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Numerical simulation of moving contact line in wetting phenomena using the Generalized Navier Boundary Condition

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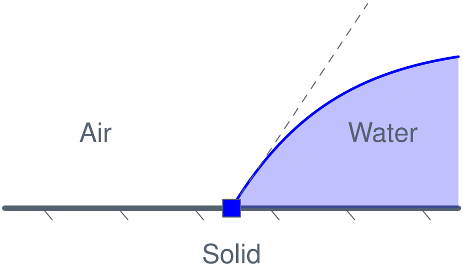
Outline

(a) Raindrops gracing on the leaf.



(b) Static contact line.

Figure: Contact line description.

Background

- The contact line (CL) is the intersection between fluid interface and solid wall.

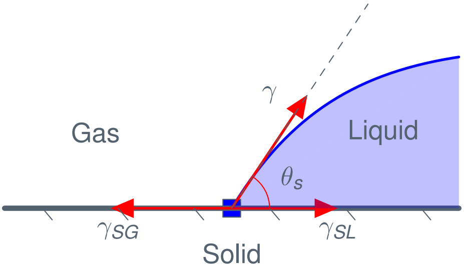


Figure: Contact line description.

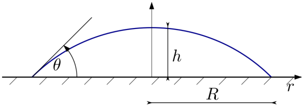
Surface tension: γ (liquid-gas), γ_{SG} (solid-gas), γ_{SL} (solid-liquid)

Static contact line - Young's equation

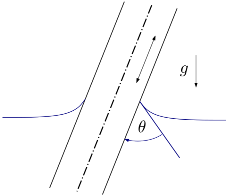
$$\cos \theta_s = \frac{\gamma_{SG} - \gamma_{SL}}{\gamma}$$

Dynamic contact line

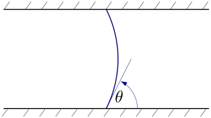
- Capillary and wetting phenomena
- Capillary number $Ca = \frac{\textit{viscous forces}}{\textit{surface tension}}$



(a) Droplet spreading (DS)



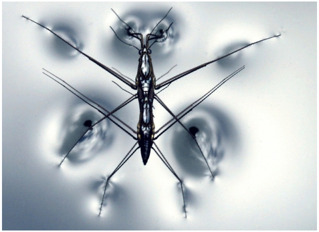
(b) Forced wetting (FW)

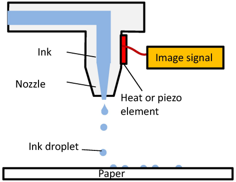


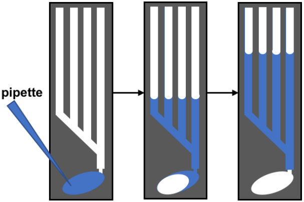
(c) Capillary spreading (in tube or between two plates) (CS)

Why study contact lines?

- Important in nature and in many industrial applications.







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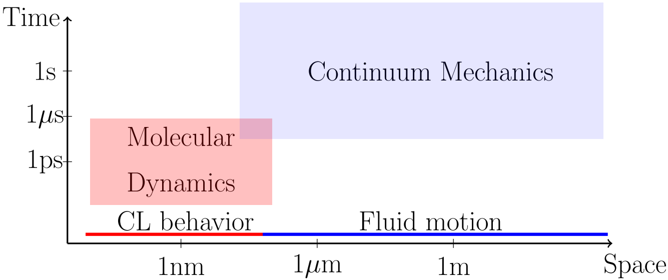
Why study contact lines?

- Important in nature and in many industrial applications.
- Great challenges in both modeling and experiments.

1. Multiscale problem

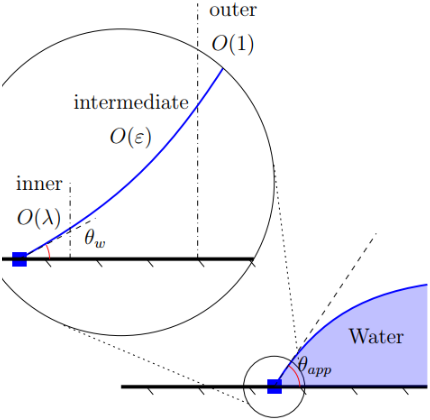


Cox's model (1986) [1]

- For a solid/liquid/gas system with $\theta < 3\pi/4$ and $Ca << 1$.

  $$(\theta_d^{macro})^3 = (\theta_d^{micro})^3 + 9Ca\ln(L/\lambda)$$

  L: outer length (Capillary length),
  λ: inner length (Slip length).
- Well-defined the contact velocity which fits with many experimental results.



[1] R. G. Cox. The dynamics of the spreading of liquids on a solid surface. J. of Fluid Mechanics, July 1986

Generalize Navier Boundary Condition (GNBC)

- Qian et al. (2003) [2] from MD simulation:

$$\beta u_{slip} = \tau_{wall}^{visc} + \tilde{\tau}^{Young}$$

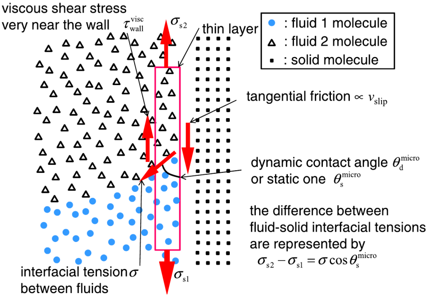
slip coefficient β :,

viscous stress $\tau_{wall}^{visc} = \mu \frac{\partial u}{\partial n}\Big|_{wall}$,

uncompensated Young stress

$\int_{int} \tilde{\tau}^{Young} = \sigma(\cos\theta_s - \cos\theta_d^{micro})$.

- Validate by the diffused interface method with $Ca << 0.1$.



[2] T. Qian et al., Molecular scale contact line hydrodynamics of immiscible flows, Phys. Rev. E, July 2003.

The governing equations are described in a one-fluid formulation as:

- Navier-Stokes equations:

$$\nabla \cdot \mathbf{u} = 0, \tag{1}$$

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \nabla \cdot \left(\mu (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \right) + \rho \mathbf{g} + \mathbf{F}_\sigma . \tag{2}$$

- GNBC:

$$\beta u_{slip} = \tau_{wall}^{visc} + \tilde{\tau}^{Young} \tag{3}$$

The physical properties such as local density and dynamic viscosity:

$$\phi = C\phi_1 + (1 - C)\phi_2 .$$

Front tracking method (J. Glimm .et .al [3]) is used to represent and evolve the interface.

Numerical model

Procedure

- Advect interface markers.
- Update density and viscosity.
- Compute the interfacical surface force $\mathbf{F}_\sigma$.
- Impose the slip velocity.
- Solve the NS equations with the BC and then update the flow fields.

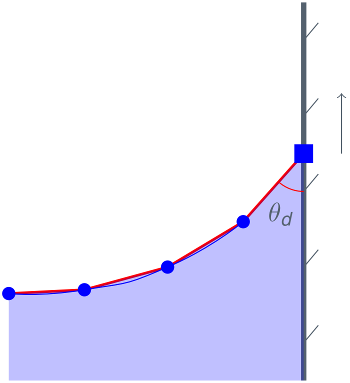


Figure: Interface tracking by markers.

The geometry and dynamics of the interface is tracked by the set of linked marker points.

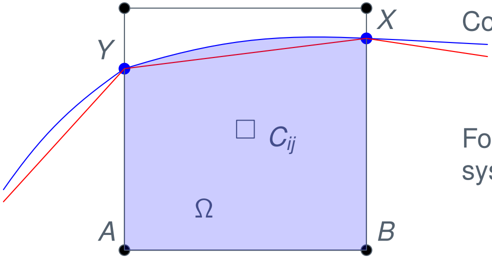
- Updating the front by the Runge-Kutta method.
- Redistributing the front.
- Computing the $\mathbf{t}, \kappa$ and θ_d by the position of markers.

The open-source FronTier++ library package.

The CSF approximation: $\mathbf{F}_\sigma = \sigma\kappa\mathbf{n}\delta_\mathbf{I} = \sigma\kappa\nabla\mathbf{C}$.
The $\mathbf{F}_\sigma$ is discretized on at the velocity nodes as follows

$$F_{\sigma i+1/2,j} = \sigma\kappa_{i+1/2,j}\frac{C_{i+1,j} - C_{i,j}}{\Delta x}, \quad (4)$$

$$F_{\sigma i,j+1/2} = \sigma\kappa_{i,j+1/2}\frac{C_{i,j+1} - C_{i,j}}{\Delta x}. \quad (5)$$



Computation volume fraction

$$C_{ij} \approx |ABXY|/|Cell_{ij}|.$$

For the axisymmetric coordinate system $\kappa = \kappa^{2D} + \kappa^{axis}$.

Mathematical model

Interface curvature fields

The hybrid formulation (Shin et al. [4]):

$$\sigma\kappa = \frac{\mathbf{F}' \cdot \mathbf{G}}{\mathbf{G} \cdot \mathbf{G}}, \tag{6}$$

where

$$\mathbf{F}'_{i+1/2,j} = \sum_e \mathbf{f}_e D_{i+1/2,j}(\mathbf{x}_e)|e|, \tag{7}$$

$$\mathbf{G}_{i+1/2,j} = \sum_e \mathbf{n}_e D_{i+1/2,j}(\mathbf{x}_e)|e|. \tag{8}$$

Here, $\mathbf{x}_e$ is a parameterization of the element e of the interface, $\mathbf{f}_e$ is the capillary force contribution of element e, $\mathbf{n}_e$ is a unit normal and $D_{i+1/2,j}(\mathbf{x}_e)$ is the Dirac distribution function approximated by:

$$D_{i+1/2,j}(\mathbf{x}_e) = \frac{1}{\Delta x \Delta y} d\left(\frac{x_{i+1/2,j} - x_e}{\Delta x}\right) d\left(\frac{y_{i+1/2,j} - y_e}{\Delta y}\right) \tag{9}$$

GNBC: $\beta u_{slip} = \tau_{wall}^{visc} + \tilde{\tau}^{Young}$.
By $\tau_{wall}^{visc} << \tilde{\tau}^{Young}$, then GNBC is simplified to

$$\beta' u_{slip} = \tilde{\tau}^{Young} \quad (10)$$

Remember that uncompensated Young stress, satisfying

$$\int_{int} \tilde{\tau}^{Young} = \sigma(\cos\theta_s - \cos\theta_d^{micro})$$

then

$$\tilde{\tau}^{Young}(y_j) = \sigma(\cos\theta_s - \cos\theta_d^{micro}) d(y_j - y_{CL}) \quad (11)$$

where $d(r) = \begin{cases} \frac{1}{4\Delta}\left(1 + \cos\frac{\pi r}{2\Delta}\right) & \text{if } |r| \leqslant 2\Delta, \\ 0 & \text{if } |r| > 2\Delta, \end{cases}$ and Δ is the grid spacing.

$$\boxed{\beta u_{CL} = \frac{1}{2\Delta}\sigma(\cos\theta_s - \cos\theta_d^{micro})} \quad (12)$$

Notice that $Ca = \mu u_{CL}/\sigma$ and (12), it follows:

$$Ca = \chi(\cos\theta_s - \cos\theta_d^{micro}) \tag{13}$$

where $\chi = \overline{\mu}/(\beta' \Delta)$ is the nondimensional slip parameter. Then from Cox's model,

$$(\theta_d^{macro})^3 = (\theta_d^{micro})^3 + 9Ca \ln(L/\lambda)$$

by setting $L = \Delta$ and $\lambda = l^{micro}$,

$$\boxed{(\theta_d^{micro})^3 = (\theta_d^{grid})^3 - 9Ca \ln\left(\frac{\Delta}{l^{micro}}\right)}. \tag{14}$$

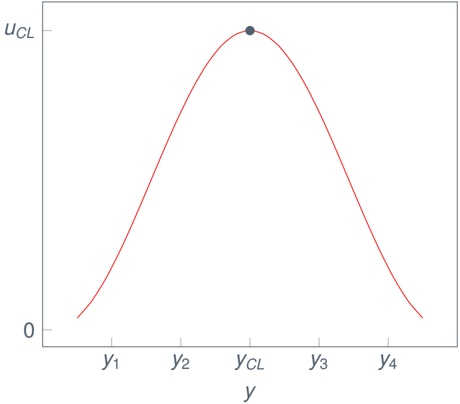
We have:

$$Ca = \chi(\cos\theta_s - \cos\theta_d^{micro})$$

$$(\theta_d^{micro})^3 = (\theta_d^{grid})^3 - 9Ca \ln\left(\frac{\Delta}{l^{micro}}\right)$$

Then

$$u_{slip}(y_j) = u_{CL} 2\Delta d(y_j - y_{CL}). \quad (15)$$



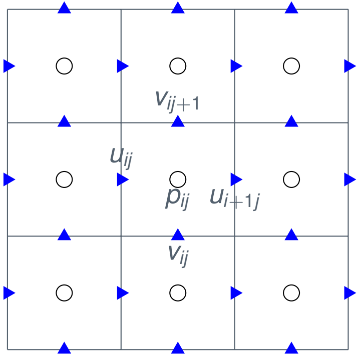


Figure: Marker and Cell discretization.

The open-source CFD code - Notus (https://notus-cfd.org) at I2M.

- Time discretization of the momentum equation is a 1st order Eulerian scheme with an implicit formulation for the viscous term.
- The velocity/pressure coupling is solved with the time splitting pressure correction method

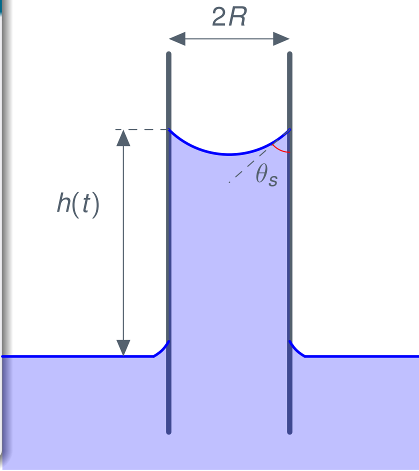
Capillary rise

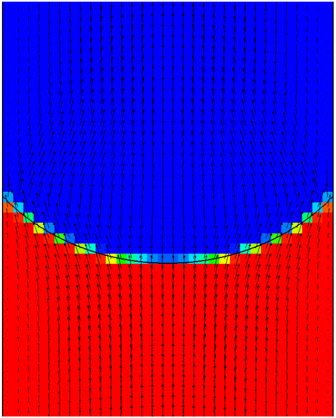
- The tendency of liquids to rise up in narrow tubes.
- The balance of forces that results in the static contact angle θ_s.
- Jurin's law:

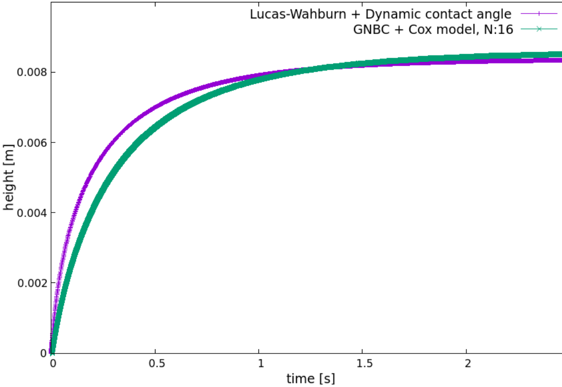
$$h = \frac{2\gamma \cos\theta_s}{\rho g R}$$

- The Lucas - Washburn - Bosanquet equation of fluid motion:

$$\frac{d}{dt}\left(\pi R^2 \rho h \frac{dh}{dt}\right) + 8\pi\mu h \frac{dh}{dt} = 2\pi R \gamma \cos\theta_s$$



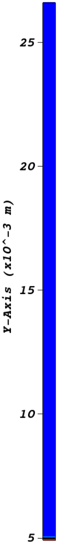




Liquid columm height as a function in time. N: number of grid points

Simulation

- Gas and glycerin 50% water.
- The axisymmetric capillary tube, $R = 0,512(mm)$.
- $\sigma = 67.9(mN/m)$
- $\theta_s = 37.08^\circ$.



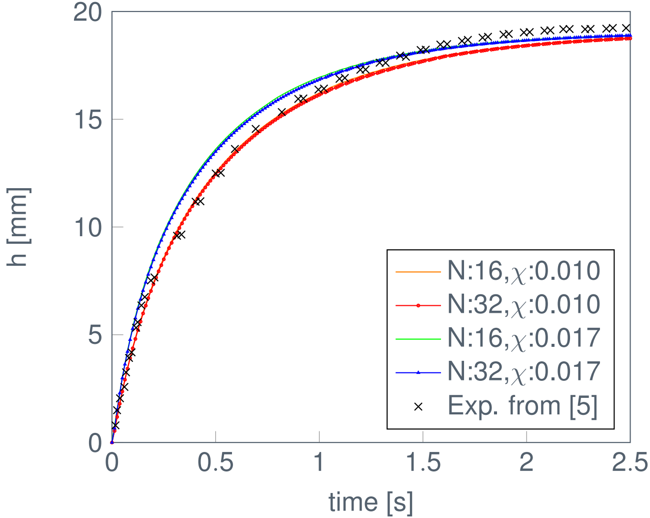


Figure: Glycerin 50% water column height with time.

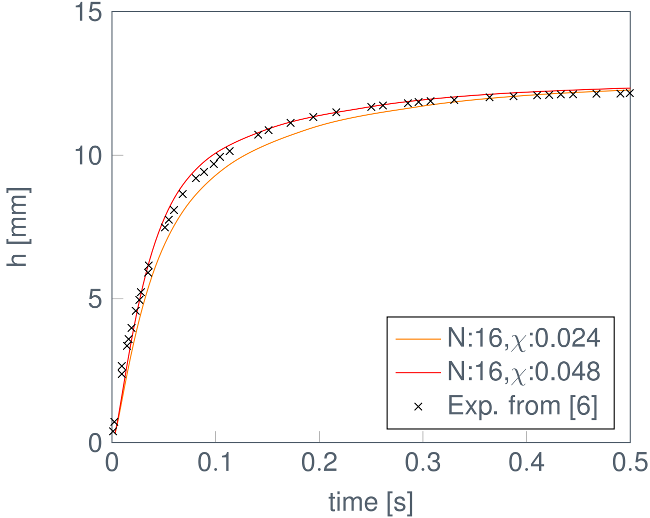
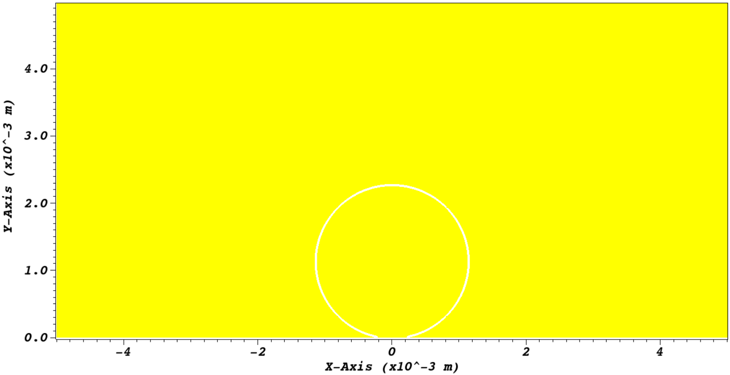


Figure: n-Dodecane column height with time, $\theta_s = 0^\circ$.

- Water and gas, with equilibrium contact angle 90°.
- The initial droplet with $R = 1.14$ (mm) and impacts to the wall with $V_{int} = 1$ (m/s).



Numerical simulation
Spreading drop

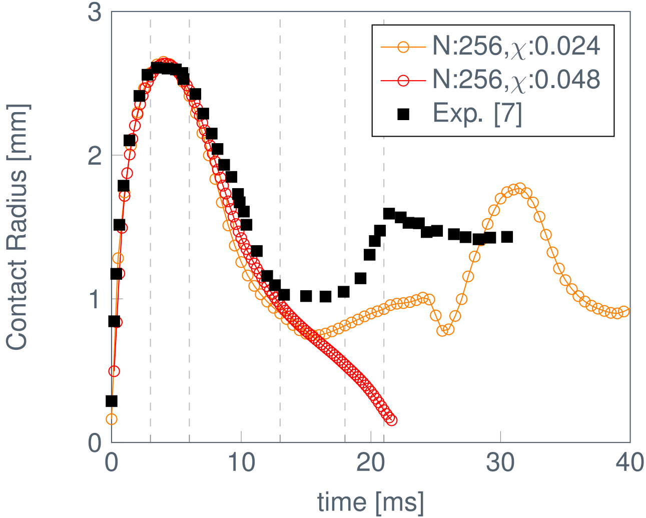


Figure: Spreading radius as a function of time.

Perspectives

- Improve the simulation of spreading drop for the receding phase up to the first equilibrium state.
- Study drop sliding down an inclined plane.
- Study complex geometries.
- Simulate the wetting phenomena to high Ca number cases ($Ca \sim 0.1$).

Thank you!

References

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References

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C_{ij} is approximated by polygon area made by the crossing points and the grid cell corners enclosed by Ω.

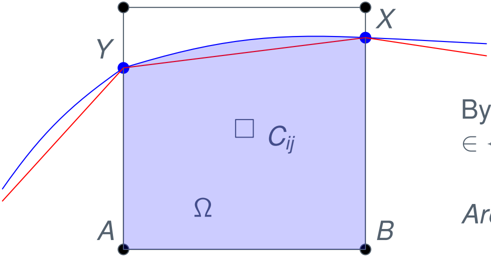

Figure: Computation volume fraction.

$$Area = \oint_{\partial\Omega} y dx = -\oint_{\partial\Omega} x dy. \quad (16)$$

By ordered vertices $(x_i, y_i) \in \{A, B, X, Y\}$ and midpoint rule:

$$Area_{2D} = \frac{1}{2}\sum_i (y_{i+1} + y_i)(x_{i+1} - x_i). \quad (17)$$

$$Area_{axisymmetric} = \frac{\pi}{3}\sum_i (y_{i+1} + y_i)(x_{i+1} - x_i)(x_i + x_{i+1}). \quad (18)$$

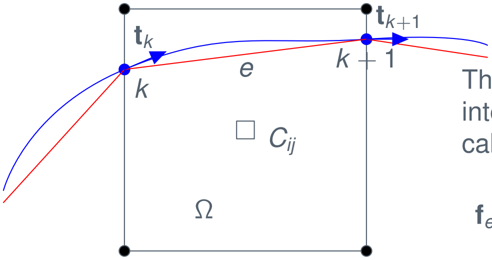

Figure: Local force $\mathbf{f}_e$ of element e is computed from tangent $\mathbf{t}_k$ and $\mathbf{t}_{k+1}$ of marker k and $k+1$.

The total tension force acting on a interface element e in 2D is calculated following:

$$\mathbf{f}_e = \int_e \sigma\kappa\mathbf{n}ds = \sigma(\mathbf{t}_{k+1} - \mathbf{t}_k). \quad (19)$$

Mathematical model
Interface curvature fields

For the axisymmetric coordinate system:

$$\mathbf{F}_\sigma = \sigma\left(\kappa^{2D} + \kappa^{axis}\right)\nabla \mathbf{C}. \tag{20}$$

The axisymetric curvature on Eulerian grid:

$$\kappa^{axis}_{i+1/2,j} = \sum_k \kappa^{axis}_k D_{i+1/2,j}(\mathbf{x}_k) / \sum_k D_{i+1/2,j}(\mathbf{x}_k) \tag{21}$$

where

$$\kappa^{axis}_k = \begin{cases} n_k / x_k & \text{if } x_k \neq 0, \\ \kappa^{2D}_k & \text{if } x_k = 0, \end{cases}$$

here, n_x: the radial component of unit normal $\mathbf{n}_k$.

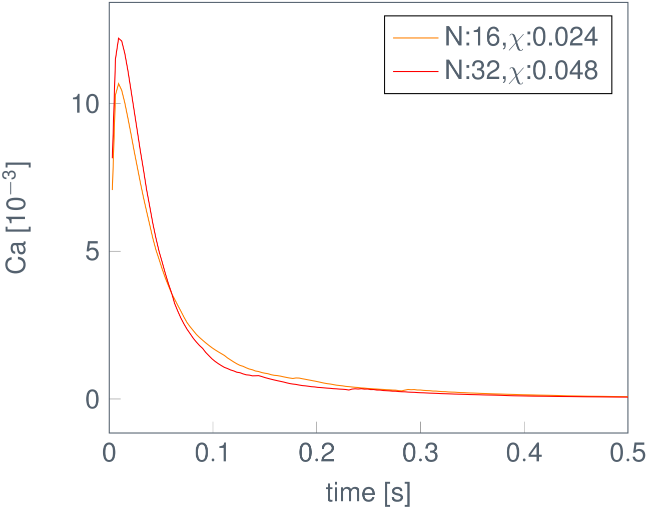

Figure: Ca number with time.