Subproject B5: Numerical computation for drop impact on textured surfaces

Martina Baggio
Institute of Aerospace Thermodynamics, University of Stuttgart

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Martina Baggio

2009 – 2012: B.Sc. in Aerospace Engineering
at the University of Padua

2013 – 2015: M.Sc. in Aerospace Engineering
at the University of Stuttgart

→ Specialization 1: mathematical and physical modeling in Aerospace Engineering
→ Specialization 2: experimental and numerical methods in Aerospace Engineering

Master Thesis at the Institute of Aerospace Thermodynamics “Numerical investigation of impingement jet cooling on a concave target”

Since 2016: Doctoral Student in DROPIT

TA A: Drop-Gas Interaction
TA B: Drop-Wall Interaction
TA C: Drop-Liquid Interaction

SP-B5: Numerical computation for drop impact on textured surfaces
Cooperation with other subprojects

**SP-B1**: Droplet collisions with solid superhydrophilic surfaces

**SP-B2**: Drop impact/deposition onto micro-structured hydrophobic and superhydrophobic surfaces

**SP-B3**: Characterization of porous media by X-ray micro computed tomography

**SP-B4**: Compressible effects in droplet interactions with textured walls

**SP-B5**: Numerical computation for drop impact on textured surfaces

Experimental data for validation of numerical models

Comparison with different numerical approaches
Why drop impact on textured surfaces?
Surface micro- and nanostructures are important in determining the wetting behavior of solid interfaces

A1/2: Droplets on a taro leaf exhibiting a contact angle of ca. 159° [1].

B: Micro- and nanometric structures on an insect (Homoptera meimuna opalifera) wing. The contact angle is 165° [1].

C: A droplet sitting on micropillars [2].


Incompressible transport equations (one field formulation):

\[ \nabla \cdot \mathbf{u} = 0 \]

mass/volume conservation

\[ \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = -\nabla p + \rho \mathbf{k} + \nabla \cdot \mathbf{\mu}[(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + f \gamma \delta_s \]

momentum transport

where: \( \rho = \rho_d f + \rho_c (1 - f) \), \( \mu = \mu_d f + \mu_c (1 - f) \) and \( f \) is the volume fraction of the disperse phase.

Volume of fluid (VoF) method for interface tracking

\[ \frac{\partial f}{\partial t} + \nabla \cdot (f \mathbf{u}) = 0 \]

transport of volume fraction

\[ f = \begin{cases} 
1 & \text{liquid} \\
0 & \text{gas} 
\end{cases} \]

0 < \( f \) < 1 in interface cells

Discretization

Finite Volume

Interface Reconstruction

Piecewise Linear Reconstruction of the Interface (PLIC)
FS3D allows only Cartesian grids → use of “dummy fields” to represent embedded solid boundaries.

**Dummy field 1:** tags the cells belonging to the wall structures

**Dummy field 2:** enables the enforcement of boundary conditions

→ Representation of solid squared boundaries easy and straightforward!
FS3D allows only Cartesian grids → use of “dummy fields” to represent embedded solid boundaries.
Current status: dealing with microscales

\[ N_{cell} = 128^3 \]
\[ \theta_{eq} = 90^\circ \]
Current status: dealing with microscales

\[
\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u \otimes u) = -\nabla p + \rho k + \nabla \cdot \mu \left( (\nabla u + (\nabla u)^T) \right) + f_\gamma \delta_s
\]

Continuum Surface Stress (CSS) model

\[
f_\gamma = \nabla \cdot \left( \sigma \left[ |n|I - \frac{n \otimes n}{|n|} \right] \right)
\]
Current status: dealing with microscales

\[
\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u) \otimes u = -\nabla p + \rho k + \nabla \cdot \mu \left[ (\nabla u + (\nabla u)^T) \right] + f_{\gamma} \delta_s
\]

Continuum Surface Force (CSF) model

\[
f_{\gamma} = \sigma k \nabla f
\]
Current status: dealing with microscales
Overview

- Implementation of structured surfaces
- Implementation of correct boundary conditions for curvature calculation near the wall
- Implementation of models for the dynamic contact angle $\theta_{dyn} = \theta_{dyn}(U_{cl}, \theta_{eq})$


Appendix A -- Current status: dealing with microscales

\[ U_0 = 20 \frac{cm}{s} \rightarrow We = \frac{\rho_d D U_0^2}{\sigma} = 0.656 \]
\[ \theta_{eq} = 135^\circ \]
Appendix B -- Modeling of surface tension: Continuum Surface Force (CSF) balanced

Parasitic currents: to reduce parasitic currents, pressure drop and surface tension should be discretized in the same way (“balanced algorithm” see [3]).

\[
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u}) \otimes \mathbf{u} = \rho \mathbf{k} + \nabla \cdot \mu[(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + (f \gamma \delta_s - \nabla p)
\]

\[f \gamma = \sigma \kappa \nabla f\]

\(\kappa\) is the interface curvature. \(\kappa\) is calculated with Height Functions (HF) or, when HFs fail, with paraboloid fitting (see Popinet [4]).

1) Calculate stencil height functions \((-1 < l < 1, l \in \mathbb{Z})\):

\[h_{i+l} = \sum_{j=j_{bottom(l)}}^{j_{top(l)}} f(i + l, j)\]

2) Set common origin

\[h_{i+l} \leftarrow h_{i+l} \Delta y + (y(j_{bottom(l)}) - y(j_{bottom(0)}))\]

3) Obtain curvature \(\kappa\) from \(h\)-derivatives

\[\kappa = \frac{h_{xx}}{(1 + h_x)^{3/2}} \bigg|_{x=0}\]


Boundary conditions for height functions should take the contact angle $\theta$ into account. According to Afkhami and Bussmann [5] (here 2D):

$$h_0 = h_1 + \frac{\Delta h}{\tan \theta}$$

Not all interface cells next to a solid boundary are contact line cells $\rightarrow$ boundary conditions should be applied only to contact line cells and adjacent cells (see [5]).