Accurate numerical surface tension computation for the simulation of diphasic flows...

... and application to the study of rain drops impact

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CPU
Le monde numérique au service
de la certification et de la
sécurisation des systèmes

Accurate numerical method for computing surface tension

CONTEXT AND MOTIVATIONS

Context: ocean waves attenuation by falling rain drops

10^1s, 10^1m

© J. Dekort

10^0s, 10^0m

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10^{-2}s, 10^{-2}m

Waves
10 000 drops/s

→

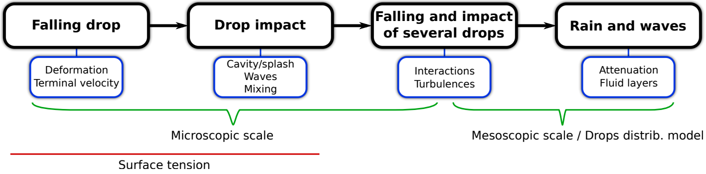
Small waves
100 drops/s

→

Flat plane
0.1 drop/s

←

Context: ocean waves attenuation by **falling rain drops**



Difficulties

- Large time and spatial scales
- Sensitive (many different behaviours), turbulent
- Measures

Needs (for simulations)

- Macro and meso numerical **models**
- **Appropriate** numerical methods for **micro** scales simulations
  - **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**?

©Jackson Carson

©M.-C. Guérout

Classical numerical methods

- Fail to solve (1) ⇒ **challenging** problem
- Introduce errors in (2) ⇒ incorrect **dynamics**

Numerical convergence, surface tension and fluid dynamics

What we expect

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

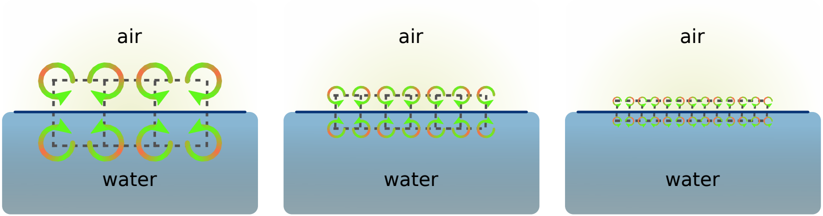
Precision $\Rightarrow$ **Accuracy**

Numerical convergence, surface tension and fluid dynamics

What we expect

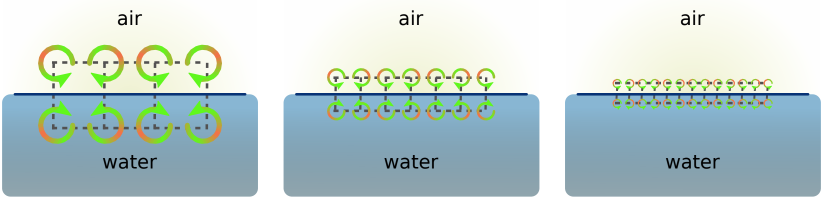
Refine the discretization/*mesh* ⇒ Get better results

Precision ⇒ **Accuracy**



The equilibrium of a flat surface problem: **parasitic currents** (numerical)
As $h \to 0 \Rightarrow \mathbf{error} \to 0$
Order 1: as $h/2 \to \mathrm{error}/2$

Numerical convergence, surface tension and fluid dynamics



Why is it *touchy*?

Smallest wave captured: $\lambda_{min} = 2h$

Fastest capillary wave velocity: $v_\sigma = O(\lambda_{min}^{-1/2}) \Rightarrow \Delta t_{CFL} = O(h^{3/2})$

Ex: $h = 10^{-4} m \Rightarrow v_{\lambda_{min}} \simeq 1.5\, m.s^{-1} \Rightarrow \Delta t_{CFL} < 6 \cdot 10^{-5} s$

Why is it *touchy*? (cont.)

More complex dynamics expected:

- Waves interactions
- Small scale topological changes (bubbles, drops)
- Low energy (eventually damped at macro scale)... but **numericaly sensitive**

NUMERICAL METHODS AND SIMULATIONS

Modelling surface tension

A boundary condition between 2 fluids

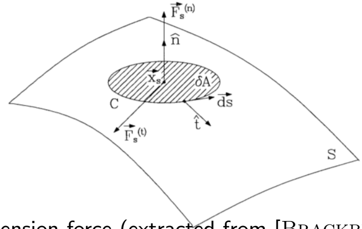
1. Young-Laplace law:

$$[p] = \sigma \kappa$$

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

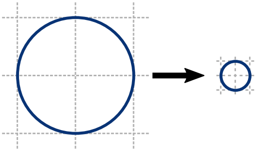
2. Surface force

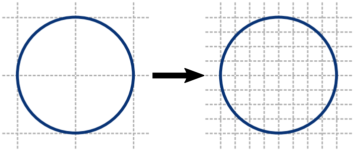
$$\mathbf{F}_s = \sigma \mathbf{n} \kappa$$



Surface tension force (extracted from [BRACKBILL1990])

Numerical convergence and the surface tension force





Diving into details

$$\text{As } R \to 0, \kappa \to \infty$$

$$\text{Also as h}\to 0, \lambda_{min} \to 0$$

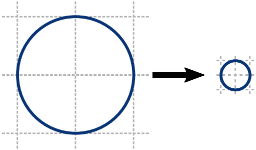
$$\text{And } \lambda_{min} \to 0 \iff \kappa_{max} \to \infty$$

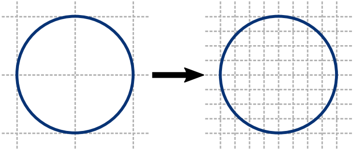
$$\kappa \to \infty \Rightarrow [p] \to \infty$$

Barriers

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

Numerical convergence and the surface tension force





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In fact, when surface tension is important...

- *Big* errors in κ $\Rightarrow$ **severe** errors in the simulation
    - (numerical) **parasitic/spurious currents** are $O(\kappa^2)$ [Denner et al. 2014]
- *Polutes* simulation results
- Leads to wrong solutions/analysis

Three things to remember

First thing to remember

The problem is essentially **geometry related** (whatever the fluid dynamic model)

Three things to remember

Second thing to remember

The **absolute** need to **compute accurately** the curvature

Three things to remember

Geometry memo

1. **Surface** S spatially derivates to...
   1. **Normal** vector $\mathbf{n}$ (eq. the tangent plane) spatially derivates to...
   2. **Curvature** κ

Moving/Tracking/Transporting the interface

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

$$\Downarrow$$

Curvature κ computed with (spatial) precision $O(h^{M-2})$

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The surface (transport methods) have to be **at least 3^{rd} order accurate** for κ to converge

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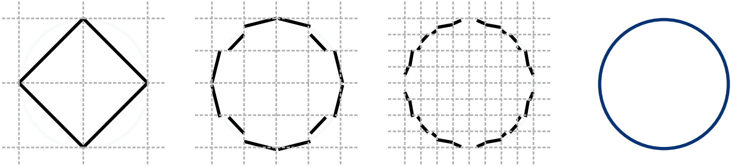
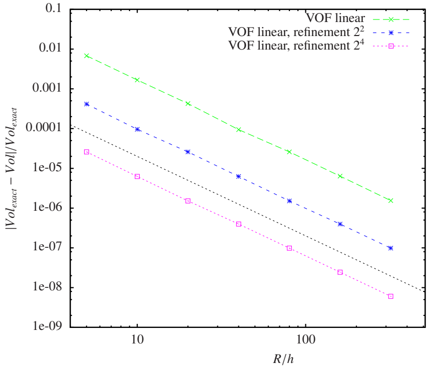
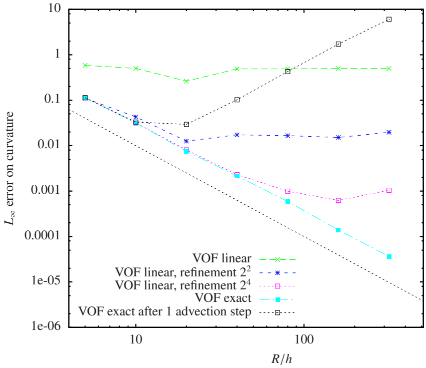
“Traditional” Volume Of Fluid (VOF-PLIC)





Distance to the surface



Curvature error (as in [CUMMINS2005] ,but continued)

(non) convergence of geometric computations

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The incompressible Navier-Stokes equations (1-fluid method)

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}\right)=-\nabla p+\nabla\cdot(2\mu\mathbf{D}(\mathbf{u}))+\mathbf{f}+\underline{\sigma\kappa\mathbf{n}\delta_S}$$

$$\nabla\cdot\mathbf{u}=0 \quad \text{and} \quad \frac{\partial\rho}{\partial t}+\mathbf{u}\cdot\nabla\rho=0$$

What we propose

Model choice

- Within **Continuum Surface-Force (CSF)** [Brackbill1990]

$$\sigma \kappa \mathbf{n} \delta_S \Rightarrow \sigma \kappa \nabla c$$

Proposed method

An **accurate curvature extension**

Interface/Surface

Level Set representation

- transport: 5^{th} order accurate (WENO5+RK)

Achievement

(at least) 3^{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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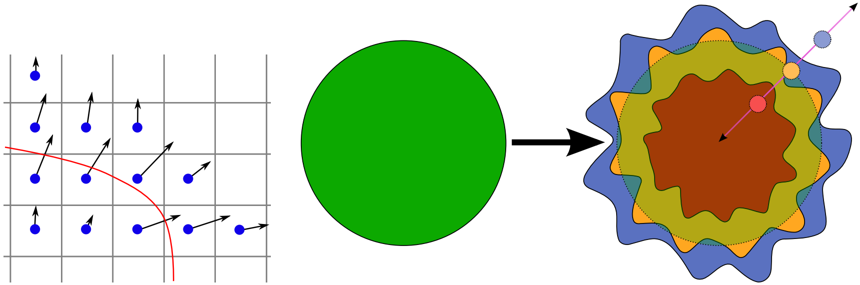
An accurate numerical method for curvature computation

Principal difficulty

The curvature is needed **around** the surface...
... but it is only defined **on** the surface



CSF discretization

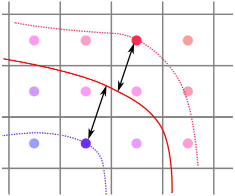
Effect on the dynamics

Curvature around the surface

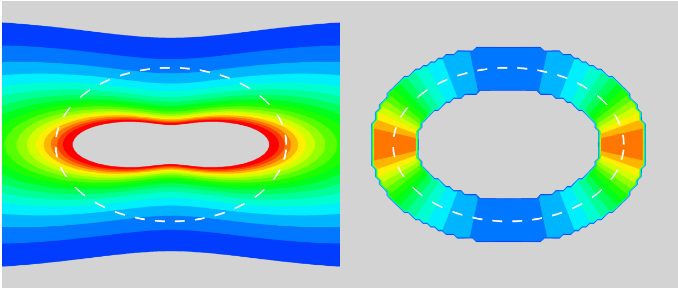
An accurate numerical method for curvature computation

Proposed solution

Curvature **extension** along **n** $\Rightarrow$ minimal variation along **n**
$\Rightarrow$ Use and extend the *Closest Point* method



Closest Point principle



Curvature field without (left) and with (right) the extension

An accurate numerical method for curvature computation

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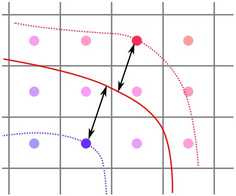

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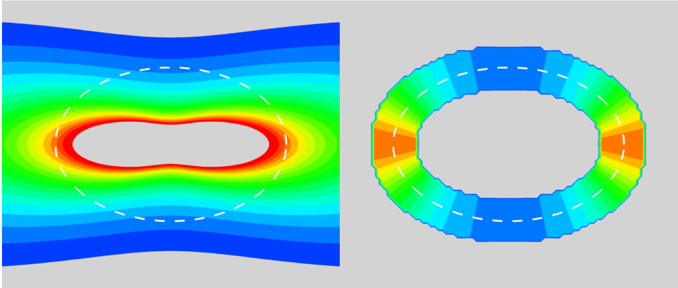
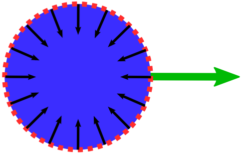
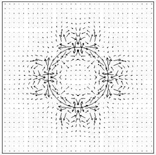


Curvature field without (left) and with (right) the extension

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right) = -\nabla \mathrm{p} + \nabla\cdot(2\mu\mathbf{D}(\mathbf{u})) + \mathbf{f} + \underline{\sigma\kappa_{CP}\nabla c}$$

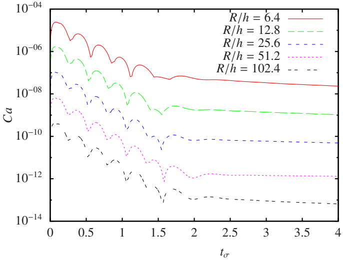
Numerical validation



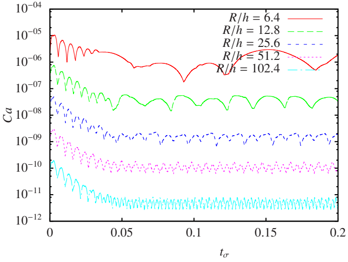


Study case : static and translating drop at equilibrium

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



Static column

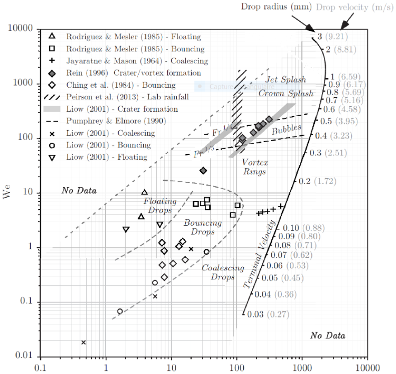


Translating column

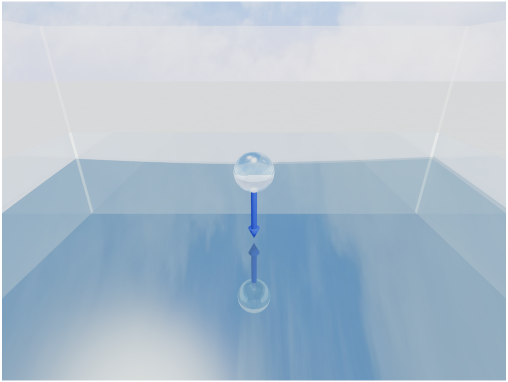
Application to rain drop impact

Back to our original problem : the **falling of a rain drop**

1. What is its **terminal velocity** ? ⇒ **shape** and **internal currents** (prelim. results)
2. What is the **dynamic of the impact** ?
   1. Wide range of parameters (We and Fr)
   2. Many complex regimes/dynamics



We/Fr map



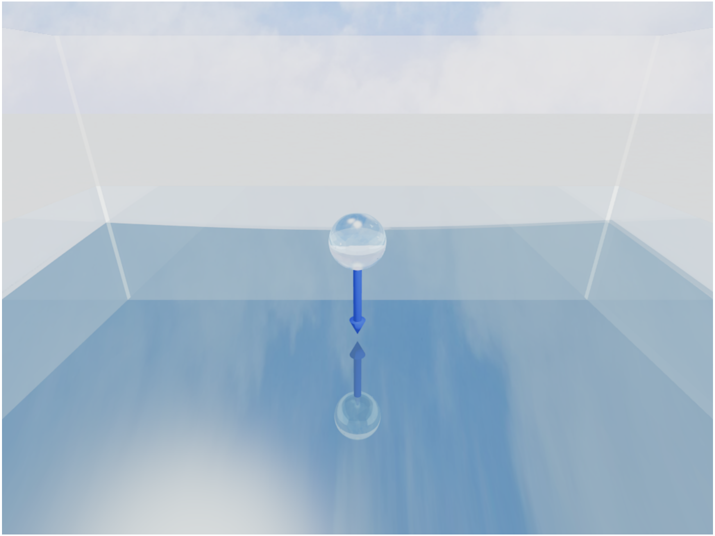
Simulation setup (realistic rendering)

Adequate numerical methods

Numerical methods : Finite Volume based

- **Navier-Stokes : 1-fluid method**
  - Velocity-pressure splitting
  - Inertial term : WENO5Z-RK3
- **Surface tension**
  - CSF [Brackbill1990]
  - Curvature extension w/ Closest Point [Coquerelle2016]
- **Interface : Level Set representation**
  - Transport : WENO5Z-RK3
  - Regularized ($3\Delta x$) volume fraction
  - Reinitialization : HCR2 (second order) [Hartmann2010]
  - Semi-implicit treatment (prediction) [Cottet2015]

Selected result : Fr=650, We=600



Falling drop, Fr=650, We=600.
8.5M cells, 32 comp. nodes. 8 days for 6000 iterations.

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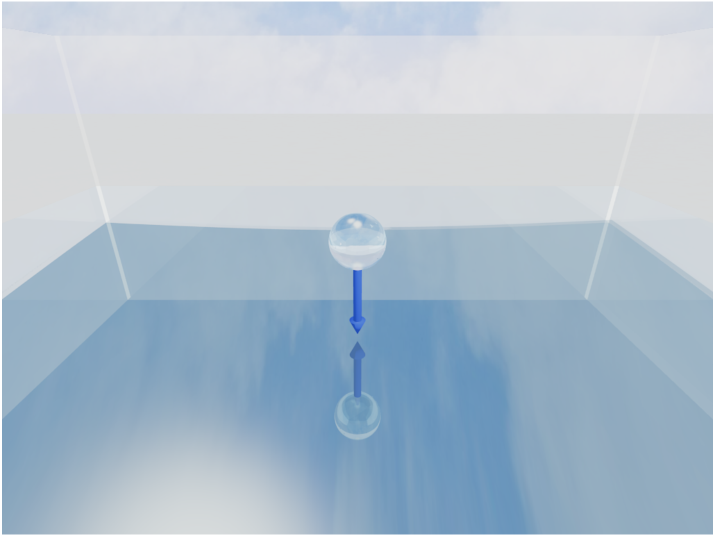

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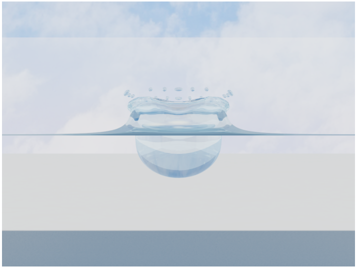
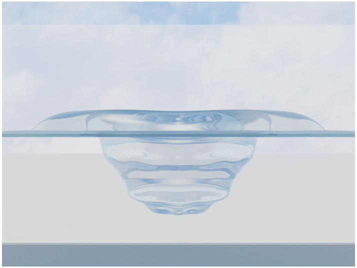
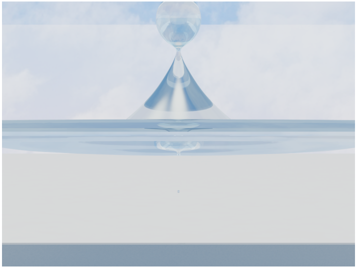
Principle phenomena



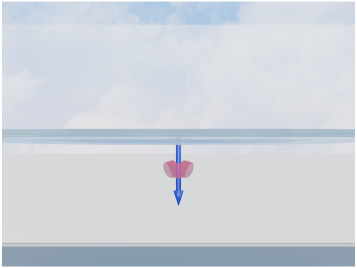
Cavity and crown



Capillary waves

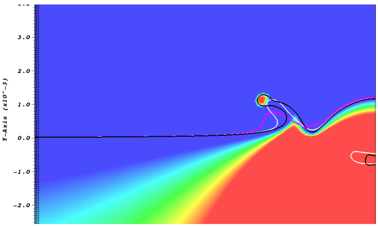


Jet and secondary drop ejection

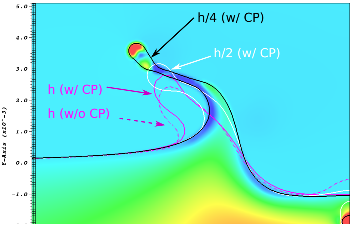


Vortex ring(s)

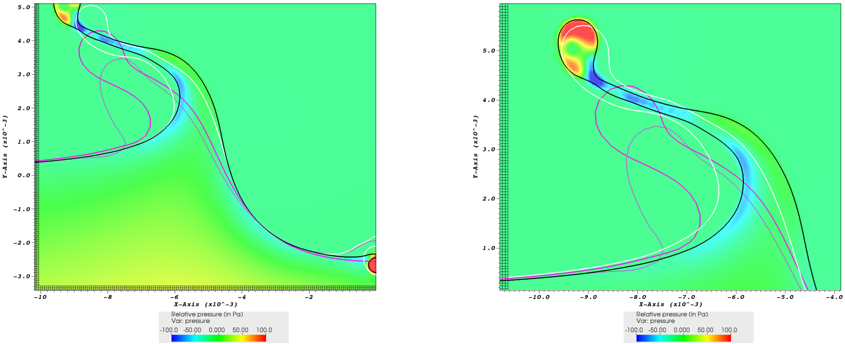
Closest Point accuracy demonstration



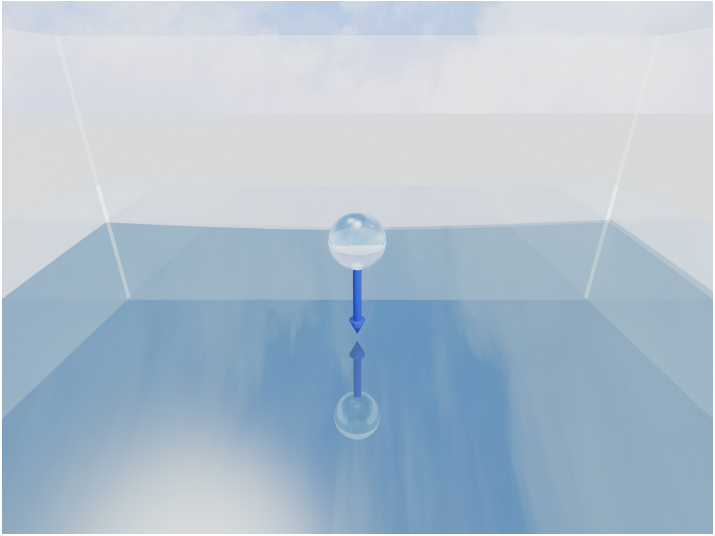
$t = 3.1\,ms$



$t = 5.5\,ms$

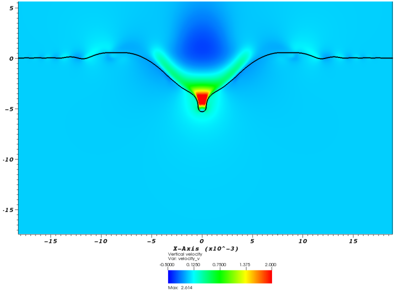


Selected result : Fr=124, We=117

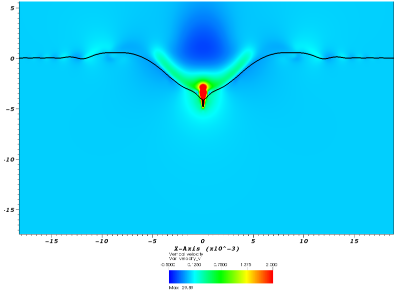


Falling drop, Fr=124, We=117.
$24M$ cells, 128 comp. nodes. 6 days for 7000 iterations.

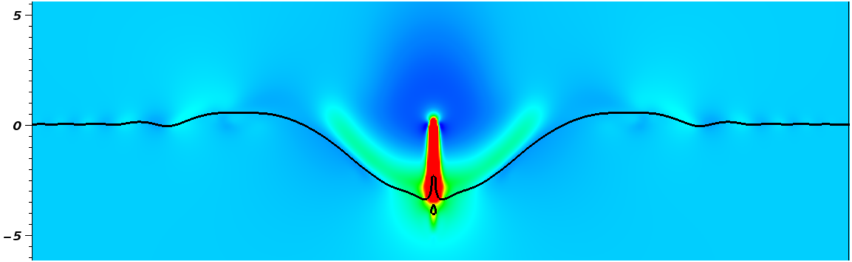
Small features, big impact



The “pinch”



Air ejection ($30\,m.s^{-1}$)



Jet formation and bubble entrapment

Simulations results

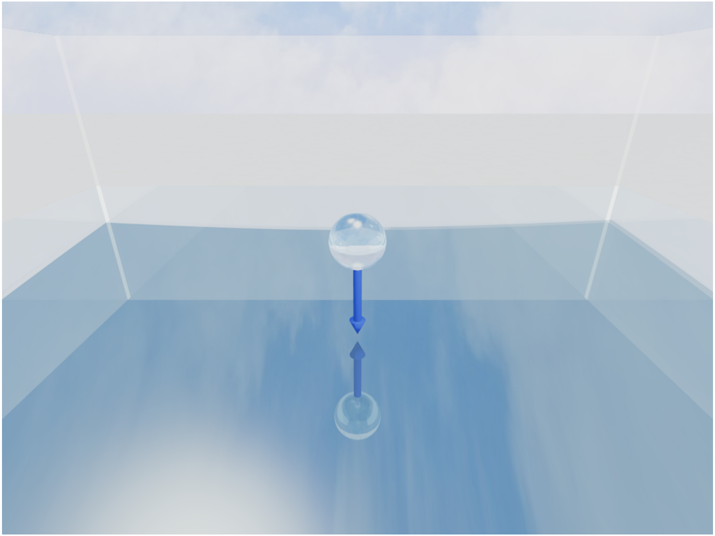
Achievements

- Around 20 simulations : $10<Fr<800$, $10<We<800$
- **Good agreement** with experiments [COLE,LIOW]
  - Cavity and multiple capillary waves
  - Thin/thick jet
  - Secondary drops and bubble entrapment
  - Simple to more complex vortex rings
- $\Rightarrow$ ongoing quantitative study $\Rightarrow$ **article**

Computational cost

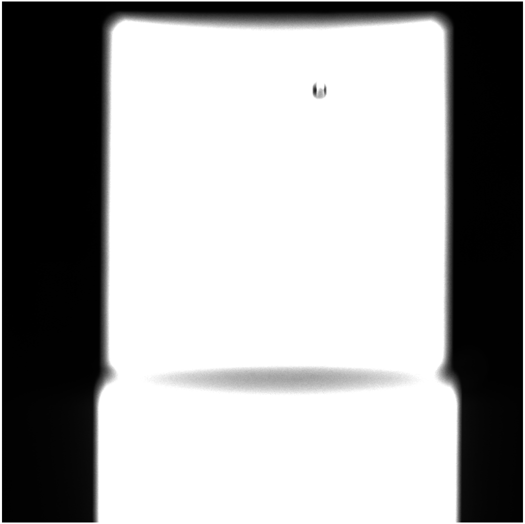
- Good scalability
  - 8.5M cells $\Rightarrow$ 7 days on 32 comp. nodes
  - 24M cells $\Rightarrow$ 7 days on 128 comp. nodes (28 on 32 nodes)
- **Worth it** to use the **proposed CP method**
  - For relevant small features
  - Avoid fine discretization
  - $5-10\%$ CPU cost

Going farther... terminal velocity



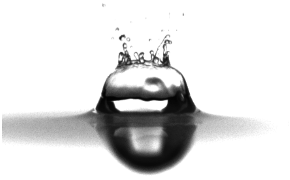
Falling drop
Fr=1200, We=1200
8.5M cells, 32 comp. nodes. 6 days for 8000 iterations

Goingfarther... terminal velocity



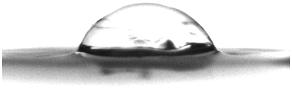
Falling drop at terminal velocity
$Fr \sim 1000$, $We \sim 1000$
Experiment by F. Veron (U. of Delaware)

The canopy : a tough challenge

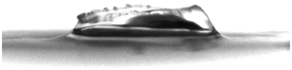


Formation

Donut



Canopy bubble



Collapse ($< 1ms$)

Conclusion

Keep in mind

- Numerical convergence is **mandatory** for simulation analysis
    - industrial codes might not converge...
    - ...viscous damping can hide the problem.
    - ⇒ the **translating drop test**
- The **smaller the scale**
    - the **more severe the problems**
    - the **more costly** ⇒ **high-order methods** help !

Perspectives / challenges

- Numerical
    - Algorithm efficiency
    - Mass conservation (LS reinitialization)
- Mechanics
    - Rain drop shape and internal currents
    - Bubbles, secondary drops, thin films
    - Contact line

notus
Computational Fluid Dynamics

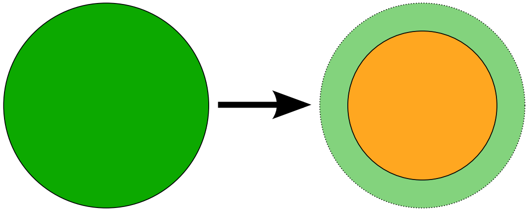
Errors on curvature ⇒ wrong interface dynamic

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 :



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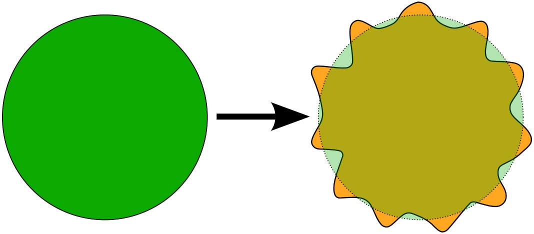

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