Modelling and computation of non-isothermal interfacial flow with OpenFOAM®

Dr. Edin Berberović

Polytechnic faculty, University of Zenica

eberberovic@ptf.unze.ba

CEEPUS III Network
Building Knowledge and Experience Exchange in CFD

Overview

Not only beautiful to observe...[1]

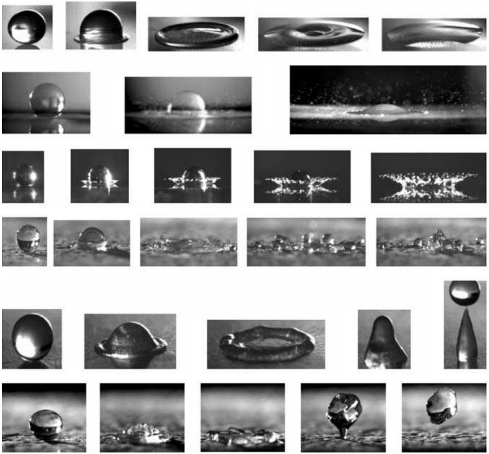
[1] http://medex.basecent.com/admin/resources/images/1/1/1911.pdf

… but also very important in engineering

- Flows with free surfaces occur in many industrial applications: important to understand the underlying physics
    - paint spraying
    - agriculture spray deposition
    - cosmetic sprays
    - internal combustion engines
    - spray cooling
    - cooling towers
    - icing on airplanes
- Numerical simulations provide a detailed insight into the phenomena and dynamic behavior of such flows
- Intended for investigations of flows with free surfaces
- The amount of information obtained is beyond the scope of experimental and theoretical methods
    - requires sharp interface capturing: expensive to compute

Limitations in experiments[2]

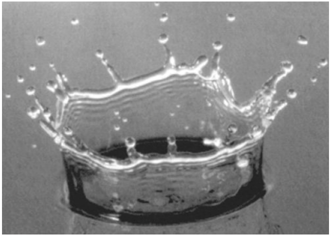
- Three-dimensional phenomenon, highly transient

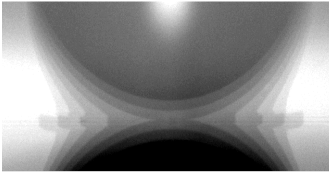


[2] [Rioboo et al., 2001]

Limitations in experiments[3]

- Complex physics, a variety of phenomena produced by single-drop impacts and their interactions
  - emerging of uprising sheets, breakup of sheets, crater formation in the wall film, emerging of jets and capillary waves

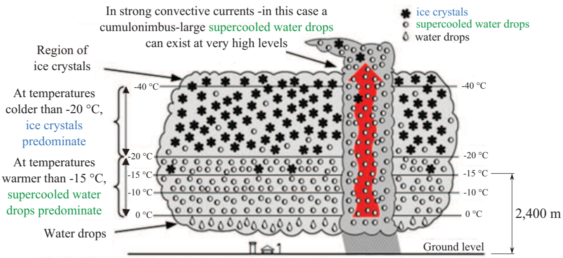




3 [Cossali et al., 1997]

Droplet Dynamics Under Extreme Ambient Conditions

- Aircraft icing[4]



(a)

(b)

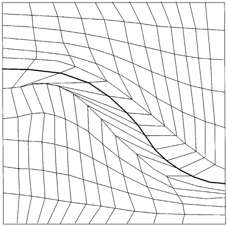
4 [Criscione, 2014]

Aircraft icing

- Impact of supercooled droplets onto cold surfaces
- A lack of understanding the fundamentals
- Model of the impact and solidification process which describes the impact of supercooled single drops on cold walls in detail
- In addition to predicting the hydrodynamics, a special challenge is to predict the observed morphology of icing (thermodynamics)
  - numerical simulations provide a detailed distributions of field variables in space and time: a valuable database that cannot be collected in experiments
  - determination and understanding the physics (parameters) that govern the flows at different stages
  - development of simple and reliable theoretical models able to predict the outcome of the phenomena
  - eventually enable the control of processes involving such flows

Interface tracking vs. interface capturing

- Interface tracking (surface or front tracking)
  - a computational mesh moving with the free surface
  - free surface treated as a boundary (boundary conditions)



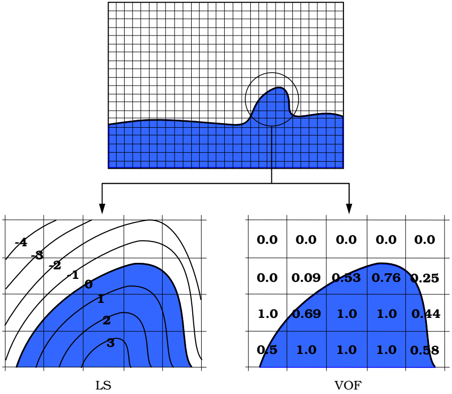
- Interface capturing (volume tracking)
  - by introducing a level-set function[5]
  - by tracking fluid volumes using an indicator function[6]

[5] [Osher and Sethian, 1988]

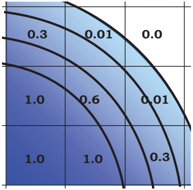
[6] [Hirt and Nichols, 1981]

Interface capturing models

- Level-Set (LS) Method
  - a level-set function embedded in the flow (signed distance)
- Volume Of Fluid (VOF)
  - indicator function for tracking phases by occupied subdomains



VOF model hydrodynamics: a mixture approach



$$\alpha = \frac{\int_{V \to \partial x^3} \alpha_l \mathrm{d}V}{\int_{V \to \partial x^3} (\alpha_l + \alpha_g) \mathrm{d}V} \begin{cases} = 0, & \text{gas} \\ = 1, & \text{liquid} \\ > 0, < 1, & \text{interface} \end{cases}$$

$$\rho = \rho_l \alpha + \rho_g (1 - \alpha), \quad \mu = \mu_l \alpha + \mu_g (1 - \alpha)$$

$$\nabla \cdot \mathbf{U} = 0$$

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\mathbf{U} \alpha) = 0$$

$$\frac{\partial (\rho \mathbf{U})}{\partial t} + \nabla \cdot (\rho \mathbf{U} \mathbf{U}) = -\nabla p + \nabla \cdot \mathbf{T} + \mathbf{f}_b$$

$$\mathbf{T} = \mu \left[\nabla \mathbf{U} + (\nabla \mathbf{U})^T \right], \mathbf{f}_b = \rho \mathbf{g} + \mathbf{f}_\sigma$$

Mixture as incompressible fluid

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0$$

$$\frac{\partial [\rho_l \alpha + \rho_g (1-\alpha)]}{\partial t} + \nabla \cdot \{[\rho_l \alpha + \rho_g (1-\alpha)]\mathbf{U}\} = 0$$

$$\frac{\partial \rho_l}{\partial t}\alpha + \rho_l \frac{\partial \alpha}{\partial t} + \frac{\partial \rho_g}{\partial t}(1-\alpha) + \rho_g \frac{\partial (1-\alpha)}{\partial t} +$$

$$\nabla \rho_l \alpha \mathbf{U} + \rho_l \nabla \alpha \mathbf{U} + \nabla \rho_g (1-\alpha)\mathbf{U} + \rho_g \nabla (1-\alpha)\mathbf{U} + [\rho_l \alpha + \rho_g (1-\alpha)]\nabla \cdot \mathbf{U}$$

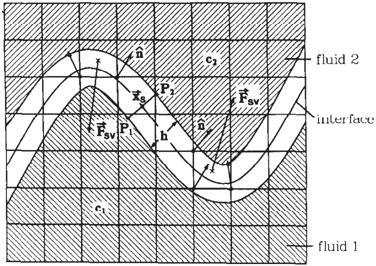
$$= \alpha \underbrace{\left[\frac{\partial \rho_l}{\partial t} + \mathbf{U}\nabla \rho_l\right]}_{\mathrm{D}\rho_l/\mathrm{D}t = 0} + (1-\alpha) \underbrace{\left[\frac{\partial \rho_g}{\partial t} + \mathbf{U}\nabla \rho_g\right]}_{\mathrm{D}\rho_g/\mathrm{D}t = 0} + (\rho_l - \rho_g) \underbrace{\left[\frac{\partial \alpha}{\partial t} + \mathbf{U} \cdot \nabla \alpha\right]}_{\mathrm{D}\alpha/\mathrm{D}t = 0}$$

$$+ [\rho_l \alpha + \rho_g (1-\alpha)]\nabla \cdot \mathbf{U} = 0$$

$$\nabla \cdot \mathbf{U} = 0$$

Surface tension effects at the interface

- Kinematic and dynamic conditions at the interface



$$\mathbf{v}_1 - (\mathbf{n} \cdot \mathbf{v}_1)\mathbf{n} = \mathbf{v}_2 - (\mathbf{n} \cdot \mathbf{v}_2)\mathbf{n}$$

$$\mathbf{n} \cdot (\mathbf{T}_1 - \mathbf{T}_2) = \sigma\kappa\mathbf{n} - \nabla_s\sigma$$

$$\nabla_s = \nabla - \nabla_n$$

$$(p_2 - p_1)\mathbf{n} = \sigma\kappa\mathbf{n}$$

- Continuum Surface Force (CSF) model[7]

$$\mathbf{f}_\sigma \approx \sigma\kappa\nabla\alpha = \sigma(-\nabla \cdot \mathbf{n})\nabla\alpha$$

7 [Brackbill et al., 1992]

Reformulation of the momentum equation

- Modifications in the momentum equation
  - modified pressure, stress tensor, surface tension CSF model

$$p_d = p - \rho \mathbf{g} \cdot \mathbf{x}$$

$$-\nabla p = -\nabla p_d - \rho \mathbf{g} - \mathbf{g} \cdot \mathbf{x} \nabla \rho$$

$$\nabla \cdot \mathbf{T} = \nabla \cdot \mu \left[\nabla \mathbf{U} + (\nabla \mathbf{U})^T \right] = \nabla \cdot (\mu \nabla \mathbf{U}) + (\nabla \mathbf{U}) \cdot \nabla \mu$$

$$\begin{aligned} \frac{\partial(\rho \mathbf{U})}{\partial t} &+ \nabla \cdot (\rho \mathbf{U}\mathbf{U}) - \nabla \cdot (\mu \nabla \mathbf{U}) - (\nabla \mathbf{U}) \cdot \nabla \mu \\ &= -\nabla p_d - \mathbf{g} \cdot \mathbf{x} \nabla \rho + \sigma \left[-\nabla \cdot \left(\frac{\nabla \alpha}{|\nabla \alpha|} \right) \right] \nabla \alpha \end{aligned}$$

Sharp interface capturing

- Not geometrically reconstructive, requires some modelling to numerically *compress* the interface
  - modifications in the phase fraction equation, compression term

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\mathbf{U}\alpha) + \nabla \cdot [\mathbf{U}_c \alpha(1-\alpha)] = 0$$

- the *compression* velocity
  - shrinking the interphase, not related to compressible flow
  - acting only in the interface region, normal to the interface
  - does not bias the solution elsewhere
  - limited by the largest value of the velocity in the domain
  - model parameter C_α between 0 and 1[8]

$$\mathbf{U}_c = \min[C_\alpha|\mathbf{U}|, \max(|\mathbf{U}|)]\frac{\nabla\alpha}{|\nabla\alpha|}$$

[8] [foam-extend, 2016]

Energy equation

- In terms of specific enthalpy $h = u + \frac{p}{\rho}$

$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\rho \mathbf{U} h) = \nabla \cdot (k \nabla T) + \frac{\mathrm{D}p}{\mathrm{D}t} + (\mathbf{T} : \nabla \mathbf{U}) + \dot{q}_V$$

- In terms of temperature $(\mathrm{d}h = (\frac{\partial h}{\partial T})_p \mathrm{d}T + (\frac{\partial h}{\partial p})_T \mathrm{d}p)$

$$\frac{\partial(\rho c_p T)}{\partial t} + \nabla \cdot (\rho c_p \mathbf{U} T)$$

$$= \nabla \cdot (k \nabla T) + \rho T \frac{\mathrm{D}c_p}{\mathrm{D}t} - \left[\frac{\partial(\ln \rho)}{\partial(\ln T)}\right]_p \frac{\mathrm{D}p}{\mathrm{D}t} + (\mathbf{T} : \nabla \mathbf{U}) + \dot{q}_V$$

  - neglecting viscous dissipation and sources

$$\frac{\partial(\rho c_p T)}{\partial t} + \nabla \cdot (\rho c_p \mathbf{U} T) = \nabla \cdot (k \nabla T)$$

$$k = k_l \alpha + k_g (1 - \alpha), \rho c_p = (\rho c_p)_l \alpha + (\rho c_p)_g (1 - \alpha)$$

Complete model for the non-isothermal free-surface flow

$$\nabla \cdot \mathbf{U} = 0$$

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\mathbf{U}\alpha) + \nabla \cdot [\mathbf{U}_c \alpha (1-\alpha)] = 0$$

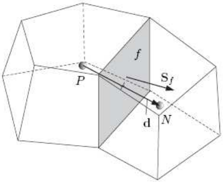
$$\begin{aligned} \frac{\partial (\rho \mathbf{U})}{\partial t} &+ \nabla \cdot (\rho \mathbf{U}\mathbf{U}) - \nabla \cdot (\mu \nabla \mathbf{U}) - (\nabla \mathbf{U}) \cdot \nabla \mu \\ &= -\nabla p_d - \mathbf{g} \cdot \mathbf{x} \nabla \rho + \sigma \left[-\nabla \cdot \left(\frac{\nabla \alpha}{|\nabla \alpha|} \right) \right] \nabla \alpha \end{aligned}$$

$$\frac{\partial (\rho c_p T)}{\partial t} + \nabla \cdot (\rho c_p \mathbf{U} T) = \nabla \cdot (k \nabla T)$$

$$\rho, \mu, k, \rho c_p = f(\text{liquid and gas properties}, \alpha)$$

Discretization of space and time

- Discretization of the solution domain



- Discretization/integration of transport equations

$$\frac{\partial(\rho\phi)}{\partial t} + \nabla \cdot (\rho \mathbf{U} \phi) = \nabla \cdot (\Gamma \nabla \phi) + S_\phi(\phi)$$

$$\int_t^{t+\Delta t} \left[\frac{\partial}{\partial t} \int_{V_P} \rho\phi \mathrm{d}V + \int_{V_P} \nabla \cdot (\rho \mathbf{U} \phi) \mathrm{d}V \right] \mathrm{d}t$$

$$= \int_t^{t+\Delta t} \left[\int_{V_P} \nabla \cdot (\Gamma \nabla \phi) \mathrm{d}V + \int_{V_P} S_\phi(\phi) \mathrm{d}V \right] \mathrm{d}t$$

Gradient, divergence, laplacian

- Spatial derivatives: Gauss's theorem

$$\int_{V_P} \nabla \phi \mathrm{d}V = \int_{S_P} \mathrm{d}\mathbf{S}\phi \approx \sum_f \mathbf{S}_f \phi_f$$

$$\int_{V_P} \nabla \cdot \phi \mathrm{d}V = \int_{S_P} \mathrm{d}\mathbf{S} \cdot \phi \approx \sum_f \mathbf{S}_f \cdot \phi_f$$

- Laplacian term

$$\int_{V_P} \nabla \cdot (\Gamma \nabla \phi) \mathrm{d}V = \int_{S_P} \mathrm{d}\mathbf{S} \cdot (\Gamma \nabla \phi) \approx \sum_f \Gamma_f \mathbf{S}_f \cdot (\nabla \phi_f)$$

$$(\nabla \phi)_f^{\perp} \approx \frac{\phi_N - \phi_P}{|\mathbf{d}|}$$

Convection term

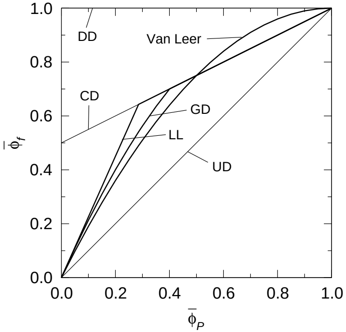
- Convection term linearization

$$\int_{V_P} \nabla\cdot(\rho\mathbf{U}\phi)\mathrm{d}V = \int_{S_P} \mathrm{d}\mathbf{S}\cdot(\rho\mathbf{U}\phi) \approx \sum_f \mathbf{S}_f\cdot(\rho\mathbf{U})_f\phi_f = \sum_f F\phi_f$$

  - NVD-TVD approach

$$\overline{\phi}_f = \frac{\phi_f - \phi_U}{\phi_D - \phi_U}$$

$$\overline{\phi}_P = \frac{\phi_P - \phi_U}{\phi_D - \phi_U}$$



Cell-face interpolation

- A combination of upwind (UD) and central differencing (CD)

$$\phi_{f,UD} = \mathrm{pos}(\mathbf{U}_f \cdot \mathbf{S}_f)\phi_P + [1 - \mathrm{pos}(\mathbf{U}_f \cdot \mathbf{S}_f)]\phi_N$$

$$\phi_{f,CD} = f_{\mathbf{d}}\phi_P + (1 - f_{\mathbf{d}})\phi_N, f_{\mathbf{d}} = \overline{f\mathrm{N}}/\overline{\mathrm{PN}}$$

$$\mathrm{pos}(\mathbf{U}_f \cdot \mathbf{S}_f) = \begin{cases} 1, & \text{for } \mathbf{U}_f \cdot \mathbf{S}_f > 0, \text{flow from P to N} \\ 0, & \text{for } \mathbf{U}_f \cdot \mathbf{S}_f < 0, \text{flow from N to P} \end{cases}$$

$$\phi_f = \psi\phi_{f,CD} + (1 - \psi)\phi_{f,UD}$$

$$\phi_f = \lambda(\phi_P - \phi_N) + \phi_N$$

$$\lambda = \psi f_{\mathbf{d}} + (1 - \psi) \cdot \mathrm{pos}(\mathbf{U}_f \cdot \mathbf{S}_f)$$

  - except for conductivity: harmonic interpolation

$$k_f = \left(\frac{1 - f_{\mathbf{d}}}{k_P} + \frac{f_{\mathbf{d}}}{k_N}\right)^{-1}$$

Source term handling

- Source terms linearization

$$\int_{V_P} S_\phi(\phi)\mathrm{d}V \approx S_{\phi_1} V_P + S_{\phi_2}\phi_P V_P$$

- Source terms reconstruction

$$\phi_P = \left(\sum_f \frac{\mathbf{S}_f \mathbf{S}_f}{|\mathbf{S}_f|}\right)^{-1} \cdot \left(\sum_f \frac{\mathbf{S}_f}{|\mathbf{S}_f|} \cdot \phi_f |\mathbf{S}_f|\right)$$

  - cell-centre value recovered as weighted average of the (staggered) cell-face values

$$(\nabla p_d)_P = \left(\sum_f \frac{\mathbf{S}_f \mathbf{S}_f}{|\mathbf{S}_f|}\right)^{-1} \cdot \left(\sum_f \frac{\mathbf{S}_f}{|\mathbf{S}_f|} \cdot (\nabla p_d)_f^{\perp} |\mathbf{S}_f|\right)$$

Time integration

- Euler implicit

$$\frac{\partial}{\partial t}\int_{V_P}(\rho\phi)\mathrm{d}V \approx \frac{(\rho_P\phi_P V_P)_{(t+\Delta t)} - (\rho_P\phi_P V_P)_t}{\Delta t}$$

$$\int_t^{t+\Delta t}\left[\frac{\partial}{\partial t}\int_{V_P}\rho\phi\mathrm{d}V\right]\mathrm{d}t \approx (\rho_P\phi_P V_P)_{(t+\Delta t)} - (\rho_P\phi_P V_P)_t$$

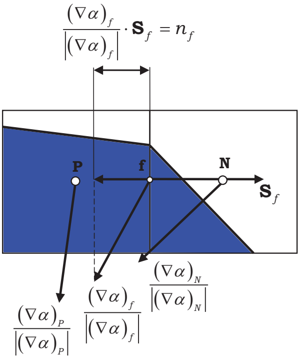
$$\int_t^{t+\Delta t}\left[\int_{V_P}\mathcal{L}\phi\mathrm{d}V\right]\mathrm{d}t \approx \mathcal{L}^*(\phi_P)_{(t+\Delta t)}\Delta t$$

$$\int_t^{t+\Delta t}\left[\int_{V_P}S_\phi(\phi)\mathrm{d}V\right]\mathrm{d}t \approx (S_{\phi_1}V_P + S_{\phi_2}\phi_P V_P)_{(t+\Delta t)}\Delta t$$

Evaluation of the *compression* term

- The *compression* fluxes

$$(\mathbf{U}_{c,f}\cdot\mathbf{S}_f) = n_f \cdot \min\left[C_\alpha\frac{|\mathbf{U}_f\cdot\mathbf{S}_f|}{|\mathbf{S}_f|}, \max\left(\frac{|\mathbf{U}_f\cdot\mathbf{S}_f|}{|\mathbf{S}_f|}\right)\right]$$



$$n_f = \frac{(\nabla\alpha)_f}{|(\nabla\alpha)_f + \delta_n|}\cdot\mathbf{S}_f$$

$$\delta_n = \frac{\varepsilon}{\left(\frac{\sum_N V_i}{N}\right)^{1/3}},\quad \varepsilon = 10^{-8}$$

Time step control and sub-cycling

- Adaptive time step control

$$\mathrm{Co} = \frac{|\mathbf{U}_f \cdot \mathbf{S}_f|}{\mathbf{d} \cdot \mathbf{S}_f} \Delta t$$

$$\Delta t = \min \left[\frac{\mathrm{Co}_{\max}}{\mathrm{Co}_o} \Delta t_o, (1 + \lambda_1 \frac{\mathrm{Co}_{\max}}{\mathrm{Co}_o}) \Delta t_o, \lambda_2 \Delta t_o, \Delta t_{\max} \right]$$

$$\mathrm{Co}_{\max} \approx 0.2, \lambda_1 = 0.1, \lambda_2 = 1.2$$

- Temporal sub-cycling

$$\Delta t_{sc} = \frac{\Delta t}{n_{sc}}$$

$$F = \rho \mathbf{U}_f \cdot \mathbf{S}_f = \sum_{i=1}^{n_{sc}} \frac{\Delta t_{sc}}{\Delta t} F_{sc,i}$$

Boundary conditions

- Basic boundary conditions
  - Dirichlet, specifies the values of the dependent variable on all boundaries at all times

$$\phi_b = f(\mathbf{x}_b, t)$$

  - Neumann, specifies the normal derivative of the dependent variable on all boundaries at all times

$$\left(\frac{\partial \phi}{\partial n}\right)_b = \mathbf{n} \cdot \nabla \phi = f(\mathbf{x}_b, t)$$

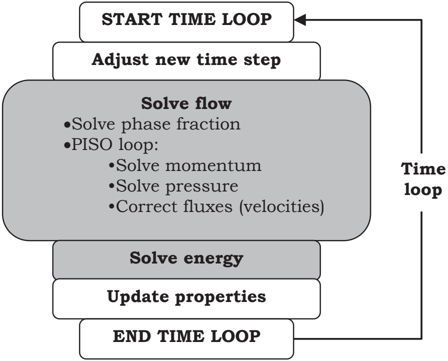
- Derived boundary conditions
  - various combinations

Solution procedure

- Iterative solution of linear systems

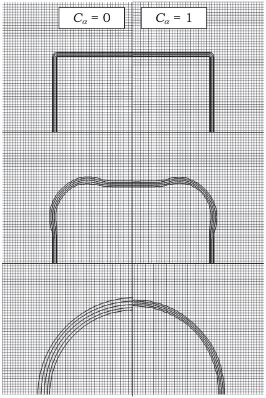
$$a_P \phi_{P(t+\Delta t)} + \sum_N a_N \phi_{N(t+\Delta t)} = b$$

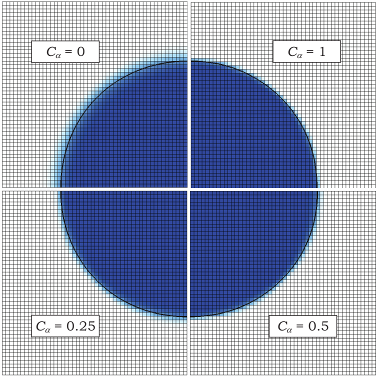
$$\mathbf{A} \cdot \Phi = \mathbf{b}$$



Some of the previous results[9]

- Droplet shape evolution in zero gravity

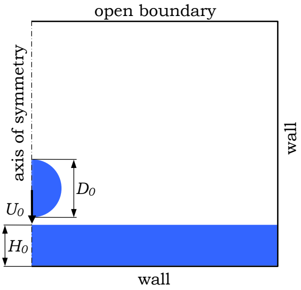


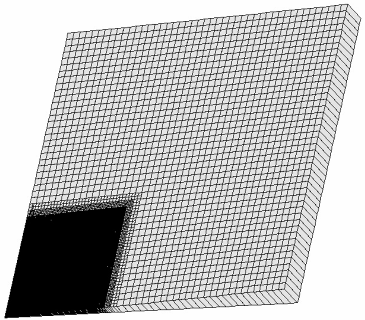


[9] [Berberovic, 2010]

Some of the previous results

- Droplet impact onto a liquid layer





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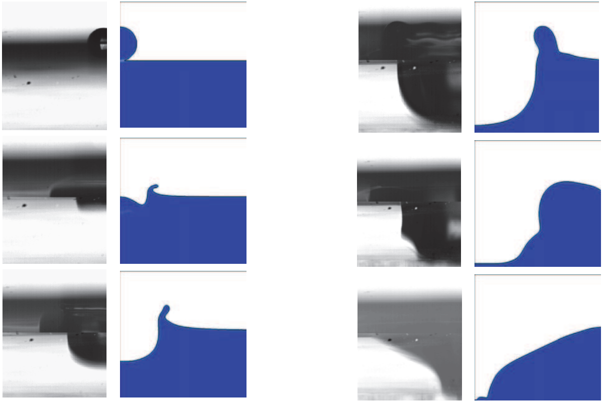

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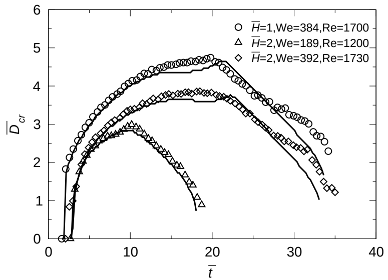
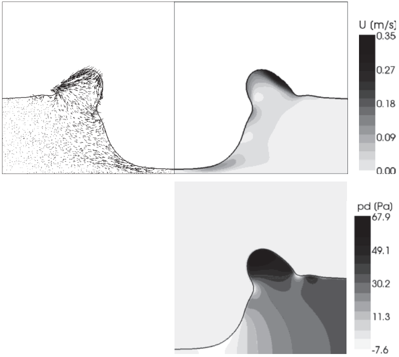
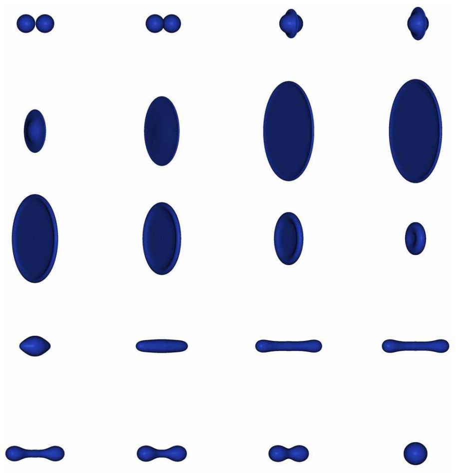




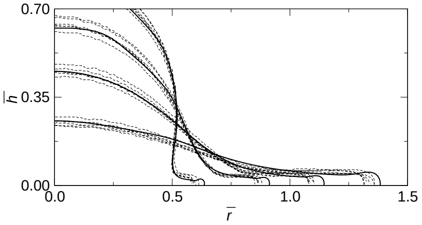
Some of the previous results

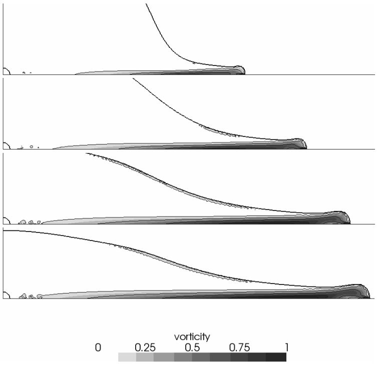
- Collisions of droplets



Some of the previous results

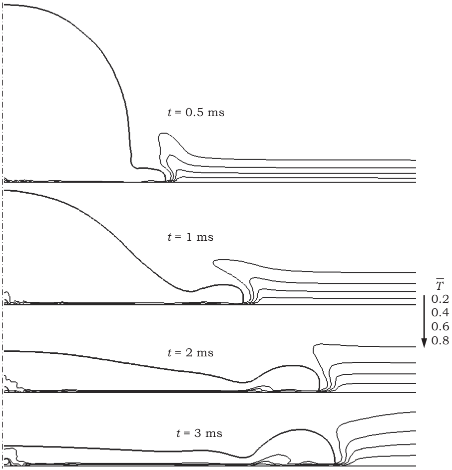
- Droplet impact onto a solid wall





Some of the previous results

- Droplet impact onto a solid wall: non-isothermal case



foam-extend release[11]

- The Extend Project of OpenFOAM®[10]
- To be done in the workshop
    - preparing and running the cases using the existing solver `interFOAM`
    - extending the `transportModels` library to enable thermal treatment
    - extending the solver to include the temperature equation
    - modifying and preparing the cases for non-isothermal flow

[10] [OpenFOAM, 2016]
[11] [foam-extend, 2016]

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