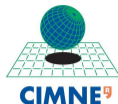




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Computation of transient viscoelastic flow problems
approximated by a VMS stabilized Finite Element formulation
using time-dependent subgrid-scales for monolithic and
fractional step schemes

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Outline

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What is a viscoelastic fluid?

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- Viscoelastic fluids are a specific type of **non-Newtonian fluids** that exhibit a combination of **elastic** and **viscous** effects.
 - **Visco**: friction, irreversibility, loss of memory.
 - **Elastic**: recoil, internal energy storage.
- This combination of properties is explained by a **complex internal structure**.
- They have **memory**. The state-of-stress depends on the flow history.



wikipedia

Modelling of polymeric fluid flows

- Momentum equation:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} - \nabla \cdot \mathbf{T} + \nabla p = \mathbf{f}$$

Deviatoric extra stress tensor

$$\mathbf{T} = 2\eta(\nabla^s \mathbf{u})$$

Newtonian viscous fluids

- Continuity equation:

$$\nabla \cdot \mathbf{u} = 0$$

$$\mathbf{T} = 2\eta_s(\nabla^s \mathbf{u}) + \sigma$$

Polymeric fluids

- Constitutive equation:

$$\frac{1}{2\eta_p}(1 + \mathfrak{h}(\sigma)) \cdot \sigma - \nabla^s \mathbf{u} + \frac{\lambda}{2\eta_p} \left(\frac{\partial \sigma}{\partial t} + \mathbf{u} \cdot \nabla \sigma - \sigma \cdot \nabla \mathbf{u} + (\nabla \mathbf{u})^T \cdot \sigma \right) = \mathbf{0}$$

$$\mathfrak{h}(\sigma) = 0$$

Oldroyd-B

$$\mathfrak{h}(\sigma) = \frac{\varepsilon \lambda}{\eta_p} \sigma$$

Giesekus

$$\mathfrak{h}(\sigma) = \frac{\varepsilon \lambda}{\eta_p} \text{tr}(\sigma)$$

Phan-Thien-Tanner

The Weissenberg number and HWNP

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- We is small: viscous effect relevant, elastic behavior small.
- If $We > 1$: problems become extremely complicated.

Weissenberg number

$$We = \frac{\lambda U}{L}$$

Problem: The High Weissenberg Number Problem (HWNP)

"Solution": the Log-Conformation Reformulation (LCR)

Motivation and goal

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

- Bochev et al. demonstrate that $\delta t > Ch^2$ is a **sufficient condition** to avoid instabilities.
- For anisotropic space-time discretizations, this inequality **is not necessarily satisfied**.

Goal

- 1 **Design of new stabilization techniques.**
- 2 Design **fractional step schemes** in order to reduce the expensive computational cost.

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Spatial and temporal discretizations

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Spatial discretization

Galerkin finite element approximation. It consists in finding $\mathbf{U}_h : (0, T) \rightarrow \mathcal{X}_h$,

$$\underbrace{(\mathcal{G}(\mathbf{U}_h), \mathbf{V}_h)}_{\text{Temporal terms}} + \underbrace{B(\mathbf{u}_h; \mathbf{U}_h, \mathbf{V}_h)}_{\text{Semi-linear form}} = L(\mathbf{V}_h),$$

for all $\mathbf{V}_h \in \mathcal{X}_h$.

Time discretization

Monolithic and **fractional step** time discretization. BDF1 and BDF2 schemes have been employed in this work.

Stabilization technique: Variational Multi-Scale (VMS) Methods

- Objective: to approximate the components of the continuous problem solution that cannot be resolved by the finite element mesh.
- Unknown splitting: $\mathbf{U} = \underbrace{\mathbf{U}_h}_{\in \mathcal{X}_h} + \underbrace{\tilde{\mathbf{U}}}_{\in \tilde{\mathcal{X}}}$ and $\mathcal{X} = \mathcal{X}_h \oplus \tilde{\mathcal{X}}$.

$$\underbrace{(\mathcal{G}(\mathbf{U}_h), \mathbf{V}_h) + B(\mathbf{u}_h; \mathbf{U}_h, \mathbf{V}_h)}_{\text{Galerkin terms}} + \underbrace{\langle \mathcal{G}(\tilde{\mathbf{U}}), \mathbf{V}_h \rangle + \sum_K \langle \tilde{\mathbf{U}}, \underbrace{\mathcal{L}^*(\mathbf{u}_h; \mathbf{V}_h)}_{\text{adjoint operator of } \mathcal{L}} \rangle_K}_{\text{Stabilization terms}} = L(\mathbf{V}_h)$$

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

Sub-grid scale

- \tilde{P} is the L^2 – projection onto the space of sub-grid scales,
- α is a matrix computed within each element,
- \mathcal{L} is the operator associated with the problem.

Dynamic subscales for residual-based stabilized formulation

$$\underbrace{\mathcal{G}(\mathbf{U}_h, \mathbf{V}_h) + B(\mathbf{u}_h; \mathbf{U}_h, \mathbf{V}_h)}_{\text{Galerkin terms}} + \underbrace{(\mathcal{G}(\tilde{\mathbf{U}}), \mathbf{V}_h) + S_1(\mathbf{u}_h; \mathbf{U}_h, \mathbf{V}_h) + S_2(\mathbf{U}_h, \mathbf{V}_h) + S_3(\mathbf{u}_h; \mathbf{U}_h, \mathbf{V}_h)}_{\text{Stabilization terms}} = \underbrace{L(\mathbf{V}_h)}_{\text{Gal. term}}$$

$$S_1(\hat{\mathbf{u}}_h; \mathbf{U}_h, \mathbf{V}_h) = \sum_K \langle \tilde{\mathbf{u}}, -\nabla \cdot \boldsymbol{\chi}_h + \underbrace{2\beta\eta_0 \nabla \cdot (\nabla^s \mathbf{v}_h) + \rho \hat{\mathbf{u}}_h \cdot \nabla \mathbf{v}_h + \nabla q_h}_{\text{Momentum eq. residual}} \rangle_K$$

$$\rho \frac{\partial \tilde{\mathbf{u}}}{\partial t} + \alpha_1^{-1} \tilde{\mathbf{u}} = \tilde{P}(\mathbf{F}_1 - \rho \frac{\partial \mathbf{u}_h}{\partial t} - \mathcal{L}_1(\mathbf{u}_h; \mathbf{U}_h)),$$

$$\tilde{\mathbf{u}}^{n+1} = \underbrace{\left(\rho \frac{1}{\delta t} + \frac{1}{\alpha_1^{n+1}} \right)^{-1}}_{\alpha_{1\text{dyn}}} \left(\rho \frac{1}{\delta t} \tilde{\mathbf{u}}^n - \rho \tilde{P}(\mathbf{F}_1 - \rho \frac{\partial \mathbf{u}_h}{\partial t} - \mathcal{L}_1(\mathbf{u}_h; \mathbf{U}_h)) \right)$$

Discretization using a BDF1 scheme

Stabilized formulation: Residual-based vs Split OSS

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$$\underbrace{(\mathcal{G}(\mathbf{U}_h), \mathbf{V}_h) + B(\mathbf{u}_h; \mathbf{U}_h, \mathbf{V}_h)}_{\text{Galerkin terms}} + \underbrace{(\mathcal{G}(\tilde{\mathbf{U}}), \mathbf{V}_h) + S_1(\mathbf{u}_h; \mathbf{U}_h, \mathbf{V}_h) + S_2(\mathbf{U}_h, \mathbf{V}_h) + S_3(\mathbf{u}_h; \mathbf{U}_h, \mathbf{V}_h)}_{\text{Stabilization terms}} = \underbrace{L(\mathbf{V}_h)}_{\text{Gal. term}}$$

$$S_1(\hat{\mathbf{u}}_h; \mathbf{U}_h, \mathbf{V}_h) = \sum_K \alpha_{1\text{dyn}} \left\langle \rho \frac{1}{\delta t} \tilde{\mathbf{u}}^n + \tilde{P} \left[\rho \frac{\partial \mathbf{u}_h}{\partial t} \underbrace{- \frac{\eta_p}{\lambda_0} \nabla \cdot (\exp(\psi_h))}_{\tilde{u}_1} \right. \right. \\ \left. \left. \underbrace{+ \rho \hat{\mathbf{u}}_h \cdot \nabla \mathbf{u}_h}_{\tilde{u}_2}, \right. \right. \\ \left. \left. \underbrace{+ \nabla p_h}_{\tilde{u}_3} \right] \left[-\nabla \cdot \chi_h \right. \right. \\ \left. \left. + 2\eta_s \nabla \cdot (\nabla^s \mathbf{v}_h) \right. \right. \\ \left. \left. + \rho \hat{\mathbf{u}}_h \cdot \nabla \mathbf{v}_h \right. \right. \\ \left. \left. + \nabla q_h \right] \right\rangle_K$$

- 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. In that case $\tilde{P} = P_h^\perp$.

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Fractional step. Algebraic system

Momentum $M_{\mathbf{u}} \frac{\delta_k}{\delta t} \mathbf{U}^{n+1} + K_{\mathbf{u}} (\mathbf{U}^{n+1}) \mathbf{U}^{n+1} + G \mathbf{P}^{n+1} - D_{\psi}^E \boldsymbol{\Psi}^{n+1} = \mathbf{F}_{\mathbf{u}}^E,$ (1)

Continuity $D \mathbf{U}^{n+1} = \mathbf{0},$ (2)

Constitutive $M_{\psi}^E \frac{\delta_k}{\delta t} \boldsymbol{\Psi}^{n+1} + K_{\psi}^E (\mathbf{U}^{n+1}) \boldsymbol{\Psi}^{n+1} - S \mathbf{U}^{n+1} = \mathbf{F}_{\psi}^E.$ (3)

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & 0 \\ A_{31} & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{U}^{n+1} \\ \boldsymbol{\Psi}^{n+1} \\ \mathbf{P}^{n+1} \end{bmatrix} = \begin{bmatrix} \mathbf{F}_1^{n+1} \\ \mathbf{F}_2^{n+1} \\ \mathbf{F}_3^{n+1} \end{bmatrix}$$

$$A_{11} = \frac{1}{\gamma_k \delta t} M_{\mathbf{u}} + K_{\mathbf{u}} (\mathbf{U}^{n+1}),$$

$$A_{12} = -D_{\psi}^E,$$

$$A_{21} = -S,$$

$$A_{22} = \frac{1}{\gamma_k \delta t} M_{\psi}^E + K_{\psi}^E (\mathbf{U}^{n+1}),$$

$$A_{13} = G,$$

$$A_{31} = D,$$

$$\mathbf{F}_1 = \mathbf{F}_{\mathbf{u}}^E + \frac{1}{\delta t \gamma_k} \left(\sum_{i=0}^{k-1} \varphi_k^i \mathbf{U}^{n-i} \right), \quad \mathbf{F}_3 = 0,$$

$$\mathbf{F}_2 = \mathbf{F}_{\psi}^E + \frac{1}{\delta t \gamma_k} \left(\sum_{i=0}^{k-1} \varphi_k^i \boldsymbol{\Psi}^{n-i} \right).$$

Fractional step. Equivalent form

$$M_{\mathbf{u}} \frac{\delta_k}{\delta t} \tilde{\mathbf{U}}^{n+1} + K_{\mathbf{u}} \left(\tilde{\mathbf{U}}^{n+1} \right) \tilde{\mathbf{U}}^{n+1} + G \hat{\mathbf{P}}_{k'-1}^{n+1} - D_{\psi}^E \hat{\Psi}_{k'-1}^{n+1} = \mathbf{F}_{\mathbf{u}}^E, \quad (4)$$

$$M_{\mathbf{u}} \frac{\delta_k}{\delta t} \left(\mathbf{U}^{n+1} - \tilde{\mathbf{U}}^{n+1} \right) + N_{\mathbf{u}} + G \left(\mathbf{P}^{n+1} - \hat{\mathbf{P}}_{k'-1}^{n+1} \right) - D_{\psi}^E \left(\Psi^{n+1} - \hat{\Psi}_{k'-1}^{n+1} \right) = \mathbf{0}, \quad (5)$$

$$M_{\psi}^E \frac{\delta_k}{\delta t} \tilde{\Psi}^{n+1} + K_{\psi}^E \left(\tilde{\mathbf{U}}^{n+1} \right) \tilde{\Psi}^{n+1} - S \tilde{\mathbf{U}}^{n+1} = \mathbf{F}_{\psi}^E, \quad (6)$$

$$M_{\psi}^E \frac{\delta_k}{\delta t} \left(\Psi^{n+1} - \tilde{\Psi}^{n+1} \right) + \mathbf{N}_{\psi}^{n+1} - S \left(\mathbf{U}^{n+1} - \tilde{\mathbf{U}}^{n+1} \right) = \mathbf{0}, \quad (7)$$

$$\begin{aligned} -D \tilde{\mathbf{U}}^{n+1} + \gamma_k \delta t D M_{\mathbf{u}}^{-1} \mathbf{N}_{\mathbf{u}}^{n+1} + \gamma_k \delta t D M_{\mathbf{u}}^{-1} G \left(\mathbf{P}^{n+1} - \hat{\mathbf{P}}_{k'-1}^{n+1} \right) \\ - \gamma_k \delta t D M_{\mathbf{u}}^{-1} D_{\psi}^E \left(\Psi^{n+1} - \hat{\Psi}_{k'-1}^{n+1} \right) = \mathbf{0}, \end{aligned} \quad (8)$$

$\tilde{\mathbf{U}}^{n+1}$ and $\tilde{\Psi}^{n+1}$ are the **auxiliary variables** that later must be corrected.

$\hat{\mathbf{g}}_{k'-1}^{n+1}$ are the **extrapolated variables**, where the order of the extrapolation is $k' - 1$ at time t^{n+1} .

(4) + (5) \longrightarrow (1) Momentum

(6) + (7) \longrightarrow (3) Constitutive

(8) + $\gamma_k \delta t D$ (5) \longrightarrow (2) Continuity

Fractional step. Algorithm (I). Intermediate steps

- 1 Compute the intermediate velocity** using extrapolated values of the pressure and ψ variable.

$$(4) M_u \frac{\delta_k}{\delta t} \tilde{\mathbf{U}}^{n+1} + K_u \left(\tilde{\mathbf{U}}^{n+1} \right) \tilde{\mathbf{U}}^{n+1} + G \hat{\mathbf{P}}_{k'-1}^{n+1} - D_\psi^E \hat{\Psi}_{k'-1}^{n+1} = \mathbf{F}_u^E \longrightarrow \tilde{\mathbf{U}}^{n+1}$$

- 2 Compute the intermediate ψ** using the intermediate velocity computed in the previous step.

$$(6) M_\psi^E \frac{\delta_k}{\delta t} \tilde{\Psi}^{n+1} + K_\psi^E \left(\tilde{\mathbf{U}}^{n+1} \right) \tilde{\Psi}^{n+1} - S \tilde{\mathbf{U}}^{n+1} = \mathbf{F}_\psi^E \longrightarrow \tilde{\Psi}^{n+1}$$

- 3 Compute the intermediate pressure** using both intermediate velocities and ψ computed in the two previous steps:

$$(8) -D \tilde{\mathbf{U}}^{n+1} + \gamma_k \delta t D M_u^{-1} \mathbf{N}_u^{n+1} + \gamma_k \delta t D M_u^{-1} G \left(\tilde{\mathbf{P}}^{n+1} - \hat{\mathbf{P}}_{k'-1}^{n+1} \right) - \gamma_k \delta t D M_u^{-1} D_\psi^E \left(\tilde{\Psi}^{n+1} - \hat{\Psi}_{k'-1}^{n+1} \right) = \mathbf{0} \longrightarrow \tilde{\mathbf{P}}^{n+1}$$

Fractional step. Algorithm (II). Correction steps

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4 Compute the velocity correction:

$$(5) M_{\mathbf{u}} \frac{\delta_k}{\delta t} \left(\mathbf{U}^{n+1} - \tilde{\mathbf{U}}^{n+1} \right) + \mathbf{N}_{\mathbf{u}}^{n+1} + G \left(\tilde{\mathbf{P}}^{n+1} - \hat{\mathbf{P}}_{k'-1}^{n+1} \right) - D_{\psi}^E \left(\tilde{\Psi}^{n+1} - \hat{\Psi}_{k'-1}^{n+1} \right) = \mathbf{0} \longrightarrow \mathbf{U}^{n+1}$$

5 Compute the ψ correction:

$$(7) M_{\psi}^E \frac{\delta_k}{\delta t} \left(\Psi^{n+1} - \tilde{\Psi}^{n+1} \right) + \mathbf{N}_{\psi}^{n+1} - S \left(\mathbf{U}^{n+1} - \tilde{\mathbf{U}}^{n+1} \right) = \mathbf{0} \longrightarrow \Psi^{n+1}$$

6 Pressure correction: $\mathbf{P}^{n+1} = \tilde{\mathbf{P}}^{n+1} \longrightarrow \mathbf{P}^{n+1}$

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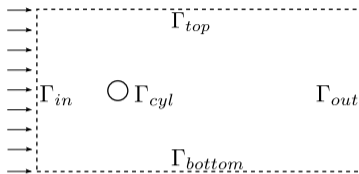
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Flow over a cylinder. Main features.



- The computational domain is a rectangle of length 16 and width 8, with a unitary cylinder centered vertically.
- The boundary conditions of the problem are:
 - The inflow velocity is $u_x = 1$ and $u_y = 0$.
 - The top and the bottom boundaries are considered fictitious walls.
 - For the outflow boundary the velocity is free in both components.
 - Non-slip conditions are set in the wall of the cylinder .
- The viscoelastic fluid parameters are: $\rho = 1$, $\beta = 0.5$ and $\eta_0 = 0.01$.
- $Re=100$, $We \in \{0.125, 0.165, 0.25, 0.5\}$.
- Spatial discretization: Coarse mesh. $h_{min} = 0.01$ and $h_{max} = 0.4$.
- Temporal discretization: $\delta t \in \{0.05, 0.025, 3.125 \times 10^{-3}, 1.562 \times 10^{-3}\}$

Flow over a cylinder. Monolithic scheme

Comparing stabilizations

P1 elements Method	Time step (δt)			
	0.050	0.0250	3.125×10^{-3}	1.562×10^{-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 $We = 0.125$,
 $\alpha_{1,\min} \approx 1.156 \times 10^{-3}$.

Comparing formulations

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

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

Conclusions

- The **most unstable** stabilization is the **quasi-static + OSS** stabilization.
- **Dynamic formulations** are more efficient avoiding **elastic instabilities**.

Lid-driven cavity flow problem. Main features

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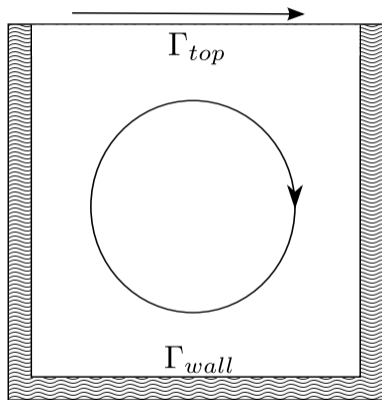
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- The computational domain: fluid confined in the unit square.
- The boundary conditions are:
 - On the top boundary, velocity is prescribed in the x direction.
 - At the walls, velocity is set to zero in both components.
- $We = 1.0$ and $Re = 0$.
- Spatial discretization: a structured mesh composed of 10000 bilinear Q1 elements.
- Temporal discretization: $\delta t = 0.0025$



Lid-driven cavity flow problem. Case $Re=0$

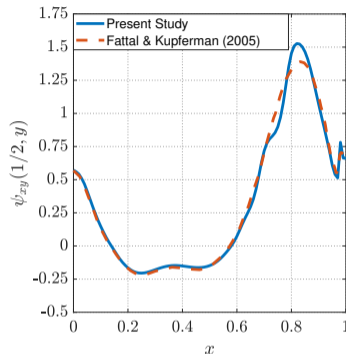
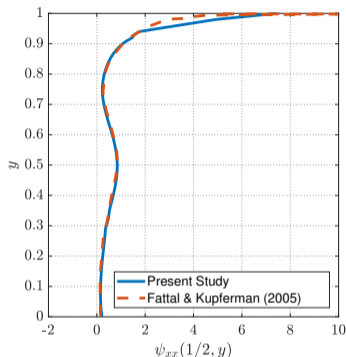
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Formulation	Stabilization S-OSS	
	Quasi-static	Dynamic
Standard	Failed - time step 265	Failed - time step 1316
Logarithmic	Failed - time step 340	Solved

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

Lid-driven cavity flow problem. Monolithic vs Fractional schemes

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		Stabilization S-OSS	
Scheme	Formulation	Quasi-static	Dynamic
Monolithic	Standard	Failed - time step 265	Failed - time step 1316
Monolithic	LCR	Failed - time step 340	Solved
Fractional Step	Standard	Failed - time step 692	Failed - time step 1781
Fractional Step	LCR	Failed - time step 593	Solved

Table: Comparison between different formulations and schemes with $We = 0.5$, $Re = 0$, $\delta t = 0.0025$ considering a mesh of 35×35 . The time step at which convergence fails is indicated in each case.

Case	Total time ratio	Solver time ratio
$We=0.5, Re=0.0$	0.48	0.10
$We=1.0, Re=100$	0.49	0.07

Table: Ratio of CPU times. Computational mesh 100×100 .

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- **Dynamic sub-scales** allow solving problems where two different sources of instability can appear simultaneously.
- **Combination of LCR and dynamic subscales** in term-by-term stabilization is capable of solving problems with **higher elasticity than other options**.
- **Fractional step methods** for the LCR have been designed using a purely algebraic approach in order to **reduce the computational cost**.

Related publications

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- 1 Moreno L., Codina R., Baiges J. & Castillo E. (2019). Logarithmic conformation reformulation in viscoelastic flow problems approximated by a VMS-type stabilized finite element formulation. *Computer Methods in Applied Mechanics and Engineering*, 354, 706-731.
- 2 Moreno L., Codina R. & Baiges J. (2020). Solution of transient viscoelastic flow problems approximated by a term-by-term VMS stabilized finite element formulation using time-dependent subgrid-scales. *Computer Methods in Applied Mechanics and Engineering*, 367, 113074.
- 3 Codina, R., & Moreno, L. Stability Analysis of time dependent linearized viscoelastic flow problems using a stabilized finite element formulation in space. *ESAIM. Mathematical Modelling and Numerical Analysis*, Submitted.
- 4 Castillo, E., Moreno, L., Baiges, J., & Codina, R. (2021). Stabilised Variational Multi-Scale Finite Element Formulations for Viscoelastic Fluids. *Archives of Computational Methods in Engineering*, 1-33.

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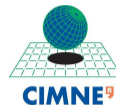
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Thank you for your attention!!

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