Parametric finite element approximation of two-phase Navier–Stokes flow with viscoelasticity

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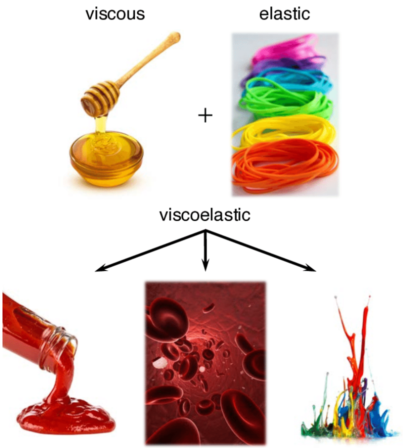
Motivation

Why are viscoelastic materials interesting?



picture from J. Brenner

Motivation

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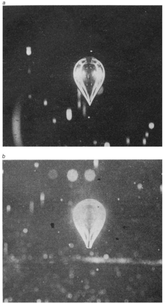
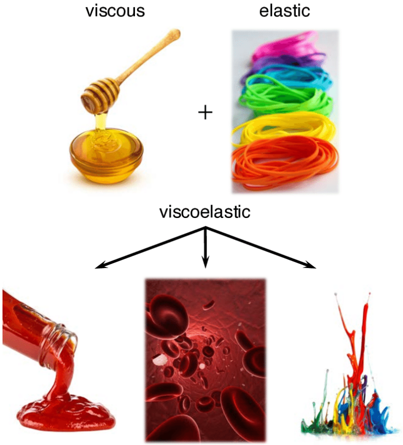


Negative wake behind bubbles in viscoelastic fluids (Hassager '79)



picture from J. Brenner

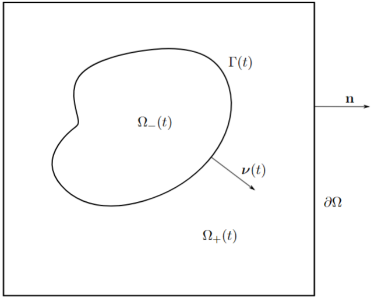
Incompressible Navier–Stokes model

In the two phases $\Omega_+(t)$ and $\Omega_-(t)$:

$$\varrho_\pm(\partial_t \mathrm{u} + \mathrm{u}\cdot\nabla \mathrm{u}) + \nabla p = \operatorname{div}(2\eta_\pm \mathrm{D}\mathrm{u}) + \mathrm{f}$$
$$\operatorname{div} \mathrm{u} = 0$$

Notation:

- u: velocity
- p: pressure
- $\varrho_\pm$: densities
- $\eta_\pm$: viscosities
- Du: symmetrized velocity gradient
- f: force



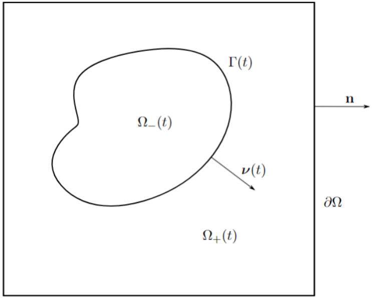
Jump conditions on the free boundary

On the interface $\Gamma(t) = \partial\Omega_-(t)$:

$$\begin{aligned} [\![\, \mathrm{u} \,]\!] &= 0 \\ -[\![\, 2\eta \mathrm{Du} - p\mathbb{I} \,]\!]\,\boldsymbol{\nu} &= \gamma\kappa\,\boldsymbol{\nu} \\ \mathcal{V} &= \mathrm{u}\cdot\boldsymbol{\nu} \end{aligned}$$

Notation:

- $\boldsymbol{\nu}$: unit normal on interface
- $[\![\, \cdot \,]\!]$: jump across interface
- γ: surface tension
- κ: mean curvature
- $\mathcal{V}$: normal velocity



Physical properties

- Energy inequality: (with b.c., without forces)

$$\frac{d}{dt}\Big(\underbrace{\int_\Omega \frac{\varrho}{2}|\mathrm{u}|^2}_{\text{kinetic energy}} + \underbrace{\int_{\Gamma(t)} \gamma}_{\text{surface energy}} \Big) = -\int_\Omega 2\eta|\mathrm{Du}|^2 \leq 0$$

- Volume preserving, i.e., volume of $\Omega_-(t)$, $\Omega_+(t)$ do not change in time:

$$\frac{d}{dt}\mathrm{Vol}\,(\Omega_-(t)) = \int_{\Gamma(t)} \mathcal{V} = \int_{\Gamma(t)} \mathrm{u}\cdot\boldsymbol{\nu} = \int_\Omega \mathrm{div}\,(\mathrm{u})\,\chi_{|\Omega_-(t)} = 0$$

$$\frac{d}{dt}\mathrm{Vol}\,(\Omega_+(t)) = \frac{d}{dt}\mathrm{Vol}\,(\Omega \setminus \Omega_-(t)) = 0$$

Goals

- Design a structure preserving discretization
  1. Energy inequality
  2. Geometric conservation properties
- Good mesh properties for the evolving interface mesh
- Avoid spurious velocities

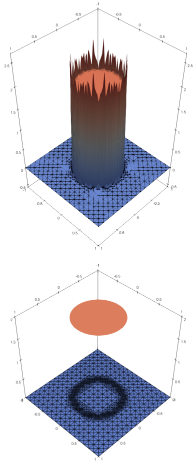


Figure: Two-phase Stokes flow $-\mathrm{div}\,(2\eta Du) + \nabla p = 0$ with free boundary conditions. Pressure oscillations (top) can lead to artificial velocities. XFEM-approaches can avoid pressure oscillations (bottom).

Interface mesh properties

Traditional parametric approaches have problems:

- Mesh quality can degrade
- Mesh coalescence is possible

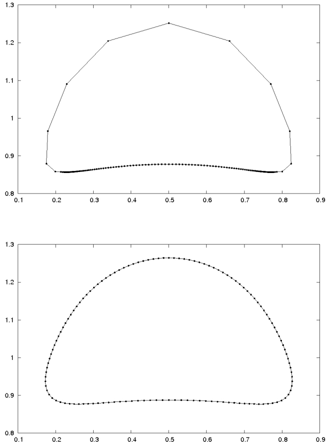
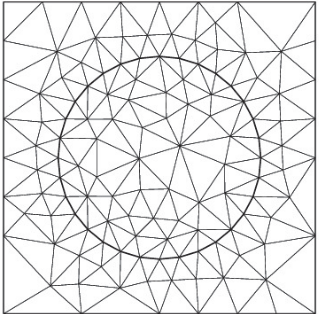


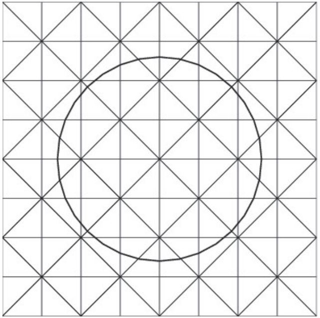
Figure: Example for two-phase flow.
Top: very nonuniform interface mesh.
Bottom: equidistributed nodes.

Two different approaches

Parametric approach works both for fitted or unfitted bulk meshes:

- Fitted approach needs remeshing of bulk mesh
- Unfitted approach is flexible w.r.t. mesh movement





Discretization of two-phase (Navier–)Stokes flow

Treatment of curvature and normal velocity:

- First approach for the curvature by Dziuk '91: discretize

$$\Delta_s \mathrm{id} = \kappa \boldsymbol{\nu} \quad \text{on } \Gamma(t)$$

  with linear finite elements
- Only prescribe normal velocity $\mathcal{V} = \partial_t \mathrm{x} \cdot \boldsymbol{\nu} \stackrel{!}{=} \mathrm{u} \cdot \boldsymbol{\nu}$. Tangential velocity adjusts itself such that good mesh properties are attained.
- Weak formulation:

$$\begin{aligned} \langle \partial_t \mathrm{x} \cdot \boldsymbol{\nu}, \chi \rangle_{\Gamma(t)} &= \langle \mathrm{u} \cdot \boldsymbol{\nu}, \chi \rangle_{\Gamma(t)} && \forall \chi \\ \langle \kappa \boldsymbol{\nu}, \boldsymbol{\xi} \rangle_{\Gamma(t)} + \langle \nabla_s \mathrm{x}, \nabla_s \boldsymbol{\xi} \rangle_{\Gamma(t)} &= 0 && \forall \boldsymbol{\xi} \end{aligned}$$

Discretization of two-phase (Navier–)Stokes flow

Treatment of flow variables:

- LBB stable velocity–pressure discretization, e.g., P2-P1, P2-P0, P2-(P0+P1)
- Weak formulation for Stokes:

$$(2\eta \mathrm{Du}\,,\,\mathrm{Dw}) - (p\,,\,\mathrm{div}\,\mathrm{w}) = \gamma\,\langle \kappa\,\boldsymbol{\nu}\,,\,\mathrm{w}\rangle_{\Gamma(t)} + (\mathrm{f}\,,\,\mathrm{w}) \qquad \forall\,\mathrm{w}$$

$$(\mathrm{div}\,\mathrm{u}\,,\,q) = 0 \qquad \forall\,q$$

- Extension to Navier–Stokes: use appropriate discretization of $\varrho(\partial_t \mathrm{u} + \mathrm{u}\cdot\nabla\mathrm{u})$

Mass conservation

- Typical unphysical problem: volume loss for bubble due to surface tension effect.
- An XFEM-approach of Barrett-Garcke-Nürnberg '13: extend ansatz functions of pressure by *only one* function

$$\chi_{|\Omega_-^h(t)} = \begin{cases} 1 & \text{in } \Omega_-^h(t) \\ 0 & \text{in } \Omega \setminus \Omega_-^h(t) \end{cases}$$

  (characteristic function of the bubble)
- *Semi-discrete* version: exact volume conservation (e.g. Barrett-Garcke-Nürnberg '13)

$$\frac{d}{dt}\mathrm{Vol}\,(\Omega_-^h(t)) = \langle \partial_t \mathrm{X}^h \,,\, \boldsymbol{\nu}^h \rangle_{\Gamma^h(t)}^h = \langle \mathrm{u}^h \,,\, \boldsymbol{\nu}^h \rangle_{\Gamma^h(t)} = 0$$

- XFEM-approach avoids spurious velocities! (semi-discrete *and* fully-discrete)

Oldroyd-B model

Consider the model with an additional stress tensor T:

- In the two phases $\Omega_\pm(t)$:

$$\varrho_\pm(\partial_t \mathrm{u} + \mathrm{u}\cdot\nabla\mathrm{u}) + \nabla p = \operatorname{div}(2\eta_\pm \mathrm{D}\mathrm{u}) + \operatorname{div}(\mathrm{T}) + \mathrm{f}$$
$$\operatorname{div}\mathrm{u} = 0$$
$$\mathrm{T} = G\,(\mathbb{B} - \mathbb{I})$$
$$\partial_t\mathbb{B} + \mathrm{u}\cdot\nabla\mathbb{B} - \nabla\mathrm{u}\mathbb{B} - \mathbb{B}(\nabla\mathrm{u})^\top = -\frac{1}{\lambda_\pm}(\mathbb{B} - \mathbb{I})$$

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- On the interface $\Gamma(t)$:

$$[\![\,\mathrm{u}\,]\!] = 0, \quad -[\![\,2\eta\mathrm{D}\mathrm{u} - p\mathbb{I} + \mathrm{T}\,]\!]\boldsymbol{\nu} = \gamma\kappa\,\boldsymbol{\nu}, \quad \mathcal{V} = \mathrm{u}\cdot\boldsymbol{\nu}$$

Notation:

- $\mathbb{B}$: left Cauchy–Green tensor
- G: elastic shear modulus (constant)
- $\lambda_\pm$: relaxation time
- λ small $\approx$ Newtonian fluid ($\mathrm{T} \approx 0$), λ large $\approx$ (visco-)elastic solid

Model properties

- Energy inequality: (with b.c., without forces)

$$\frac{d}{dt}\Big(\underbrace{\int_\Omega \frac{\varrho}{2}|\mathrm{u}|^2}_{\text{kinetic energy}} + \underbrace{\int_\Omega \frac{G}{2}(\mathrm{Tr}\,\mathbb{B} - \ln\det(\mathbb{B}) - d)}_{\text{elastic energy}} + \underbrace{\int_{\Gamma(t)} \gamma}_{\text{surface energy}} \Big)$$

$$= -\int_\Omega 2\eta|\mathrm{Du}|^2 - \int_\Omega \frac{G}{2\lambda}\mathrm{Tr}\,(\mathbb{B} + \mathbb{B}^{-1} - 2\mathbb{I}) \leq 0$$

- Requirement: $\mathbb{B}$ positive definite
- as before: conservation of volume of $\Omega_+(t)$, $\Omega_-(t)$

Goal: analogue properties on the discrete level

The Oldroyd-B model with stress diffusion

- Find a discretization that also works with possible stress diffusion:

$$\partial_t \mathbb{B} + \mathbf{u} \cdot \nabla \mathbb{B} - \nabla \mathbf{u} \mathbb{B} - \mathbb{B}(\nabla \mathbf{u})^\top + \frac{1}{\lambda_\pm}(\mathbb{B} - \mathbb{I}) = \alpha \Delta \mathbb{B}, \quad \alpha \geq 0$$

- Physical justification of $\alpha \Delta \mathbb{B}$:
  - macroscopic closure of a Fokker–Planck type equation (Barrett-Süli '07)
  - nonstandard thermodynamical processes (Málek-Průša-Skřivan-Süli '18)
- With $\alpha > 0$:
  - additional dissipation $\int_\Omega \alpha |\nabla \ln \det \mathbb{B}|^2$

Discretization of the Oldroyd-B model

Fully-discrete approximation with linear finite elements: (Barrett-Boyaval '11)

$$0 = \frac{1}{\Delta t}\left(\mathbb{B}^{n+1} - \mathbb{B}^{n}\,,\,\mathbb{G}\right)^{h} - \sum_{i,j=1}^{d}\left((\mathrm{u}^{n})_i\,\Lambda_{i,j}(\mathbb{B}^{n+1})\,,\,\partial_{x_j}\mathbb{G}\right)$$
$$+\left(\tfrac{1}{\lambda}(\mathbb{B}^{n+1} - \mathbb{I})\,,\,\mathbb{G}\right)^{h} - 2\left(\nabla \mathrm{u}^{n+1}\,,\,\mathbb{I}_1\left[\mathbb{G}\mathbb{B}^{n+1}\right]\right)$$
$$+\,\alpha\left(\nabla\mathbb{B}^{n+1}\,,\,\nabla\mathbb{G}\right) \qquad \forall\,\mathbb{G}$$

- $(\cdot\,,\,\cdot)^h$: mass lumping, $\mathbb{I}_1$: P1 interpolation operator
- $\Lambda_{i,j}(\mathbb{B}^{n+1}) \approx \delta_{i,j}\,\mathbb{B}^{n+1}$ needed for discrete energy inequality

A fully-discrete approximation

Find $(\mathrm{u}^{n+1}, p^{n+1}, \mathbb{B}^{n+1}, \mathrm{X}^{n+1}, \kappa^{n+1})$ with $\mathbb{B}^{n+1}$ positive definite such that

N.St.
$$\begin{cases} 0 &= \frac{1}{2\Delta t}\left(\rho^n \mathrm{u}^{n+1} - \rho^{n-1}\mathrm{u}^n\,,\, \mathrm{w}\right) + \frac{1}{2\Delta t}\left(\rho^{n-1}(\mathrm{u}^{n+1} - \mathrm{u}^n)\,,\, \mathrm{w}\right) \\ & \quad + \frac{1}{2}\left(\rho^n\,,\, [(\mathrm{u}^n \cdot \nabla)\mathrm{u}^{n+1}] \cdot \mathrm{w}\right) - \frac{1}{2}\left(\rho^n\,,\, \mathrm{u}^{n+1} \cdot [(\mathrm{u}^n \cdot \nabla)\mathrm{w}]\right) \\ & \quad + \left(2\eta^n \mathrm{D}\mathrm{u}^{n+1}\,,\, \mathrm{D}\mathrm{w}\right) - \left(p^{n+1}\,,\, \operatorname{div}\mathrm{w}\right) + G\left(\mathbb{B}^{n+1}\,,\, \nabla \mathrm{w}\right) - \gamma\left\langle \kappa^{n+1}\boldsymbol{\nu}^n\,,\, \mathrm{w}\right\rangle_{\Gamma^n}, \\ 0 &= \left(\operatorname{div}\mathrm{u}^{n+1}\,,\, q\right), \end{cases}$$

interface $\{$

Oldr.-B $\{$

for all test functions w, q, $\mathbb{G}$, χ, ζ, and set $\Gamma^{n+1} = \mathrm{X}^{n+1}(\Gamma^n)$.

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$$\text{interface}\begin{cases} 0 &= \frac{1}{\Delta t}\left\langle (\mathrm{X}^{n+1} - \mathrm{id}) \cdot \boldsymbol{\nu}^n\,,\,\chi\right\rangle_{\Gamma^n}^h - \left\langle \mathrm{u}^{n+1} \cdot \boldsymbol{\nu}^n\,,\,\chi\right\rangle_{\Gamma^n}, \\ 0 &= \left\langle \kappa^{n+1}\boldsymbol{\nu}^n\,,\,\boldsymbol{\zeta}\right\rangle_{\Gamma^n}^h + \left\langle \nabla_s \mathrm{X}^{n+1}\,,\,\nabla_s \boldsymbol{\zeta}\right\rangle_{\Gamma^n}, \end{cases}$$

$$\text{Oldr.-B}\begin{cases} \\ \end{cases}$$

for all test functions w, q, $\mathbb{G}$, χ, $\boldsymbol{\zeta}$, and set $\Gamma^{n+1} = \mathrm{X}^{n+1}(\Gamma^n)$.

A fully-discrete approximation

Find $(\mathrm{u}^{n+1}, p^{n+1}, \mathbb{B}^{n+1}, \mathrm{X}^{n+1}, \kappa^{n+1})$ with $\mathbb{B}^{n+1}$ positive definite such that

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$$\text{Oldr.-B}\begin{cases} 0 &= \frac{1}{\Delta t}\left(\mathbb{B}^{n+1} - \mathbb{B}^n\,,\, \mathbb{G}\right)^h - \sum_{i,j=1}^d \left((\mathrm{u}^n)_i \Lambda_{i,j}(\mathbb{B}^{n+1})\,,\, \partial_{x_j}\mathbb{G}\right) \\ &\quad + \left(\frac{1}{\lambda^n}(\mathbb{B}^{n+1} - \mathbb{I})\,,\, \mathbb{G}\right)^h - 2\left(\nabla \mathrm{u}^{n+1}\,,\, \mathbb{I}_1^n\left[\mathbb{G}\mathbb{B}^{n+1}\right]\right) + \alpha\left(\nabla\mathbb{B}^{n+1}\,,\, \nabla\mathbb{G}\right), \end{cases}$$

for all test functions w, q, $\mathbb{G}$, χ, $\boldsymbol{\zeta}$, and set $\Gamma^{n+1} = \mathrm{X}^{n+1}(\Gamma^n)$.

Numerical analysis

Theorem: (HG-Nürnberg-Trautwein '24)
Let $\alpha \geq 0$. For $n = 0, 1, 2, \ldots$ assume that Γ^n, u^n and $\mathbb{B}^n$ positive definite are given.

- There exists at least one solution with $\mathbb{B}^{n+1}$ positive definite.
- The following discrete energy inequality holds

$$
\begin{aligned}
&\frac{1}{2}\|\sqrt{\rho^n}\mathrm{u}^{n+1}\|_{L^2}^2 + \frac{G}{2}\left(\mathrm{Tr}\,\mathbb{B}^{n+1} - \ln\det\mathbb{B}^{n+1} - d\,,\,1\right)^h + \gamma\mathrm{Area}\left(\Gamma^{n+1}\right) \\
&\quad + 2\Delta t\|\sqrt{\eta^n}\mathrm{D}\mathrm{u}^{n+1}\|_{L^2}^2 + \Delta t\Big(\frac{G}{2\lambda^n}\,,\,\mathrm{Tr}\left(\mathbb{B}^{n+1} + (\mathbb{B}^{n+1})^{-1} - 2\mathbb{I}\right)\Big)^h \\
&\quad + \Delta t\frac{\alpha G}{2d}\|\nabla\mathrm{I}_1\ln\det\mathbb{B}^{n+1}\|_{L^2}^2 \\
&\leq \frac{1}{2}\|\sqrt{\rho^{n-1}}\mathrm{u}^n\|_{L^2}^2 + \frac{G}{2}\left(\mathrm{Tr}\,\mathbb{B}^n - \ln\det\mathbb{B}^n - d\,,\,1\right)^h + \gamma\mathrm{Area}\left(\Gamma^n\right)
\end{aligned}
$$

Sketch of the proof

1. Absorb pressure to the velocity function space
2. Introduce regularizations ($\delta > 0$) in the system
3. Energy estimates uniformly in δ (and in $h, \Delta t, \alpha$)

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1. Absorb pressure to the velocity function space
2. Introduce regularizations ($\delta > 0$) in the system
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$$\frac{1}{2}\|\sqrt{\rho^n}\mathrm{u}^{n+1}\|_{L^2}^2 + \frac{G}{2}\left(\mathrm{Tr}\,\mathbb{B}^{n+1} - \mathrm{Tr}\,g_\delta(\mathbb{B}^{n+1}) - d\,,\,1\right)^h + \gamma\mathrm{Area}\,(\Gamma^{n+1})$$
$$+ 2\Delta t\|\sqrt{\eta^n}\mathrm{Du}^{n+1}\|_{L^2}^2 + \Delta t\left(\frac{G}{2\lambda^n}\,,\,\mathrm{Tr}\,(\beta_\delta(\mathbb{B}^{n+1}) + \beta_\delta(\mathbb{B}^{n+1})^{-1} - 2\mathbb{I})\right)^h$$
$$+ \Delta t\frac{\alpha G}{2d}\|\nabla \mathrm{I}_1 \ln\det\beta_\delta(\mathbb{B}^{n+1})\|_{L^2}^2$$
$$\leq \frac{1}{2}\|\sqrt{\rho^{n-1}}\mathrm{u}^n\|_{L^2}^2 + \frac{G}{2}\left(\mathrm{Tr}\,\mathbb{B}^n - \mathrm{Tr}\,g_\delta(\mathbb{B}^n) - d\,,\,1\right)^h + \gamma\mathrm{Area}\,(\Gamma^n)$$

- $g_\delta(\cdot)$ is a linear extension of $\ln(\cdot)$
- $\beta_\delta(\cdot)$ is a cut-off from below

Sketch of the proof

- uniform control of negative eigenvalues: (Barrett-Boyaval '11)

$$\mathrm{Tr}\left(\mathbb{B} - g_\delta(\mathbb{B})\right) \geq \frac{1}{4}|\mathbb{B}| + \frac{1}{4\delta}\left|[\mathbb{B}]_-\right|, \qquad [\cdot]_- : \; s \mapsto \min\{0, s\}$$

- discrete "chain rule": (Barrett-Boyaval '11)

$$\begin{aligned} &- \left((\mathrm{u} \cdot \nabla)\mathbb{B}\,,\, \mathbb{B}^{-1}\right) \\ &\approx \sum_{i,j=1}^{d} \left((\mathrm{u}^n)_i\, \Lambda_{i,j}(\mathbb{B}^{n+1})\,,\, \partial_{x_j} \mathbb{I}_1(\mathbb{B}^{n+1})^{-1}\right) = \left(\mathrm{u}^n\,,\, \nabla \mathrm{I}_1 \ln \det(\mathbb{B}^{n+1})^{-1}\right) = 0 \end{aligned}$$

- discrete analogue of the inequality: (e.g. Barrett-Boyaval '11, HG-Trautwein '24)

$$-\nabla\mathbb{B} : \nabla\mathbb{B}^{-1} \geq \frac{1}{d}|\nabla \ln \det \mathbb{B}|^2$$

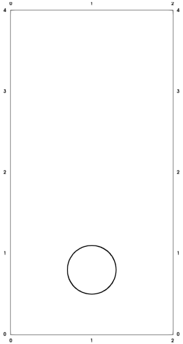
Sketch of the proof

4. Existence of solutions ($\delta > 0$) with a fixed point argument
5. Limit passing $\delta \to 0$, recover limit function with $\mathbb{B}^{n+1}$ positive definite
6. Reconstruction of pressure (if LBB stable)

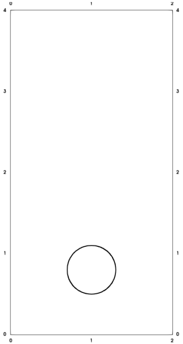
Example: rising bubble in a viscoelastic fluid

Setting: Newtonian bubble in a viscoelastic fluid. (e.g. Pillapakkam et al '07)

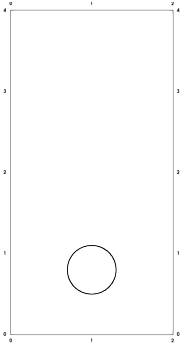
Vary the viscosity fraction $\eta/(\eta + \lambda G)$ of the outer phase:



viscosity fraction $= 1$



viscosity fraction $= 0.5$



viscosity fraction ≈ 0.05

Example: rising bubble in a viscoelastic fluid

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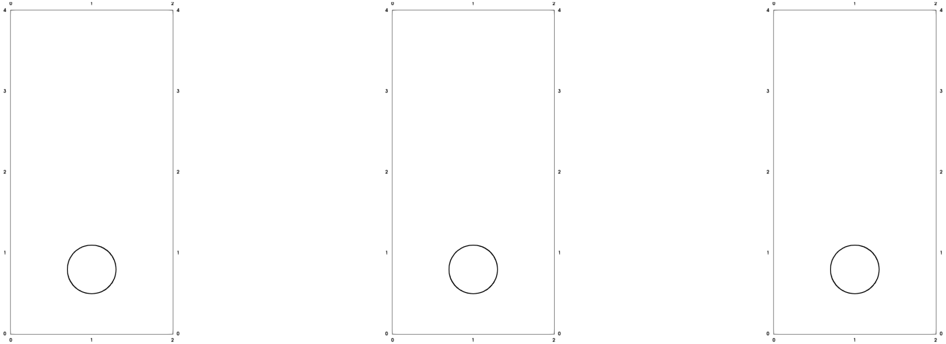
Vary the viscosity fraction $\eta/(\eta + \lambda G)$ of the outer phase:

Observations: oscillatory behaviour $\rightarrow$ development of a tail $\rightarrow$ stationary shape



viscosity fraction $= 1$ | viscosity fraction $= 0.5$ | viscosity fraction ≈ 0.05

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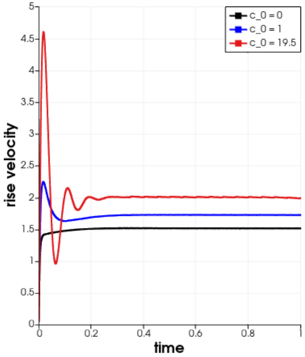
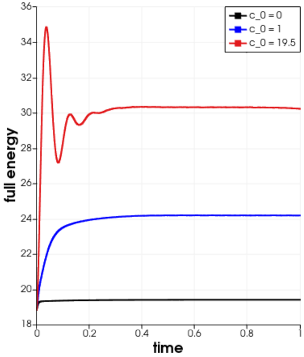


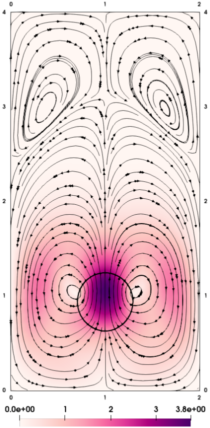
rise velocity



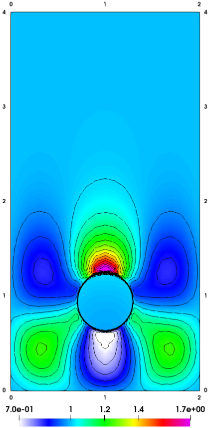
energy plot

Example: rising bubble in a viscoelastic fluid

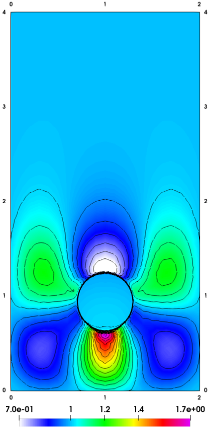
For the highly viscoelastic case: highest energy ($t = 0.04$)



velocity field



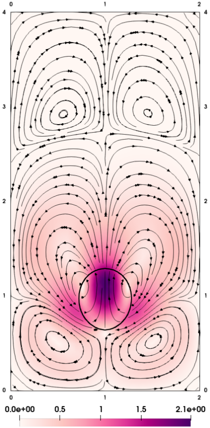
diagonal component $\mathbb{B}_{11}$



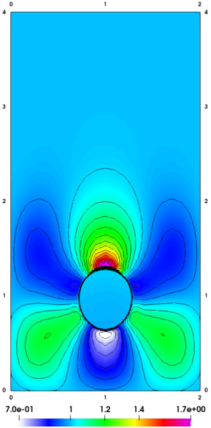
diagonal component $\mathbb{B}_{22}$

Example: rising bubble in a viscoelastic fluid

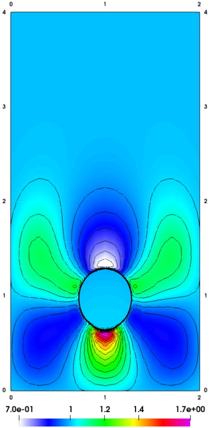
For the highly viscoelastic case: negative wake below the bubble ($t = 0.06$)



velocity field



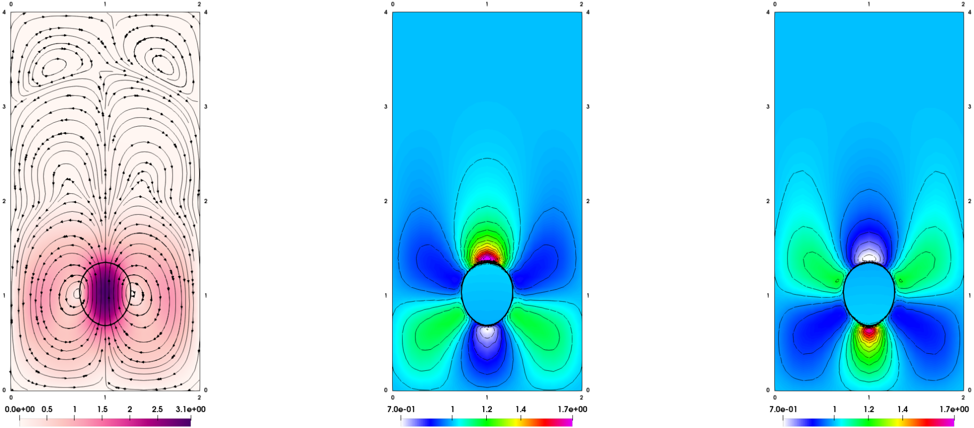
diagonal component $\mathbb{B}_{11}$



diagonal component $\mathbb{B}_{22}$

Example: rising bubble in a viscoelastic fluid

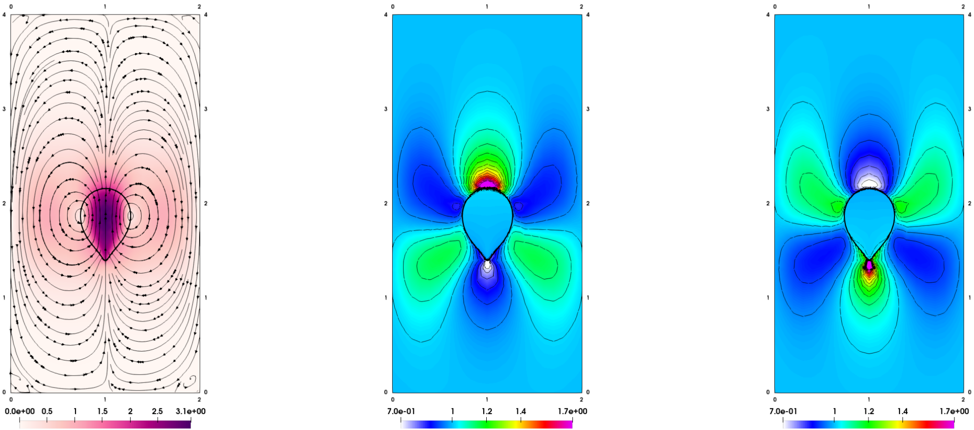
For the highly viscoelastic case: rapid acceleration of the bubble ($t = 0.10$)



velocity field | diagonal component $\mathbb{B}_{11}$ | diagonal component $\mathbb{B}_{22}$

Example: rising bubble in a viscoelastic fluid

For the highly viscoelastic case: stationary shape ($t = 0.50$)



velocity field — diagonal component $\mathbb{B}_{11}$ — diagonal component $\mathbb{B}_{22}$

Summary

- Parametric finite element method
  1. General idea
  2. Structure preserving discretization (energy, volume)
  3. Good mesh quality
- Viscoelastic two-phase models
  1. Difficulties in the Oldroyd-B model
  2. Stable numerical discretization
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Thank you for your attention