

CIMNE Coffee Talk

Simulating viscoelastic fluid flows with high Weissenberg number

Laura Moreno Martínez Advisors: Ramon Codina and Joan Baiges

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- [Viscoelasticity and heat](#page-2-0) [transfer](#page-2-0)
- **[Models of polymeric fluids](#page-4-0)**
- 2 [Logarithmic formulation](#page-7-0)
	- **[Main features](#page-8-0)**
	- [New problem to solve](#page-9-0)
	- **[Discretization](#page-11-0)**
- **3** [Stabilization](#page-12-0)
	- **Wariational Multiscale** [methods](#page-13-0)
- [Split OSS method](#page-15-0)
- **[Validation](#page-17-0)**
- 4 [Dynamic subscales](#page-19-0)
	- **[Introduction](#page-20-0)**
	- **[Design](#page-22-0)**
	- **[Results](#page-24-0)**
- **5** [Thermal coupling](#page-27-0)
	- [Coupling model](#page-28-0)
	- **[Validation](#page-29-0)**

6 [Conclusions](#page-31-0)

- Fluids depending on their behaviour under the action of shear stress, can be classified as $\sqrt{\sqrt{\frac{1}{N}}$ Newtonian and non-Newtonian
- Viscoelastic fluids are a specific type of non-Newtonian fluids that exhibits a combination of elastic and viscous effects.
	- **Visco:** friction, irreversibility, loss of memory.
	- **Elastic:** recoil, internal energy storage.
- They have "memory": the state-of-stress depends on the flow history.

- Viscoelastic fluids have very advantageous properties for heat transfer and transport:
- As the Weissenberg number increases, the dynamics of viscoelastic fluid change. This turn out in a higher mixing capacity, with benefits in the heat transfer between the fluid and the pipe transporting it.
- **Examples:** Fire brigades water tanks, petroleum extraction, reducing the drag forces in submarines, chemical reactors.

Introduction: The Weissenberg number

- **1** Computational rheology: 1970s. FEM steady 2D flows.
- 2 All methods, were found to **breakdown** at a low Weissenberg number.
- **3** The breakdown occurs for a **critical value** of the Weissenberg number, but it is specific to each problem.
- 4 For approximately 30 years, the reason for this breakdown has been a **mystery**, although it had been associated to a numerical phenomenon.

- **Niscoelasticity and heat** [transfer](#page-2-0)
- **[Models of polymeric fluids](#page-4-0)**
- **2** [Logarithmic formulation](#page-7-0)
	- **[Main features](#page-8-0)**
	- [New problem to solve](#page-9-0)
	- **[Discretization](#page-11-0)**

3 [Stabilization](#page-12-0)

National Multiscale [methods](#page-13-0)

- [Split OSS method](#page-15-0)
- [Validation](#page-17-0)
- 4 [Dynamic subscales](#page-19-0)
	- [Introduction](#page-20-0)
	- **■** [Design](#page-22-0)
	- **[Results](#page-24-0)**
- 5 [Thermal coupling](#page-27-0)
	- [Coupling model](#page-28-0)
	- [Validation](#page-29-0)
- **6** [Conclusions](#page-31-0)

Main features

- Proposed by Fattal and Kupferman (2004).
- Treats the exponential growth of the elastic stresses when the elastic component becomes dominant.
- Allows to extend the range of Weissenberg numbers. √
- More computational expensive than the standard formulation. χ

Elastic stress tensor
$$
\sigma = \frac{\eta_p}{\lambda}(\tau - I) \longrightarrow \tau = \frac{\lambda \sigma}{\eta_p} + I
$$
 [Conformation tensor]

Conformation tensor is replaced by $\psi = \log(\tau)$.

$$
-\frac{\eta_{p}}{\lambda_{0}}\nabla \cdot \exp(\psi) - 2\eta_{e}\nabla \cdot (\nabla^{s} \mathbf{u}) + \rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p = \mathbf{f}
$$

Continuity equation:

$$
\nabla \cdot \mathbf{u} = 0
$$
 New non-linearities!

Constitutive equation: \sim

$$
\frac{1}{2\lambda_0}(\exp(\psi) - \mathbf{I}) - \nabla^s \mathbf{u} + \frac{\lambda}{2\lambda_0} (\mathbf{u} \cdot \nabla \exp(\psi)) \n+ \frac{\lambda}{2\lambda_0} \left(-\exp(\psi) \cdot \nabla \mathbf{u} - (\nabla \mathbf{u})^T \cdot \exp(\psi) + 2\nabla^s \mathbf{u} \right) = \mathbf{0}
$$

Laura Moreno Martínez **Simulating viscoelastic fluid flows** 10/ 36

$$
\exp(\psi) = \underbrace{\exp(\hat{\psi} + \delta\psi)}_{\text{exp}(\delta\psi)} = \exp(\hat{\psi}) \cdot \underbrace{\exp(\delta\psi)}_{\text{exp}(\delta\psi)} \\
\left\{\n\begin{array}{c}\n\text{exp}(\delta\psi) \approx I + \delta\psi \\
\hline\n\text{exp}(\delta\psi) \approx I + \delta\psi\n\end{array}\n\right\}
$$
\nConsequently,

\n
$$
\exp(\psi) \approx \exp(\hat{\psi}) \cdot (I + \delta\psi) = \exp(\hat{\psi}) \cdot \psi + \exp(\hat{\psi}) \cdot (I - \hat{\psi}).
$$

Galerkin FE approximation. Consists in finding U_h : $(0, t_f)$ → \mathcal{X}_h ,

$$
(\underbrace{\mathcal{D}_{t}(\boldsymbol{U}_{h}),\boldsymbol{V}_{h}}_{\text{Temporal terms}})+\underbrace{\mathcal{B}(\boldsymbol{u},\boldsymbol{U}_{h},\boldsymbol{V}_{h})}_{\text{Bilinear form}}=\mathcal{L}(\boldsymbol{V}_{h}),
$$

for all $\boldsymbol{V}_h = [\boldsymbol{v}_h, q_h, \boldsymbol{\chi}_h] \in \boldsymbol{\mathcal{X}}_h$

Monolithic time discretization the simplest BDF1 scheme

$$
\frac{\delta_1 f^{n+1}}{\delta t} = \frac{f^{n+1} - f^n}{\delta t} = \frac{\partial f}{\partial t}\bigg|_{t^{n+1}} + \mathcal{O}(\delta t).
$$

$$
\frac{\partial (\exp(\psi))}{\partial t}\bigg|_{t^{n+1}} = \frac{1}{\delta t} \Big[\exp(\hat\psi^{n+1}) \cdot \psi^{n+1} + \exp(\hat\psi^{n+1}) - \exp(\hat\psi^{n+1}) \cdot \hat\psi^{n+1} \\ - \exp(\psi^n) \Big] + \mathcal{O}(\delta t) + \mathcal{O}((\delta \psi^{n+1})^2).
$$

- **Niscoelasticity and heat** [transfer](#page-2-0)
- **[Models of polymeric fluids](#page-4-0)**

2 [Logarithmic formulation](#page-7-0)

- **[Main features](#page-8-0)**
- [New problem to solve](#page-9-0)
- **[Discretization](#page-11-0)**

3 [Stabilization](#page-12-0)

National Multiscale [methods](#page-13-0)

■ [Split OSS method](#page-15-0) **[Validation](#page-17-0)**

- 4 [Dynamic subscales](#page-19-0)
	- [Introduction](#page-20-0)
	- **■** [Design](#page-22-0)
	- **[Results](#page-24-0)**
- 5 [Thermal coupling](#page-27-0)
	- [Coupling model](#page-28-0)
	- [Validation](#page-29-0)

6 [Conclusions](#page-31-0)

To approximate the components of the continuous problem solution that cannot be resolved by the finite element mesh.

$$
\overbrace{(\mathcal{D}_{t}(\boldsymbol{U}_{h}), \boldsymbol{V}_{h}) + \mathcal{B}(\boldsymbol{u}_{h}; \boldsymbol{U}_{h}, \boldsymbol{V}_{h})}^{\text{Galerkin terms}} + \overbrace{\sum_{K} \langle \underbrace{\alpha \tilde{\mathcal{P}}[\textbf{F} - \mathcal{D}_{t}(\boldsymbol{U}_{h}) - \mathcal{L}(\boldsymbol{u}_{h}; \boldsymbol{U}_{h})]}_{\boldsymbol{U}}, \mathcal{L}_{0}^{*}(\boldsymbol{u}_{h}; \boldsymbol{V}_{h}) \rangle_{K}}^{\text{Galerkin terms}} = L(\boldsymbol{V}_{h})
$$

$$
\mathcal{L}(\hat{u}; U) := \begin{pmatrix}\n-\frac{\eta_p}{\lambda_0} \nabla \cdot (\exp(\psi)) - 2\eta_e \nabla \cdot (\nabla^s u) + \rho \hat{u} \cdot \nabla u + \nabla \rho\n\end{pmatrix}
$$
\n
$$
\mathcal{L}(\hat{u}; U) := \begin{pmatrix}\n-\frac{1}{\lambda_0} \exp(\psi) - \nabla^s u + \frac{\lambda}{2\lambda_0} (\hat{u} \cdot \nabla (\exp(\psi)) \\
-\exp(\psi) \cdot \nabla \hat{u} - (\nabla \hat{u})^T \cdot \exp(\psi) + 2\nabla^s u\n\end{pmatrix}
$$
\nConstitutive

$$
\mathcal{L}_0^*(\hat{\mathbf{u}};\mathbf{V}) := \left(\begin{array}{c} \nabla\cdot\mathbf{X} - 2\eta_e\nabla\cdot(\nabla^s\mathbf{v}) - \rho\hat{\mathbf{u}}\cdot\nabla\mathbf{v} - \nabla q \\ -\nabla\cdot\mathbf{v} \\ \frac{1}{2\eta_p}\mathbf{X} + \nabla^s\mathbf{v} - \frac{\lambda}{2\eta_p}\left(\hat{\mathbf{u}}\cdot\nabla\mathbf{X} + \mathbf{X}\cdot(\nabla\hat{\mathbf{u}})^T + \nabla\hat{\mathbf{u}}\cdot\mathbf{X}\right) \end{array}\right)
$$

Laura Moreno Martínez **Simulating viscoelastic fluid flows** 15/ 36

- The **residual** based stabilization contemplates all terms.
- 2 Split OSS stabilization: neglect the cross local inner-product terms as well as some other terms that do not contribute to stability.

Benefits of Split vs Residual stabilization

- Simpler than the residual. √
- For smooth solutions, it presents optimal convergence. \checkmark
- More robust if the solutions has strong gradients. \checkmark

Remarks: Linearized problem and algorithm

- Non-linear terms are linearized with the Newton-Raphson's method.
- Tensors $\hat{\psi}$ and $\hat{\mu}$ are obtained from the previous iteration of the current time step.
- The **orthogonal projection** of any function f has been approximated as $P_h^{\perp}(f^i) \approx \overline{f}^i - P_h(f^{i-1}).$

Profile of the first component stress (σ_{xx})
along a cylinder and downstream.

Comparison of drag force coefficient.

Standard formulation break down around We=0.9. The logarithmic formulation shows good stability for higher values.

Laura Moreno Martínez **Simulating viscoelastic fluid flows** 18/ 36

Validation: Contraction 4:1

Streamlines patterns in the contraction planar for different Weissenberg number and $Re = 0.01$

Corner vortex length comparison with finer mesh.

- Standard form. is able to simulate until We=6.5 approx.
- **Logarithmic formulation until** We=15 with the coarsest mesh.

Laura Moreno Martínez **Simulating viscoelastic fluid flows** 19/ 36

- **[Viscoelasticity and heat](#page-2-0)** [transfer](#page-2-0)
- **[Models of polymeric fluids](#page-4-0)**

2 [Logarithmic formulation](#page-7-0)

- **[Main features](#page-8-0)**
- [New problem to solve](#page-9-0)
- **[Discretization](#page-11-0)**

3 [Stabilization](#page-12-0)

National Multiscale [methods](#page-13-0)

■ [Split OSS method](#page-15-0) ■ [Validation](#page-17-0)

4 [Dynamic subscales](#page-19-0)

- **[Introduction](#page-20-0)**
- **[Design](#page-22-0)**
- **[Results](#page-24-0)**
- 5 [Thermal coupling](#page-27-0)
	- [Coupling model](#page-28-0)
	- [Validation](#page-29-0)

6 [Conclusions](#page-31-0)

Classical residual-based stabilized methods for unsteady incompressible flows may experience difficulties when the time step is small relative to the spatial grid size.

- Bochev et al. argue that $\delta t > C h^2$ a sufficient condition to avoid instabilities.
- For anisotropic space-time discretizations, this inequality is not necessarily satisfied: a very common issue in viscoelastic flow formulations.

Consequently...

New stabilization techniques must be designed to compute time-dependent viscoelastic flow problems with high elasticity and anisotropic space-time discretization.

$$
\underbrace{(\mathcal{D}_t(\boldsymbol{U}_h), \boldsymbol{V}_h)}_{\substack{\text{temporal terms} \\ \text{Galerkin terms}}} + \underbrace{B(\boldsymbol{u}_h; \boldsymbol{U}_h, \boldsymbol{V}_h)}_{\text{Bilinear terms}} + \underbrace{\sum_{K} \langle \tilde{\boldsymbol{U}}, \sum_{\substack{\mathcal{L}^*(\boldsymbol{u}_h; \boldsymbol{V}_h) \\ \text{adjoint operator of } \mathcal{L}}} \rangle_K}_{\text{Stabilization terms}} = L(\boldsymbol{V}_h)
$$

Quasi-static subscales:

$$
\alpha^{-1}\tilde{\boldsymbol{U}} = \tilde{P}[\boldsymbol{F} - \mathcal{D}_t(\boldsymbol{U}_h) - \mathcal{L}(\boldsymbol{u}_h; \boldsymbol{U}_h)]
$$

Dynamic subscales:

$$
\frac{\partial \tilde{\bm{U}}}{\partial t} + \bm{\alpha}^{-1} \tilde{\bm{U}} = \tilde{P}[\bm{F} - \mathcal{D}_t(\bm{U}_h) - \mathcal{L}(\bm{u}_h; \bm{U}_h)]
$$

Discretization using a BDF1 scheme

Laura Moreno Martínez **Simulating viscoelastic fluid flows** 23/ 36

$$
S_1(\hat{\boldsymbol{u}}_h; \boldsymbol{U}_h, \boldsymbol{V}_h) = \boxed{\sum_K \langle \tilde{u}_1, -\rho \boldsymbol{u}_h \cdot \nabla \boldsymbol{v}_h \rangle_K} + \sum_K \langle \tilde{u}_2, -\nabla q_h \rangle_K
$$

+
$$
\sum_K \langle \tilde{u}_3, \nabla \cdot \chi_h \rangle_K + \sum_K \langle \tilde{p}, -\nabla \cdot \boldsymbol{v}_h \rangle_K
$$

$$
\rho \frac{\partial \tilde{u}_1}{\partial t} + \alpha_1^{-1} \tilde{u}_1 = -P_h^{\perp}(\rho \boldsymbol{u}_h \cdot \nabla \boldsymbol{u}_h),
$$

$$
\hat{\boldsymbol{u}}_1^{n+1} = \underbrace{\left(\rho \frac{1}{\delta t} + \frac{1}{\alpha_1^{n+1}}\right)^{-1}}_{\alpha_{1\text{dyn}}} \left(\rho \frac{1}{\delta t} \tilde{\boldsymbol{u}}_1^n - \rho P_h^{\perp}(\boldsymbol{u}_h^{n+1} \cdot \nabla \boldsymbol{u}_h^{n+1})\right)
$$

Coarse mesh $\delta t = 0.1$

Table: Solved and failed cases $\text{We} = 0.125$, $\alpha_{1,\text{min}} \approx 1.156 \times 10^{-3}$.

The most unstable stabilization is the quasi-static $+$ OSS stabilization.

Coarse mesh $\delta t = 0.1$

	Weissenberg (We)			
Formulation	0.125	0.165	0.25	0.5
Std-Static	Solved	Failed		
Std-Dyn	Solved	Solved	Solved	Failed
Log-Static	Solved	Solved	Failed	
Log-Dyn	Solved	Solved	Solved	Solved

Table: Solved and failed cases for S-OSS formulations, dynamic and quasi-static, $\delta t = 0.1$

Dynamic formulations are more efficient avoiding elastic instabilities.

Laura Moreno Martínez **Simulating viscoelastic fluid flows** 26/ 36

	Stabilization S-OSS			
Formulation	Quasi-static	Dynamic		
Standard	Failed - time step 265	Failed - time step 1316		
Logarithmic	Failed - time step 340	Solved		

Table: Comparison between different formulations, $\text{We} = 1.0$, $\delta t = 0.0025$. The time step at which convergence fails is indicated.

- **[Viscoelasticity and heat](#page-2-0)** [transfer](#page-2-0)
- **[Models of polymeric fluids](#page-4-0)**

2 [Logarithmic formulation](#page-7-0)

- **[Main features](#page-8-0)**
- [New problem to solve](#page-9-0)
- **[Discretization](#page-11-0)**

3 [Stabilization](#page-12-0)

National Multiscale [methods](#page-13-0)

- [Split OSS method](#page-15-0)
- [Validation](#page-17-0)
- 4 [Dynamic subscales](#page-19-0)
	- [Introduction](#page-20-0)
	- **■** [Design](#page-22-0)
	- **[Results](#page-24-0)**
- **5** [Thermal coupling](#page-27-0)
	- [Coupling model](#page-28-0)
	- [Validation](#page-29-0)

[Conclusions](#page-31-0)

Energy equation is added:

$$
\rho C_p \left(\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta \right) = k \Delta \theta + \underbrace{\sigma : \nabla^s \mathbf{u}}_{\text{Viscous dissipation}}
$$

Viscosity and relaxation time parameters now will be temperature dependent: $\lambda(\theta) = \lambda(\theta_0) f(\theta)$, and $\eta_0(\theta) = \eta_0(\theta_0) f(\theta)$

Algorithm: iterative, non-monolithic, executed in a partitioned manner П

- Distribution of temperature (K) (below) and stress component (top) around the cylinder for We=4.
- \blacksquare Temperature rise as function of the Weissenberg number.
- Reduction of the stress when temperature increase, due to the heating of the material.

Temperature on the walls (563 K) is greater than the fluid temperature at the inlet (463 K).

However, viscous dissipation generates thermal energy in the flowing fluid.

Highest temperature is reached in the central zone.

k.

- **[Viscoelasticity and heat](#page-2-0)** [transfer](#page-2-0)
- **[Models of polymeric fluids](#page-4-0)**

2 [Logarithmic formulation](#page-7-0)

- **[Main features](#page-8-0)**
- [New problem to solve](#page-9-0)
- **[Discretization](#page-11-0)**

3 [Stabilization](#page-12-0)

National Multiscale [methods](#page-13-0)

- [Split OSS method](#page-15-0)
- [Validation](#page-17-0)
- 4 [Dynamic subscales](#page-19-0)
	- [Introduction](#page-20-0)
	- **■** [Design](#page-22-0)
	- **[Results](#page-24-0)**
- **5** [Thermal coupling](#page-27-0)
	- [Coupling model](#page-28-0)
	- [Validation](#page-29-0)
- **6** [Conclusions](#page-31-0)

- **1** The convergence of the proposed method has a strong dependency on the treatment of the exponential function.
- 2 The resulting method allows to obtain globally stable solutions, validated in different benchmarks.
- 3 It shows accuracy, optimal convergence for smooth solutions and robustness.
- **4 Dynamic subscales** allow to solve problems where two different sources of instability can appear simultaneouly: one originated by a time step small and the other the exponential growth typical of high Weissenberg numbers.
- **5** In thermal coupling the **viscous dissipation effect** is significant, especially for high-velocity flows or highly viscous flows even at moderate velocities.

Presentation based on the next papers:

- L.Moreno, R. Codina, J.Baiges and E. Castillo. Logarithmic conformation reformulation in viscoelastic flow problems approximated by a VMS-type stabilized finite element formulation. Computer Methods in Applied Mechanics and Engineering. 2019 Sep 1;354:706-31
- L. Moreno, R. Codina and J.Baiges. Solution of transient viscoelastic flow problems aproximated by a term-by-term VMS stabilized finite element formulation using time-dependent subgrid-scales.

- R. Fattal and R. Kupferman. Constitutive laws for the matrix-logarithm of the conformation tensor. Journal of Non-Newtonian Fluid Mechanics, 123(2-3):281–285, 2004.
- Variational multi-scale stabilized formulations for the stationary three-field incompressible viscoelastic flow problem. Computer Methods in Applied Mechanics and Engineering, 279:579–605, 2014.
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- P. B. Bochev, M. D. Gunzburger, and J. N. Shadid. "On inf-sup stabilized finite element methods for transient problems." Computer Methods in Applied Mechanics and Engineering 193.15-16: 1471-1489, 2004.
- E. Castillo and R. Codina. Dynamic term-by-term stabilized finite element formulation using orthogonal subgrid-scales for the incompressible Navier–Stokes problem. Computer Methods in Applied Mechanics and Engineering, 349, 701-721. 2019

[Introduction](#page-2-0) [Logarithmic formulation](#page-7-0) [Stabilization](#page-12-0) [Dynamic subscales](#page-19-0) [Thermal coupling](#page-27-0) [Conclusions](#page-31-0)

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Thank you for your attention!!

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Laura Moreno Martínez **Simulating viscoelastic fluid flows** 36/ 36 36/ 36