Complex-Fluid/Solid Interaction Simulations based on Diffuse-Interface Binary-Fluid Models

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océ

Outline

Elasto-capillarity: *capillary origami*

Play/Pause | Rewind

source: https://youtu.be/6gYb2fOnMvM

Applications

- Novel micro-fluidic concepts
  - durotaxis[1]
  - capillary origami[2]
- Additive manufacturing
- Inkjet printing

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[1] R.W. Style et al., PNAS 110 (2013), no. 31, 12541-12544.

[2] C. Py et al., Phys. Rev. Lett. 98 (2007), 156103.

Properties and Applications

Properties

- Wealth of complicated physical phenomena
  - contact-line pinning[1]
  - stick-slip behavior[2]
  - singularities
  - ...
- Multi-physics / multi-field
- Multiscale in space / time
- Free-boundary character
- Surface transport (surfactants)
- Phase changes (evaporation)
- Poro-mechanics
- ...

[1] S. Karpitschka et al., *Dynamic contact angle of a soft linear viscoelastic solid*, (2015)
[2] S. Karpitschka et al., Nat Commun 6 (2015)

Stick-slip behavior on visco-elastic substrates

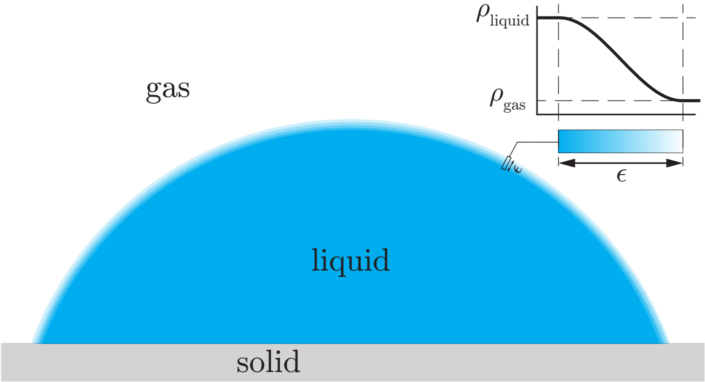
Play/Pause Rewind

source: https://youtu.be/62cd6oGX8HM

Modeling paradigm

Interaction of a complex (binary) fluid with an elastic solid substrate

1. *diffuse-interface* model for the fluid-fluid interface
2. *sharp-interface* model for the fluid-solid interface



Modeling paradigm: motivation

Diffuse-interface binary-fluid model

1. Allows for topological changes (incl. contact-line motion)
2. Rigorous thermodynamic basis (conservation/dissipation)
3. Not necessary to conform mesh to fluid-fluid interface

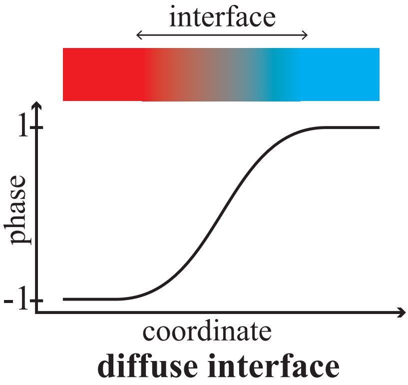
Sharp-interface model for fluid-solid interface

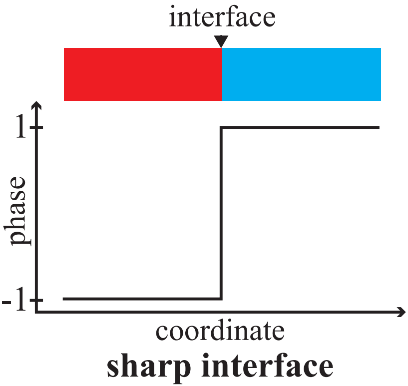
1. *Lagrangian formulation* of solid must be accommodated
2. No topological changes of fluid-solid interface
3. Conforming approaches generally more accurate

Outline

Phase-field models of interface problems

A phase-field model* provides a model for interface problems, in which the interface is represented by a finite transition layer, and interface conditions are accounted for as additional terms in the PDE.





*Also called *diffuse-interface model*

Phase-field models of interface problems

A phase-field model* provides a model for interface problems, in which the interface is represented by a finite transition layer, and interface conditions are accounted for as additional terms in the PDE.

Dual interpretations

1. Diffuse-interface models are *regularizations* of sharp-interface models[1]
2. Sharp-interface models are *limits* of diffuse-interface models[2,3,4]

[1] J.U. Brackbill et al. J. Comput. Phys. 100 (1992), 335-354
[2] B.E.E. Stoth, J. Diff. Eqs. 125 (1996), 154-183
[3] K. Hermsdörfer et al., Interfaces and Free Boundaries 13 (2011), 239-254
[4] W. Dreyer and C. Kraus, Proc. Roy. Soc. Edinburgh Sect. A. 140 (2010), 1161-1186

Phase-field models of interface problems

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Dual interpretations

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Diffuse-interface models are more comprehensive and versatile than sharp-interface models in that they can account for topological changes

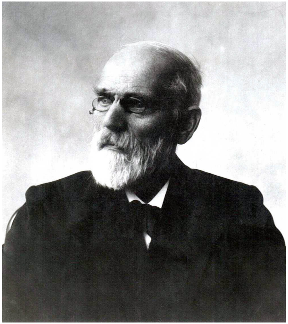
[1] J.U. Brackbill et al. J. Comput. Phys. 100 (1992), 335-354

[2] B.E.E. Stoth, J. Diff. Eqs. 125 (1996), 154-183

[3] K. Hermsdörfer et al., Interfaces and Free Boundaries 13 (2011), 239-254

[4] W. Dreyer and C. Kraus, Proc. Roy. Soc. Edinburgh Sect. A. 140 (2010), 1161-1186

Diffuse-interface models: history



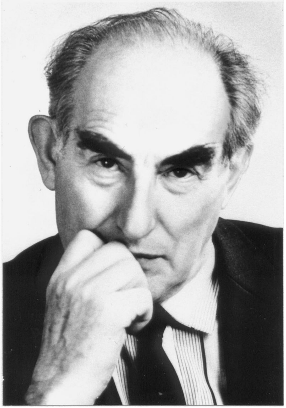
J.D. van der Waals

Lord Rayleigh (J.W. Strutt)

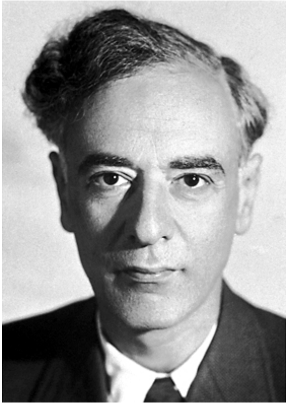
"... *the density of the body varies continuously at and near its transition layer*" (J.D. van der Waals)

J.D. van der Waals, Verhand. Kon. Akad. V Wetensch. Amst. Sect. 1, 1893
Lord Rayleigh, Phil. Mag. V 30 (1890), 285-298.

Diffuse-interface models: history



V.L. Ginzburg



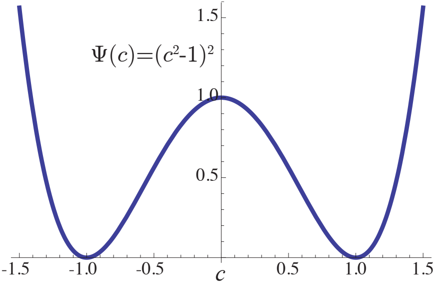
L.D. Landau

Ginzburg-Landau theory for phase transitions based on an order parameter and an energy functional

Diffuse-interface models: history

J.W. Cahn

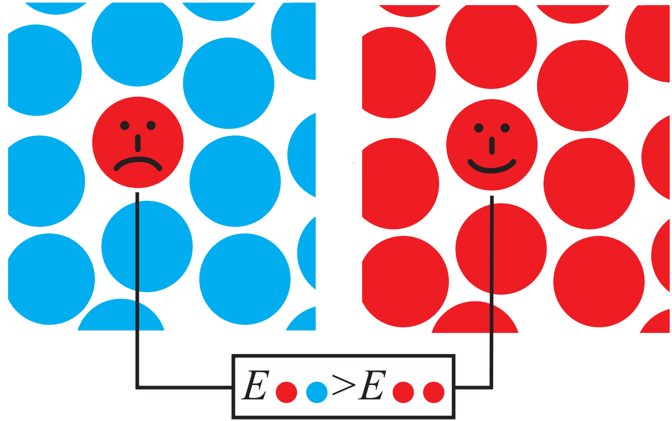
$$E(c) = \int_\Omega \Psi(c) + \varepsilon^2 |\nabla c|^2$$



$$\begin{aligned} d_t c + \mathrm{div} c\boldsymbol{u} &= \mathrm{Pe}^{-1}\Delta\mu \\ \mu &= \Psi'(c) - \varepsilon^2 \Delta c \big(= \delta E / \delta c \big) \end{aligned} \qquad \text{(CH)}$$

J.W. Cahn and J.E. Hilliard, J. Chem. Phys. 28 (1958), 258–267

Diffuse-interface models: molecular-scale cartoon



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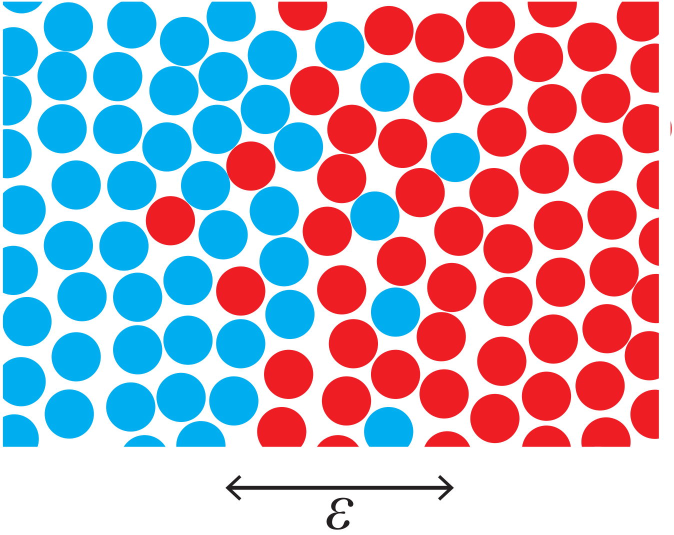


Cahn–Hilliard model of phase separation: dynamics

Play/Pause Rewind

Navier-Stokes-Cahn-Hilliard model of two-species flows

The NSCH equations are not (yet) one system of equations, but a class of models. 2×2 subclasses can be distinguised, depending on the choice of the order parameter (=phase) and the mixture velocity.

Remarks

- Derivation via *mixture theory*
- A mixture of two incompressible species is not incompressible[1]
- If mixture velocity $\boldsymbol{v}$ is defined as *mass-averaged* velocity then $\operatorname{div}\boldsymbol{v} \neq 0$ but conservation of momentum of the mixture is compatible with conservation of momentum for the components: only a capillary term appears
- If mixture velocity is defined as *volume-averaged* velocity then $\operatorname{div}\boldsymbol{v} = 0$ but conservation of momentum for the mixture must include a mass-flux term[2]

[1] J. Lowengrub and L. Truskinovsky, Phys. Engng. Sci. 454 (1998), 2617–2654.

[2] H. Abels, H. Garcke, and G. Grün, M3AS 22 (2012), 1150013.

Navier-Stokes-Cahn-Hilliard model of two-species flows

The NSCH equations are not (yet) one system of equations, but a class of models. 2×2 subclasses can be distinguised, depending on the choice of the order parameter (=phase) and the mixture velocity.

	c=mass fraction	c=volume fraction
$\boldsymbol{v}$=mass-averaged $(\mathrm{div}\boldsymbol{v} \neq 0)$	1,2	3
$\boldsymbol{v}$=volume-averaged $(\mathrm{div}\boldsymbol{v} = 0)$	-	4,5

[1] J. Lowengrub and L. Truskinovsky, Phys. Engng. Sci. 454 (1998), 2617-2654.
[2] Z. Guo, P. Lin, and J.S. Lowengrub, J. Comput. Phys. 276 (2014), 486-507.
[3] G. Şimşek, K.G. van der Zee, and E.H. van Brummelen (in preparation).
[4] H. Abels, H. Garcke, and G. Grün, M3AS 22 (2012), 1150013.
[5] H. Garcke, M. Hinze, and C. Kahle, Applied Numerical Mathematics 99 (2016), 151-171.

Energy-dissipation structure

The NSCH equations (are supposed to) dissipate the convex functional:

$$E(c,\boldsymbol{v}) = \underbrace{\int_\Omega \frac{1}{2}\rho|\boldsymbol{v}|^2}_{\text{kinetic}} + \tilde{\sigma}\underbrace{\int_\Omega \frac{\varepsilon}{2}|\boldsymbol{\nabla} c|^2 + \frac{1}{\varepsilon}\Psi(c)}_{\text{Ginzburg-Landau}}$$

with $\Psi(c) = \frac{1}{4}(c^2-1)^2$ a double-well potential. The following equivalences hold:

$$\begin{aligned} d_t(c,\boldsymbol{v}) = 0 \quad &\Leftrightarrow \quad E(c,\boldsymbol{v}) \stackrel{!}{=} \min \\ &\Leftrightarrow \quad (c,\boldsymbol{v}) = \text{‘meaningful equilibrium’} \end{aligned}$$

Navier-Stokes-Cahn-Hilliard model of two-species flows

$$\left.\begin{aligned} d_t\rho\boldsymbol{u} + \mathrm{div}\rho\boldsymbol{u}\otimes\boldsymbol{u} + \boldsymbol{\nabla}p - \mathrm{div}\boldsymbol{\tau} + \underbrace{\tilde{\sigma}\varepsilon\mathrm{div}(\boldsymbol{\nabla}c\otimes\boldsymbol{\nabla}c)}_{\text{surface tension}} &= 0 \\ \mathrm{div}\,\boldsymbol{u} &= 0 \\ d_tc + \underbrace{\mathrm{div}c\boldsymbol{u}}_{\text{transport}} - \gamma\Delta\mu &= 0 \\ \mu - (\tilde{\sigma}/\varepsilon)\Psi'(c) + \tilde{\sigma}\varepsilon\Delta c &= 0 \end{aligned}\right\} \text{ in } \Omega_t^f$$

- $\rho := \rho_1(1+c)/2 + \rho_2(1-c)/2$
- $2\sqrt{2}\tilde{\sigma} = 3\sigma$ with σ as surface tension
- $\boldsymbol{\tau} = \mu\boldsymbol{\nabla}^s\boldsymbol{u}$ as viscous stress tensor
- refinements possible

Conventional boundary conditions

Typical BCs for the NSCH equations are:

Dirichlet		Neumann	
$u = g_{\mathrm{D}}^{u}$	on Γ_{D}^{u}	$-pn + \tau n - \tilde{\sigma}\epsilon\partial_n c \boldsymbol{\nabla} c = g_{\mathrm{N}}^{u}$	on Γ_{N}^{u}
$c = g_{\mathrm{D}}^{c}$	on Γ_{D}^{c}	$-\tilde{\sigma}\epsilon\partial_n c = g_{\mathrm{N}}^{c}$	on Γ_{N}^{c}
$\mu = g_{\mathrm{D}}^{\mu}$	on $\Gamma_{\mathrm{D}}^{\mu}$	$\gamma\partial_n \mu = g_{\mathrm{N}}^{\mu}$	on $\Gamma_{\mathrm{N}}^{\mu}$

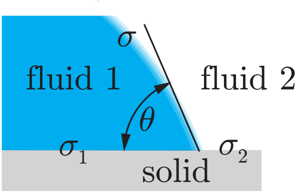
In principle, 'mix-and-match' between left and right column, one from each row

Preferential wetting boundary condition

In the presence of fluid-solid surface tension, with different surface tensions for the two phases, the fluid-solid interface carries an energy:

$$E_{\mathrm{fs}}(c) = \int_{\Gamma_{\mathrm{fs}}} \sigma_{\mathrm{fs}}(c)$$

- $\sigma_{\mathrm{fs}}(c) = \frac{1}{4}(c^3 - 3c)(\sigma_2 - \sigma_1) + \frac{1}{2}(\sigma_1 + \sigma_2)$ is a mixture surface tension that interpolates the fluid-solid surface energies of the two species[1,2]
- $\theta_s = \arccos((\sigma_2 - \sigma_1)/\sigma)$ is static contact angle (interior to fluid 1)



[1] D. Jacqmin, J. Fluid Mech. 402 (2000), 57-88

[2] P. Yue and J.J. Feng, Phys. Fluids 23 (2011), 012106

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$$E_{\mathrm{fs}}(c) = \int_{\Gamma_{\mathrm{fs}}} \sigma_{\mathrm{fs}}(c)$$

Differentiation of the fluid-solid surface energy leads to the preferential wetting boundary condition

$$\tilde{\sigma}\varepsilon\partial_n c + \sigma'_{\mathrm{fs}}(c) = 0 \quad \text{on } \Gamma_{\mathrm{fs}}$$

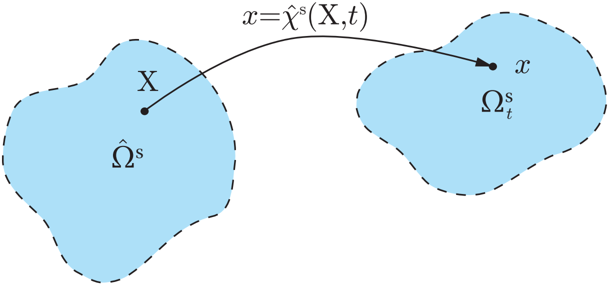
[1] D. Jacqmin, J. Fluid Mech. 402 (2000), 57-88

[2] P. Yue and J.J. Feng, Phys. Fluids 23 (2011), 012106

Outline

Large-deformation elasticity

Reference configuration $\hat{\Omega}^s \subset \mathbb{R}^d$ and deformation $\hat{\chi}^s : \hat{\Omega}^s \to \Omega_t^s$:



The deformation satisfies the equation of motion

$$\hat{\rho}\frac{\partial^2 \hat{\chi}^s}{\partial t^2} - \widehat{\mathrm{div}}\hat{P} = 0 \qquad \text{in } \hat{\Omega}^s$$

- $\hat{\rho} : \hat{\Omega}^s \to \mathbb{R}_{>0}$ is density in reference configuration
- $\hat{P}$ is first Piola-Kirchhoff stress tensor

Hyperelastic material with St.-Venant–Kirchhoff constitutive behavior

Hyperelastic material: stress results as variational derivative of stored energy functional to deformation:

$$-\int_{\hat{\Omega}^s} \hat{x} \cdot \widehat{\mathrm{div}} \hat{P} = \mathscr{W}'(\hat{\chi}^s; \hat{x})$$

- $\mathscr{W}$ the *stored-energy functional* and $\mathscr{W}'(\hat{\chi}^s; \hat{x})$ the Fréchet derivative at $\hat{\chi}^s$ acting on $\hat{x}$

St.-Venant–Kirchhoff constitutive behavior:

$$\mathscr{W}(\hat{\chi}^s) = \int_{\hat{\Omega}^s} \frac{\lambda_{\mathrm{L}}}{2} (\mathrm{tr} E)^2 + \mu_{\mathrm{L}} \mathrm{tr} E^2$$

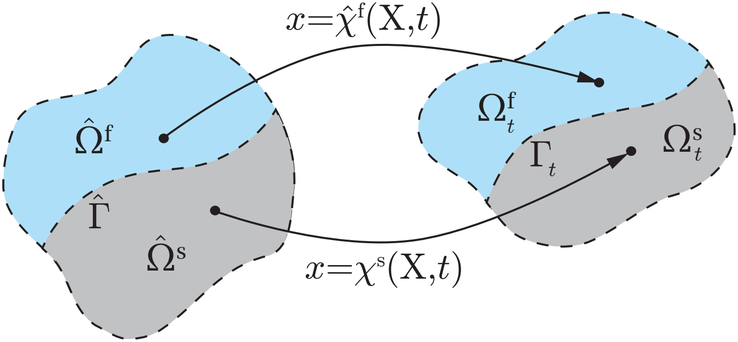
- $E = \frac{1}{2}(F^T F - I)$ the Green-Lagrange strain tensor
- $F = F(\hat{\chi}^s) = \hat{\boldsymbol{\nabla}} \hat{\chi}^s$ the deformation gradient
- λ_{L} and μ_{L} the Lamé parameters

Outline

Kinematic conditions

1. Continuity of motion: if the fluid domain is obtained as deformation acting on reference configuration, $\Omega_t^f = \hat{\chi}^f \hat{\Omega}^f$, then:

$$\hat{\chi}^f\big|_{\hat{\Gamma}} = \hat{\chi}^s\big|_{\hat{\Gamma}}$$



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$$\hat{\chi}^f\big|_{\hat{\Gamma}} = \hat{\chi}^s\big|_{\hat{\Gamma}}$$

2. Continuity of velocity: the complex-fluid mixture velocity coincides with the domain velocity

$$\boldsymbol{u} = \partial_t \hat{\chi}^s \circ \hat{\chi}^{-1} \quad \text{on } \Gamma_t$$

$\Rightarrow$ fluid conforms to Dirichlet boundary condition on interface, with data corresponding to solid velocity

Dynamic condition

Equilibrium of fluid and solid tractions +fluid-solid surface tension at interface (in distributional form)

$$\int_{\hat\Gamma} \hat v \cdot (-\hat P \hat n)\, d\hat S = -\int_{\Gamma_t} (\hat v \circ \hat\chi^{-1}) \cdot \underbrace{(p\boldsymbol{n} - \boldsymbol{\tau}\boldsymbol{n} + \tilde\sigma \epsilon \partial_n c \boldsymbol{\nabla} c)}_{\text{fluid traction}}\, dS$$

$$- \int_{\Gamma_t} (\hat v \circ \hat\chi^{-1}) \cdot \underbrace{(\sigma_{\mathrm{fs}}(c)\kappa\boldsymbol{n} + \boldsymbol{\nabla}_\Gamma \sigma_{\mathrm{fs}}(c))}_{\text{surface tension}}\, dS \qquad \forall \hat v \in C_0^\infty(\hat\Gamma)$$

- Structure in reference configuration, fluid in actual configuration
- $\boldsymbol{\nabla}_\Gamma$ is surface gradient
- κ is curvature
- Additional contribution from non-constant surface tension[1]
- Structure satisfies Neumann boundary condition on interface

[1] H. Gouin, Mathematics and Mechanics of Complex Systems 2 (2014), 23-43

Outline

Arbitrary-Lagrangian-Eulerian formulation of NSCH

To accommodate motion of fluid domain, we apply weak ALE[1,2,3] formulation. Consider arbitrary $\hat{z} \in C^\infty(\hat{\Omega}^f)$ and $\psi \in C^\infty(\Omega_t^f)$:

$$\begin{aligned}\int_{\Omega_t^f} (\hat{z} \circ \hat{\chi}^{-1}) \partial_t \psi &= \frac{d}{dt} \int_{\Omega_t^f} (\hat{z} \circ \hat{\chi}^{-1}) \psi - \int_{\Omega_t^f} \operatorname{div}\big(\boldsymbol{w} (\hat{z} \circ \hat{\chi}^{-1}) \psi \big) \\ &\quad - \int_{\Omega_t^f} \partial_t (\hat{z} \circ \hat{\chi}^{-1}) \psi \\ &= \frac{d}{dt} \int_{\Omega_t^f} (\hat{z} \circ \hat{\chi}^{-1}) \psi - \int_{\Omega_t^f} (\hat{z} \circ \hat{\chi}^{-1}) \operatorname{div}(\boldsymbol{w} \psi)\end{aligned}$$

- $\boldsymbol{w} = \partial_t \hat{\chi}^f \circ \hat{\chi}^{-1}$ is domain velocity
- 1st identity: product rule + Reynolds transport thm.
- 2nd identity: $\partial_t (\hat{z} \circ \hat{\chi}^{-1}) = -\boldsymbol{w} \cdot \boldsymbol{\nabla} (\hat{z} \circ \hat{\chi}^{-1})$

[1] J. Donea, Comput. Methods Appl. Mech. Engrg. 33 (1982), 689-723
[2] Y. Bazilevs et al., Computational Mechanics 43 (2008), 3-37
[3] E.H. van Brummelen et al., ArXiv 1510.02441v1 (2015), 1-8

Arbitrary-Lagrangian-Eulerian formulation of NSCH

Denote by ℓ a lifting/extension of the structure velocity at FS interface (+other Dirichlet data). Then $c = \boldsymbol{u}_0 + \ell$, $\boldsymbol{u}_0 \in \boldsymbol{H}^1_{0,\Gamma_t}(\Omega^f_t)$ s.t.

$$\frac{d}{dt}\int_{\Omega^f_t} \boldsymbol{v}\cdot\rho\boldsymbol{u} - \int_{\Omega^f_t} \boldsymbol{\nabla}\boldsymbol{v} : (\rho\boldsymbol{u}\otimes(\boldsymbol{u}-\boldsymbol{w}) - \boldsymbol{\tau} + \tilde{\sigma}\varepsilon\boldsymbol{\nabla}c\otimes\boldsymbol{\nabla}c) - \int_{\Omega^f_t} p\,\mathrm{div}\boldsymbol{v} = \text{r.h.s.}$$

for all $\boldsymbol{v} \in \{\boldsymbol{v} = \hat{\boldsymbol{v}}\circ\hat{\chi}^{-1} : \hat{\boldsymbol{v}} \in \boldsymbol{H}^1_{0,\Gamma_t}(\hat{\Omega}^f)\}$

1. Identical to fixed-domain NS(CH), except domain-velocity term $\boldsymbol{w}$
2. ... and the time derivative acts on time-dependent domain
3. Lift ensures that velocity is continuous across interface

Arbitrary-Lagrangian-Eulerian formulation of NSCH

Similar for CH part: denote by ℓ a lifting/extension of Dirichlet data. Then $c = c_0 + \ell$, $c_0 \in H^1_{0,\Gamma_D}(\Omega^f_t)$ s.t.

$$\frac{d}{dt}\int_{\Omega^f_t} zc + \int_{\Omega^f_t} \nabla z \cdot (\gamma \nabla \mu - c(\boldsymbol{u} - \boldsymbol{w})) = \text{r.h.s.}$$

for all $z \in \{z = \hat{z} \circ \hat{\chi}^{-1} : \hat{z} \in H^1_{0,\Gamma_D}(\hat{\Omega}^f)\}$

1. Identical to fixed-domain (NS)CH, except domain-velocity term $\boldsymbol{w}$
2. ... and the time derivative acts on time-dependent domain

Weak formulation of solid

Given a lift ℓ of the Dirichlet data, $\hat{\chi}^s = \hat{\chi}_0^s + \ell$ with $\hat{\chi}_0^s \in \boldsymbol{H}^1_{0,\hat{\Gamma}_D}(\hat{\Omega}^s)$:

$$\frac{d^2}{dt^2} \int_{\hat{\Omega}^s} (\hat{x} \cdot \hat{\rho} \hat{\chi}^s) + \mathscr{W}(\hat{\chi}^s; \hat{x}) = \cdots + \int_{\hat{\Gamma}} \hat{x} \cdot \hat{P} \hat{n} \qquad \forall \hat{x} \in \boldsymbol{H}^1_{0,\hat{\Gamma}_D}(\hat{\Omega}^s)$$

- Stress term appears naturally as Fréchet derivative of stored-energy functional
- The rhs term represents the fluid traction + FS surface tension

Weak evaluation of tractions

The traction on the solid is to be understood in a weak sense[1,2]:

$$
\begin{aligned}
\int_{\hat\Gamma} \hat{x}\cdot\hat{P}\hat{n}\,d\hat{S} &= \int_{\Gamma_t} x\cdot(p\boldsymbol{n} - \boldsymbol{\tau}\boldsymbol{n} + \tilde\sigma\varepsilon\partial_n c\boldsymbol{\nabla} c)\,dS \\
&\quad + \int_{\Gamma_t} x\cdot(\sigma_{\mathrm{fs}}(c)\kappa\boldsymbol{n} + \boldsymbol{\nabla}_\Gamma\sigma_{\mathrm{fs}}(c))\,dS \\
&= \frac{d}{dt}\int_{\Omega_t^f}(\ell_x\cdot\rho\boldsymbol{u}) - \int_{\Omega_t^f} p\,\mathrm{div}\ell_x \\
&\quad - \int_{\Omega_t^f}\boldsymbol{\nabla}\ell_x : (\rho\boldsymbol{u}\otimes(\boldsymbol{u}-\boldsymbol{w}) - \boldsymbol{\tau} + \tilde\sigma\varepsilon\boldsymbol{\nabla} c\otimes\boldsymbol{\nabla} c) \\
&\quad + \int_{\Gamma_t}\sigma_{\mathrm{fs}}(c)\boldsymbol{\nabla}_\Gamma \mathrm{Id}_{\Gamma_t} : \boldsymbol{\nabla}_\Gamma x\,dS + \int_{\partial\Gamma_t}\boldsymbol{\nu}\cdot(\sigma_{\mathrm{fs}}(c)x)\,dC
\end{aligned}
\tag{$*$}
$$

[1] E.H. van Brummelen et al., J. Appl. Mech. 79 (2012), 010904-8.

[2] E.H. van Brummelen et al., ArXiv 1510.02441v1 (2015), 1-8

Weak evaluation of tractions: Remarks (1)

- Final terms in $(*)$ follow by integration by parts on NSCH equations
- Final terms in $(*)$ represent fluid-residual functional evaluated at lift of trace of solid test function
- Final terms in $(*)$ follow from expression for curvature based on Laplace-Beltrami acting on the Identity[1,2]
- 2nd term in $(*)$ is generally unbounded, but can be suppressed without loss of consistency if appropriate BCs hold
- The final terms+terms in $(*)$ provide a proper weak formulation of the traction functional: the underlying integration-by-parts identities hold for sufficiently smooth functions, but final expression is valid for a larger class of functions
- Lift of trace of solid test function $\Rightarrow$ continuity of fluid and solid test functions for equations of motion

[1] E. Bänsch, Numer. Math. 88 (2001), 203-235

[2] G. Dziuk, Numer. Math. 58 (1991), 603-611

Weak evaluation of tractions: Remarks (2)

- Existence of integral of ∇_Γ-terms imposes additional regularity conditions on solid deformation at interface
- In the sharp interface limit $\varepsilon \to +0$, the fluid-fluid surface tension yields a point force (2D) or line force (3D) on the solid surface at the contact line. Such a localized load is unbounded without fluid-solid surface tension
- Because the fluid-fluid surface tension at the contact line is singular with respect to elastic energy, the surface shape at the contact line is determined by surface-tension contributions only (Neumann triangle) (also[1])
- Still many open question w.r.t. proper functional setting

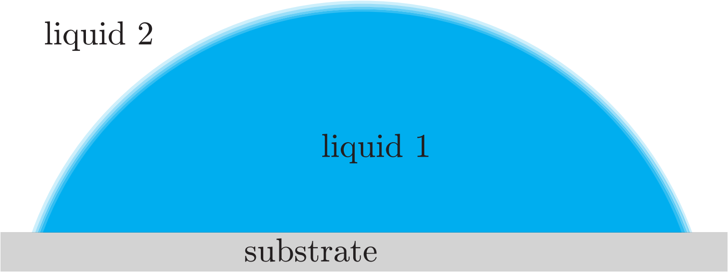
[1] S. Karpitschka et al., *Dynamic contact angle of a soft linear viscoelastic solid*, (2015)

Outline

Setup

Setup taken from Style et al.:

R.W. Style, R. Boltyanskiy, Y. Che, J.S. Wettlaufer, L.A. Wilen, and E.R. Dufresne, *Universal deformation of soft substrates near a contact line and the direct measurement of solid surface stresses*, Phys. Rev. Lett. **110** (2013), 066103.



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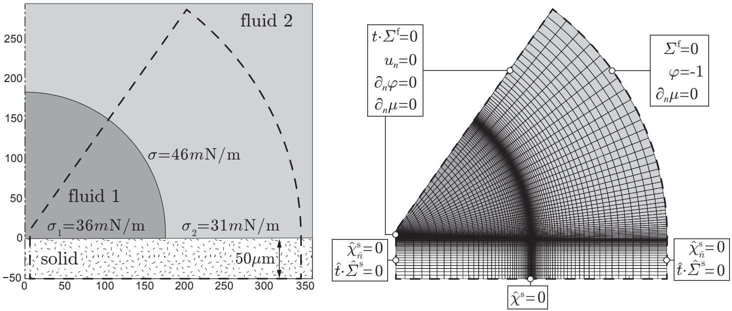
- $13.8\,p$l droplet on soft substrate
- Youngs modulus $E = 3k$Pa, Poisson ratio $\nu_{\mathrm{L}} = 0.499$
- fluid-fluid surface tension $\sigma = 46\,m$N/m, fluid-solid surface tension liquid $\sigma_1 = 36\,m$N/m, fluid-solid surface tension ambient liquid $\sigma_1 = 31\,m$N/m
- Interface thickness $\epsilon = 2\,\mu$m
- viscosities, densities, etc. mock-up (only stationary displacement)

Computational setup (1)



- Radially symmetric
- Raviart-Thomas compatible B-spline approximations for velocity and pressure with order ((3,2),(2,3)) and 2
- Order parameter and chemical potential with quadratic B-splines
- Solid deformation and fluid-domain deformation with quadratic B-splines
- Fluid-domain deformation by means of harmonic extension
- Backward-Euler in time

Computational setup (2)

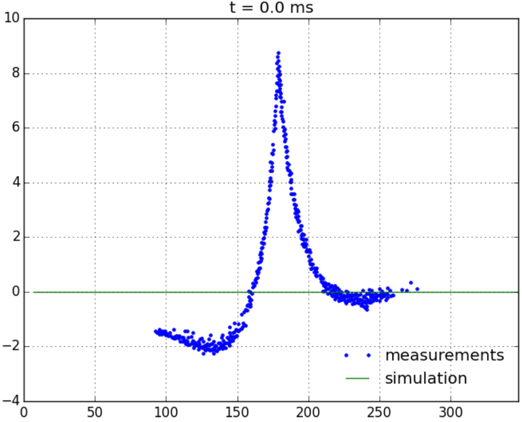
Solve fluid-solid interaction problem by means of subiteration[1] with under-relaxation: Repeat within each time step

1. Solve NSCH subproblem subject to kinematic condition with current displacement+velocity of solid
2. Solve solid subproblem subject to dynamic condition with NSCH solution from 1 (+implicit surface tension!)
3. Update solid displacement according to $\hat{\chi}_k^s = \alpha\hat{\chi}_{k,*}^s + (1-\alpha)\hat{\chi}_{k-1}^s$

[1] E.H. van Brummelen, Int. J. Numer. Meth. Fluids 65 (2011), 3-27

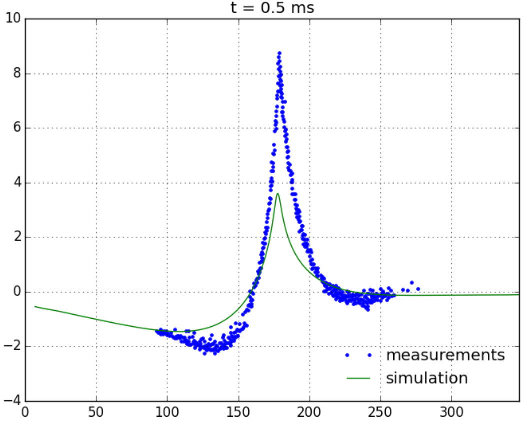
Results

Interface displacement



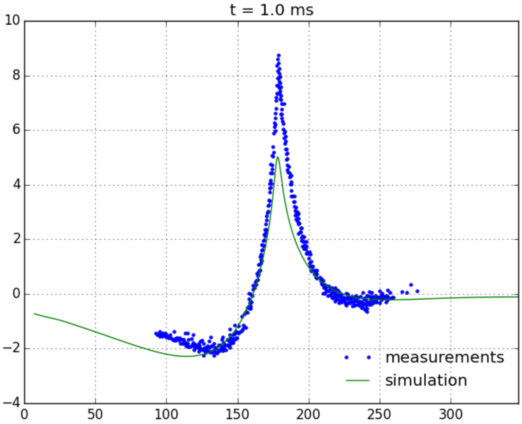
Results

Interface displacement



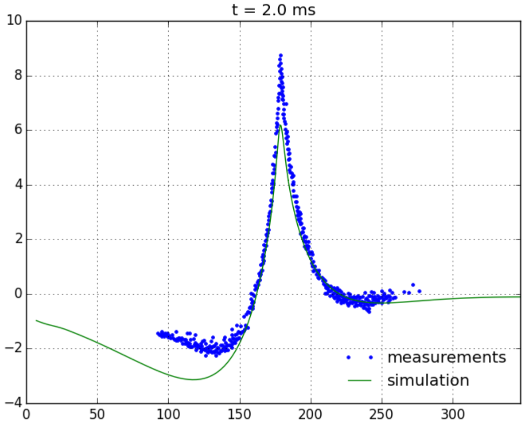
Results

Interface displacement



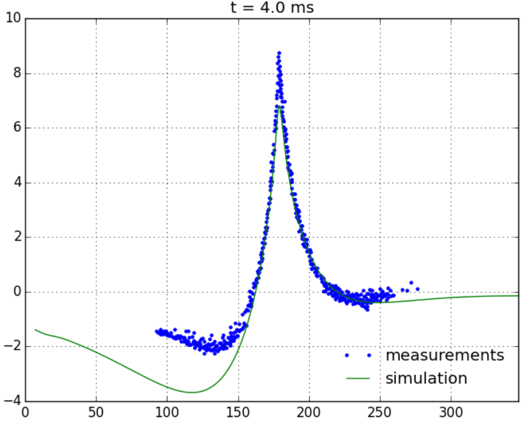
Results

Interface displacement



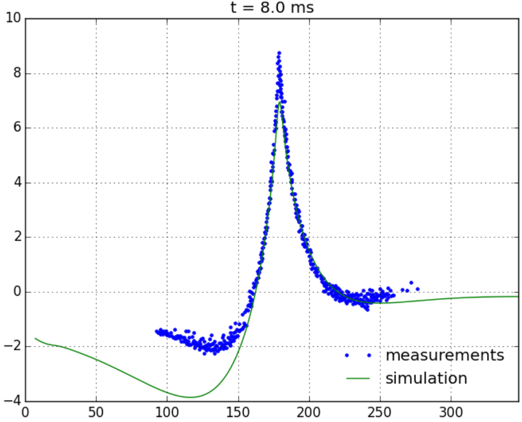
Results

Interface displacement



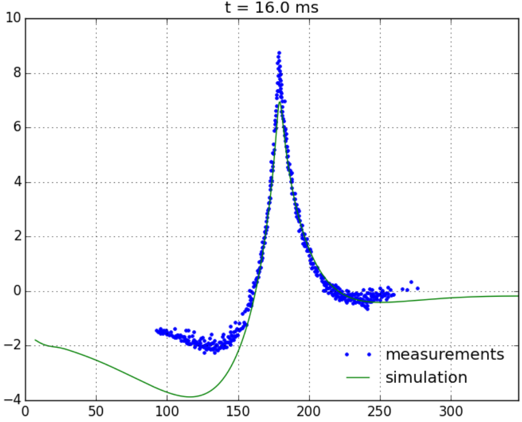
Results

Interface displacement



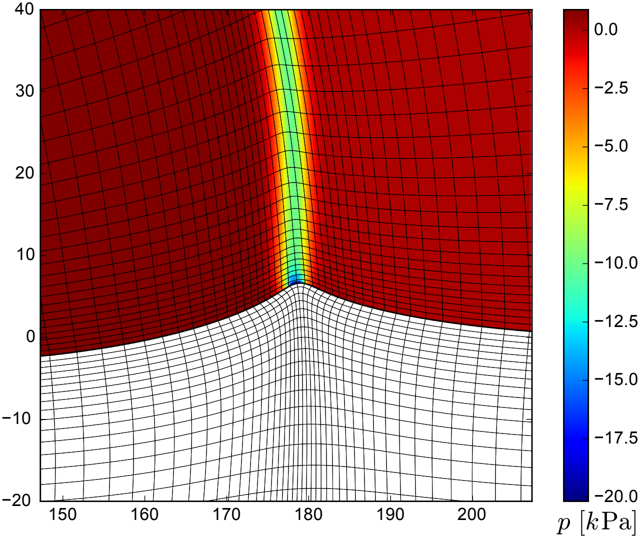
Results

Interface displacement



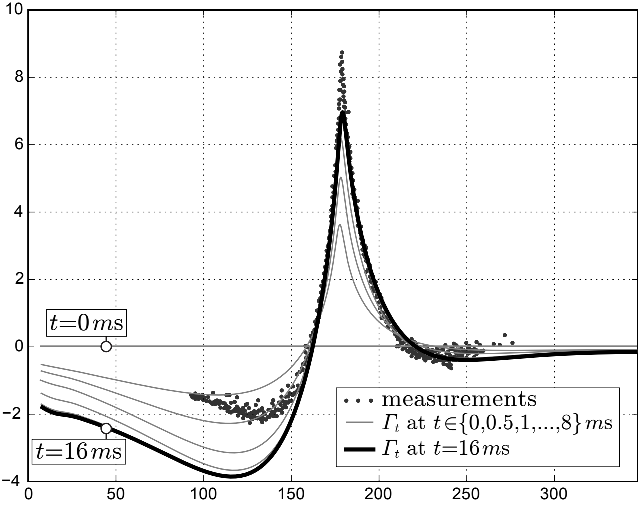
Results

Steady interface displacement ($t = 16\,m$s), fluid+solid mesh, pressure



Results

Steady interface displacement ($t = 16\,m$s), comparison to experiment



Results: discussion

1. Generally excellent agreement, especially near contact line (kink/cusp)
2. Indentation below droplet overestimated. (But comparison with corresponding analytical solution (uniform load on circular region) *spot on*)
3. Severe underrelaxation required (possibly mesh dependent)

Conclusions

1. The NSCH equations provide a comprehensive and versatile modeling framework for elasto capillarity
2. The computed results agree well with experimental data
3. Fluid-solid surface tension yields regularization of surface deformation near contact line (cusp/kink)
4. Fluid-solid interface conditions require careful treatment: weak traction evaluation and fluid-solid surface tension contribution

Discussion & open questions

1. Elasto-capillary problems are a wonderful playground for physicists and applied and numerical mathematicians: interfaces, free-boundaries, conservation/dissipation structures, stick-slip behavior, etc.
2. . . . with important technological applications!
3. What is the proper functional setting of NSCH-FSI problem?
4. What is the connection between fluid-solid surface tension and singular tractions?
5. How should the interface be resolved for dynamic problems?
6. How can the coupling strength in the FSI problem be characterized?
7. How can the stability and efficiency of the fluid-solid iteration be improved?
8. Establish dissipation of the complete coupled problem!