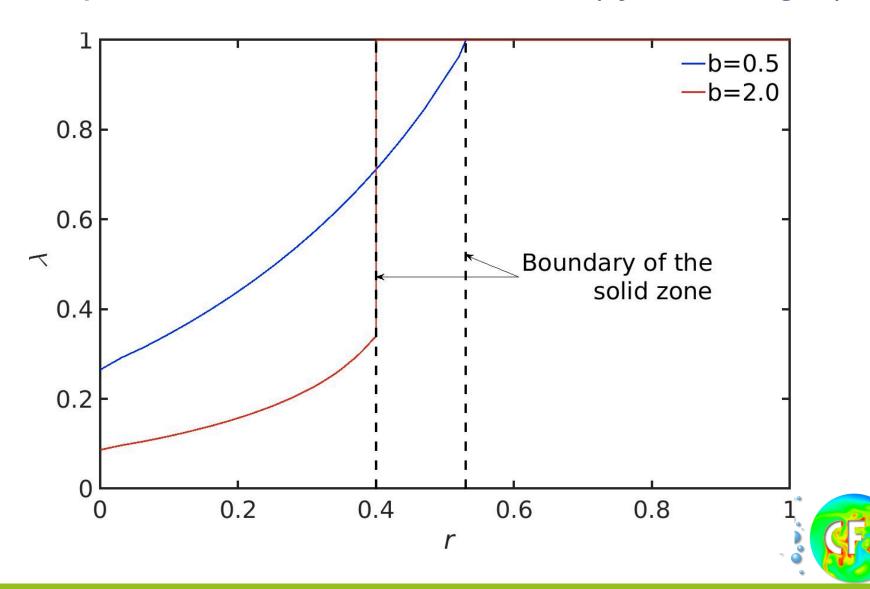
Shear rate in a couette w.r.t. breakdown parameter (by Naheed Begum)



Thixotropic flow



Structure parameter in a couette w.r.t. breakdown (by Naheed Begum)



Thixotropy flow



- √ shear history effect
- √ time history effect
- ✓ Hysteresis
- √ stress overhoots

A quasi-Newtonian model for thixotropic phenomena via a time and shear dependent viscosity



Generalized quasi-Newtonian approach



- Include the non-Newtonian stress or any extra stress in diffusion operator
- Get rid of a tensorial field
 - Less constraints for the choices of FE approximation
 - > Robust and efficient numerical algorithms
 - Simple evolution equations!

Proof of the concept and validation



Laplacian operator



Divergence form

$$\mathcal{L} u = \sum_{i,j=1}^{n} \frac{\partial}{\partial x_i} \left(a_{ij} u \frac{\partial}{\partial x_i} \right)$$

Weak form

$$\mathcal{L}_{\mathbf{w}} u = \sum_{i,j=1}^{N} A_{ij} : \left(\nabla \cdot e_{j} \otimes \nabla \cdot e_{i} \right) u$$

Benefit of the weak form representation!





Weak form representation 2D

$$\mathcal{L}_{\mathbf{W}} u = \sum_{k,l=1}^{2} \sum_{i,j=1}^{N} [A_{kl}]_{ij} : \left(\nabla \cdot e_j \otimes \nabla \cdot e_i \right) u_j^l, \quad k = 1, 2$$

Gradient formulation

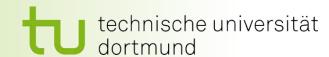
$$A_{11} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad A_{12} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$$
$$A_{21} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}, \quad A_{22} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

Deformation formulation

$$A_{11} = \begin{bmatrix} 1 & 0 \\ 0 & \frac{1}{2} \end{bmatrix}, \quad A_{12} = \begin{bmatrix} 0 & \frac{1}{2} \\ 0 & 0 \end{bmatrix}$$
 $A_{21} = \begin{bmatrix} 0 & 0 \\ \frac{1}{2} & 0 \end{bmatrix}, \quad A_{22} = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & 1 \end{bmatrix}$

Different deriviatives combinations accessibilities !

Generalized quasi-Newtonian approach



Weak form representation 2D

$$\mathcal{L}_{\mathbf{W}} u = \sum_{k,l=1}^{2} \sum_{i,j=1}^{N} [A_{kl}]_{ij} : \left(\nabla \cdot e_j \otimes \nabla \cdot e_i \right) u_j^l, \quad k = 1, 2$$

Generalized formulation I

$$A_{11} = \begin{bmatrix} a_{11} & \frac{1}{2}a_{21} \\ \frac{1}{2}a_{12} & \frac{1}{4}(a_{11} + a_{22}) \end{bmatrix}, \quad A_{12} = \begin{bmatrix} \frac{1}{2}a_{12} & \frac{1}{4}(a_{11} + a_{22}) \\ 0 & \frac{1}{2}a_{12} \end{bmatrix}$$
$$A_{21} = \begin{bmatrix} \frac{1}{2}a_{21} & 0 \\ \frac{1}{4}(a_{11} + a_{22}) & \frac{1}{2}a_{21} \end{bmatrix}, \quad A_{22} = \begin{bmatrix} \frac{1}{4}(a_{11} + a_{22}) & \frac{1}{2}a_{21} \\ \frac{1}{2}a_{12} & a_{22} \end{bmatrix}$$

More deriviatives combinations accessibilities are allowed!

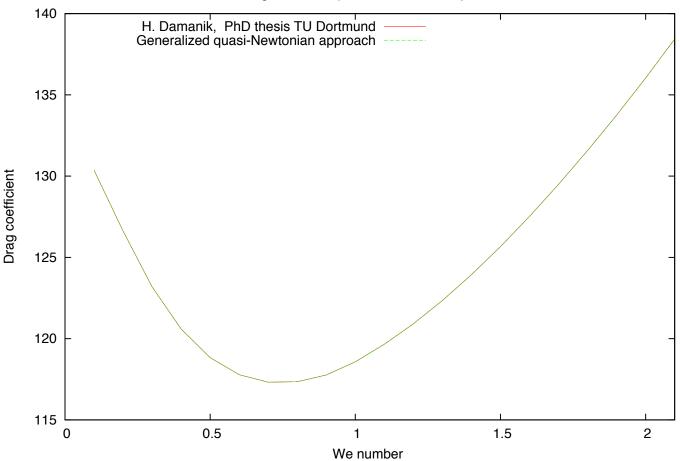


Viscoelastic benchmark



Planar flow around cylinder Oldroyd-B (by Hogenrich Damanik)

Drag coefficient planar flow around cylinder



Genalized quasi-Newtonian approach for non-Newtonian problem i.e. Oldroyd-B!



Summary



New generalized quasi-Newtonian approach for modeling and simulating complex flows is introduced and validated.

Based on new numerical and algorithmic tools using

- ✓ Monolithic FEM two-field and three-field Stokes solver.
- ✓ Generalized Newton's method w.r.t. singularities with global convergent property
- ✓ Edge Oriented stabilization (EO-FEM)
- ✓ Fast Multigrid Solver with local MPSC smoother

 Extensively tested from numerical and physical perspectives
 via the simulations of different flow problems in different
 formulations to motivate the newly introduced generalized quasiNewtonian approach.