

Numerical solution of a dumbbell-based model for dilute polymer solutions

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joint with
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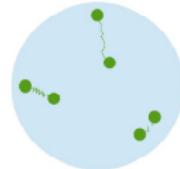


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A dumbbell model

Dilute polymer solutions: a dumbbell model

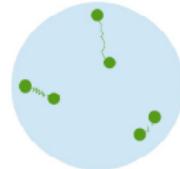
- polymer molecules surrounded by Newtonian fluid
- no interactions between molecules
- polymer molecules modeled as dumbbells



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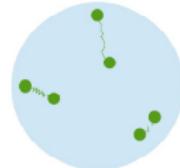
The Navier-Stokes equations

$$\begin{aligned} \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla_x) \mathbf{u} &= \nu \Delta_x \mathbf{u} + \operatorname{div}_x \mathbf{T} - \nabla_x p, & \text{in } (0, T) \times \Omega \\ \mathbf{u} = \mathbf{0} & & \text{on } (0, T) \times \partial\Omega \\ \mathbf{u}(0) = \mathbf{u}_0 & & \text{in } \Omega \\ \mathbf{T} = \gamma \int_{\mathbb{R}^d} (\mathbf{R} \otimes \mathbf{R}) \psi d\mathbf{R} - \mathbf{I} & \quad (\text{Kramer's expression}) & \text{in } (0, T) \times \Omega \end{aligned}$$

A dumbbell model

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The Navier-Stokes equations

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The Fokker-Planck equation

$$\frac{\partial \psi}{\partial t} + (\mathbf{u} \cdot \nabla_x) \psi + \operatorname{div}_R (\nabla_x \mathbf{u} \cdot \mathbf{R} \psi) = \chi \Delta_R \psi + \operatorname{div}_R (\mathbf{F}(\mathbf{R}) \psi) + \epsilon \Delta_x \psi$$

Linear vs. nonlinear spring force

Hooke's law: $\mathbf{F}(\mathbf{R}) = H\mathbf{R}$, $H > 0$

$$\frac{\partial \psi}{\partial t} + (\mathbf{u} \cdot \nabla_x) \psi + \operatorname{div}_R (\nabla_x \mathbf{u} \cdot \mathbf{R} \psi) = \Delta_R \psi + \operatorname{div}_R (H \mathbf{R} \psi) + \epsilon \Delta_x \psi$$

\approx kinetic Hookean model (γ , χ , ξ are constants)

- J.W. Barrett, E. Süli: *Existence of global weak solutions to the kinetic Hookean dumbbell model for incompressible dilute polymeric fluids*, Nonlinear Anal.-Real. (2017)

Linear vs. nonlinear spring force

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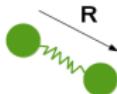
nonlinear spring law: $\mathbf{F}(\mathbf{R}) = \xi(|\mathbf{R}|^2)\mathbf{R}$

$$\frac{\partial \psi}{\partial t} + (\mathbf{u} \cdot \nabla_x) \psi + \operatorname{div}_R (\nabla_x \mathbf{u} \cdot \mathbf{R} \psi) = \chi(|\mathbf{R}|^2) \Delta_R \psi + \operatorname{div}_R (\xi(|\mathbf{R}|^2) \mathbf{R} \psi) + \epsilon \Delta_x \psi$$

+ Peterlin approximation

length of the spring is replaced by the average length

$$f(|\mathbf{R}|^2) \mapsto f(\langle |\mathbf{R}|^2 \rangle) = f(\operatorname{tr} \mathbf{C})$$



$$\operatorname{tr} \mathbf{C}(\psi) = \langle |\mathbf{R}|^2 \rangle := \int_{\mathbb{R}^d} |\mathbf{R}|^2 \psi(t, x, \mathbf{R}) d\mathbf{R}$$

$$\frac{\partial \psi}{\partial t} + (\mathbf{u} \cdot \nabla_x) \psi + \operatorname{div}_R (\nabla_x \mathbf{u} \cdot \mathbf{R} \psi) = \chi(\operatorname{tr} \mathbf{C}) \Delta_R \psi + \operatorname{div}_R (\xi(\operatorname{tr} \mathbf{C}) \mathbf{R} \psi) + \epsilon \Delta_x \psi$$

Linear vs. nonlinear spring force

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\approx kinetic Peterlin model (γ , χ , ξ functions of $\operatorname{tr} \mathbf{C}$)

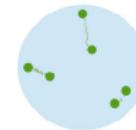
- ▶ P. Gwiazda, M. Lukáčová-Medviďová, H. Mizerová, A. Świerczewska-Gwiazda:
Existence of global weak solutions to the kinetic Peterlin model, arXiv (2017)

$$\boxed{\chi = \xi}$$

Multiscale model

The Navier-Stokes-Fokker-Planck system

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla_x) \mathbf{u} = \nu \Delta_x \mathbf{u} + \operatorname{div}_x \mathbf{T} - \nabla_x p, \quad \operatorname{div}_x \mathbf{u} = 0$$
$$\mathbf{T} = \gamma \mathbf{C}(\psi) - \mathbf{I}$$



Boundary and initial conditions: $\mathbf{u} = \mathbf{0}$ on $(0, T) \times \partial\Omega$, $\mathbf{u}(0) = \mathbf{u}_0$ in Ω

$$\frac{\partial \psi}{\partial t} + (\mathbf{u} \cdot \nabla_x) \psi + \operatorname{div}_R (\nabla_x \mathbf{u} \cdot \mathbf{R} \psi) = \chi \Delta_R \psi + \operatorname{div}_R (\xi \mathbf{R} \psi) + \epsilon \Delta_x \psi$$

Decay/boundary conditions: $\psi \rightarrow 0$ as $|\mathbf{R}| \mapsto \infty$ in $(0, T) \times \Omega$,

$$\frac{\partial \psi}{\partial \mathbf{n}} = 0 \text{ on } (0, T) \times \partial\Omega \times \mathbb{R}^d,$$

and initial condition: $\psi(0) = \psi_0$ in $\Omega \times \mathbb{R}^d$

physical space: $\mathbf{x} \in \Omega \subset \mathbb{R}^d$ configuration space: $\mathbf{R} \in \mathcal{D} = \mathbb{R}^d$

Numerical approximation

Macroscopic solvent: Navier-Stokes equations

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla_x) \mathbf{u} = \nu \Delta_x \mathbf{u} + \operatorname{div}_x \mathbf{T} - \nabla_x p, \quad \operatorname{div}_x \mathbf{u} = 0$$

Stabilized Lagrange-Galerkin method

Conforming finite element approximation: continuous piecewise linear finite elements

Method of characteristics: discretization of the material derivative

Pressure-stabilization: the Brezzi-Pitkäranta stabilization

$$\begin{aligned} \left(\frac{\mathbf{u}_h^n - \mathbf{u}_h^{n-1} \circ X^n}{\Delta t}, \mathbf{v}_h \right) &= -2\nu (\mathbf{D}(\mathbf{u}_h^n), \mathbf{D}(\mathbf{v}_h)) + (\operatorname{div} \mathbf{v}_h, p_h^n) - (\operatorname{div} \mathbf{u}_h^n, q_h) + \\ &\quad - \delta_0 \sum_K h_K^2 (\nabla p_h^n, \nabla q_h)_K - (\operatorname{tr} \mathbf{T}_h^n, \nabla \mathbf{v}_h) \end{aligned}$$

Numerical approximation

Molecular part: Fokker-Planck equation

$$\frac{\partial \psi}{\partial t} + (\mathbf{u} \cdot \nabla_x) \psi - \epsilon \Delta_x \psi = -\operatorname{div}_R (\nabla_x \mathbf{u} \cdot \mathbf{R} \psi) + \chi \Delta_R \psi + \operatorname{div}_R (\xi \mathbf{R} \psi)$$

Space splitting + Hermite spectral method:

→ configuration space ($\mathcal{D} = \mathbb{R}^2$): $\frac{\partial \psi}{\partial t} + \operatorname{div}_R (\nabla_x \mathbf{u} \cdot \mathbf{R} \psi) - \chi \Delta_R \psi - \operatorname{div}_R (\xi \mathbf{R} \psi) = 0$

→ physical space ($\Omega \subset \mathbb{R}^2$): $\frac{\partial \psi}{\partial t} + (\mathbf{u} \cdot \nabla_x) \psi - \epsilon \Delta_x \psi = 0$

$$\psi(t, \mathbf{x}, \mathbf{R}) = \sum_{z,k=0}^N \phi_{zk}(t, \mathbf{x}) \tilde{H}_z(r_1) \tilde{H}_k(r_2), \quad \mathbf{R} = (r_1, r_2)$$

$$\tilde{H}_n(r) = \frac{\omega_\alpha^{-1}(r)}{\sqrt{2^n n!}} H_n(\alpha r), \quad \omega_\alpha(r) = e^{\alpha^2 r^2}, \quad H_n(r) = (-1)^n e^{r^2} \partial_r^n(e^{-r^2}), \quad r \in \mathbb{R}$$

$$\mathcal{D}_N = \left\{ \mathbf{R}_{ij} = (r_{1,i}, r_{2,j}), i, j = 0, 1, \dots, N; H_{N+1}(r_{1,i}) = H_{N+1}(r_{2,j}) = 0 \right\}$$

Numerical approximation

Molecular part: Fokker-Planck equation

$$\frac{\partial \psi}{\partial t} + (\mathbf{u} \cdot \nabla_x) \psi - \epsilon \Delta_x \psi = -\operatorname{div}_R (\nabla_x \mathbf{u} \cdot \mathbf{R} \psi) + \chi \Delta_R \psi + \operatorname{div}_R (\xi \mathbf{R} \psi)$$

Space splitting + Hermite spectral method:

Finite difference: $\frac{\phi_{zk}^* - \phi_{zk}^{n-1}}{\Delta t} = \mathcal{L}(\phi_{zk}^*)$

Lagrange-Galerkin method: $\left(\frac{\phi_{zk}^n - \phi_{zk}^* \circ X^n}{\Delta t}, \varphi_h \right) + \epsilon (\nabla_x \phi_{zk}^n, \nabla_x \varphi_h) = 0$

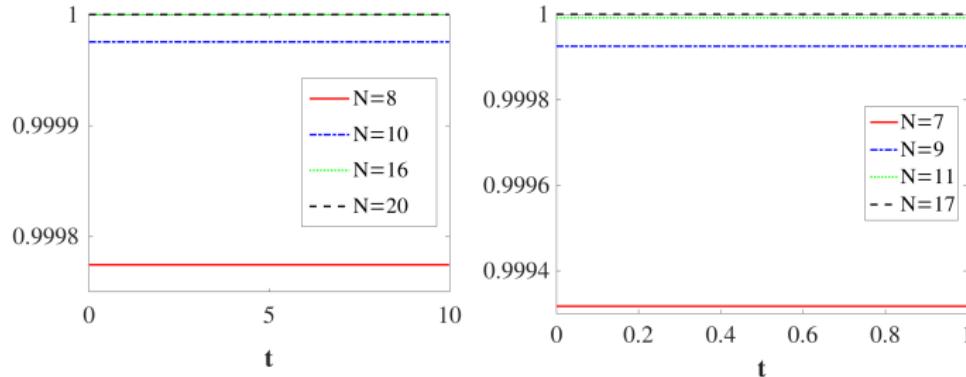
- ▶ H. Mizerová, B. She : *Multiscale simulation of dilute polymer solutions*, preprint (2017)

Conservation of discrete mass

Theorem

Let $\psi_{h,N}$ be the numerical solution of the NSFP system,
and let the initial probability density satisfy $\psi(0, \mathbf{x}, \mathbf{R}) = \psi^0(\mathbf{R})$.
Then, for any n , it holds that

$$\int_{\mathcal{D}} \psi_{h,N}^n(\mathbf{R}) d\mathbf{R} = \int_{\mathcal{D}} \psi_{h,N}^0(\mathbf{R}) d\mathbf{R}.$$

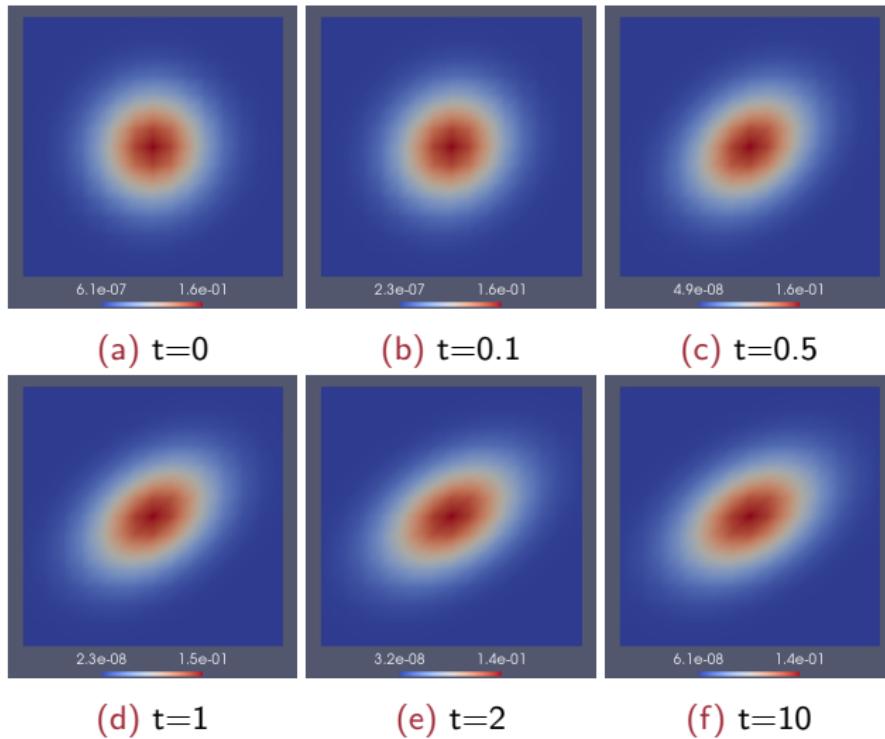


(a) FP solver: shear flow

(b) NSFP solver: Poiseulle flow

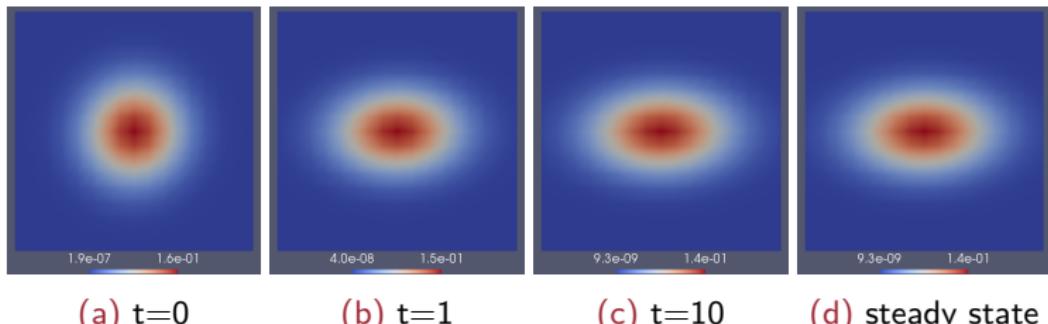
Experiment 1: shear flow

FP solver: $\mathbf{u} = (x_2, 0)^T$ $\varepsilon = \xi = \chi = 1$ $\Delta t = 0.05$ $N = 21$



Experiment 2: extensional flow

FP solver: $\nabla_x \mathbf{u} = \text{diag}\{\kappa, -\kappa\}$ $\kappa = 0.5$ $\xi = \chi = 1$ $\varepsilon = 0$ $\Delta t = 0.05$ $N = 40$



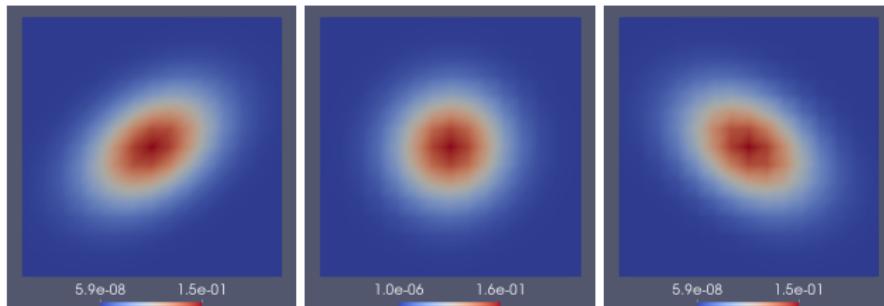
exact steady-state solution: $\psi_{\text{ref}}(\mathbf{R}) = cM e^{\mathbf{R}^T (\nabla_x \mathbf{u}) \mathbf{R}}$

numerical error: $e_\psi = \psi_{\text{ref}} - \psi_{h,N}$

N	5	8	10	16	20	30	40
$\ e_\psi\ _{L^2(\mathcal{D})}$	3.4e-2	2.1e-2	1.3e-2	3.3e-3	1.3e-3	1.5e-4	1.8e-5
$\ e_\psi\ _{L^\infty(\mathcal{D})}$	1.9e-2	7.6e-3	4.8e-3	1.2e-3	5.0e-4	5.7e-5	8.0e-6

Experiment 3: Poiseulle flow

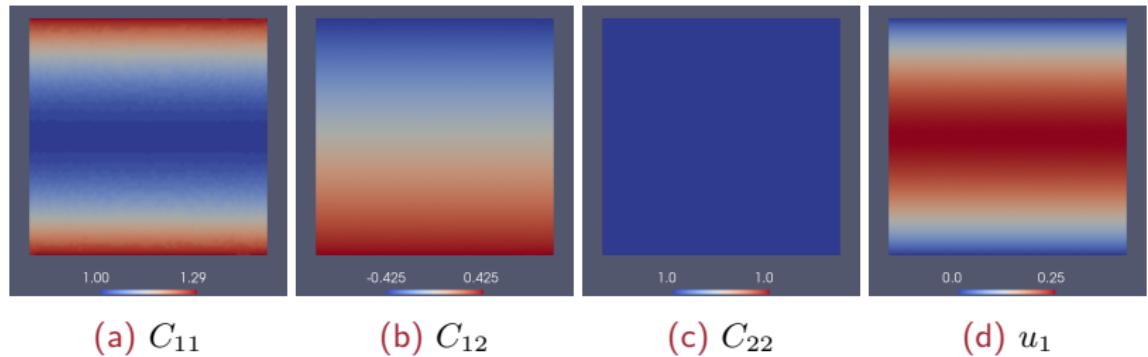
NSFP solver: $\Omega_h = [0, 1]^2$ $\mathbf{u}^0 = \left(x_2(1 - x_2), 0 \right)^T$
 $\nu = 0.5$ $\varepsilon = 0$ $\chi = \xi = \gamma = 1$ $\Delta t = h$ $T = 1$



(a) $\mathbf{x} = (0.75, 0)$ (b) $\mathbf{x} = (0.75, 0.5)$ (c) $\mathbf{x} = (0.75, 1)$

Experiment 3: Poiseulle flow

NSFP solver: $\Omega_h = [0, 1]^2$ $\mathbf{u}^0 = \left(x_2(1 - x_2), 0 \right)^T$
 $\nu = 0.5$ $\varepsilon = 0$ $\chi = \xi = \gamma = 1$ $\Delta t = h$ $T = 1$



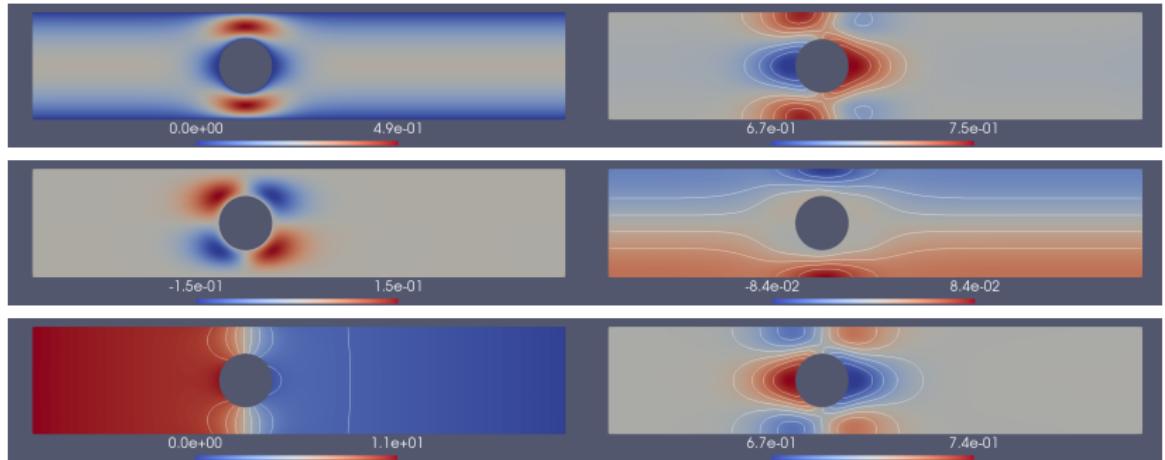
exact solution: $C_{11} = 1 + \frac{1}{2} \left| \frac{\partial u_1}{\partial x_2} \right|^2 \left(1 - (2t + 1)e^{-2t} \right)$, $C_{12} = \frac{1}{2} \frac{\partial u_1}{\partial x_2} (1 - e^{-2t})$, $C_{22} = 1$

$1/h$	N	$\ e_{\mathbf{u}}\ _{L^2(\Omega)}$	$\ e_{\mathbf{u}}\ _{H^1(\Omega)}$	$\ e_{C_{11}}\ _{L^2(\Omega)}$	$\ e_{C_{12}}\ _{L^2(\Omega)}$	$\ e_{C_{22}}\ _{L^2(\Omega)}$
16	8	2.15e-3	1.11e-2	3.17e-2	6.41e-2	2.82e-2
32	12	5.17e-4	4.33e-3	5.30e-3	1.45e-2	2.64e-3
64	16	1.30e-4	2.24e-3	2.58e-3	7.85e-3	1.53e-3

Experiment 4: flow past cylinder

NSFP solver: $\gamma = 1$ $\chi = \text{tr } \mathbf{C}$ $\xi = (\text{tr } \mathbf{C})^2$ $\varepsilon = 1$ $T = 4$ $\Delta t = 0.01$ $\nu = 0.59$

$$\text{inlet velocity } \mathbf{u} = \left(\frac{1}{4}x_2(1 - x_2), 0 \right)^T$$



solution of u_1 , u_2 , p , (left) C_{11} , C_{12} , C_{22} (right)

The Peterlin macroscopic model

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla_x) \mathbf{u} = \nu \Delta_x \mathbf{u} + \operatorname{div}_x \mathbf{T} - \nabla_x p, \quad \operatorname{div}_x \mathbf{u} = 0$$

$$\mathbf{T} = \gamma(\operatorname{tr} \mathbf{C}) \mathbf{C}$$

$$\frac{\partial \mathbf{C}}{\partial t} + (\mathbf{u} \cdot \nabla_x) \mathbf{C} - (\nabla_x \mathbf{u}) \mathbf{C} - \mathbf{C} (\nabla_x \mathbf{u})^T = \chi(\operatorname{tr} \mathbf{C}) \mathbf{I} - \xi(\operatorname{tr} \mathbf{C}) \mathbf{C} + \varepsilon \Delta_x \mathbf{C}$$

$$\text{boundary conditions: } \mathbf{u} = \mathbf{0}, \quad \varepsilon \frac{\partial \mathbf{C}}{\partial \mathbf{n}} = 0$$

$$\text{initial conditions: } \mathbf{u}(0) = \mathbf{u}_0, \quad \mathbf{C}(0) = \mathbf{C}_0$$

-
- M. Lukáčová-Medvid'ová, H. Mizerová, Š. Nečasová: *Global existence and uniqueness result for the diffusive Peterlin viscoelastic model*, Nonlinear Anal.-Theor. 120 (2015)

$$\boxed{\gamma = \chi = \operatorname{tr} \mathbf{C}, \quad \xi = (\operatorname{tr} \mathbf{C})^2}$$

- M. Lukáčová-Medvid'ová, H. Mizerová, Š. Nečasová, M. Renardy: *Global existence result for the generalized Peterlin viscoelastic model*, SIAM J. Math. Anal. 49-4 (2017)

Numerical solution

The Oseen-type Peterlin viscoelastic model

Stabilized Lagrange-Galerkin method:

I. Nonlinear scheme

Conforming finite element approximation:

Method of characteristics:

Pressure-stabilization:

Fully implicit:

continuous piecewise linear finite elements
discretization of the material derivative
the Brezzi-Pitkäranta stabilization
time discretization

$$\begin{aligned} \left(\frac{\mathbf{u}_h^n - \mathbf{u}_h^{n-1} \circ X^n}{\Delta t}, \mathbf{v}_h \right) &= -2\nu (\mathbf{D}(\mathbf{u}_h^n), \mathbf{D}(\mathbf{v}_h)) + (\operatorname{div} \mathbf{v}_h, p_h^n) - (\operatorname{div} \mathbf{u}_h^n, q_h) + \\ &\quad - \delta_0 \sum_K h_K^2 (\nabla p_h^n, \nabla q_h)_K - (\operatorname{tr} \mathbf{C}_h^n \mathbf{C}_h^n, \nabla \mathbf{v}_h) \\ \left(\frac{\mathbf{C}_h^n - \mathbf{C}_h^{n-1} \circ X^n}{\Delta t}, \mathbf{D}_h \right) &= 2 ((\nabla \mathbf{u}_h^n) \mathbf{C}_h^n, \mathbf{D}_h) + (\operatorname{div} \mathbf{u}_h^n (\mathbf{C}_h^n)^{\#}, \mathbf{D}_h) + \\ &\quad + (\operatorname{tr} \mathbf{C}_h^n \mathbf{I}, \mathbf{D}_h) - ((\operatorname{tr} \mathbf{C}_h^n)^2 \mathbf{C}_h^n, \mathbf{D}_h) - \varepsilon (\nabla \mathbf{C}_h^n, \nabla \mathbf{w}_h) \end{aligned}$$

- M. Lukáčová-Medvid'ová, H. Mizerová, H. Notuš, M. Tabata: *Numerical analysis of the Oseen-type Peterlin viscoelastic model by the stabilized Lagrange-Galerkin method, Part I: A nonlinear scheme*, ESAIM: M2AN 51 (2017)

Numerical solution

The Oseen-type Peterlin viscoelastic model

Stabilized Lagrange-Galerkin method:

II. Linear scheme

Conforming finite element approximation:

Method of characteristics:

Pressure-stabilization:

Semi-implicit:

continuous piecewise linear finite elements
discretization of the material derivative
the Brezzi-Pitkäranta stabilization
time discretization

$$\begin{aligned} \left(\frac{\mathbf{u}_h^n - \mathbf{u}_h^{n-1} \circ X^n}{\Delta t}, \mathbf{v}_h \right) &= -2\nu (\mathbf{D}(\mathbf{u}_h^n), \mathbf{D}(\mathbf{v}_h)) + (\operatorname{div} \mathbf{v}_h, p_h^n) - (\operatorname{div} \mathbf{u}_h^n, q_h) + \\ &\quad - \delta_0 \sum_K h_K^2 (\nabla p_h^n, \nabla q_h)_K - \left(\operatorname{tr} \mathbf{C}_h^n \mathbf{C}_h^{n-1}, \nabla \mathbf{v}_h \right) \\ \left(\frac{\mathbf{C}_h^n - \mathbf{C}_h^{n-1} \circ X^n}{\Delta t}, \mathbf{D}_h \right) &= 2 \left((\nabla \mathbf{u}_h^n) \mathbf{C}_h^{n-1}, \mathbf{D}_h \right) + \\ &\quad + \left(\operatorname{tr} \mathbf{C}_h^{n-1} \mathbf{I}, \mathbf{D}_h \right) - \left((\operatorname{tr} \mathbf{C}_h^{n-1})^2 \mathbf{C}_h^n, \mathbf{D}_h \right) - \varepsilon (\nabla \mathbf{C}_h^n, \nabla \mathbf{D}_h) \end{aligned}$$

- M. Lukáčová-Medvid'ová, H. Mizerová, H. Notuš, M. Tabata: *Numerical analysis of the Oseen-type Peterlin viscoelastic model by the stabilized Lagrange-Galerkin method, Part II: A linear scheme*, ESAIM: M2AN 51 (2017)

Error estimates

Scheme	nonlinear	linear
ε	≥ 0	> 0
d	2	2 and 3

Theorem (nonlinear scheme)

For any $(h, \Delta t)$ s. t. $h \in (0, h_0]$, $\Delta t \in (0, \Delta t_0]$, it holds that

$$\begin{aligned} & \| \mathbf{u}_h - \mathbf{u} \|_{\ell^\infty(L^2)}, \| \mathbf{u}_h - \mathbf{u} \|_{\ell^2(H^1)}, |p_h - p|_{\ell^2(|\cdot|_h)}, \\ & \| \mathbf{C}_h - \mathbf{C} \|_{\ell^\infty(L^2)}, \| \mathbf{C}_h - \mathbf{C} \|_{\ell^2(H^1)}, \left\| \operatorname{tr}(\mathbf{C}_h - \mathbf{C})(\mathbf{C}_h - \mathbf{C}) \right\|_{\ell^2(L^2)} \leq c_\dagger(h + \Delta t). \end{aligned}$$

Theorem (linear scheme)

For any $(h, \Delta t)$ s. t. $h \in (0, h_0]$, $\Delta t \leq \frac{c_0}{(1 + |\log h|)^{1/2}}$ ($d = 2$) or $\Delta t \leq c_0 h^{1/2}$ ($d = 3$)
it holds that

$$\begin{aligned} & \| \mathbf{u}_h - \mathbf{u} \|_{\ell^\infty(L^2)}, \| \mathbf{u}_h - \mathbf{u} \|_{\ell^2(H^1)}, |p_h - p|_{\ell^2(|\cdot|_h)}, \\ & \| \mathbf{C}_h - \mathbf{C} \|_{\ell^\infty(H^1)}, \left\| \bar{D}_{\Delta t} \mathbf{C}_h - \frac{\partial \mathbf{C}}{\partial t} \right\|_{\ell^2(L^2)} \leq c(h + \Delta t). \end{aligned}$$

Error estimates

Scheme	nonlinear	linear
ε	≥ 0	> 0
d	2	2 and 3

nonlinear, $d = 2$		
Existence	\emptyset	
Uniqueness	$\varepsilon > 0$	$\varepsilon = 0$
Optimal error estimates	$O\left((1 + \log h)^{-2}\right)$	$O(h)$
<hr/>		
linear, $\varepsilon > 0$		
Existence	\emptyset	
Uniqueness	\emptyset	
Optimal error estimates	$d = 2$	$d = 3$
	$O\left((1 + \log h)^{-1/2}\right)$	$O\left(\sqrt{h}\right)$

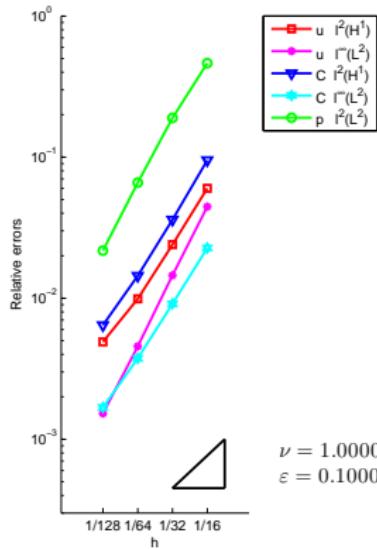
Experimental order of convergence

Semi-implicit linear scheme

- computational domain $\Omega = (0, 1)^2$
- final time $T = 0.5$
- mesh size $h = 1/16, 1/32, 1/64, 1/128$
- time step $\Delta t = h/2$
- pressure-stabilization constant $\delta_0 = 1$

h	e_u	$l^2(H^1)$	EOC	e_u	$l^\infty(L^2)$	EOC
1/16	6.01e-02	—		4.46e-02	—	
1/32	2.40e-02	1.33		1.45e-02	1.62	
1/64	9.90e-03	1.27		4.56e-01	1.67	
1/128	4.90e-03	1.02		1.52e-02	1.58	
h	e_c	$l^2(H^1)$	EOC	e_c	$l^\infty(L^2)$	EOC
1/16	9.51e-02	—		2.27e-02	—	
1/32	3.60e-02	1.40		9.13e-03	1.31	
1/64	1.44e-02	1.32		3.75e-03	1.28	
1/128	6.44e-03	1.16		1.68e-03	1.15	
h	e_p	$l^2(L^2)$	EOC			
1/16	4.64e-01	—				
1/32	1.90e-01	1.29				
1/64	6.59e-02	1.52				
1/128	2.17e-02	1.60				

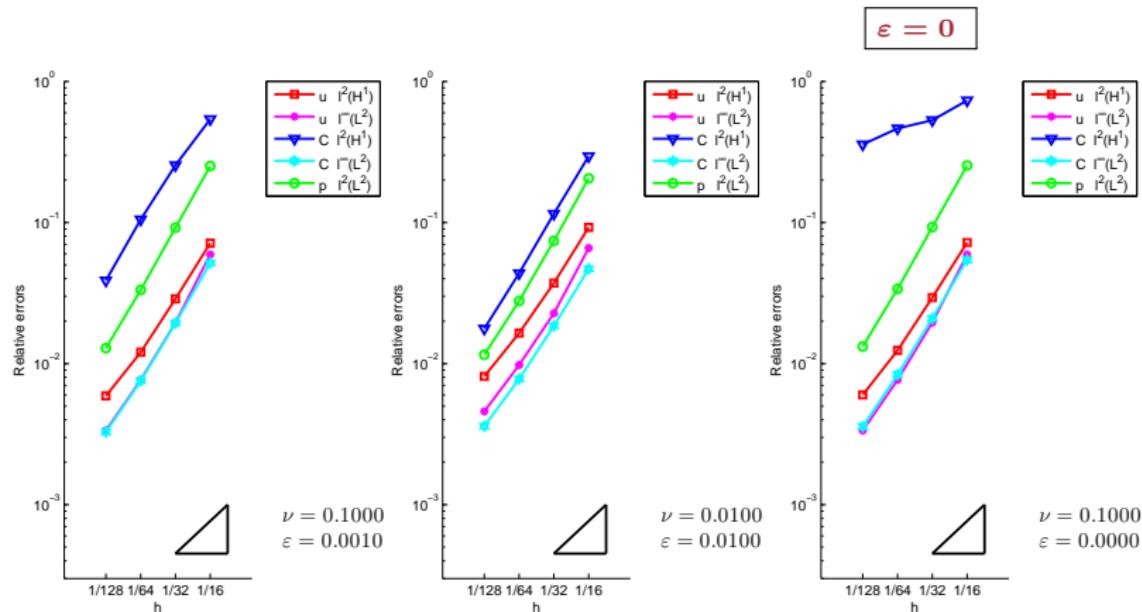
- ν = fluid viscosity
- ε = elastic stress diffusivity



Experimental order of convergence

Semi-implicit linear scheme

- computational domain $\Omega = (0, 1)^2$
 - final time $T = 0.5$
 - mesh size $h = 1/16, 1/32, 1/64, 1/128$
 - time step $\Delta t = h/2$
 - pressure-stabilization constant $\delta_0 = 1$
- ν = fluid viscosity
 - ε = elastic stress diffusivity



Thank you for your attention!