Binary mixture & evaporation

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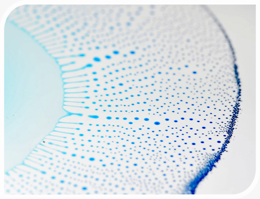
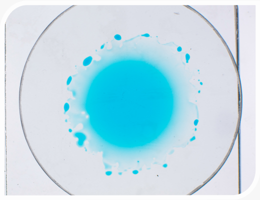
Outline





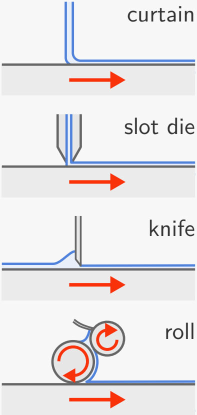
- various applications
- various substrates
- mixture liquid film ▶ coating

glass plates

flexible substrates

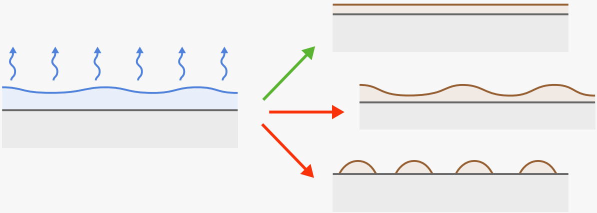
glass fabrics

Deposition methods



Drying of liquid films

▶ relaxation or destabilization?

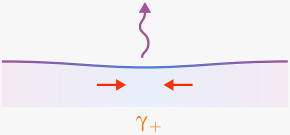


Paints, protective and functionalized layers:
defects limit the applications

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

Fluctuation of evaporation

water – ethanol



evaporation: ethanol

$\gamma_{eth} < \gamma_{water}$

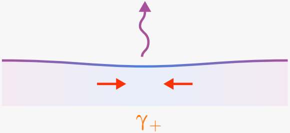
local increase of the tension

▶ healing

Introduction ▶ Marangoni flow

Fluctuation of evaporation

water – ethanol



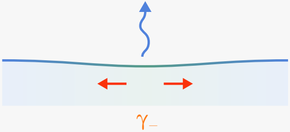
evaporation: ethanol

$\gamma_{\text{eth}} < \gamma_{\text{water}}$

local increase of the tension

▶ healing

water – polymer



evaporation: water

$\gamma_{\text{pol}} < \gamma_{\text{water}}$

local decrease of the tension

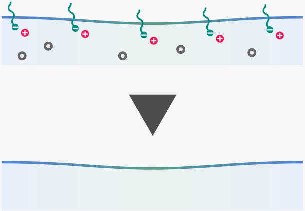
▶ break-up

Evaporation-induced Marangoni flows

- evaporation
- Marangoni stress

▶ no particle, no polymer
no thermal transfer

▶ **both** have to be **implemented** in Basilisk



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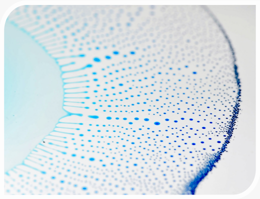
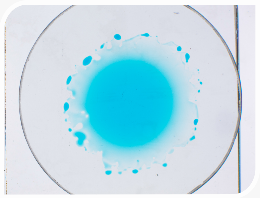
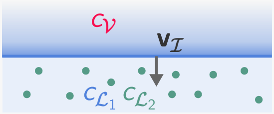




In the liquid and the vapor,
transport equation:

$$\frac{\mathrm{d}c}{\mathrm{d}t} + \nabla \cdot (c\,\mathbf{v}) = \nabla \cdot (D\,\nabla\,c)$$



at the interface,
on the vapor side:

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

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

on the liquid side:

$$\mathbf{j}^{\mathrm{D}}_{\mathcal{L}_2} = \mathbf{0} \quad \text{not evaporating}$$

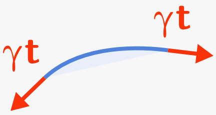
$$\mathbf{j}^{\mathrm{D}}_{\mathcal{L}_1} = \rho_{\mathcal{L}}\,\mathbf{v}_{\mathcal{I}} \quad \text{evaporating}$$

Capillary force

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

$$\mathbf{f}_S = \frac{\mathrm{d}}{\mathrm{d}s}(\gamma\,\mathbf{t})$$

$$\mathbf{f}_S = \gamma\,\kappa\,\mathbf{n} + \frac{\mathrm{d}\gamma}{\mathrm{d}s}\,\mathbf{t}$$

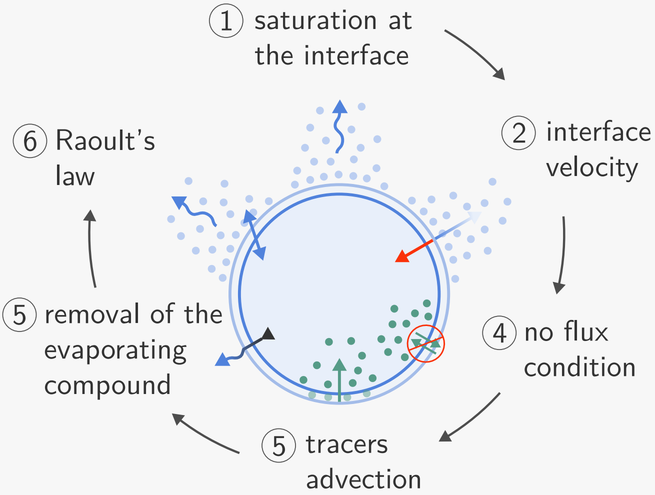


Laplace pressure
Marangoni stress

generalized in 3D:

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

Evaporation: six steps



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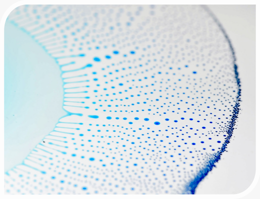

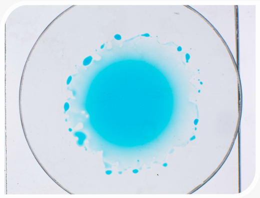

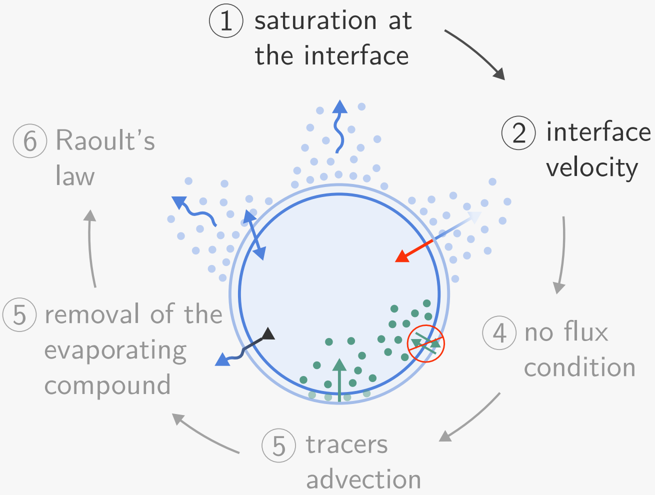
1 saturation at the interface
2 interface velocity
4 no flux condition
5 tracers advection
5 removal of the evaporating compound
6 Raoult's law

Immersed boundary condition

- **saturation** of the vapor concentration at the interface
- **immersed Dirichlet** boundary condition, **no ghost cell**

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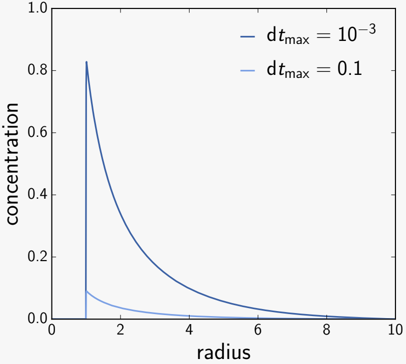
- ▶ **immersed Dirichlet** boundary condition, **no ghost cell**
- **reset** the concentration at **each step**: not sufficent

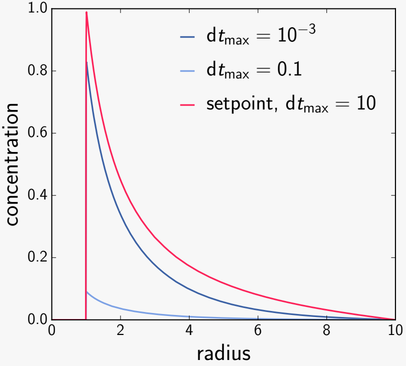


- **saturation** of the vapor concentration at the interface

▶ **immersed Dirichlet** boundary condition, **no ghost cell**

- **reset** the concentration at **each step**: not suffcent

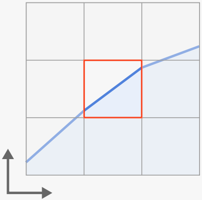
▶ **setpoint** in the diffusion equation



$$\frac{dc}{dt} = \nabla \cdot (D \nabla c) + \frac{c_s - c}{\tau}$$

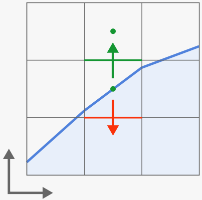
Interface velocity

$$\rho_{\mathcal{L}}\,\mathbf{v}_{\mathcal{I}} = -\mathbf{j}_{\mathcal{V}}^{\mathrm{D}} = D_{\mathcal{V}}\,\nabla\,c_{\mathcal{V}}$$



$$\rho_{\mathcal{L}} \mathbf{v}_{\mathcal{I}} = -\mathbf{j}_{\mathcal{V}}^{\mathrm{D}} = D_{\mathcal{V}} \nabla c_{\mathcal{V}}$$

- need to **offset** the computation of the **vapor gradient**



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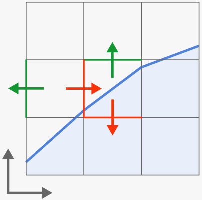
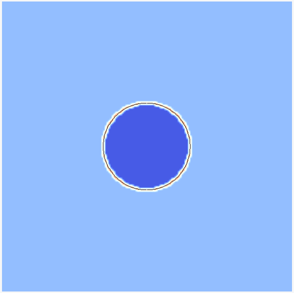


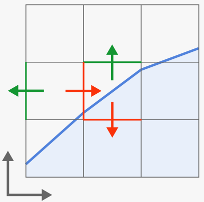


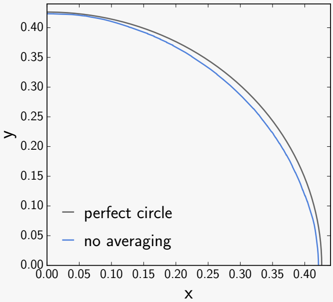
if cell[ ] or cell[-1] $\in \mathcal{I}$

$u_f.x = \nabla\, c.x[s(n.x), 0];$

$$\rho_{\mathcal{L}}\, \mathbf{v}_{\mathcal{I}} = -\mathbf{j}_{\mathcal{V}}^{\mathrm{D}} = D_{\mathcal{V}}\, \nabla\, c_{\mathcal{V}}$$

- need to **offset** the computation of the **vapor gradient**





if cell[ ] or cell[-1] $\in \mathcal{I}$

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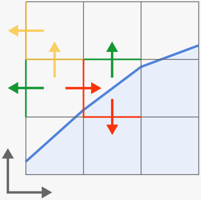
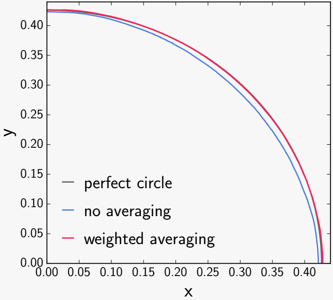
$$\rho_{\mathcal{L}}\,\mathbf{v}_{\mathcal{I}} = -\mathbf{j}^{D}_{\mathcal{V}} = D_{\mathcal{V}}\,\nabla\, c_{\mathcal{V}}$$

- need to **offset** the computation of the **vapor gradient**
- **weighted average** between neighbor vapor cells

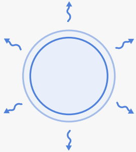




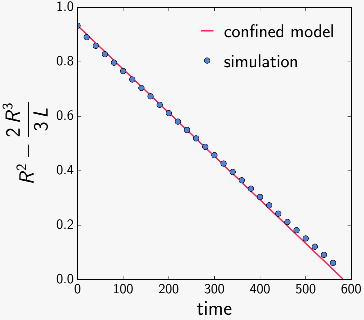
if cell[ ] or cell[-1] $\in \mathcal{I}$

$$u_f.x = |n.x|\,\nabla\, c.x[s(n.x), 0] + |n.y|\,\nabla\, c.x[s(n.x), s(n.y)];$$

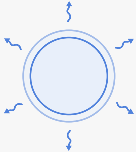
 Exemples: drop & film



$$R^2 = {R_0}^2 - 2\,D\,\frac{\Delta c}{\rho}\,t$$



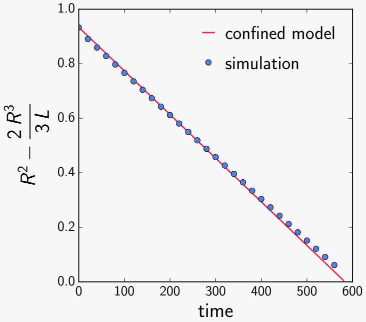
Pure liquid ▶ Exemples: drop & film

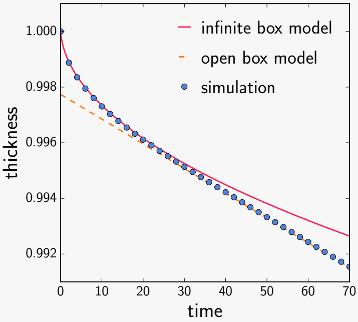


$$R^2 = {R_0}^2 - 2\,D\,\frac{\Delta c}{\rho}\,t$$

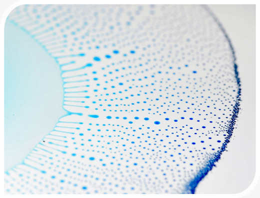
$$h_\infty = h_0 - 2\,\frac{\Delta c}{\rho}\sqrt{\frac{D\,t}{\pi}}$$

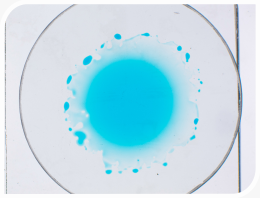
$$h_{\text{box}} \propto -\frac{\Delta c}{\rho}\,\frac{D}{L}\,t$$

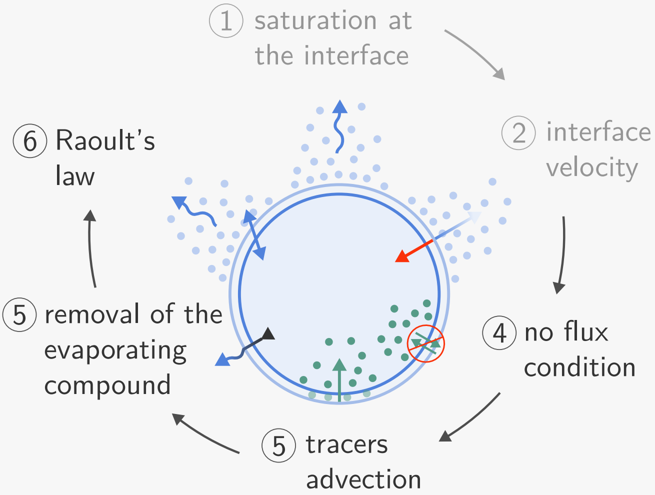




Outline

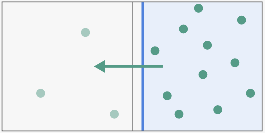




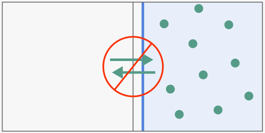


① saturation at the interface
② interface velocity
④ no flux condition
⑤ tracers advection
⑤ removal of the evaporating compound
⑥ Raoult's law

No flux condition



No flux condition



- **No diffusion** of the liquid tracers **through the interface**
- basic idea: set the **diffusion coefficient** to **zero outside** of the liquid

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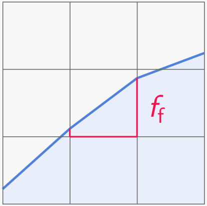
▶ **face value** of f

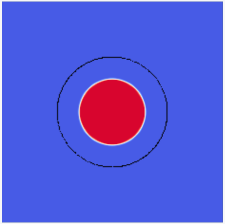


$$\frac{dc}{dt} = \nabla \cdot (D \, \nabla c), \quad \text{with} \quad \iint c \, dS \sim f \, c \, \Delta^2$$

$$\iint \frac{dc}{dt} dS = \int D \, \nabla c \cdot \mathbf{n} \, dL \quad \text{then} \quad \Delta^2 f \frac{dc}{dt} = \sum_f \Delta \, f_f \, D \, \nabla c \cdot \mathbf{n}$$

▶ $$f \frac{dc}{dt} = \nabla \cdot (f_f \, D \, \nabla c)$$

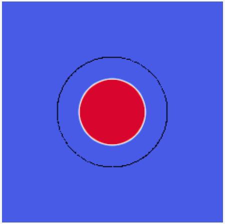
if nothing is done



$D.x = D_{\mathcal{L}}$

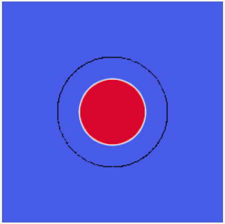
No flux condition

if nothing is done



$D.x = D_{\mathcal{L}}$

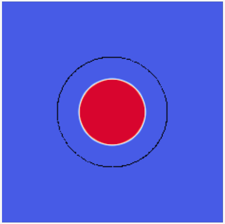
first attempt



if $f > 0$, $D.x = D_{\mathcal{L}}$
else $D.x = 0$

No flux condition

if nothing is done



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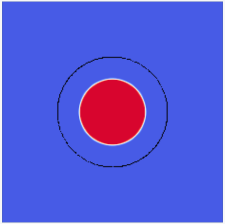

if $f > 0, \ D.x = D_{\mathcal{L}}$

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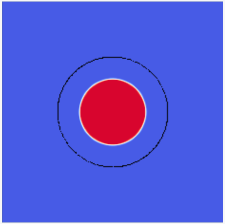
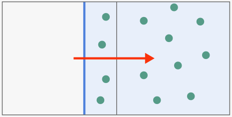
current code



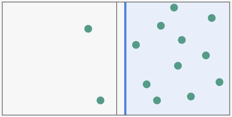
$D.x = D_{\mathcal{L}} \, f_f$

thanks to Jose-Maria!

- tracers must not be left behind



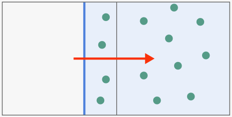
Receding interface



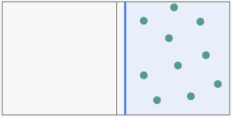
Leaving tracer behind

Tracer advection

- tracers must not be left behind
- already implemented in Basilisk
- need to advect the **quantity field** $f\,c$ instead of c



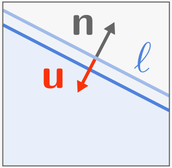
Receding interface



Clean advection

Amount to remove: $s = \rho\, \mathbf{u} \cdot \mathbf{n}\, \ell\, \mathrm{d}t$

- $\mathbf{u} \cdot \mathbf{n}$ can be computed using different approaches
- currently, **none** of them leads to a **stable interface**



▶ diffusion & advection of one compound, **deduction** of the evaporating compound:

$$c_{\mathcal{L}_1} = 1 - c_{\mathcal{L}_2}$$

To close the circle: the Raoult's law

At the interface, the Dirichlet condition has to be changed:

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

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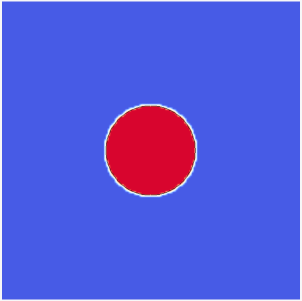
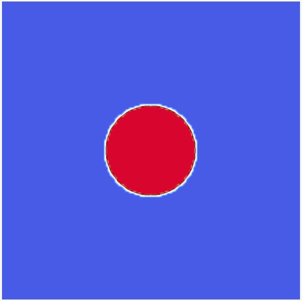
$$c_{\mathcal{V}} = c_s\left(c_{\mathcal{L}_1}\right) = c_s \frac{c_{\mathcal{L}_1}}{\rho_{\mathcal{L}}}$$

Evaporation of a mixture drop

Fast diffusion



Slow diffusion



Evaporation of a mixture drop

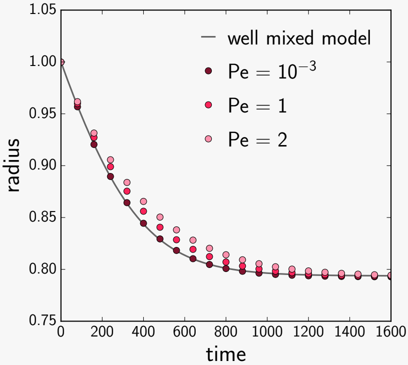
Peclet number:

$$\mathrm{Pe}_{\mathcal{L}} \sim \frac{\mathbf{v}_{\mathcal{I}}}{D_{\mathcal{L}}\, R}$$

$$\mathrm{Pe}_{\mathcal{L}} \sim \frac{D_{\mathcal{V}}}{D_{\mathcal{L}}} \frac{\Delta c_{\mathcal{V}}}{\rho_{\mathcal{L}}}$$

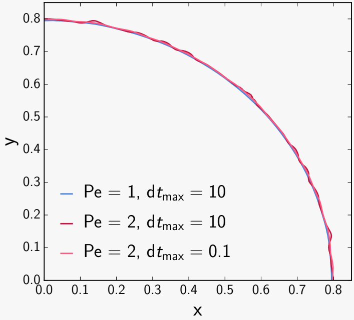
$\mathrm{Pe}_{\mathcal{L}} \ll 1$: well mixed

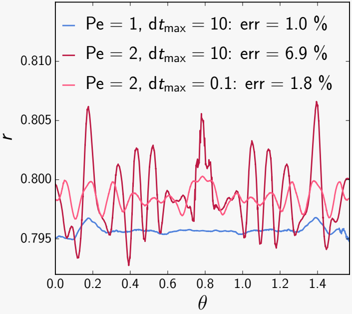
$\mathrm{Pe}_{\mathcal{L}} > 1$: slower



To close the circle: the Raoult's law

Some stability issues at large Peclet:





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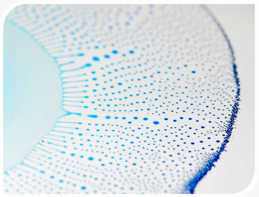
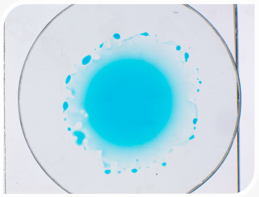
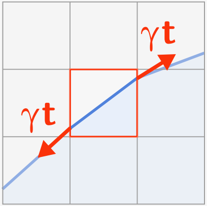




Marangoni stress in Basilisk

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

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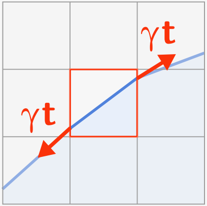

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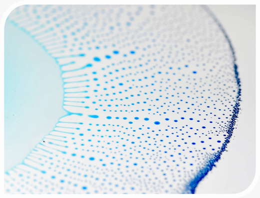
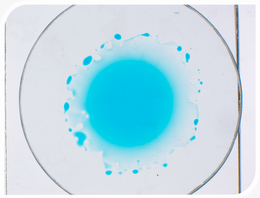
Initial formulation

Abu-Al-Saul, Popinet and Tchelepi, *submitted*

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

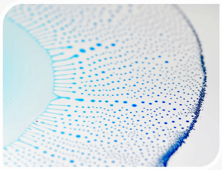
Outline

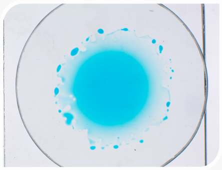




Conclusion

- Binary or more complex mixtures
  - **evaporation-induced** instability
  - **ubiquitous** in industrial **processes**





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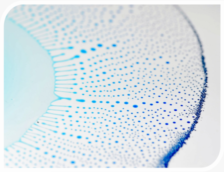

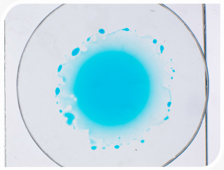

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  - **ubiquitous** in industrial **processes**
- Evaporation in Basilisk
  - most of the work is done
  - **stability issues** at large Peclet
- Marangoni in Basilisk
  - a **guiding line** to follow
  - hope for a **well-balanced** and **conservative** description of the surface tension