How to model two phase flows on arbitrary solid surfaces? (with Basilisk)

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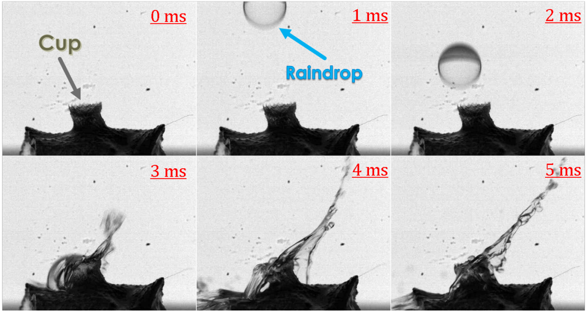
Multiphase flows without phase change



(a) Droplet impact on a leaf *[Credit: Valentin Laplaud(LadHyx)]*.

(b) Droplet hanging on fiber *[Lorenceau et al, JCI, (279) 2004]*.

Motivations

Model properly the interaction between the gas, the liquid and the solid

Multiphase flows with phase change

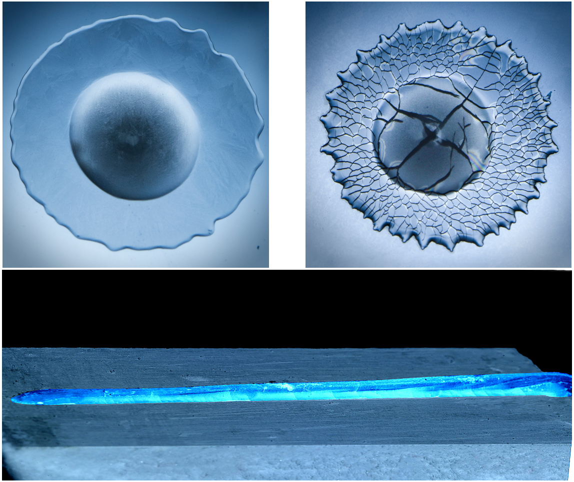


Figure: Droplet solidification *[Credit: Thievenaz and al GFM2016, Monier and al]*

Motivations

Model properly the interaction between the gas, the liquid and the solid

Interactions between a fluid and an arbitrary shape solid

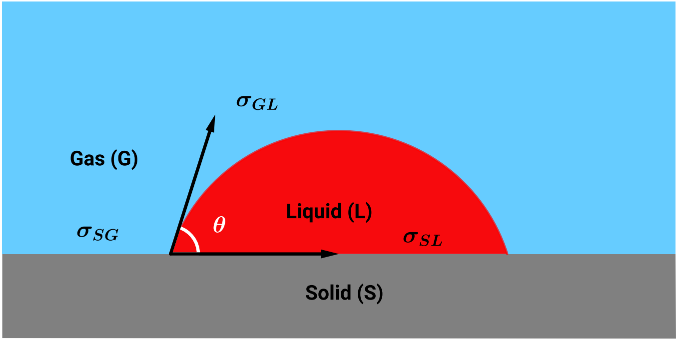


Figure: Contact angle θ and interfacial tensions σ, between solid, liquid and gas phases.

Problem

Model properly the interaction between the gas, the liquid and the solid

Interactions between a fluid and an arbitrary shape solid

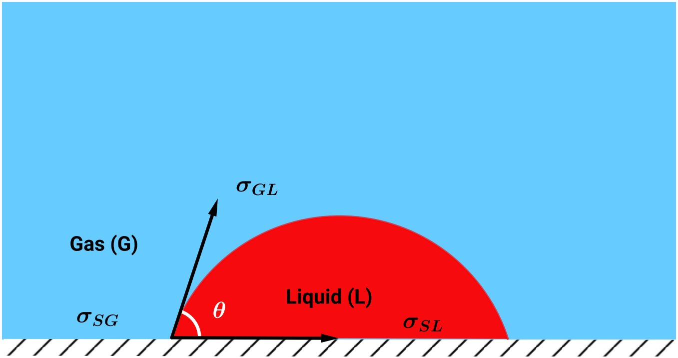


Figure: Contact angle θ and interfacial tensions σ, between solid, liquid and gas phases (*Chaudary and al Exp therm Fluid Sci 2014, Vu and al IJMF 2015, Zhang and al IJHMT 2018, Tembely and al JFM 2019, contact.h*).

Problem

Model properly the interaction between the gas, the liquid and the solid

Interactions between a fluid and an arbitrary shape solid

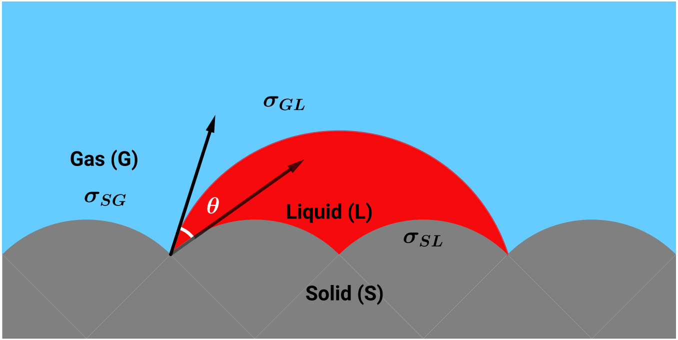


Figure: Contact angle θ and interfacial tensions σ, between solid, liquid and gas phases (*Liu and al JCP 2015, Patel and al Chem E. Sci 2017, Gohl and al IJMF 2018, Lyu and al JCP 2021*)..

Problem

Model properly the interaction between the gas, the liquid and the solid

Methodology

Goal

$\Rightarrow$ Implement a numerical method able to model multiphase flows interacting with arbitrary solids, thus taking into account the contact angle between the solid and the liquid-gas (triple point)

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$\Downarrow$

Ongoing developments

- $\Rightarrow$ Hybrid approach with Volume Of Fluid (VOF method) and the embedded boundary method
- $\Rightarrow$ Setting of the proper boundary conditions at the gas, liquid and solid intersection

Which solver?

$\Rightarrow$ **Basilisk** (Free software Program, PDE equations on adaptive Cartesian meshes (AMR))

Outline

A three phases system with **Basilisk solver** (`http://www.basilisk.fr`)

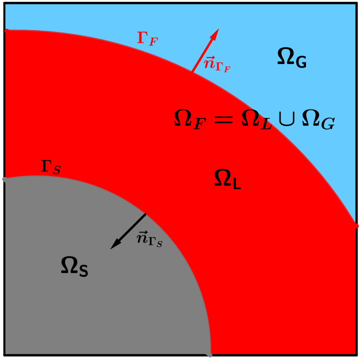


Figure: Three phases flow in a square domain

A three phases system with **Basilisk solver** (http://www.basilisk.fr)

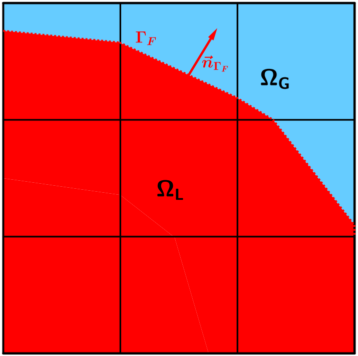


Figure: Two-phases flow discretized on a Cartesian grid

Liquid/gas phases

Navier-Stokes equations with the **Volume of Fluid method** to account for the liquid/gas interface

A three phases system with **Basilisk solver** (http://www.basilisk.fr)

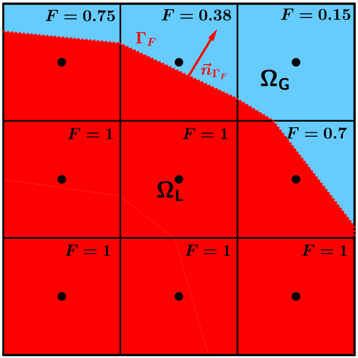


Figure: Two-phases flow discretized on a Cartesian grid

Incompressible Navier-Stokes equations for multiphase flows (One fluid model)

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

$$\frac{\partial \rho \bar{u}}{\partial t} + \bar{\nabla} \cdot (\rho \bar{u} \otimes \bar{u}) = \bar{\nabla} \cdot \bar{\bar{\mathcal{T}}} + \rho \bar{g} + \underbrace{\sigma \kappa \bar{n} \delta_s}_{\bar{F}_\sigma}$$

$$\frac{\partial \mathbf{F}}{\partial t} + \bar{u} \cdot \bar{\nabla} \mathbf{F} = 0$$

$\mathbf{F} = 0$ in G and $\mathbf{F} = 1$ in L and S

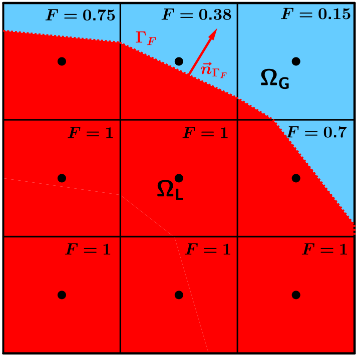
$\bar{\bar{\mathcal{T}}} \equiv -p\bar{\bar{\mathcal{I}}} + \mu(\bar{\nabla}\bar{u} + \bar{\nabla}\bar{u}^T)$ the stress tensor.

Physical properties

$$\rho = \mathbf{F}\rho_L + (1 - \mathbf{F})\rho_G$$

$$\mu = \mathbf{F}\mu_L + (1 - \mathbf{F})\mu_G$$

A three phases system with **Basilisk solver**(http://www.basilisk.fr)



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Incompressible Navier-Stokes equations

- Time staggered approximate projection method
- BCG second order scheme to discretize the advection term
- Fully implicit scheme for the viscous term
- Collocated grid for spatial discretization based on AMR

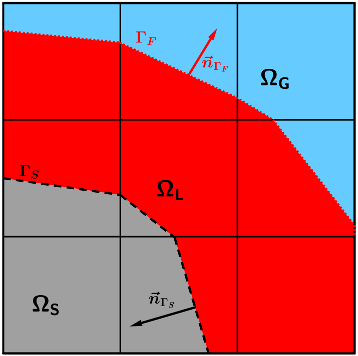
Volume of Fluid method

- VOF with a geometrical reconstruction method (PLIC) for sharp interface
- Split advection method *[Weymouth and Yue]*

Surface tension

- CSF model *[Brackbill and al]* with the well balanced surface tension calculation
- Generalized height function method for the curvature

A three phases system with **Basilisk solver** (http://www.basilisk.fr)



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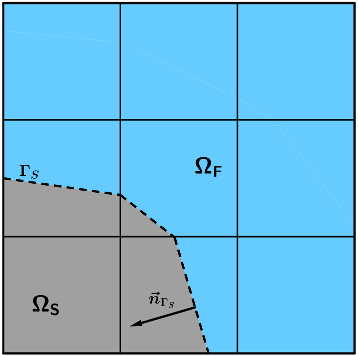


Figure: Immersed boundary flow discretized on a Cartesian grid

Solid phase

Embedded boundary method to account for the solid in the whole problem

Embedded boundary method *embed.h* *[Johansen and Colella, JCP, 1998]*

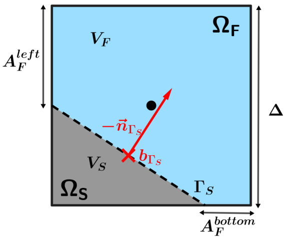


Figure: Fluid cut-cell

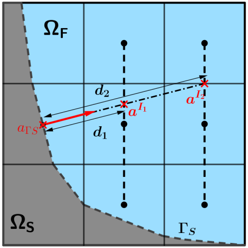


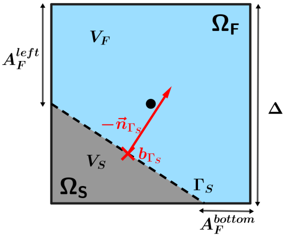
Figure: Dirichlet gradient calculation $\bar{\nabla} a|_{\Gamma_S}$ or $(\bar{\nabla} a \cdot \bar{n}_{\Gamma_S})$

Embedded fractions

$$V_F = \mathbf{C}\Delta^D \text{ with } D = \text{dimension}$$
$$A_F^d = f_F^d \Delta^{D-1} \text{ with } d = l, b, r, t$$

$$\bar{\nabla} a|_{\Gamma_S} = \frac{1}{d_2 - d_1}\left[\frac{d_2}{d_1}(a_{\Gamma_S} - a_1{}^{I_1}) - \frac{d_1}{d_2}(a_{\Gamma_S} - a_1{}^{I_2})\right]$$

Embedded boundary method *embed.h* [Johansen and Colella, JCP, 1998]



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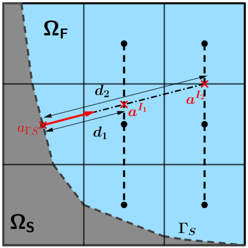


Figure: Dirichlet gradient calculation $\bar{\nabla} a|_{\Gamma_S}$ or $(\bar{\nabla} a \cdot \bar{n}_{\Gamma_S})$

Embedded fractions

$$
\begin{aligned}
V_F &= \mathbf{C}\Delta^D \text{ with } D = \text{dimension} \\
A_F^d &= f_F^d \Delta^{D-1} \text{ with } d = l, b, r, t
\end{aligned}
$$

$$\bar{\nabla} a|_{\Gamma_S} = \frac{1}{d_2 - d_1}\left[\frac{d_2}{d_1}(a_{\Gamma_S} - a_1{}^{I_1}) - \frac{d_1}{d_2}(a_{\Gamma_S} - a_1{}^{I_2})\right]$$

Discrete operator in a cut cell

$$\bar{\nabla}\cdot\bar{\Phi} \approx \frac{1}{V_F}\int_{\mathcal{V}} \bar{\nabla}\cdot\bar{\Phi}\, dV_F = \frac{1}{V_F}\int_{\delta\mathcal{V}} \bar{\Phi}.\bar{n}_d\, dA = \left(\sum_{d=l,b,r,t} f_F^d \bar{\Phi}.\bar{n}_d\right) + \bar{\Phi}_{\Gamma_S}.\bar{n}_{\Gamma_S}$$

A three phases system with **Basilisk solver**(http://www.basilisk.fr)

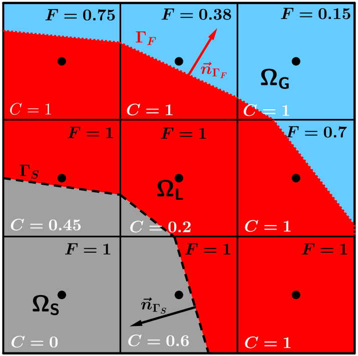


Figure: Three phases flow discretized on a Cartesian grid

Liquid/gas phases

Navier-Stokes equations with the **Volume of Fluid method** to account for the liquid/gas interface

Solid phase

Embedded boundary method to account for the solid

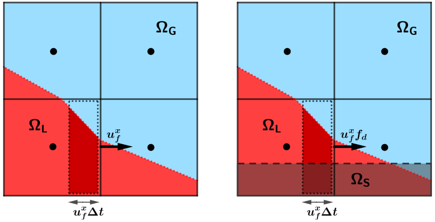
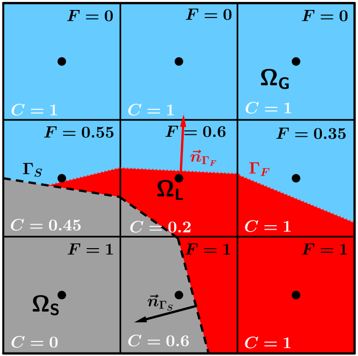


Figure: Geometrical flux estimation in a cut-cell

A three phases system with **Basilisk solver** (http://www.basilisk.fr)



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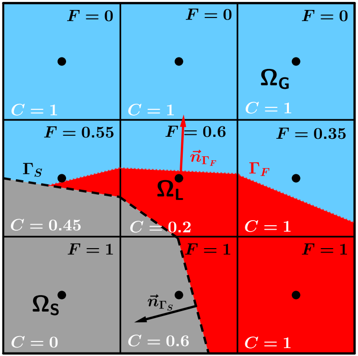

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Liquid/gas phases

Navier-Stokes equations with the **Volume of Fluid method** to account for the liquid/gas interface

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Contact angle description

Specific algorithm developed to account for the triple point at the solid/liquid/gas intersection

Algorithm description

We assume a piecewise linear reconstruction for both liquid and solid interface Γ_S and Γ_L

$$(\bar{n}_{\Gamma_{L,S}}).\bar{x} = \alpha_{L,S} \quad \text{with} \quad \alpha_{L,S} \quad \text{the intercept}$$

Algorithm 1

```
for all cells
 if (0 < C < 1 && 0 < F < 1) then //potential triple phase cell
  n̄_bound = n̄_{Γ_S} cos θ_{Γ_S} + t̄_{Γ_S} sin θ_{Γ_S}  // normal at the triple point
  α_bound = 𝓕(F, n̄_bound) //intercept at the triple point cell
 end if
end for
```

At every timestep, F is modified in the ghost-cells to account for θ_S

Algorithm 2

```
for all cells
 if (C==0) then //in the ghost cells
  w_cell = 0, w_total = 0 // weight for volume fraction reconstruction
  for all neighbors within 2 cells
   if (0 < C < 1 && 0 < F < 1) then //potential triple phase cell
    w_cell = C × (1. − C) × F × (1. − F)
    w_total = Σ w_cell
    F_G = w_cell × f(n̄_{Γ_F}, α_bound)
   end if
  end for
  F_G = F_G / w_total
 end if
end for
```

Algorithm description

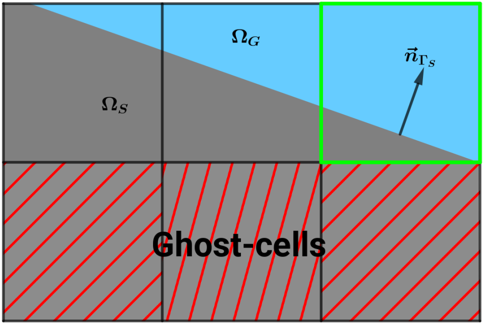


Figure: Algorithm illustration

Algorithm description

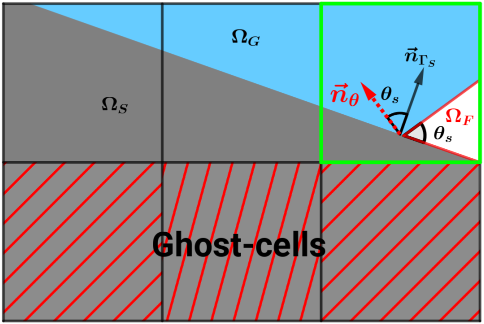


Figure: Algorithm illustration

Algorithm description

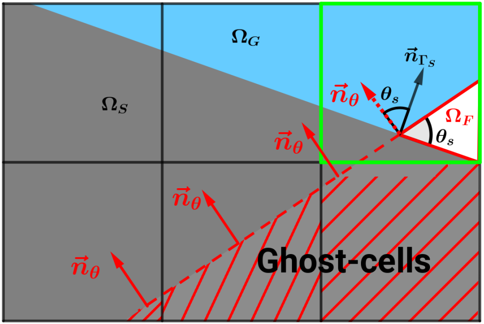


Figure: Algorithm illustration

Algorithm description

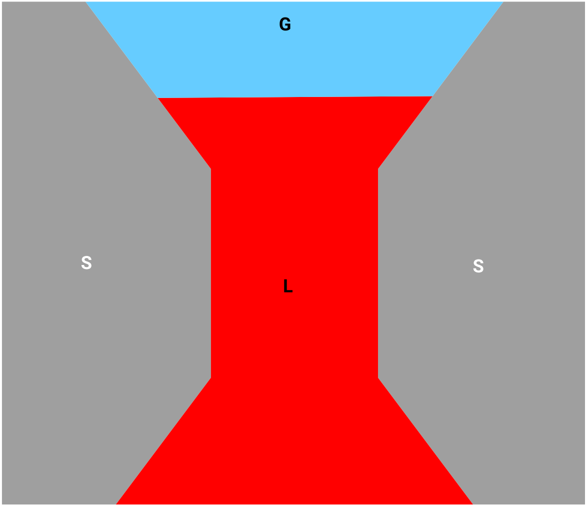
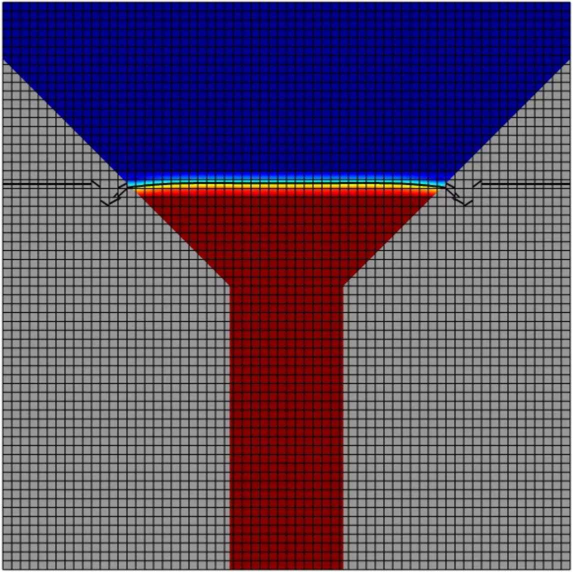


Figure: Liquid (red) initially at rest in a slot geometry (gray)

How to impose the contact angle between the liquid, the gas and the embedded solid at the triple point?

Algorithm description



Outline

Equilibrium shape of a droplet on an horizontal embedded solid

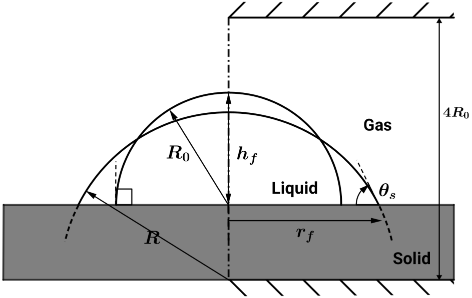


Figure: Schematic representation of the initial and equilibrium shapes of the a droplet on a flat surface with static contact angle θ_s

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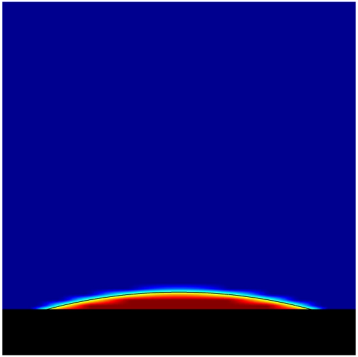
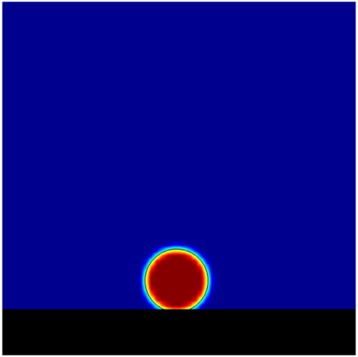
Equilibrium shapes on horizontal embed solid for 15° and 165° contact angles



(a) Equilibrium shape for 15°

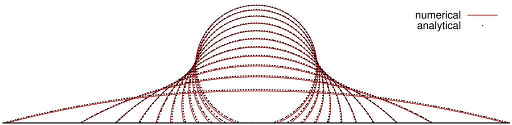


(b) Equilibrium shape for 165°

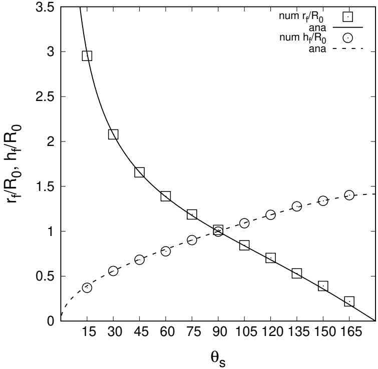
At equilibrium the radius of the circle R_f, the radius of spreading r_f, the height of the drop h_f are given by:

$$h_f = R_f(1 - \cos\theta_s), \quad r_f = R_f \sin\theta_s, \quad R_f = R_0\sqrt{\frac{\pi}{2(\theta_s - \sin\theta_s\cos\theta_s)}}$$

Equilibrium shapes on horizontal embedded solid for 15° and 165° contact angles $E = 0$

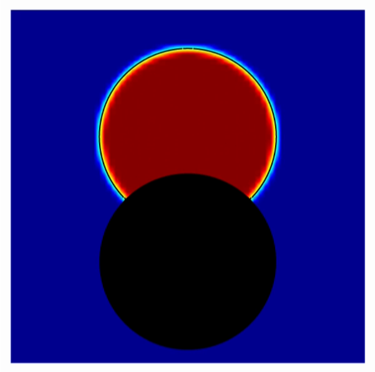


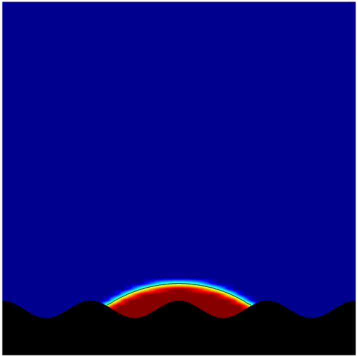
(a) Numerical equilibrium droplet shapes (-) against the analytical results (.), $R_0 = 32\Delta$



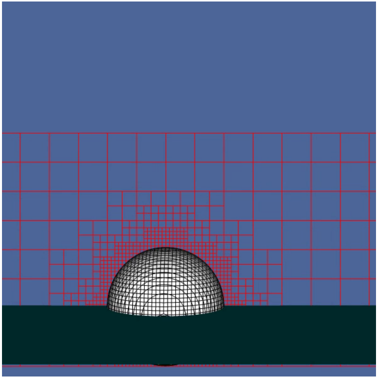
(b) Dimensionless droplet height h_f/R_0 and radius r_f/R_0 evolution, $R_0 = 32\Delta$

Equilibrium shapes on arbitrary embedded solids for 60° contact angle

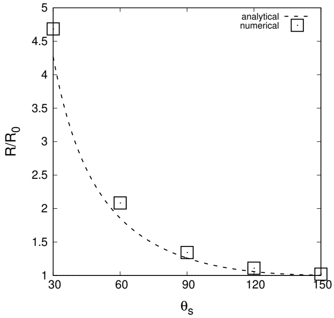

(a) Equilibrium shape for 60° (cylinder)


(b) Equilibrium shape for 120° (sinusoidal)

3D equilibrium shape



(a) Equilibrium shape for 60°



(b) Comparison of R/R_0 to the analytical expression, with $R_0 = \left(\frac{3V}{4\pi}\right)^{1/3}$, $R_{0_{min}} = 32\Delta$

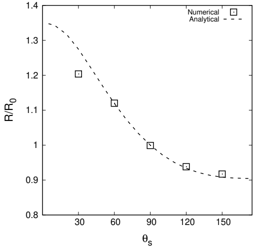
The volume of a spherical cap of radius R and (contact) angle θ:

$$V = \frac{\pi}{3} R^3 (2 + \cos\theta)(1 - cos\theta)^2$$

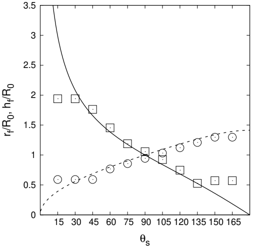
Remarks

Limitations

- We observe a pinning of the contact line in some configurations
- Mass conservation in mixed cells



(a) Embedded cylinder



(b) Embedded 45° plane

Figure: Numerical equilibrium droplet radius against the analytical results

Solutions

- Change the orientation of the solid alignment with the mesh
- Introduce Navier boundary condition on the solid to enforce the contact line motion $\lambda \frac{\partial \bar{u}_\tau}{\partial n} + (\bar{u}_\tau - \bar{U}_{s,\tau}) = 0$

Conclusion

- Coupling of VOF/embedded boundary method by imposing a contact angle at the frontier between the liquid, the gas and the solid
- Validation on 2D and 3D analitycal test cases (sessile) and other solid shapes

⇓

Ongoing works

- Validation with experimental problems (droplet flow on a fiber)
- Use this model to deal with liquid-solid phase change problems

Why?

Tavares and al : A coupling VOF/embedded boundary method to model two phase flows on arbitrary solid surfaces to be submitted

Droplet impact on a leaf cup

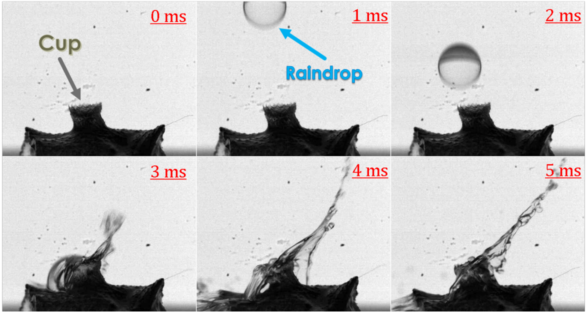


Figure: Droplet impact on a leaf

Liquid–solid phase change simulations (solidification or melting)

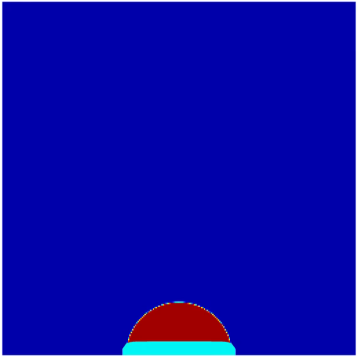
(a) Ice formation on wing plane

(b) Ice accretion on bridge cable

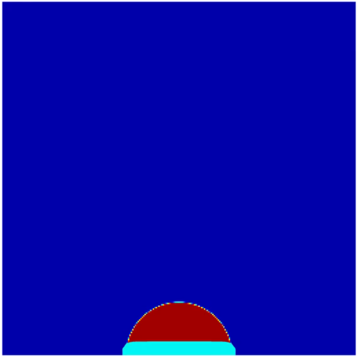
Problem

Model the phase change properly while accounting for the gas, liquid and solid interactions

A solidification test example



(a)



(b)

Figure: Water droplet solidification with $\theta_s = 20^\circ$ and $\theta_s = 60^\circ$

Apologies

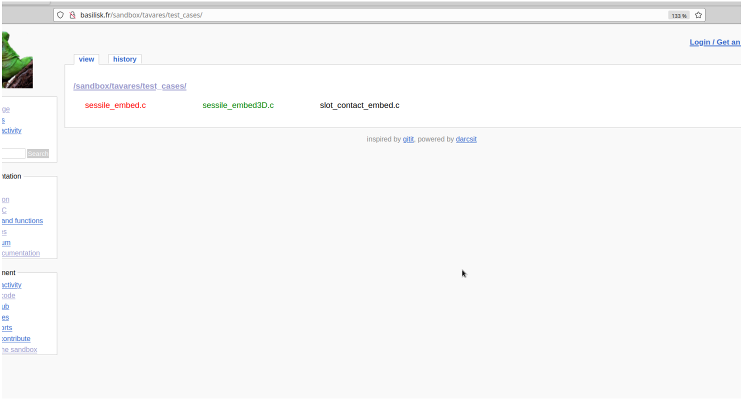


Figure: sandbox:tavares

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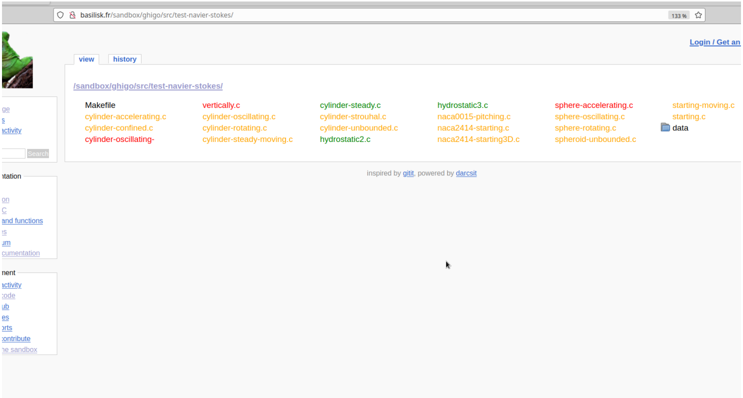

Figure: sandbox:ghigo

Thank you for your attention

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