An accurate numerical method for computing surface tension forces in CFD codes
Numerical experiments with surface tension

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Accurate numerical method for computing surface tension

1 Context and motivations
   - Context: ocean waves attenuation by falling rain drops
   - The failling drop: a (not so) simple problem
   - Simulate surface tension

2 Numerical solutions
   - Be careful...
   - What we propose
   - Numerical results
   - Applications

3 Conclusion
Context: ocean waves attenuation by falling rain drops

Figure: $10^1$ s, $10^1$ m

Figure: $10^0$ s, $10^0$ m

Figure: $10^{-2}$ s, $10^{-2}$ m

Waves 10 000 drops/s ➔ Small waves 100 drops/s ➔ Flat plane 0.1 drop/s
Context: ocean waves attenuation by falling rain drops

Difficulties
- Large time and spatial scales
- Sensitive, turbulent
- Measures

Needs (for simulations)
- Meso and micro numerical models
- Appropriate numerical methods
  - Accurate and efficient

Project leaders
M. Coquerelle (I2M), S. Glockner (I2M), P. Lubin (I2M), L. Mieussens (IMB), F. Véron (U. Delaware)
A (not so) simple problem

The falling of a rain drop: **surface tension dominated**

1. What is its **terminal velocity**?
2. What is the **dynamic of the impact**?

Classical numerical methods

- Fail to solve (1)
- Introduce errors in (2)
Aparté: what is the numerical convergence?

What we expect

Refine the discretization/mesh $\Rightarrow$ Get better results

**Precision $\Rightarrow$ Accuracy**
Aparté: what is the numerical convergence?

What we expect

Refine the discretization/mesh → Get better results

Precision → Accuracy

Example of convergence: approximation of π

<table>
<thead>
<tr>
<th>h</th>
<th>h/10^1</th>
<th>h/10^2</th>
<th>h/10^3</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>3.3</td>
<td>3.19</td>
<td>3.142</td>
</tr>
</tbody>
</table>

Example of non-convergence: approximation of π

<table>
<thead>
<tr>
<th>h</th>
<th>h/10^1</th>
<th>h/10^2</th>
<th>h/10^3</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>3.2</td>
<td>3.48</td>
<td>4.217</td>
</tr>
</tbody>
</table>
Aparté: what is the numerical convergence?

What we expect

Refine the discretization/mesh ⇒ Get better results

Precision ⇒ Accuracy

Figure: The equilibrium of a flat surface, parasitic currents
Order 1: $h/2 \rightarrow \text{error}/2$
Modeling surface tension

A boundary condition between 2 fluids

Young-Laplace law:

\[ \Delta p = \sigma \kappa \]

\[ \kappa = \left( \frac{1}{R_1} + \frac{1}{R_2} \right) / 2, \text{ the mean curvature, is purely geometric} \]

Figure: Surface tension force (extracted from [Brackbill1990])

The (1-fluid) incompressible Navier-Stokes equations

\[ \rho \left( \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = -\nabla p + \nabla \cdot (2\mu \mathbf{D}(\mathbf{u})) + \mathbf{f} + \sigma \kappa \mathbf{n} \delta S \]

\[ \nabla \cdot \mathbf{u} = 0 \quad \text{and} \quad \frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \nabla \rho = 0 \]
Computing the surface tension forces

As $R \to 0$, $\kappa \to \infty$

Also as $h \to 0$, $\kappa \to \infty$

$\kappa \to \infty \Rightarrow \Delta p \to \infty$

Barriers

- High gradients/discontinuities
  - **Tough** for numerical methods
  - Errors in computing $\kappa \Rightarrow$ errors in the simulation
Computing the surface tension forces

Diving into details

As $R \to 0, \kappa \to \infty$

Also as $h \to 0, \kappa \to \infty$

$\kappa \to \infty \Rightarrow \Delta p \to \infty$

In fact, when surface tension is important...

- Big errors in $\kappa \Rightarrow$ severe errors in the simulation
- (numerical) parasitic/spurious currents are $O(\kappa^2)$ [Denner et al. 2014]
- Polute simulation results
- Lead to wrong solutions/analysis
Two things to remember

First thing to remember
The **absolute** need to **compute accurately** the curvature
Two things to remember

Geometry memo

1. Surface $S$ spatially derivates to...
2. Normal vector $n$ (eq. the tangent plane) spatially derivates to...
3. Curvature $\kappa$

Moving/Tracking/Transporting the interface

Surface $S$ transported with (spatial) precision $O(h^M)$

$\Downarrow$

Curvature $\kappa$ computed with (spatial) precision $O(h^{M-2})$
Two things to remember

First thing to remember
The **absolute** need to **compute accurately** the curvature

Second thing to remember
The surface (transport methods) have to be **at least 3\textsuperscript{rd} order accurate** for $\kappa$ to converge
Linear Volume Of Fluid (VOF-PLIC)

(a) Distance to the surface

(b) Curvature error

Figure: (non) convergence of geometric computations
Capillary rise with VOF-PLIC + CA

Remarks
- Static contact angle model: questionable
- Errors in κ ⇒ error in equilibrium pressure ⇒ error in height

Figure: Numerical results
What we propose

Model choice

- 1-fluid incompressible Navier-Stokes equations
- With Continuum Surface-Force (CSF) [Brackbill1990]

\[ \sigma k n \delta S \Rightarrow \sigma k \nabla c \]

Interface/Surface

Level Set representation

- transport: 5\textsuperscript{th} order accurate
- curvature: 4\textsuperscript{th} order accurate based on the Closest Point method

Achievement

(at least) 3\textsuperscript{rd} order accurate surface tension force computation

More details

M. Coquerelle, S. Glockner: A fourth-order accurate curvature computation in a level set framework for two-phase flows subjected to surface tension forces. JCP 2016
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Numerical results

Study case: static and translating column at equilibrium

1. No gravity ⇒ equilibrium state ⇒ null velocity field in its ref. frame
2. Numerical errors on $\kappa$ ⇒ parasitic currents

(a) Static column

(b) Translating column
Application to our project

Falling drop, $64 \times 64 \times 640$, 32 comp. nodes

Cavity formation after impact, $256 \times 256 \times 128$, 64 comp. nodes
Application to our project

Falling drop on a surface, $150 \times 150 \times 75$, 32 comp. nodes

Falling drops on a surface, $400 \times 400 \times 200$, 128 comp. nodes
Conclusion

Warning...

- Numerical convergence is **mandatory** for simulation analysis
  - (most) state of the art surface tension methods **do not converge**
    - ... industrial codes as well
    - the **smaller the scale, the more severe the problem**
- **Reliability** of studies?
- No *all inclusive* solution, level set methods have drawbacks

... but don’t worry!

- Solutions (will) exist...
  - **Test your software:** easy minimal translating column test
- Still an opened research field
  - Next step: triple line models (Ph.D. starting)
Errors on curvature $\Rightarrow$ wrong interface dynamic

CSF methods rely on the accurate computation of curvature

### 3 criteria

1. Accuracy against exact curvature
2. Minimal deviation along the surface
3. Minimal variation along the normal

Effects on surface dynamic:

![Diagram showing effects on surface dynamic](image)
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