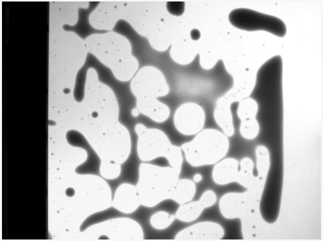
Phase change & Marangoni flows



Quentin Magdelaine

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Alban **Sauret**, Frédéric **Mondiot**
Jérémie **Teisseire**, Arnaud **Antkowiak**

I added a **slide (14)** with links toward **my sandbox**.

Applications

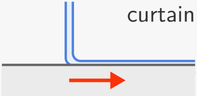
glass plates

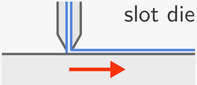
flexible substrates

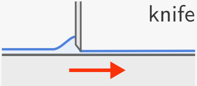
glass fabrics

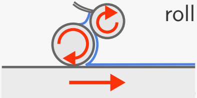
wavy substrates
Planilaque

Deposition



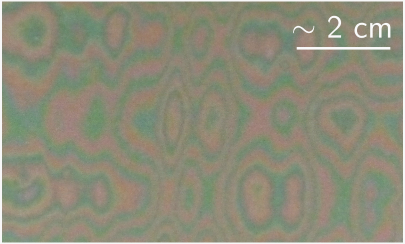






Drying of liquid films

▶ relaxation or destabilization?



Polymer-based protective coating

- $h \sim 2 - 10$ µm
- roughness: 150 nm

Paints, protective and functionalized layers:
defects limit the applications

▶ what do they have in common? ▶ **binary mixture**

Model system: water – propylene glycol

0 %
50 μm

x 6, 20 cm

Model system: water – propylene glycol

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50 µm

87 %
50 µm

x 6, 20 cm

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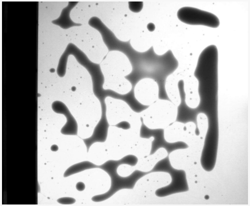

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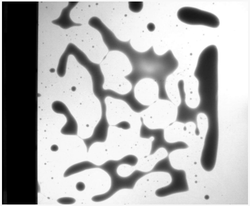

50 %
50 µm

x 6, 20 cm

Model system

- **key ingredients:** evaporation & Marangoni stress
- set of **equations**

$$\rho_{\mathcal{V}} \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} + \rho_{\mathcal{V}} \mathbf{v} \nabla \cdot \mathbf{v} = \rho_{\mathcal{V}} \mathbf{g} + \eta_{\mathcal{V}} \Delta \mathbf{v}$$

$$\frac{\mathrm{d}c_{\mathcal{V}}}{\mathrm{d}t} + \nabla \cdot (c_{\mathcal{V}} \mathbf{v}) = \nabla \cdot (D_{\mathcal{V}} \nabla c_{\mathcal{V}})$$

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1. $\mathbf{c}_{\mathcal{V}} = c_s\left(c_{\mathcal{L}_1}\right)$

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Introduction ▶ Equations

$$\rho_{\mathcal{V}} \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} + \rho_{\mathcal{V}} \mathbf{v}\ \nabla \cdot \mathbf{v} = \rho_{\mathcal{V}}\, \mathbf{g} + \eta_{\mathcal{V}}\ \Delta \mathbf{v}$$

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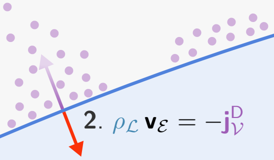

2. $\rho_{\mathcal{L}}\, \mathbf{v}_{\mathcal{E}} = -\mathbf{j}^{\mathrm{D}}_{\mathcal{V}}$

$$\rho_{\mathcal{L}} \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} + \rho_{\mathcal{L}} \mathbf{v}\ \nabla \cdot \mathbf{v} = \rho_{\mathcal{L}}\, \mathbf{g} + \eta_{\mathcal{L}}\ \Delta \mathbf{v}$$

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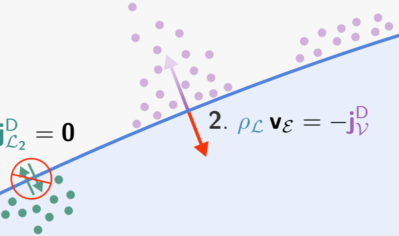

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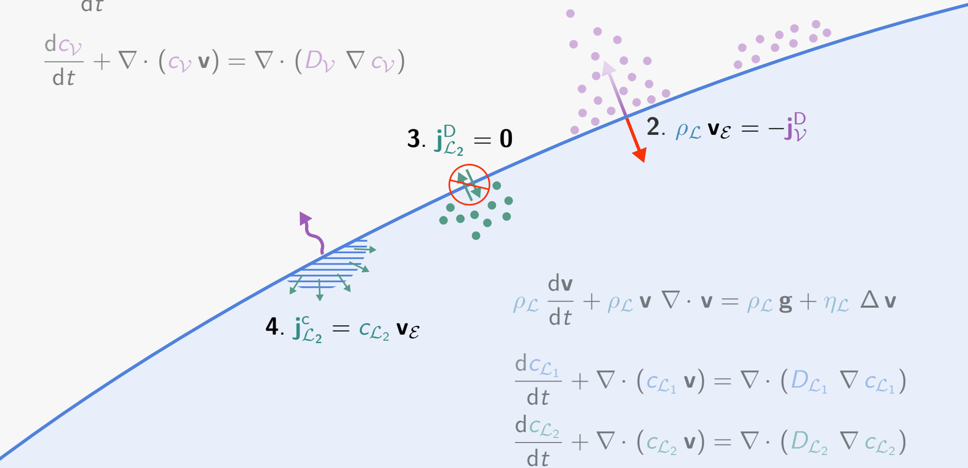

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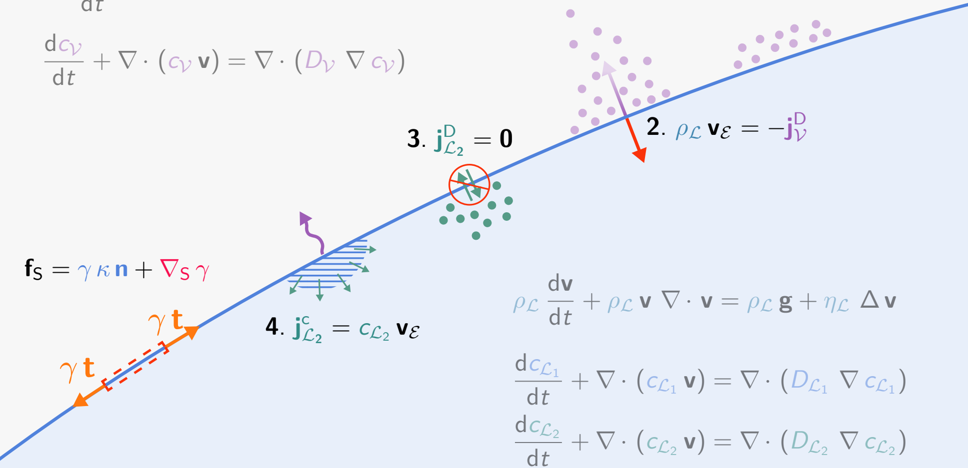

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4. $\mathbf{j}^{\mathrm{c}}_{\mathcal{L}_2} = c_{\mathcal{L}_2}\, \mathbf{v}_\mathcal{E}$

$$\mathbf{f}_\mathrm{S} = \gamma\, \kappa\, \mathbf{n} + \nabla_\mathrm{S}\, \gamma$$

$\gamma\,\mathbf{t}$ $\gamma\,\mathbf{t}$

$$\rho_\mathcal{L} \frac{d\mathbf{v}}{dt} + \rho_\mathcal{L}\, \mathbf{v}\, \nabla\cdot\mathbf{v} = \rho_\mathcal{L}\, \mathbf{g} + \eta_\mathcal{L}\, \Delta\mathbf{v}$$

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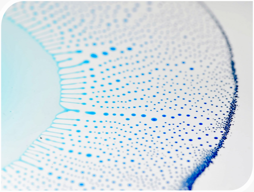
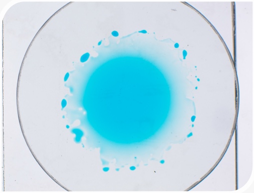
Outline

Implementations in Basilisk

Instabilities in thin films





1. Saturation of the vapor: $c_{\mathcal{V}} = c_s$

- **immersed Dirichlet** boundary condition
- **setpoint** in the diffusion equation

$$\mathrm{d}_t c_{\mathcal{V}} = \nabla \cdot (c_{\mathcal{V}} \nabla c_{\mathcal{V}}) + \frac{c_s - c_{\mathcal{V}}}{\tau}$$

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2. Evaporation velocity

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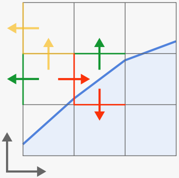

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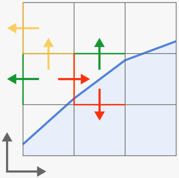
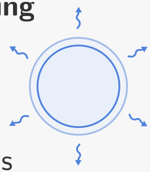
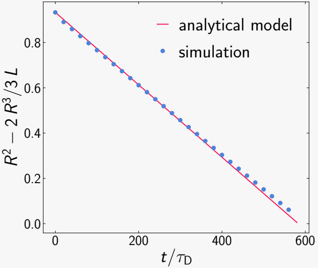


Evaporating drop



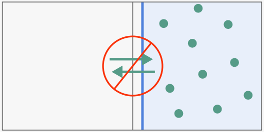
drop radius in function of time



I. Langmuir, Phys. rev., 1918

3. No flux condition
at the interface:

$$\mathbf{j}^{D}_{\mathcal{L}_2} = D_{\mathcal{L}}\, \nabla\, c_{\mathcal{L}_2} = \mathbf{0}$$



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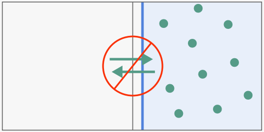


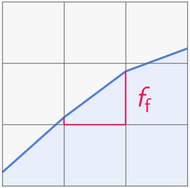
Diffusion equation

$$\mathrm{d}_t c_{\mathcal{L}_2} = \nabla \cdot (D_{\mathcal{L}} \nabla c_{\mathcal{L}_2})$$

$$\& \quad \overline{c}_{\mathcal{L}_2} = \frac{1}{\Delta^2} \iint c_{\mathcal{L}_2} \, \mathrm{d}S$$

$$f \, \mathrm{d}_t \overline{c}_{\mathcal{L}_2} = \nabla \cdot (f_{\mathrm{f}} D_{\mathcal{L}} \nabla \overline{c}_{\mathcal{L}_2})$$

▶ **face** value f_{f}
of the liquid tracer f



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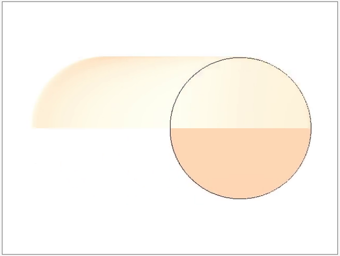

naive way: $f_{\mathrm{f}} = \left(f_n + f_{n-1}\right)/2$
nice way: VOF reconstruction
Thank Jose-Maria **López Herrera**

Diffusion equation

$$\mathrm{d}_t c_{\mathcal{L}_2} = \nabla \cdot \left(D_{\mathcal{L}}\ \nabla\, c_{\mathcal{L}_2}\right)$$

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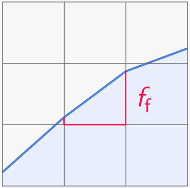
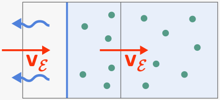


4. Tracer advection: the **net** allegory



t_1

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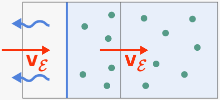
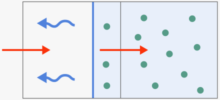


t_1

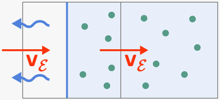
Advecting $c_{\mathcal{L}_2}$ along with f with $\mathbf{v}_{\mathcal{E}}$.



t_2

We concentrate the solute in the **next** cell. $\mathbf{v}_{\mathcal{E}}$ is **not** a flow.

4. Tracer advection: the **net** allegory



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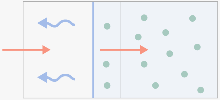
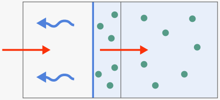


The interface is more acting as a **net**.



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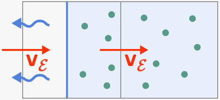

t_1

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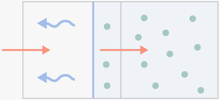

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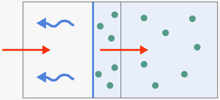
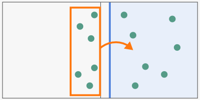


t_2

Redistribution of the solute of the **dry** cells.



t_3

Raoult law

$$c_{\mathcal{V}} = c_s\left(c_{\mathcal{L}_1}\right) = c_s\,\frac{c_{\mathcal{L}_1}}{\rho_{\mathcal{L}}}$$

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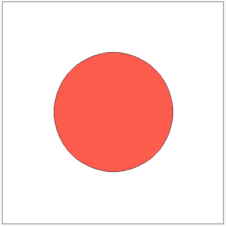
Fast diffusion



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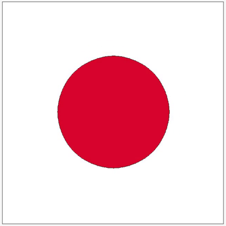
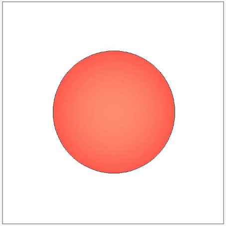
Fast diffusion



Moderate

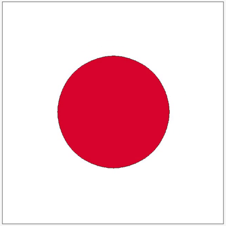


Implementations ▶ Evaporation of mixtures

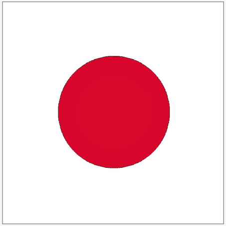
Raoult law

$$c_{\mathcal{V}} = c_s\left(c_{\mathcal{L}_1}\right) = c_s \frac{c_{\mathcal{L}_1}}{\rho_{\mathcal{L}}}$$

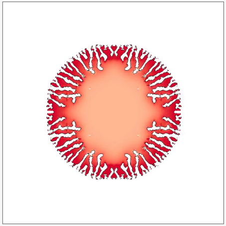
Fast diffusion



Moderate



Slow

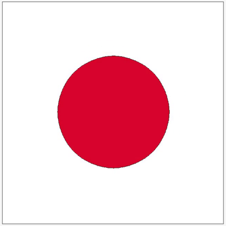


no surface tension

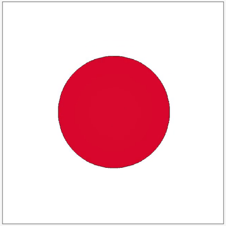
Raoult law

$$c_{\mathcal{V}} = c_s\left(c_{\mathcal{L}_1}\right) = c_s \frac{c_{\mathcal{L}_1}}{\rho_{\mathcal{L}}}$$

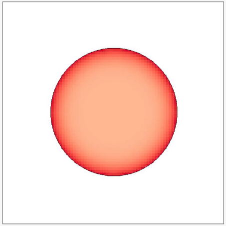
Fast diffusion



Moderate



Slow



surface tension

Implementations ▶ Evaporation of mixtures

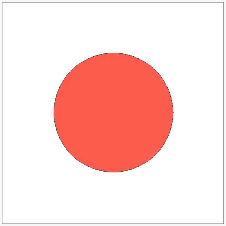
Raoult law

$$c_{\mathcal{V}} = c_s\left(c_{\mathcal{L}_1}\right) = c_s \frac{c_{\mathcal{L}_1}}{\rho_{\mathcal{L}}}$$

Péclet number

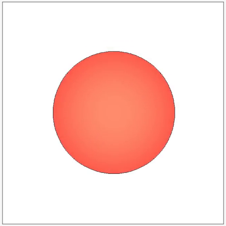
$$\mathrm{Pe}_{\mathcal{E}} = \frac{\mathbf{v}_{\mathcal{E}}\, R}{D_{\mathcal{L}}}$$

Fast diffusion



$\mathrm{Pe}_{\mathcal{E}} = 10^{-3}$

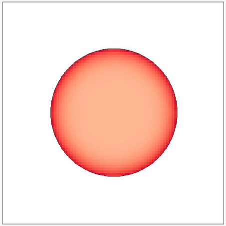
Moderate



$\mathrm{Pe}_{\mathcal{E}} = 2$

water – ethanol

Slow



$\mathrm{Pe}_{\mathcal{E}} = 10^{2}$

paint

Capillary force

$$\mathrm{d}\mathbf{F}_\ell = (\gamma\,\mathbf{t})(s) - (\gamma\,\mathbf{t})(s+\mathrm{d}s)$$
$$\mathbf{f}_\mathrm{S} = \mathrm{d}_s(\gamma\,\mathbf{t})$$
$$\mathbf{f}_\mathrm{S} = \gamma\,\kappa\,\mathbf{n} + \mathrm{d}_s\gamma\,\mathbf{t}$$

Laplace pressure
Marangoni stress

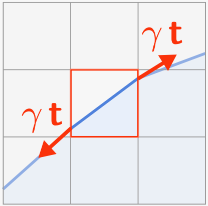
generalized in 3D:

$$\mathbf{f}_\mathrm{S} = \gamma\,\kappa\,\mathbf{n} + \nabla_\mathrm{S}\,\gamma$$

Capillary force, two formulations

$$\mathbf{F}_\ell = (\gamma\,\mathbf{t})(s) - (\gamma\,\mathbf{t})(s + \Delta s)$$

$$\mathbf{f}_\mathsf{S} = \gamma\,\kappa\,\mathbf{n} + \nabla_\mathsf{S}\,\gamma$$



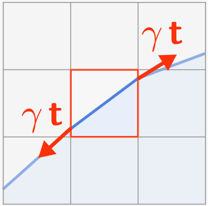
Brackbill formulation

Brackbill, Kothe, Zemach, 1992

Seric, Afkhami, Kondic, 2017

- δ_S is added to make it volumetric
- not easy to evaluate the surface gradient ∇_S

Capillary force, two formulations



$$\mathbf{F}_\ell = (\gamma\,\mathbf{t})(s) - (\gamma\,\mathbf{t})(s + \Delta s)$$

$$\mathbf{f}_S = \gamma\,\kappa\,\mathbf{n} + \nabla_S\,\gamma$$

Brackbill formulation

Brackbill, Kothe, Zemach, 1992

Seric, Afkhami, Kondic, 2017

- δ_S is added to make it volumetric
- not easy to evaluate the surface gradient ∇_S

Integral formulation

Abu-Al-Saul, Popinet and Tchelepi, 2018

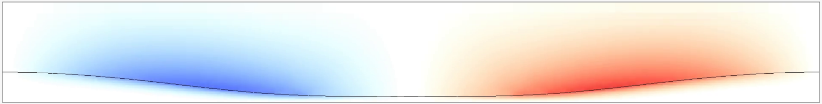
- already **discrete**
- **well-balanced** and **momentum conservative**

Evaporation of a liquid mixture layer with Marangoni stress

Evaporation of a liquid mixture layer with Marangoni stress

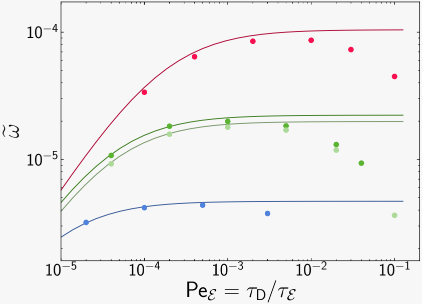
horizontal velocity

Evaporation of a liquid mixture layer with Marangoni stress



horizontal velocity

Growth rate ω in function of $\mathrm{Pe}_{\mathcal{E}} = \tau_{\mathrm{D}}/\tau_{\mathcal{E}}$

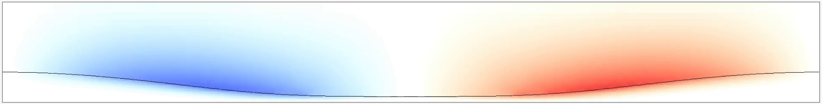


high $\mathbf{v}_{\mathcal{E}}$
moderate $\mathbf{v}_{\mathcal{E}}$
low $\mathbf{v}_{\mathcal{E}}$

- agreement at small Péclet

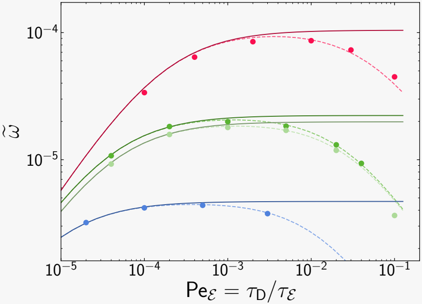
Instabilities ▶ Simulations & lubrication

Evaporation of a liquid mixture layer with Marangoni stress



horizontal velocity

Growth rate ω in function of $\mathrm{Pe}_{\mathcal{E}} = \tau_{\mathrm{D}}/\tau_{\mathcal{E}}$



high $\mathbf{v}_{\mathcal{E}}$
moderate $\mathbf{v}_{\mathcal{E}}$
low $\mathbf{v}_{\mathcal{E}}$

- agreement at small Péclet
- **cross-diffusion limited** at high Péclet: $\tau_{\mathcal{I}} = \tau_{\mathrm{D}} + \tau_{\mathcal{I},\mathrm{th}}$ *dashed line*

Links toward the sandbox

Phase change

- header file for **pure liquid**
- examples: **static**, **oscillating**, **falling**, and **blown** drops
- additional header file for **mixtures**
- mwe: **diffusion** in a domain, **advection** with respect to a phase change velocity
- example: **digitations** at slow solute diffusion

Marangoni stress

- header files: **straight line** or **circle arc** extrapolations
- **capwave** mwe
- contact angles with **straight line** or **circle arc** extrapolations
- mwe with **adaptive mesh**
- **Marangoni flow** example

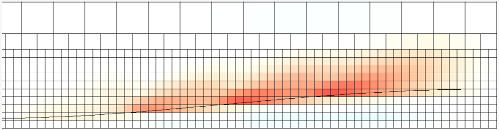
Phase change

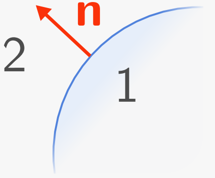
- **Stefan flow** and recoil pressure
  ▶ Cécile **Lalanne** & Jose-Maria **Fullana**
- **Embedded boundaries** would ensure more precise conditions
  ▶ Alexandre **Limare** & Christophe **Josserand**

Marangoni stress

- switch between height functions
- extend to **3D**
- jump of the **tangential viscous stress**

Close up on a simulation
horizontal velocity





$$[A] = A_2 - A_1$$

$\underline{\underline{\sigma}}$: stress tensor

Tangential stress continuity: $\left[\mathbf{t}\,\underline{\underline{\sigma}}\,\mathbf{n}\right] = \nabla_S\,\gamma\cdot\mathbf{t}$

- ▶ $\partial_t\gamma = \mu_2\left(\partial_t u_n|_2 + \partial_n u_t|_2\right) - \mu_1\left(\partial_t u_n|_1 + \partial_n u_t|_1\right)$

Normal stress continuity: $\left[\mathbf{n}\,\underline{\underline{\sigma}}\,\mathbf{n}\right] = \gamma\,\kappa$