



### CIMNE Coffee Talk

# Simulating viscoelastic fluid flows with high Weissenberg number

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- Fluids depending on their behaviour under the action of shear stress, can be classified as 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.
  - **<u>Elastic</u>**: 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.
- For approximately 30 years, the reason for this breakdown has been a mystery, although it had been associated to a numerical phenomenon.

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#### 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.  $\checkmark$
- More computational **expensive** than the standard formulation. X



Elastic stress tensor

$$=rac{\eta_p}{\lambda}( au-\mathbf{I})\longrightarrow au=rac{\lambdaoldsymbol{\sigma}}{\eta_p}+rac{\lambdaoldsymbol{\sigma}}{\eta_p}+rac{\lambdaoldsymbol{\sigma}}{\eta_p}$$

Conformation tensor

Conformation tensor is replaced by

$$\psi = \log( au).$$



Continuity equation:

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

Constitutive equation:

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

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**Galerkin FE** approximation. Consists in finding  $\boldsymbol{U}_h: (0, t_f) \longrightarrow \boldsymbol{\mathcal{X}}_h$ ,

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

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

Monolithic time discretization the simplest BDF1 scheme

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

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

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



•  $\mathcal{L}$  is the operator associated to the problem.

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### Stabilized formulation: Main operators

$$\overbrace{\left(\mathcal{D}_{t}(\boldsymbol{U}_{h}),\boldsymbol{V}_{h}\right)+B(\boldsymbol{u}_{h};\boldsymbol{U}_{h},\boldsymbol{V}_{h})}^{\text{Galerkin terms}} + \overbrace{K}^{\text{Stabilization terms}} \underbrace{\underbrace{\left(\Delta \tilde{\boldsymbol{\mu}}[\boldsymbol{F}-\mathcal{D}_{t}(\boldsymbol{U}_{h})-\mathcal{L}(\boldsymbol{u}_{h};\boldsymbol{U}_{h})]}_{\tilde{\boldsymbol{U}}}, \mathcal{L}_{0}^{*}(\boldsymbol{u}_{h};\boldsymbol{V}_{h})\right)_{K}}^{\text{Galerkin terms}} = L(\boldsymbol{V}_{h})$$

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

$$\mathcal{L}_{0}^{*}(\hat{\boldsymbol{a}};\boldsymbol{V}) := \begin{pmatrix} \nabla \cdot \boldsymbol{\chi} - 2\eta_{e}\nabla \cdot (\nabla^{s}\boldsymbol{v}) - \rho\hat{\boldsymbol{a}} \cdot \nabla \boldsymbol{v} - \nabla q \\ -\nabla \cdot \boldsymbol{v} \\ \frac{1}{2\eta_{p}}\boldsymbol{\chi} + \nabla^{s}\boldsymbol{v} - \frac{\lambda}{2\eta_{p}} \left(\hat{\boldsymbol{a}} \cdot \nabla\boldsymbol{\chi} + \boldsymbol{\chi} \cdot (\nabla\hat{\boldsymbol{a}})^{T} + \nabla\hat{\boldsymbol{a}} \cdot \boldsymbol{\chi} \right) \end{pmatrix}$$

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- **1** 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.

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### Stabilized formulation: Some remarks

#### Benefits of Split vs Residual stabilization

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

#### Remarks: Linearized problem and algorithm

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



We = 0.7

 $\mathrm{We}=0.9$ 

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

Comparison of drag force coefficient.

We

0 0.2 0.4 0.6 0.8

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

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 $1.2 \ 1.4 \ 1.6 \ 1.8 \ 2 \ 2.2 \ 2.4 \ 2.6$ 

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Validat	ion: Contracti	on $1.1$			

### Validation: Contraction 4:1





Streamlines patterns in the contraction planar for different Weissenberg number and  ${
m Re}=0.01.$ 



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.

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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  $\delta t > Ch^2$  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.



$$\underbrace{\underbrace{(\mathcal{D}_{t}(\boldsymbol{U}_{h}),\boldsymbol{V}_{h})}_{\text{Temporal terms}} + \underbrace{B(\boldsymbol{u}_{h};\boldsymbol{U}_{h},\boldsymbol{V}_{h})}_{\text{Bilinear terms}} + \underbrace{\sum_{K} \langle \tilde{\boldsymbol{U}}, \quad \mathcal{L}^{*}(\boldsymbol{u}_{h};\boldsymbol{V}_{h}) \\ \text{adjoint operator of } \mathcal{L}}_{\text{Stabilization terms}} \rangle_{K} = L(\boldsymbol{V}_{h})$$

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:

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



Discretization using a BDF1 scheme

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$$S_{1}(\hat{\boldsymbol{u}}_{h};\boldsymbol{U}_{h},\boldsymbol{V}_{h}) = \boxed{\sum_{K} \langle \tilde{\boldsymbol{u}}_{1}, -\rho \boldsymbol{u}_{h} \cdot \nabla \boldsymbol{v}_{h} \rangle_{K}} + \sum_{K} \langle \tilde{\boldsymbol{u}}_{2}, -\nabla q_{h} \rangle_{K}} + \sum_{K} \langle \tilde{\boldsymbol{u}}_{3}, \nabla \cdot \boldsymbol{\chi}_{h} \rangle_{K} + \sum_{K} \langle \tilde{\boldsymbol{p}}, -\nabla \cdot \boldsymbol{v}_{h} \rangle_{K}} \rho \frac{\partial \tilde{\boldsymbol{u}}_{1}}{\partial t} + \alpha_{1}^{-1} \tilde{\boldsymbol{u}}_{1} = -P_{h}^{\perp}(\rho \boldsymbol{u}_{h} \cdot \nabla \boldsymbol{u}_{h}),$$
$$\boxed{\tilde{\boldsymbol{u}}_{1}^{n+1} = \left(\rho \frac{1}{\delta t} + \frac{1}{\alpha_{1}^{n+1}}\right)^{-1} \left(\rho \frac{1}{\delta t} \tilde{\boldsymbol{u}}_{1}^{n} - \rho P_{h}^{\perp}(\boldsymbol{u}_{h}^{n+1} \cdot \nabla \boldsymbol{u}_{h}^{n+1})\right)}$$

 $\alpha_{1dvn}$ 





Coarse mesh

 $\delta t = 0.1$ 

P1 elements		Т	ime step ( $\delta t$ )	
Method	0.050	0.0250	$3.125 imes10^{-3}$	$1.562 imes10^{-3}$
Static-OSS	Solved	Failed	-	-
Dyn-OSS	Solved	Solved	Solved	Solved
Static-SOSS	Solved	Solved	Solved	Failed
Dyn-SOSS	Solved	Solved	Solved	Solved

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

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.

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Renchm	ark: Lid-drive	en cavity	flow proble	m	



	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, We = 1.0,  $\delta t$  = 0.0025. The time step at which convergence fails is indicated.

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Therma	al coupling				

Energy equation is added:

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

• 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



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

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Validatio	on: Extension	1:3			





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**.

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- 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.
- In thermal coupling the viscous dissipation effect is significant, especially for high-velocity flows or highly viscous flows even at moderate velocities.

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Referen	ces				

#### Presentation based on the next papers:

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- 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.
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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.
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### Thank you for your attention!!

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