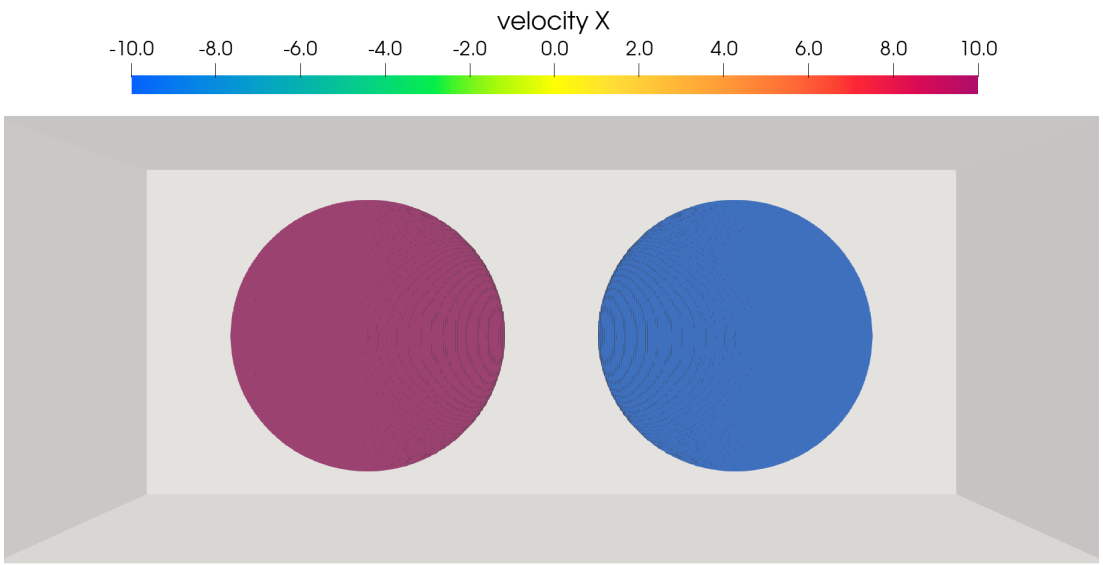
Numerical simulation of multiple phases of incompressible viscous and elastic flows with free surfaces

Alexandre Caboussat, Léo Diserens and Marco Picasso
Institute of Mathematics, Ecole Polytechnique Fédérale de Lausanne
HEG, University of Applied Sciences Western Switzerland (HES-SO)

June 14, 2022

Introduction



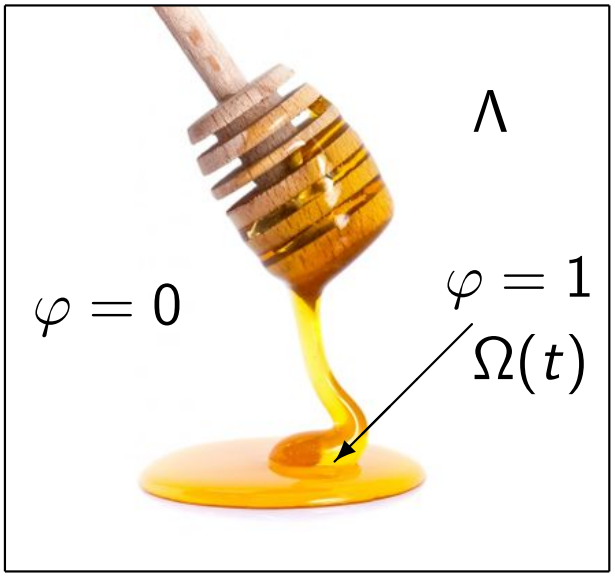
Goals:

- Simulation of multiple phases interactions with free surfaces: from Newtonian fluids to elastic solids.
- Possible applications: fluid-structure interaction (fluid-fluid, fluid-structure, structure-structure) in Eulerian coordinates with large deformations and topology changes.

Main equations for one viscoelastic fluid / elastic solid with free surfaces

In the whole cavity (characteristic function):

$$\frac{\partial \varphi}{\partial t} + \boldsymbol{u} \cdot \nabla \varphi \quad = 0.$$



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In the fluid / elastic domain:

$$\begin{aligned}
\rho \left(\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla) \boldsymbol{u} \right) - \nabla \cdot (2\eta_s \boldsymbol{\epsilon}(\boldsymbol{u}) - p \boldsymbol{I}_d + \boldsymbol{\sigma}) &= \rho \boldsymbol{g}, \\
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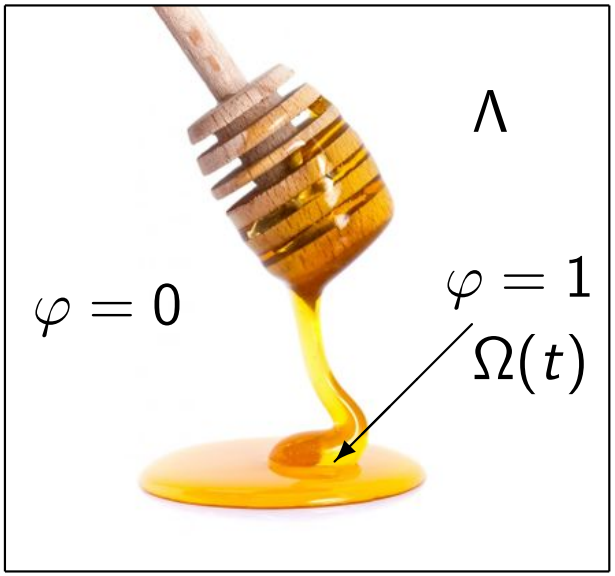
\alpha \boldsymbol{\sigma} + \lambda \left(\frac{\partial \boldsymbol{\sigma}}{\partial t} + (\boldsymbol{u} \cdot \nabla) \boldsymbol{\sigma} - \nabla \boldsymbol{u} \boldsymbol{\sigma} - \boldsymbol{\sigma} \nabla \boldsymbol{u}^T \right) &= 2\eta_p \boldsymbol{\epsilon}(\boldsymbol{u}).
\end{aligned}$$

$(2\eta_s \boldsymbol{\epsilon}(\boldsymbol{u}) + \boldsymbol{\sigma})\boldsymbol{n} - p\boldsymbol{n} = 0$, on free surface.



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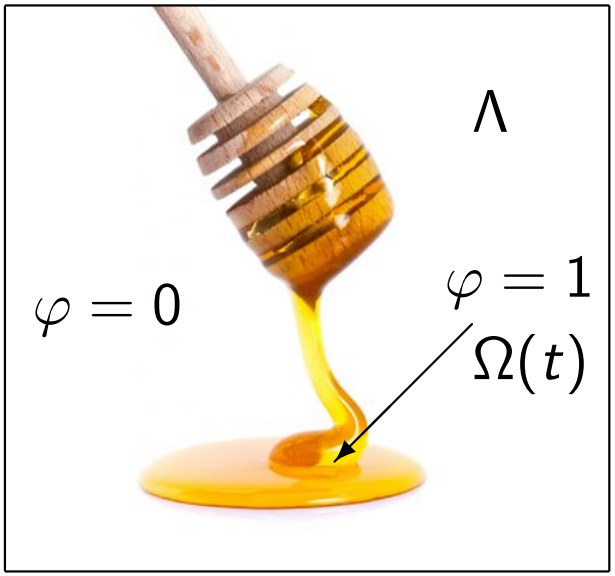
2. Viscoelastic fluid: $\alpha = 1, \lambda > 0$ (Bonito et al. 2006)
3. Elastic solid: $\alpha = 0, \lambda > 0, \eta_s = 0$ (Picasso 2016)



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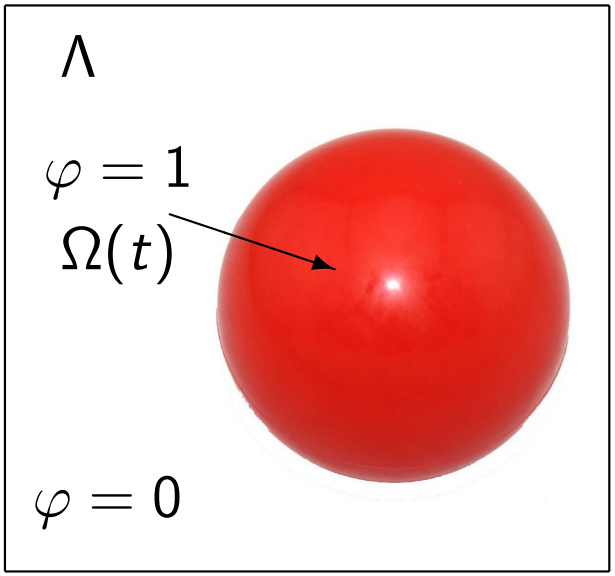
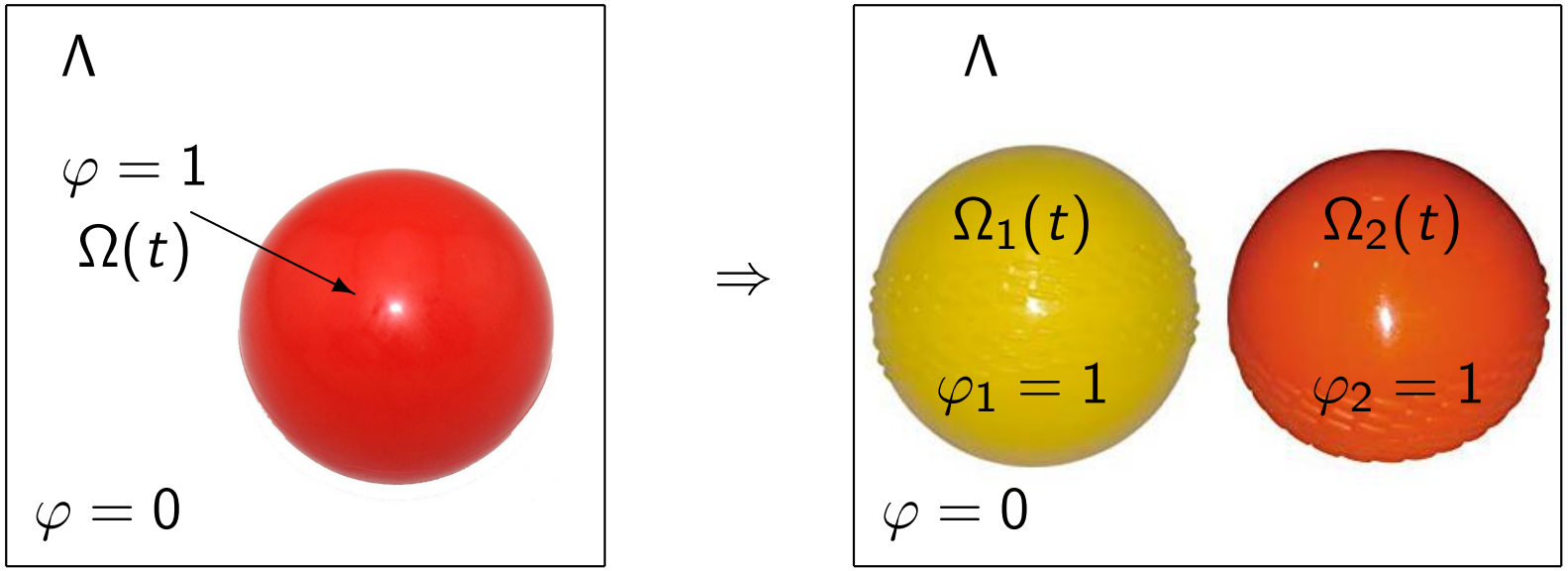


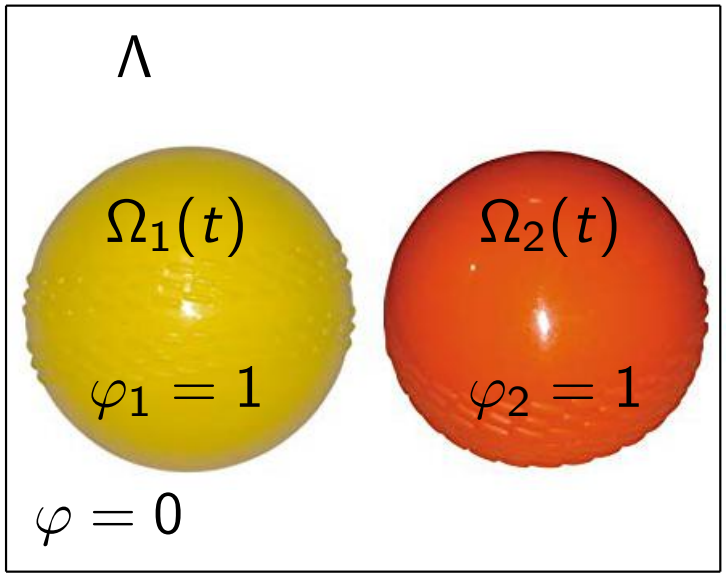
From one phase to multiple phases with free surfaces



Main equations for multiple viscoelastic fluid / elastic solid phases with free surfaces

In the whole cavity (characteristic functions):

$$\frac{\partial \varphi_\ell}{\partial t} + \boldsymbol{u} \cdot \nabla \varphi_\ell \quad = 0, \quad \ell = 1, \ldots, N, \quad \varphi = \sum_{\ell=1}^{N} \varphi_\ell, \quad \Omega = \bigcup_{\ell=1}^{N} \Omega_\ell$$



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In the whole fluid / elastic domain ($\varphi = 1$):

$$\begin{aligned} \rho(\varphi) \left(\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} \right) - \nabla \cdot (2\eta_s(\varphi)\boldsymbol{\epsilon}(\boldsymbol{u}) - p\boldsymbol{I}_d + \boldsymbol{\sigma}) &= \rho \mathbf{g}, \\ \nabla \cdot \boldsymbol{u} &= 0, \\ \alpha(\varphi)\boldsymbol{\sigma} + \lambda(\varphi) \left(\frac{\partial \boldsymbol{\sigma}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{\sigma} - \nabla \boldsymbol{u}\boldsymbol{\sigma} - \boldsymbol{\sigma}\nabla \boldsymbol{u}^T \right) &= 2\eta_p(\varphi)\boldsymbol{\epsilon}(\boldsymbol{u}). \end{aligned}$$

Parameters discontinuity:

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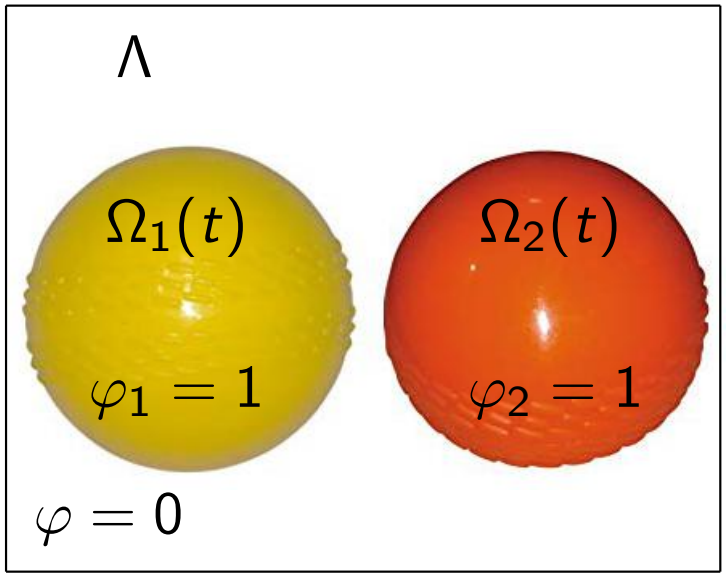

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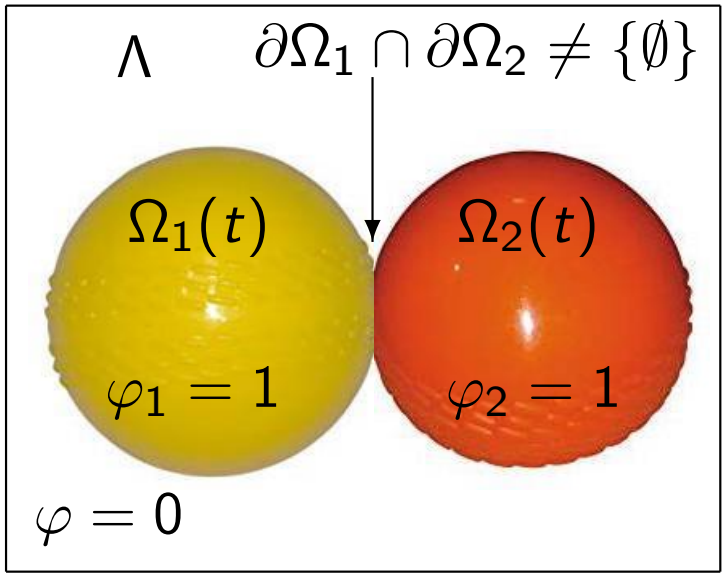
Interface conditions:



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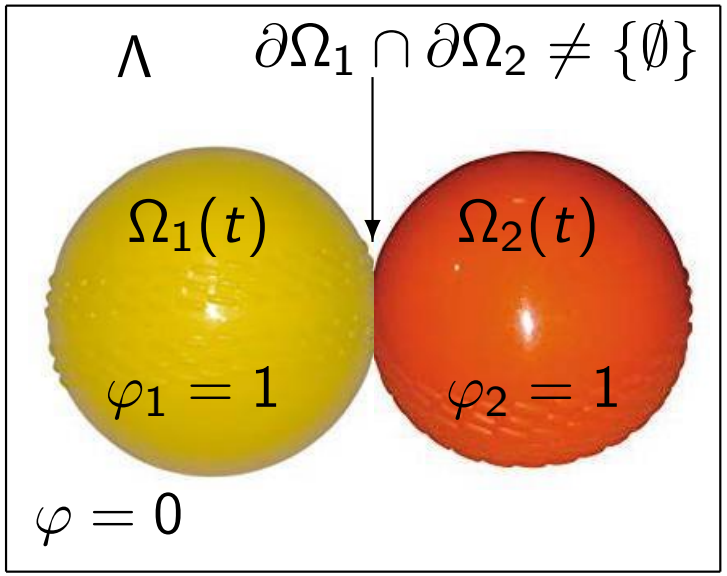

Time discretization - Splitting strategy

- Order one time splitting strategy for time discretization.
- Decoupling advection terms from the set of equations:

$$
\begin{aligned}
\frac{\partial \varphi_\ell}{\partial t} + \boldsymbol{u} \cdot \nabla \varphi_\ell &= 0, \quad \ell = 1, \ldots, N \\
\rho(\varphi)\left(\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u}\right) - \nabla \cdot (2\eta_s(\varphi)\boldsymbol{\epsilon}(\boldsymbol{u}) - p\boldsymbol{I}_d + \boldsymbol{\sigma}) &= \rho \mathbf{g}, \\
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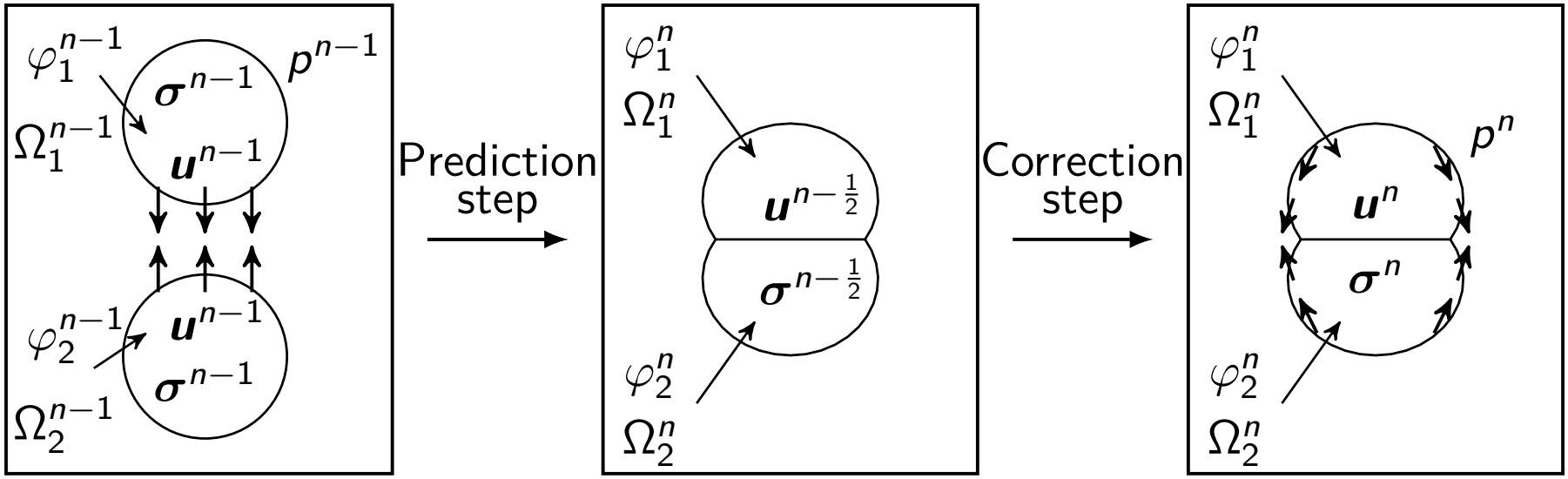
\end{aligned}
$$

$$\Downarrow$$

Advection terms & Stokes terms + Oldroyd-B terms

Time discretization: splitting advection and diffusion

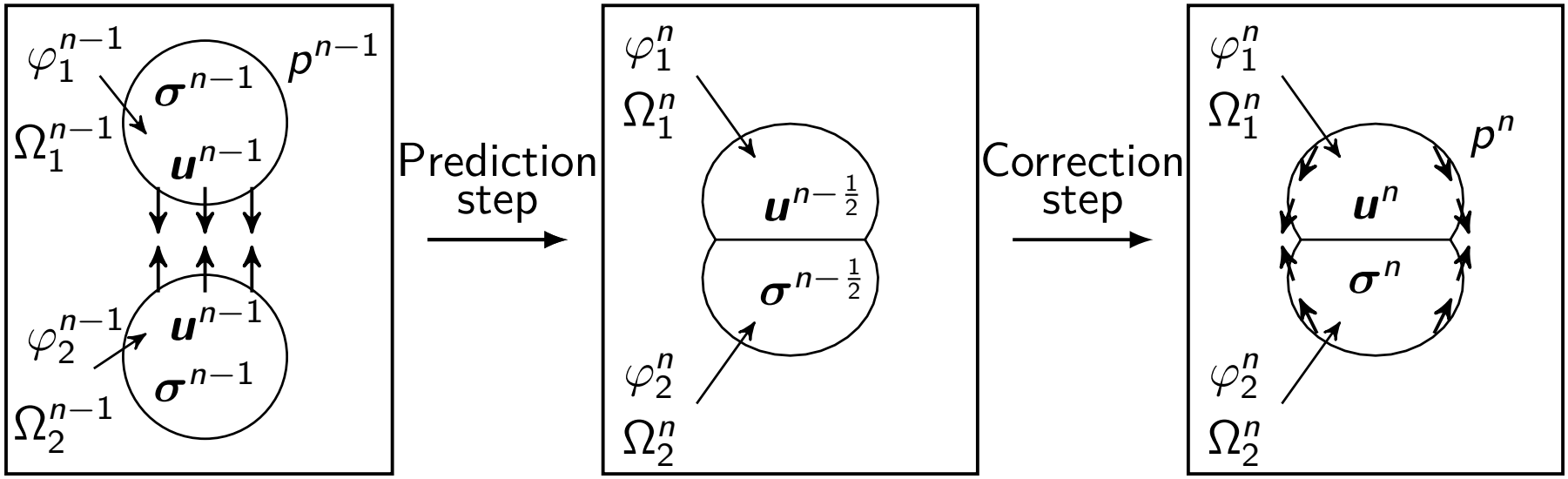


- Prediction step : solve between t^{n-1} and t^n the advection problems

$$\frac{\partial \varphi_\ell}{\partial t} + \boldsymbol{u} \cdot \nabla \varphi_\ell = 0, \quad \frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = 0, \quad \frac{\partial \boldsymbol{\sigma}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{\sigma} = 0.$$

Update of $\varphi_\ell^n, \varphi^n$ and Ω_ℓ^n, Ω^n and the predictions $\boldsymbol{u}^{n-\frac{1}{2}}$ and $\boldsymbol{\sigma}^{n-\frac{1}{2}}$ in Ω^n.

Time discretization: splitting advection and diffusion



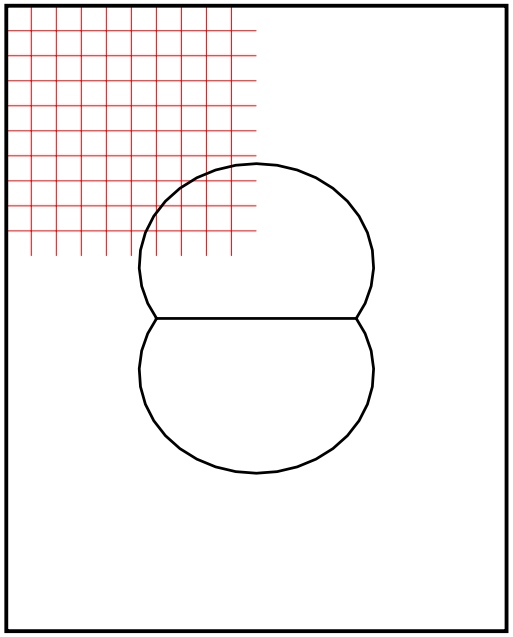
- Correction step : solve between t^{n-1} and t^n in Ω^n:

$$\rho(\varphi)\frac{\partial \boldsymbol{u}}{\partial t} - \nabla \cdot (2\eta_s(\varphi)\boldsymbol{\epsilon}(\boldsymbol{u}) - p\boldsymbol{I}_d + \boldsymbol{\sigma}) = \rho g,$$

$$\nabla \cdot \boldsymbol{u} = 0,$$

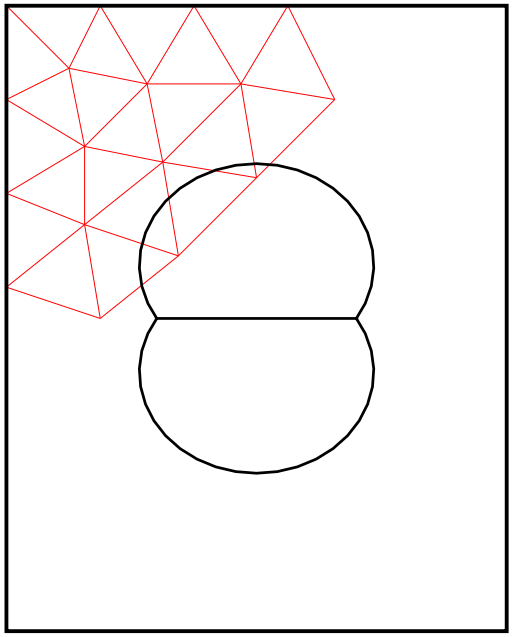
$$\alpha(\varphi)\boldsymbol{\sigma} + \lambda(\varphi)\left(\frac{\partial \boldsymbol{\sigma}}{\partial t} - \nabla \boldsymbol{u}\boldsymbol{\sigma} - \boldsymbol{\sigma}\nabla \boldsymbol{u}^T\right) = 2\eta_p(\varphi)\boldsymbol{\epsilon}(\boldsymbol{u}).$$

Two grids



Prediction step

Advection terms



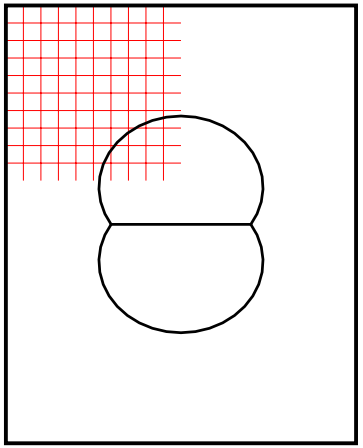
Correction step

Stokes terms
+ Oldroyd-B terms

- Structured grid of small cells (fine): Reduce numerical diffusion of characteristic function φ.
- Unstructured FE mesh (coarse): allows complex geometries and computational time efficiency.

Prediction step

Splitting strategy : prediction and correction
Grid diameter of size h.

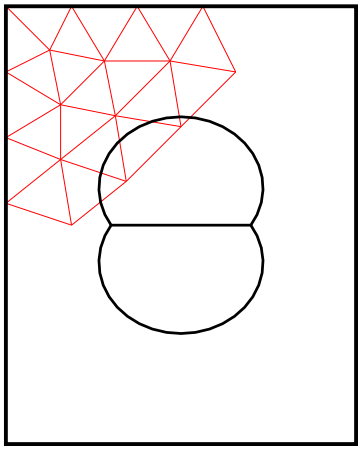


Prediction step. Solved on a structured fine grid with the characteristics method (Pironneau 89).

$$\boldsymbol{u}^{n-\frac{1}{2}}(x+\Delta t\boldsymbol{u}^{n-1}(x)) = \boldsymbol{u}^{n-1}(x), \quad x \in \Omega^{n-1},$$
$$\boldsymbol{\sigma}^{n-\frac{1}{2}}(x+\Delta t\boldsymbol{u}^{n-1}(x)) = \boldsymbol{\sigma}^{n-1}(x), \quad x \in \Omega^{n-1},$$
$$\varphi_\ell^{n-\frac{1}{2}}(x+\Delta t\boldsymbol{u}^{n-1}(x)) = \varphi_\ell^{n-1}(x), \quad x \in \Omega^{n-1}.$$

Correction step

Splitting strategy : prediction and correction
Mesh diameter of size H, with $3 \leq H/h \leq 5$.



Correction step. Solved with unstructured coarse finite elements.

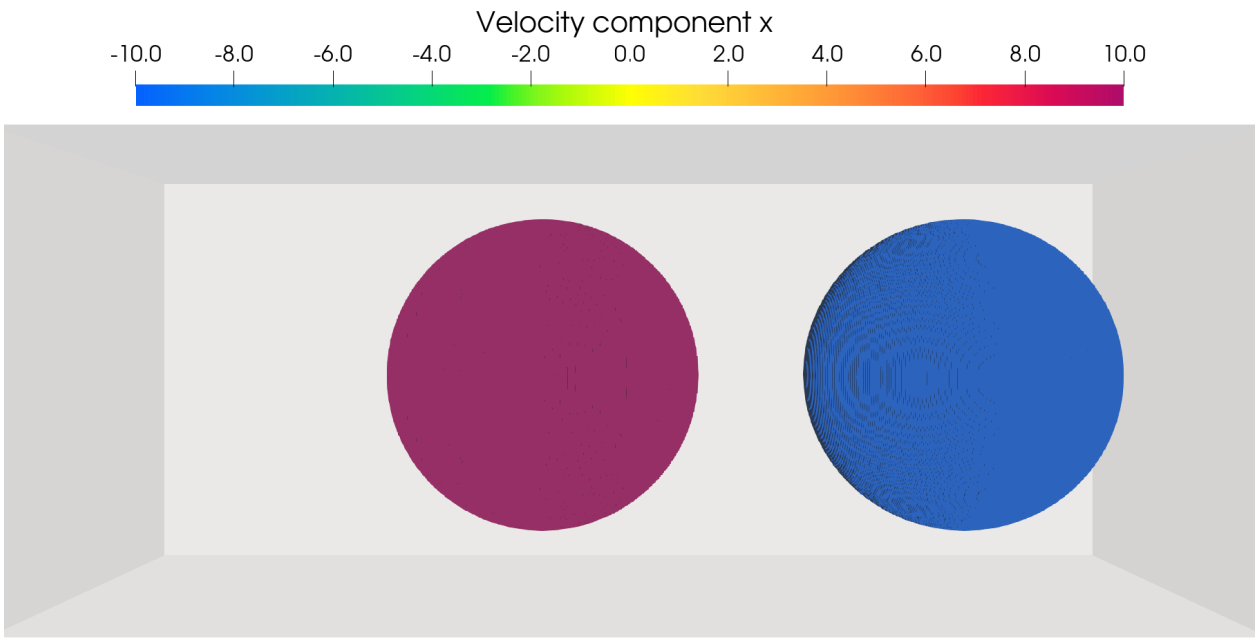
- Stokes equations

$$\begin{aligned} \rho(\varphi^n)\frac{\partial \boldsymbol{u}}{\partial t} - 2\eta_s(\varphi^n)\nabla\cdot\boldsymbol{\epsilon}(\boldsymbol{u}) + \nabla p - \nabla\cdot\boldsymbol{\sigma} &= \rho(\varphi^n)\mathbf{g}, \\ \nabla\cdot\boldsymbol{u} &= 0. \end{aligned}$$

- Oldroyd-B equation

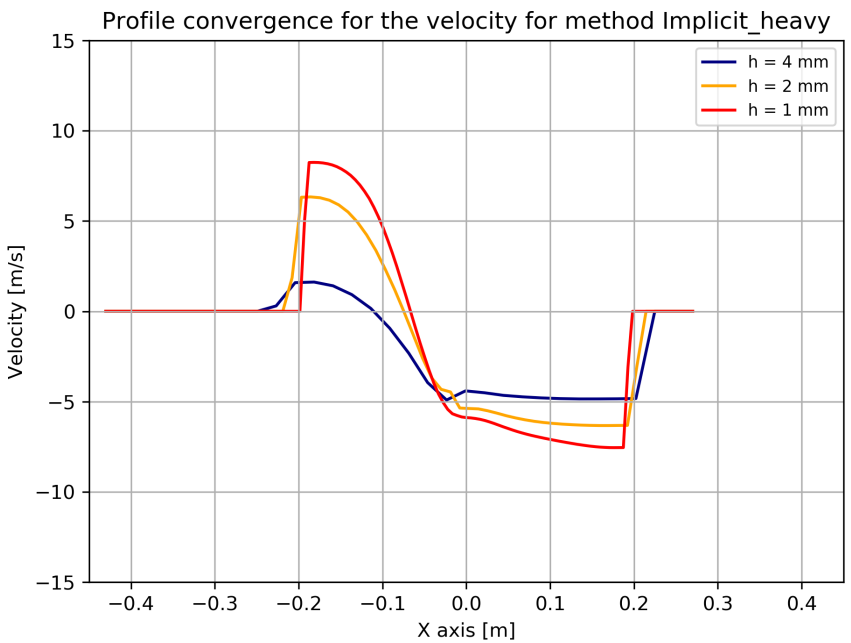
$$\alpha(\varphi^n)\boldsymbol{\sigma} + \lambda(\varphi^n)\left(\frac{\partial\boldsymbol{\sigma}}{\partial t} - \nabla\boldsymbol{u}\boldsymbol{\sigma} - \boldsymbol{\sigma}\nabla\boldsymbol{u}^T\right) = 2\eta_p(\varphi^n)\boldsymbol{\epsilon}(\boldsymbol{u}).$$

Colliding rubber balls of different densities and rigidity.

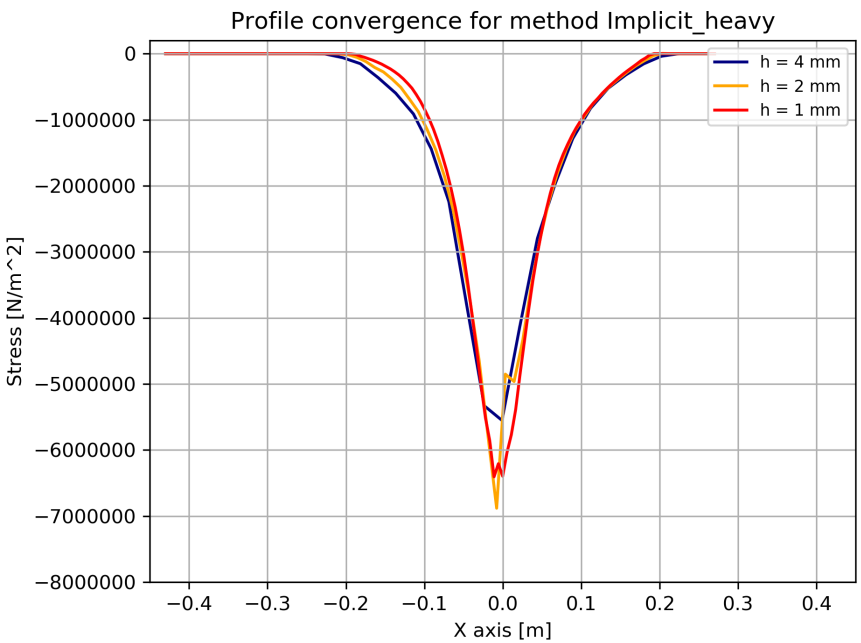


Parameters: $\eta_s = 0, \rho_1 = 1000$ kg m^{-3}, $\rho_2 = 2000$ kg m^{-3}, $\lambda_1 = \lambda_2 = 10^{-2}$ s, $\eta_{p,1} = 4 * 10^4$ Pa s, $\eta_{p,2} = 2 * 10^5$ Pa s.

Convergence with respect to mesh size and time step for a constant CFL.



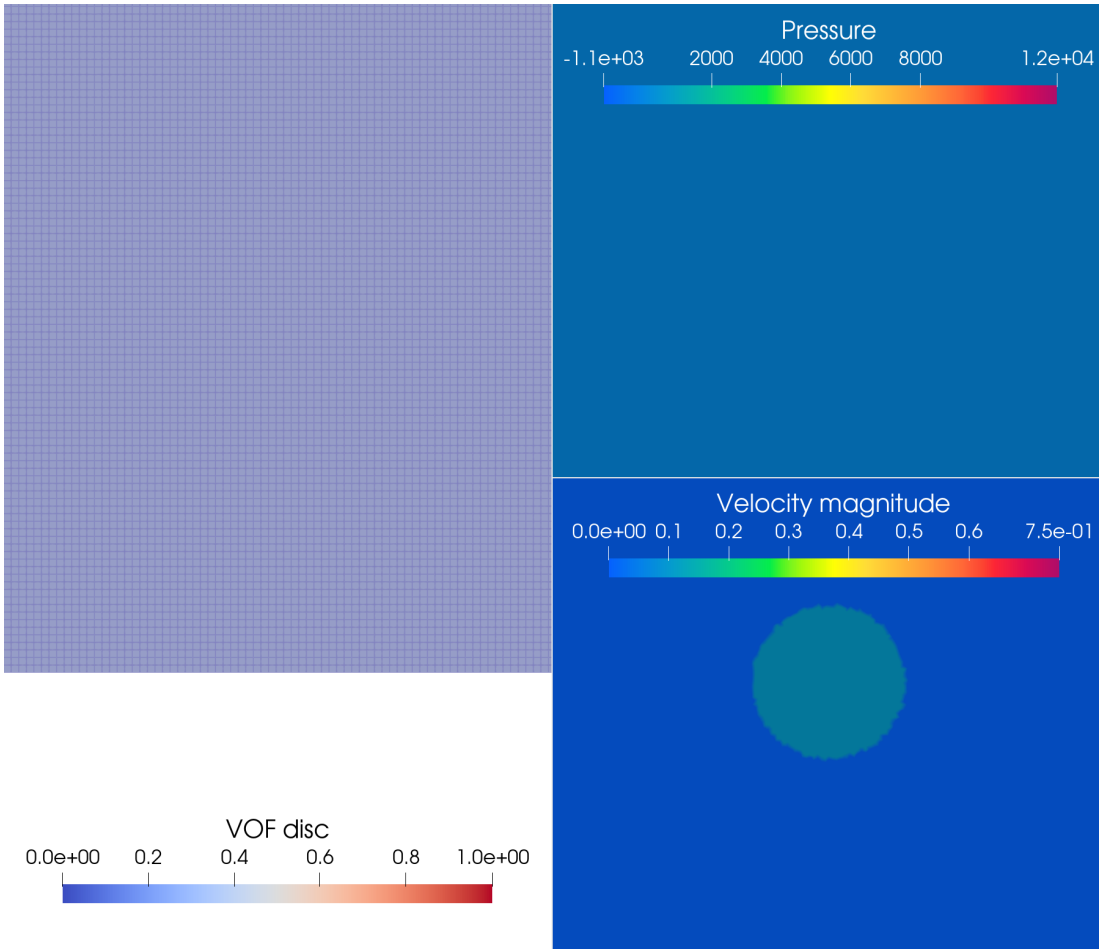
Velocity component $\boldsymbol{u}_x$ on a horizontal profile



Stress component $\boldsymbol{\sigma}_{xx}$ on a horizontal profile

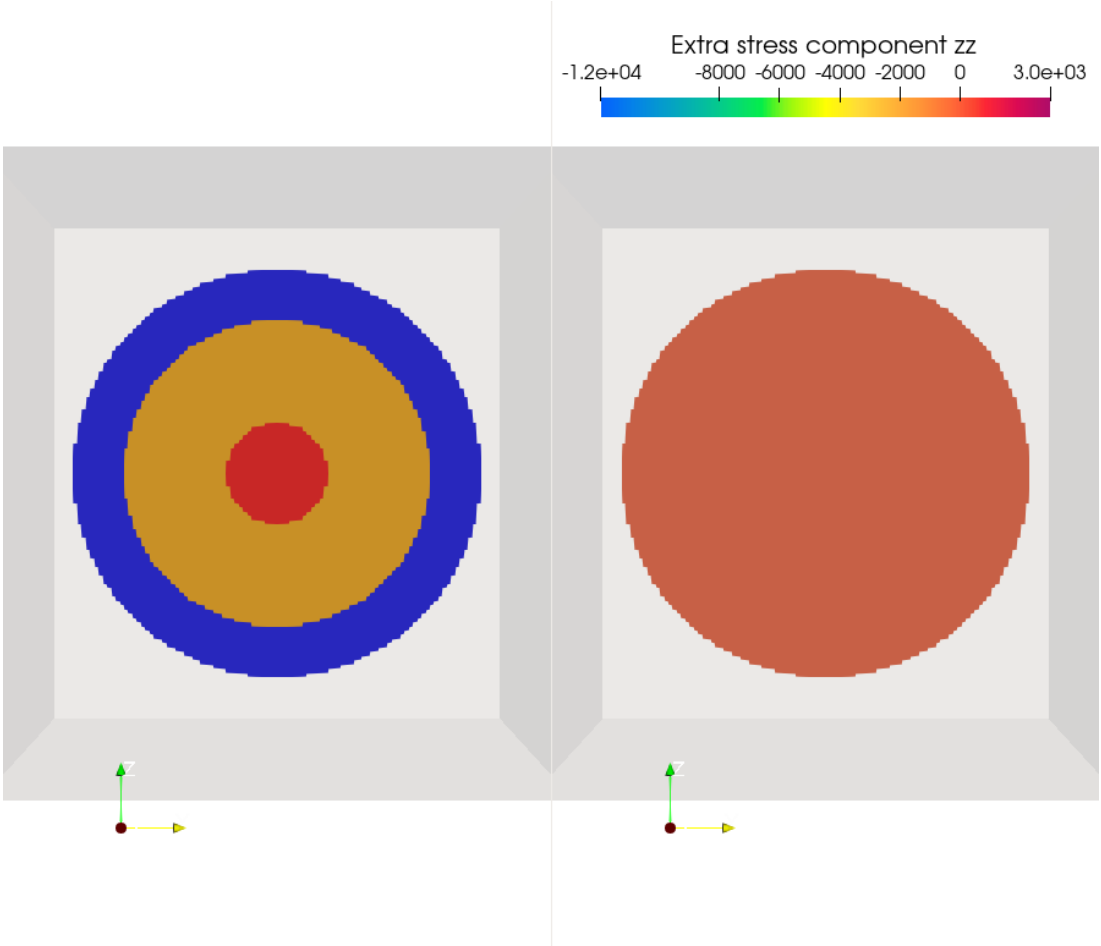
Rigid ball falling into a Newtonian fluid never reaches the bottom (Hillairet 2007)

What happens for a deformable ball ?



Left: VOF elastic solid φ_1. Right: Pressure p and Velocity $\|\boldsymbol{u}\|$.

Shock absorber simulation.



VOF function for hull (blue), viscoelastic shock absorber (orange), and protected mechanism (red).

Stress component $\boldsymbol{\sigma}_{zz}$.

Conclusion

- Mathematical modelling of incompressible viscoelastic fluids / Neo-Hookean elastic solids deformations with free surfaces
- Multiple incompressible and immiscible phases free surfaces flow formulation.
- Numerical approximation using
  - a time splitting algorithm for time for the time discretization
  - and a two grid approach for space discretization.
- Application to several numerical experiments (collision of rubber materials, lack of collision of an elastic ball in a Newtonian fluid and shock absorber).

References

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Numerical simulation of 3D viscoelastic flows with free surfaces
Journal of Computational Physics, 215(2):691–716, 2006.

N. James, S. Boyaval and A. Caboussat
Numerical simulation of 3D free surface flows, with multiple incompressible immiscible phases. Applications to impulse waves
International Journal for Numerical Methods in Fluids, pages 1004–1024, Wiley Online Library, 2014.

M. Picasso
From the free surface flow of a viscoelastic fluid towards the elastic deformation of a solid
Comptes Rendus Mathematique, 354(5):543–548, 2016.

Elastic solid formulation

Let $\mathbf{F}$ be the deformation tensor in Eulerian coordinates. It satisfies

$$\frac{\partial \mathbf{F}}{\partial t} + \boldsymbol{u} \cdot \nabla \mathbf{F} = \nabla \boldsymbol{u} \mathbf{F}. \qquad (\star)$$

The stress tensor $\boldsymbol{\sigma}$ of an incompressible Neo-Hookean elastic material (Dunne Rannacher 2006) is given by:

$$\boldsymbol{\sigma} = \frac{\eta_p}{\lambda}(\mathbf{F}\mathbf{F}^T - \boldsymbol{I}_d).$$

Then by using $(\star)$, $\boldsymbol{\sigma}$ satisfies

$$\frac{\partial \boldsymbol{\sigma}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{\sigma} - \nabla \boldsymbol{u} \boldsymbol{\sigma} - \boldsymbol{\sigma} \nabla \boldsymbol{u}^T = \frac{2\eta_p}{\lambda} \boldsymbol{\epsilon}(\boldsymbol{u}).$$

Numerical approach - common for all three models

Order one splitting strategy is applied for time discretization.

$$\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} + A\boldsymbol{u} + B\boldsymbol{u} = \mathbf{f} \quad \Leftrightarrow \quad \begin{aligned} \frac{\partial \varphi}{\partial t} + \boldsymbol{u}\cdot\nabla\varphi &= 0 \\ \rho\frac{\partial \boldsymbol{u}}{\partial t} + \rho(\boldsymbol{u}\cdot\nabla)\boldsymbol{u} - \nabla\cdot(2\eta_s\boldsymbol{\epsilon}(\boldsymbol{u}) - p\boldsymbol{I}_d + \boldsymbol{\sigma}) &= \rho\mathbf{g}, \\ \nabla\cdot\boldsymbol{u} &= 0, \\ \alpha\boldsymbol{\sigma} + \lambda\left(\frac{\partial\boldsymbol{\sigma}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{\sigma} - \nabla\boldsymbol{u}\boldsymbol{\sigma} - \boldsymbol{\sigma}\nabla\boldsymbol{u}^T\right) &= 2\eta_p\boldsymbol{\epsilon}(\boldsymbol{u}). \end{aligned}$$

$$\Downarrow$$

$$\begin{aligned} \frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} + A\boldsymbol{u} &= 0 \\ \frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} + B\boldsymbol{u} &= \mathbf{f} \end{aligned}$$

$$\Downarrow$$

Advection terms + Diffusion terms

Semi-implicit scheme

$$\rho^n \frac{\boldsymbol{u}^n - \boldsymbol{u}^{n-1}}{\Delta t} - 2\eta_s^n \nabla \cdot \boldsymbol{\epsilon}(\boldsymbol{u}^n) + \nabla p^n - \nabla \cdot \boldsymbol{\sigma}^n = \rho^n \mathbf{g},$$

$$\nabla \cdot \boldsymbol{u}^n = 0,$$

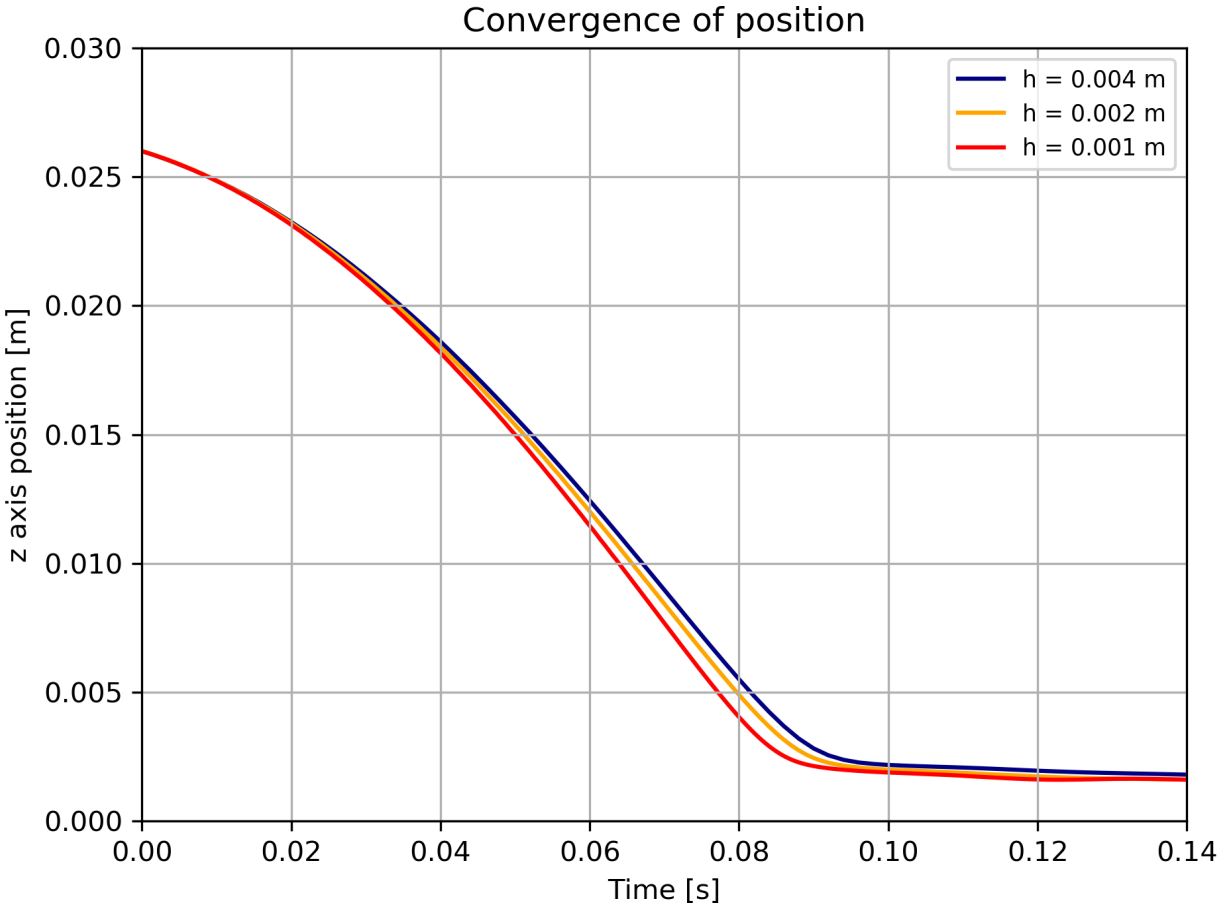
$$\alpha^n \boldsymbol{\sigma}^n + \lambda^n \left(\frac{\boldsymbol{\sigma}^n - \boldsymbol{\sigma}^{n-1}}{\Delta t} - \nabla \boldsymbol{u}^{n-1} \boldsymbol{\sigma}^{n-1} - \boldsymbol{\sigma}^{n-1} (\nabla \boldsymbol{u}^{n-1})^T \right) = 2\eta_p^n \boldsymbol{\epsilon}(\boldsymbol{u}^n).$$

The computation of $\boldsymbol{u}^n, p^n, \boldsymbol{\sigma}^n$ can be decoupled in momentum equation:

$$\rho^n \frac{\boldsymbol{u}^n - \boldsymbol{u}^{n-1}}{\Delta t} - 2\left(\eta_s^n + \frac{\eta_p^n \Delta t}{\lambda^n + \alpha^n \Delta t} \right) \nabla \cdot \boldsymbol{\epsilon}(\boldsymbol{u}^n) + \nabla p^n = \frac{\lambda^n}{\lambda^n + \alpha^n \Delta t} \nabla \cdot \boldsymbol{\sigma}^{n-1}$$

$$+ \frac{\lambda^n \Delta t}{\lambda^n + \alpha^n \Delta t} \nabla \cdot (\nabla \boldsymbol{u}^{n-1} \boldsymbol{\sigma}^{n-1} + \boldsymbol{\sigma}^{n-1} (\nabla \boldsymbol{u}^{n-1})^T) + \rho^n \mathbf{g}.$$

Convergence of position for the lack of collision.



Convergence of position of the monitored bottom of the ball