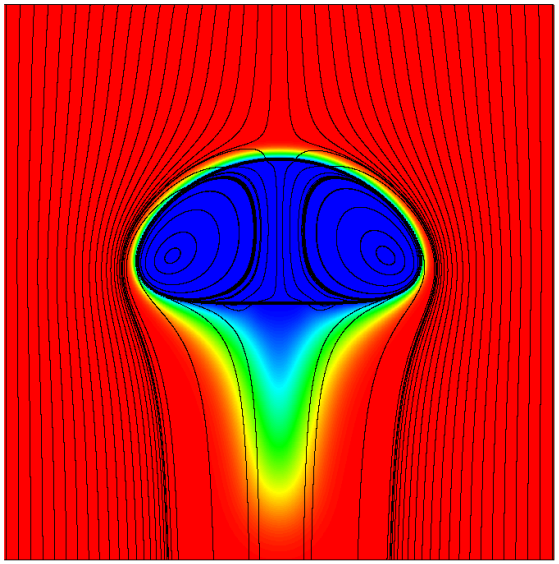
Direct Numerical Simulation of Two-Phase Flows with phase change. Applications to Nucleate Boiling and Leidenfrost Droplets

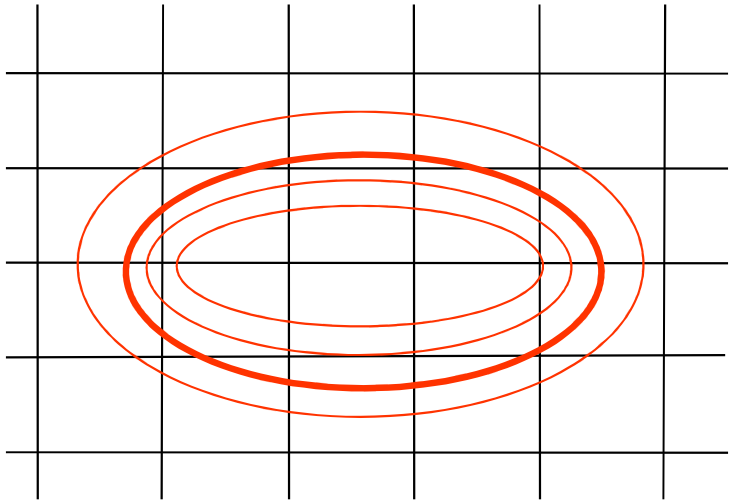


Sébastien Tanguy

Institut de Mécanique des Fluides de Toulouse

Maître de conférence Université Paul Sabatier (Toulouse 3)

1. Level Set Method



ϕ : signed distance function

$\phi < 0$ Gas phase

$\phi = 0$ Liquid-gas interface

$\phi > 0$ Liquid phase

Convection equation :

$$\frac{\partial \phi}{\partial t} + \boldsymbol{V}.\nabla\phi = 0$$

(Osher & Sethian, JCP 1989)

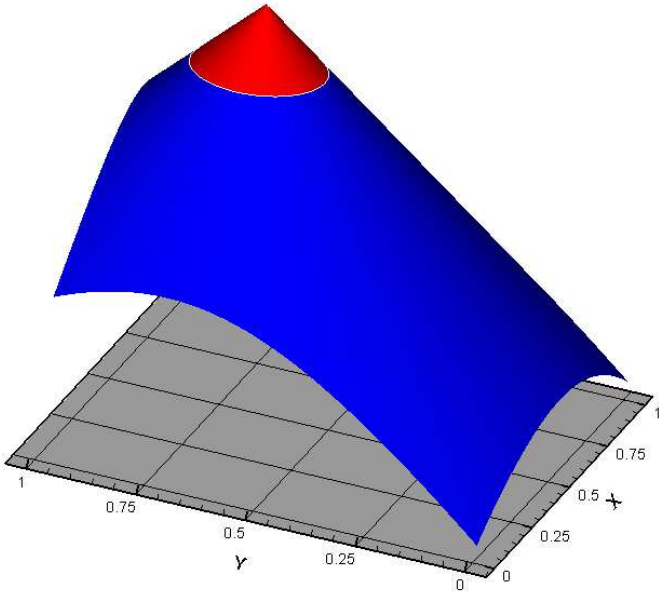
Redistance equation :

$$\frac{\partial d}{\partial \tau} = sign(\phi)(1 - |\nabla d|)$$

(Sussman et al, JCP 1994)

Geometrical properties :

$$|\nabla\phi| = 1 \quad \begin{cases} \boldsymbol{n} = \dfrac{\nabla\phi}{|\nabla\phi|} = \nabla\phi \\ \kappa(\phi) = -\nabla \cdot \boldsymbol{n} \end{cases}$$



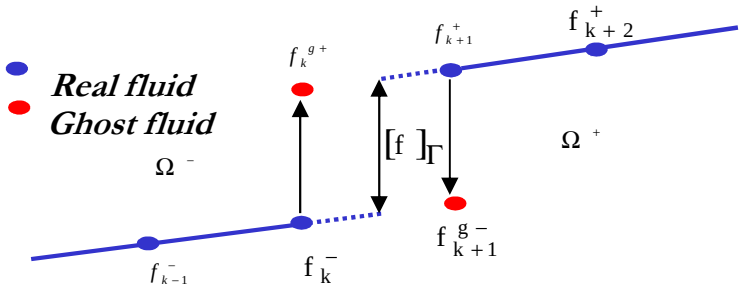
Numerical schemes : Runge-Kutta 2 or 3 and fifth order WENO-Z

2. The Ghost Fluid Method : a Sharp Interface Method

Ghost Fluid Method (Fedkiw et al, JCP 1999)

- Locate meshes crossed by interface

- Extend continuously discontinuous variables before discretization



- No fictitious interface thickness

- reduce parasitic currents and can be used with more complex problems as phase change.

The Ghost Fluid tool-box

- Sharp but first order discretization for jump conditions (Liu et al, JCP 2000)

- Sharp and second order discretization for immersed Dirichlet boundary condition (Gibou et al, JCP 2002)

- Sharp and second order discretization for immersed Neumann boundary condition (Ng et al, JCP 2009)

- Sharp and second order discretization for immersed Robin boundary condition (Papac et al, JCP 2010)

- Constant, linear and quadratic extrapolation by solving iterative PDE (Aslam et al, JCP 2003)

3. Conservation laws and jump conditions

Conservation law	Jump conditions
$\nabla \cdot \vec{V} = 0$	$\left[\vec{V}\right]_\Gamma = \dot{m}\left[\frac{1}{\rho}\right]_\Gamma \vec{n}$
$\rho \frac{D\vec{V}}{Dt} = -\nabla p + \nabla \cdot (2\mu \boldsymbol{D}) + \rho\vec{g}$	$[p]_\Gamma = \sigma\kappa + 2\left[\mu \frac{\partial V_n}{\partial n}\right]_\Gamma - \dot{m}^2\left[\frac{1}{\rho}\right]_\Gamma$
$\rho C_p \frac{DT}{Dt} = \nabla \cdot (k\nabla T)$	$[k\nabla T \cdot \vec{n}]_\Gamma = \dot{m}\left(L_{vap} + \left(C_{pliq} - C_{pvap}\right)(T_{sat} - T\Big\vert_\Gamma)\right)$
$\rho \frac{DY_1}{Dt} = \nabla \cdot (\rho D_m \nabla Y_1)$	$[\rho D_m \nabla Y_1 \cdot \vec{n}]_\Gamma = -\dot{m}[Y_1]_\Gamma$

- 4. Ghost Fluid Thermal Solver for Boiling GFTSB (Gibou et al, JCP 2007, Tanguy et al JCP 2014)

Step 1 : Update the temperature field in the liquid phase with a prescribed uniform Dirichlet boundary condition at the interface

$$\rho_l Cp_l T_l^{n+1} - \Delta t \nabla \cdot \left(k_l \nabla T_l^{n+1}\right) = \rho_l Cp_l \left(T_l^n - \Delta t \vec{V}_l^n \cdot \nabla T_l^n\right) \qquad if \phi > 0$$
$$T|_\Gamma = T_{sat}$$

Step 2 : Update the temperature field in the gas phase with a prescribed uniform Dirichlet boundary condition at the interface

$$\rho_g Cp_g T_g^{n+1} - \Delta t \nabla \cdot \left(k_g \nabla T_g\right) = \rho_g Cp_g \left(T_g^n - \Delta t \vec{V}_g^n \cdot \nabla T_g^n\right) \qquad if \phi < 0$$
$$T\Big|_\Gamma = T_{sat}$$

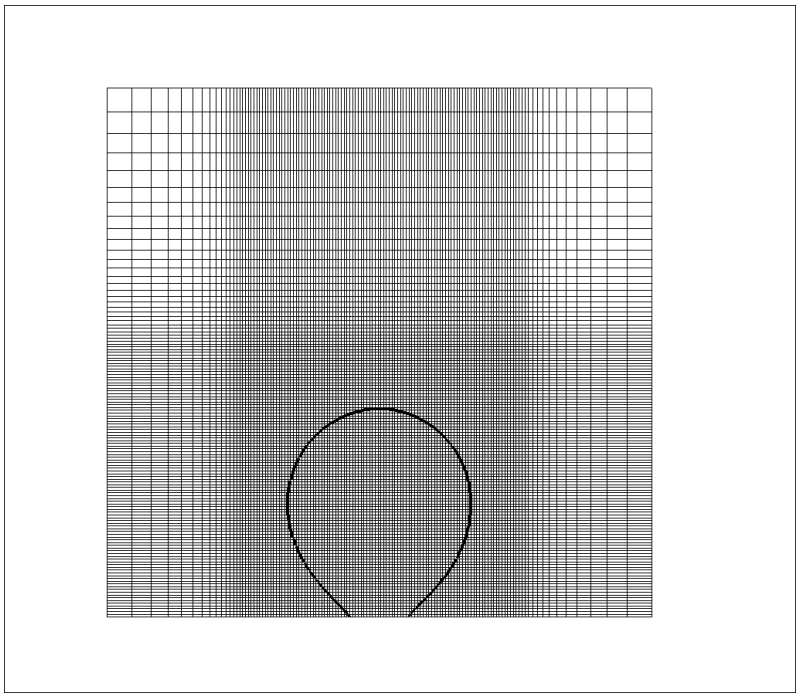
Step 3 : Compute the boiling mass flow rate from the discontinuity of thermal flux

$$\dot{m} = \frac{[k \nabla T \cdot \vec{n}]_\Gamma}{L_{vap}}$$

5. Nucleate Boiling : numerical simulation

- 2D axisymetric non-uniform mesh.
- Wall thermal conduction.
- Initial thermal boundary layer (Kays and Crawford, 1980).
- *Ja = 21* (ΔT=7 K) , θ_{app} = 50° , ρ_{liq}/ρ_{vap} = 1604

$$Ja = \frac{\rho_l Cp_l (T_{paroi} - T_{sat})}{\rho_v L_v}$$



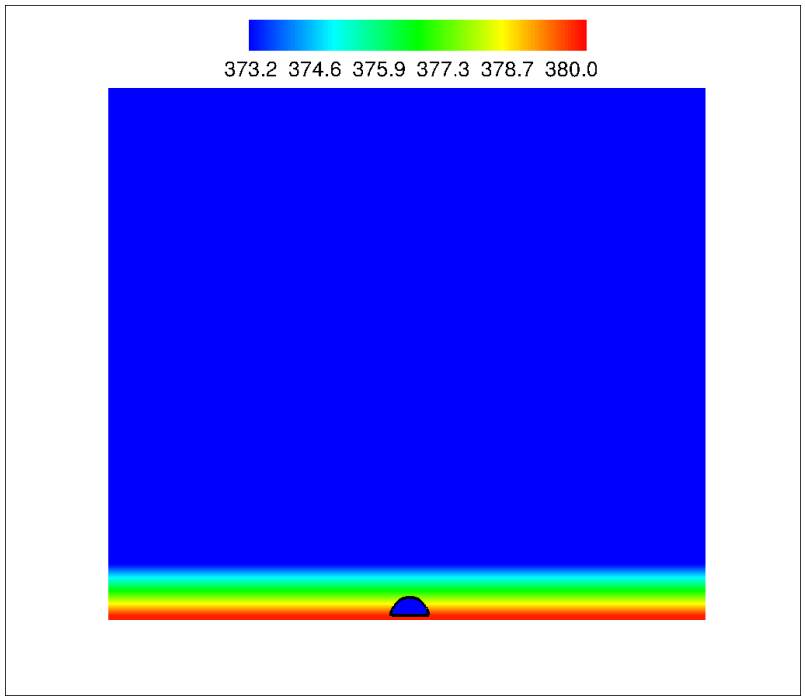
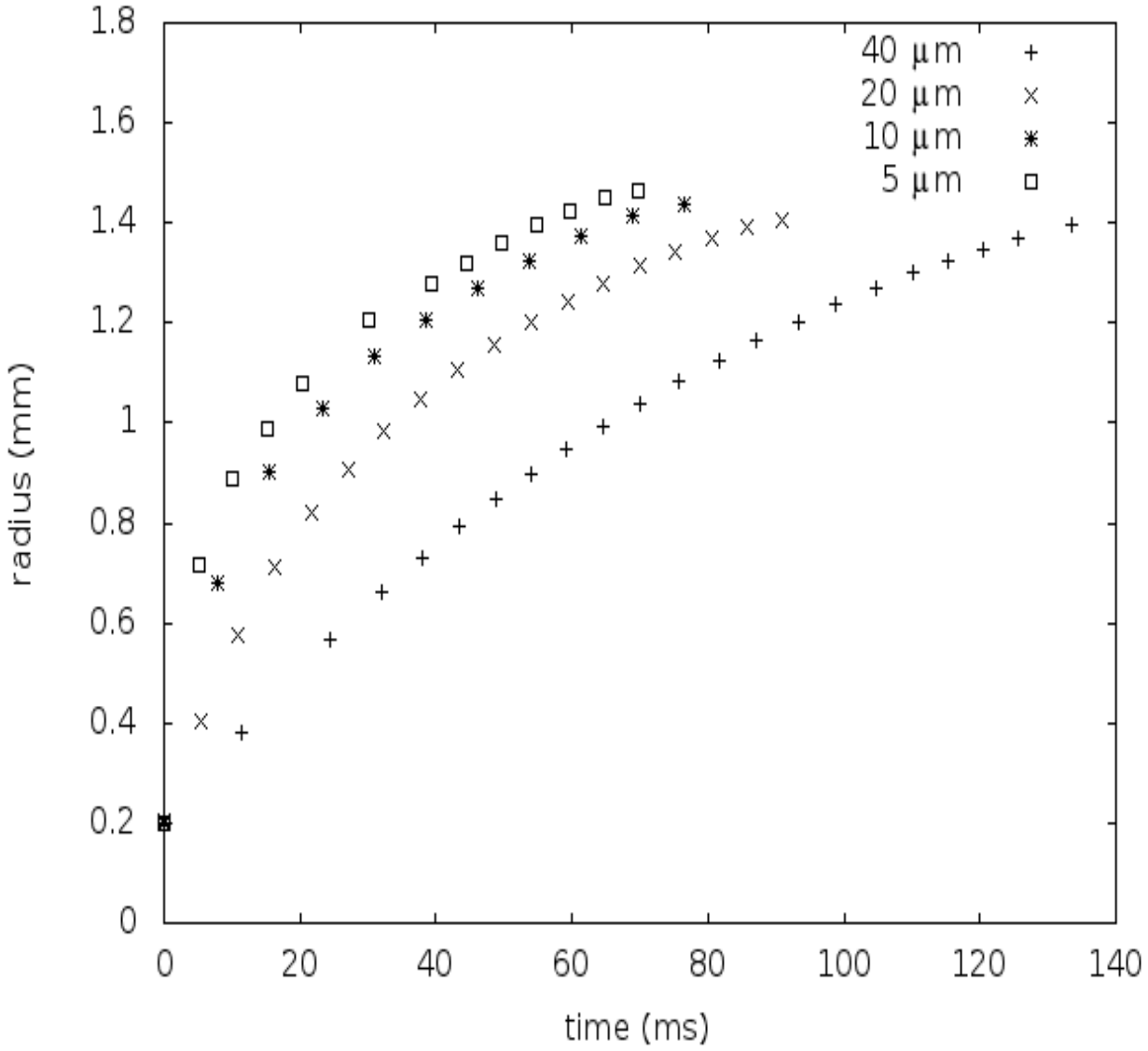


Figure : Example of a Non-uniform axisymetric mesh

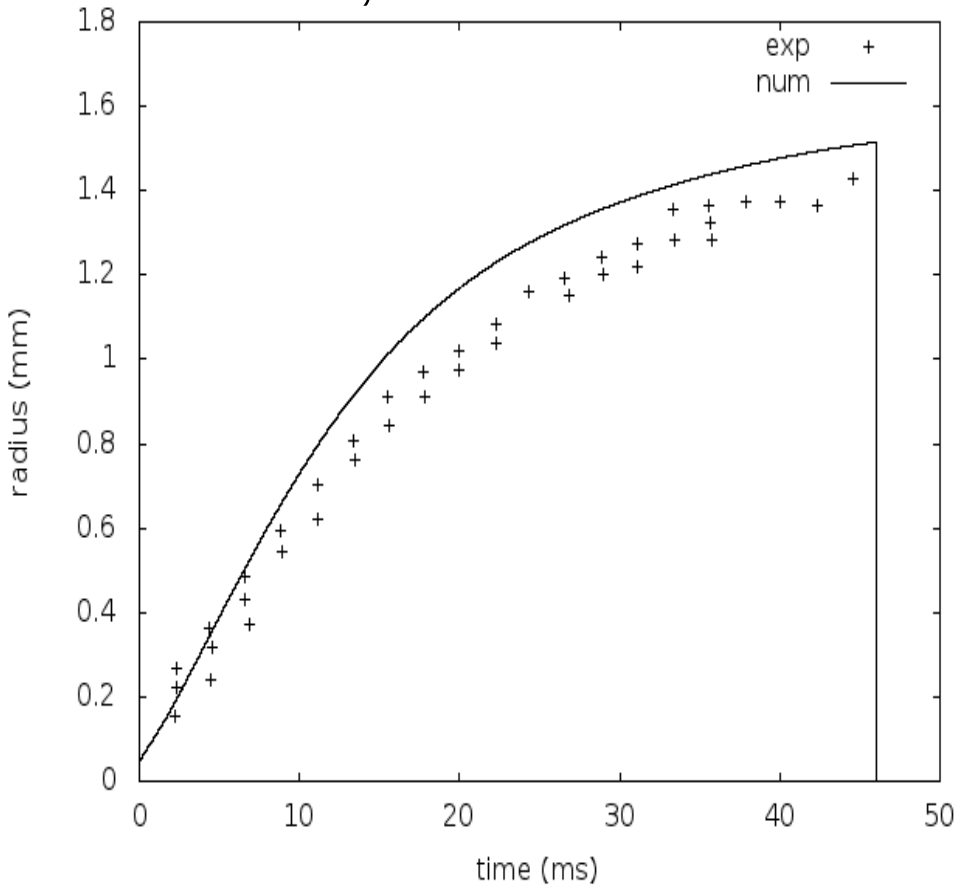
- 6. Nucleate Boiling : spatial convergence



Grid sensitivity study on the bubble radius

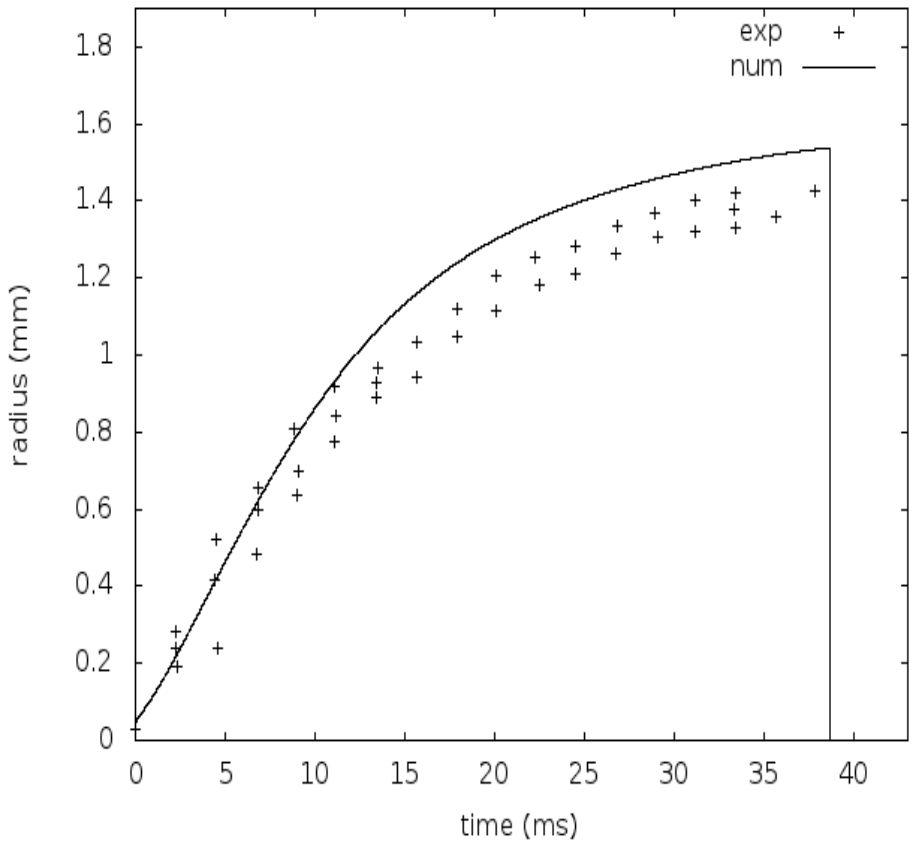
- 7. Nucleate Boiling : Comparisons between simulations and experimental results

Ja = 21 , ΔT=7 K



Departure radius relative error: 5.94%
Departure period relative error: 4.90%

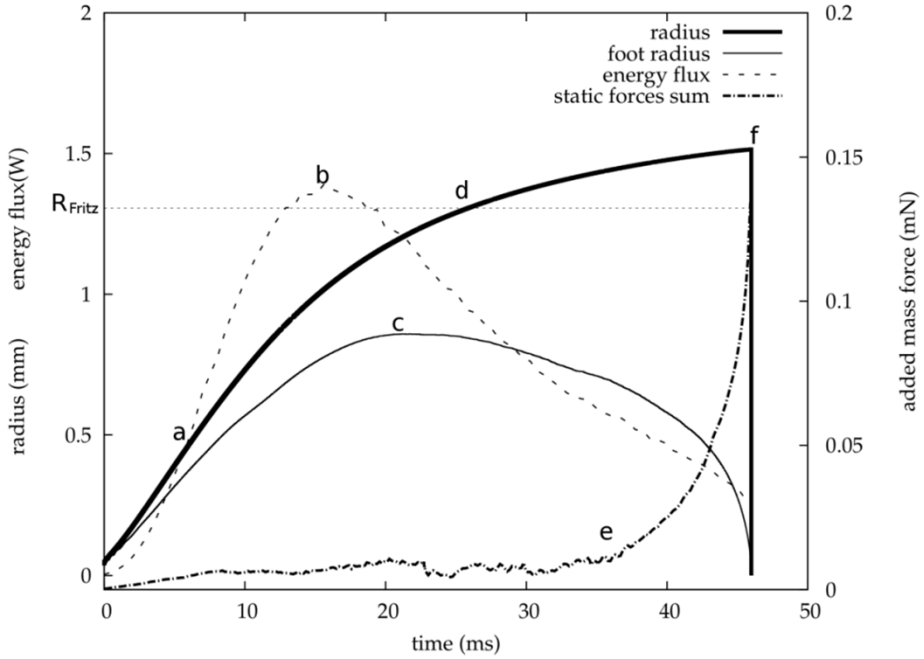
Ja = 25.5 , ΔT=8.5 K



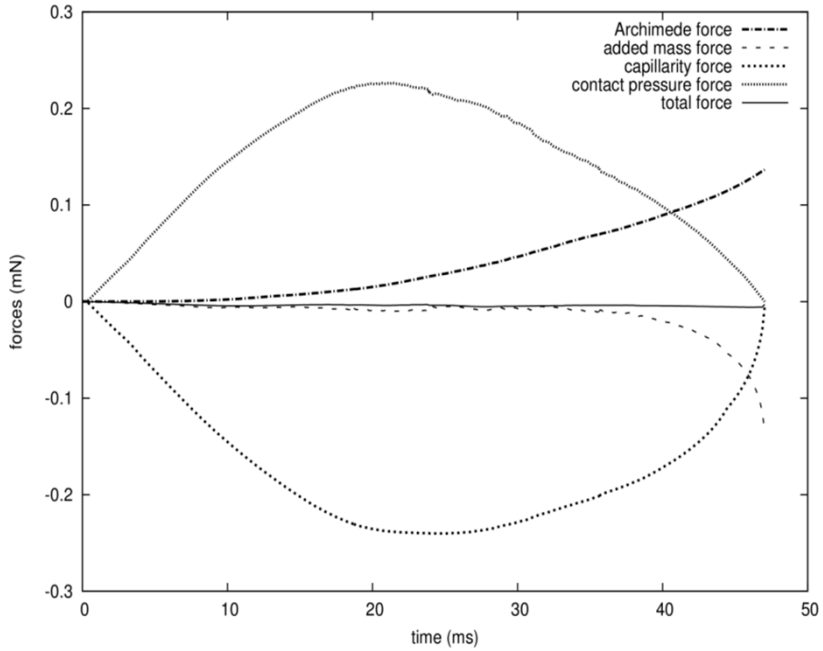
Departure radius relative error: 7.78%
Departure period relative error: 3.59%

Comparison between numerical results and experimental results (Son & Dhir, 1999).

8. Nucleate Boiling : analysis on the forces acting on the bubble



Evolution of the equivalent radius, of the foot radius, of the heat flux received by the vapor bubble and of the forces sum acting on the bubble



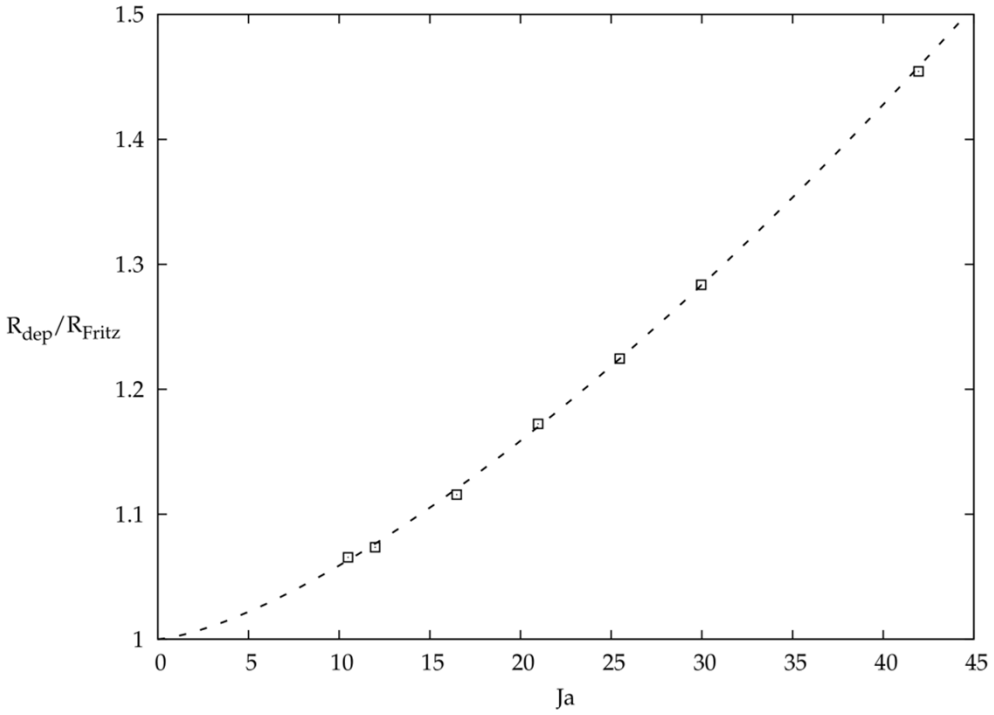
Temporal evolution of the forces acting on the bubble during one growth cycle

$$R_{Fritz} = 0.104\theta \sqrt{\frac{\sigma}{g(\rho_L - \rho_V)}} .$$

- 9. Nucleate Boiling: a simplified correlation on bubble radius departure

$$\frac{R_{dep}}{R_{Fritz}} = 1 + f\left(Ja, Pr, \theta_{micro}, \frac{\delta}{R_{fritz}}, \frac{\rho_l}{\rho_v} \ldots\right)$$

$$R_{Fritz} = 0.104\theta \sqrt{\frac{\sigma}{g(\rho_L - \rho_V)}}\,.$$



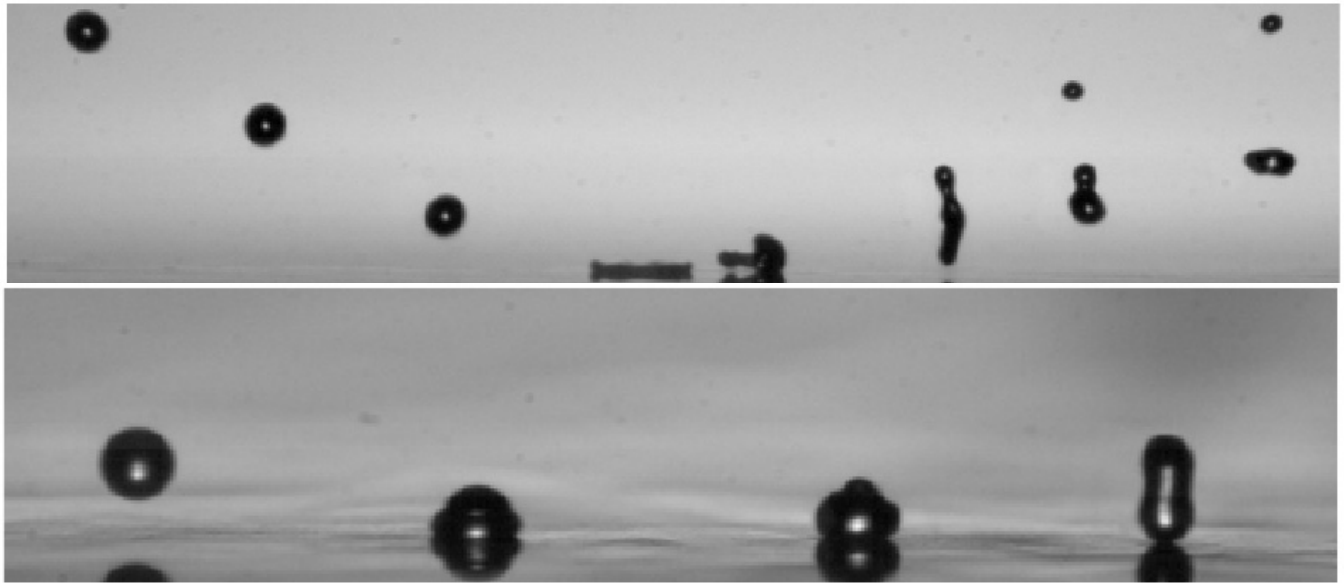
Variation of the dimensionless departure radius with the Jakob number

$$\frac{R_{dep}}{R_{Fritz}} = 1 + \alpha Ja^n$$

$\alpha = 0.00219$ and $n = 1.43$

G. Huber, S. Tanguy, M. Sagan, C. Colin, Direct Numerical Simulation of Nucleate Pool Boiling at large microscopic contact angle and moderate Jakob number . *Submitted IJHMT*

10. Leidenfrost droplets : evaporation and boiling



Experiments from
Dunand, Lemoine &
Castanet
Experiments in Fluids
2013

Many physical processes involved in this phenomenon :

- Formation of a very thin vapor layer between the plate and the bottom of the droplet
- Strong droplet deformation
- Phase change : transition between boiling and two components evaporation
- Marangoni convection
- Compressibility effects

Performing fully resolved Direct Numerical Simulations of this phenomenon is challenging

- 11. Ghost Fluid Thermal Solver for Evaporation (S. Tanguy, T. Menard, A. Berlemont, JCP 2007)

Step 1 : Update mass fraction field in the gas phase with a prescribed Dirichlet boundary condition at the interface

$$\rho_g Y_1^{n+1} - \Delta t \nabla \cdot \left(\rho_g D_m \nabla Y_1^{n+1}\right) = \rho_g \left(Y_1^n - \Delta t \vec{V}_g^n \cdot \nabla Y_1^n\right) \qquad if \phi < 0$$

$$Y_1\Big|_\Gamma = \frac{P_1|_\Gamma M_1}{P_1|_\Gamma M_1 + (P_0 - P_1|_\Gamma) M_2}$$

$$P_1|_\Gamma = P_0 e^{-\frac{L_{vap} M_1}{R}\left(\frac{1}{T|_\Gamma} - \frac{1}{T_{sat}}\right)}$$

Step 2 : Deduce the mass flow rate of evaporation from the mass fraction field in the gas phase

$$\dot{m} = \frac{\rho_g D_m \nabla Y_1 \cdot \vec{n}|_\Gamma}{1 - Y_1|_\Gamma}$$

Step 3 : Compute simultaneously in the two phases the temperature field with an imposed jump condition on the thermal flux

$$\rho Cp T^{n+1} - \Delta t \nabla \cdot \left(k \nabla T^{n+1}\right) = \rho Cp \left(T^n - \Delta t B\left(\vec{V}^n, T^n\right)\right)$$

$$[k \nabla T \cdot \vec{n}]_\Gamma = \dot{m}\left(L_{vap} + \left(C_{pliq} - C_{pvap}\right)\left(T_{sat} - T\Big|_\Gamma\right)\right)$$

- 12. Ghost Fluid Thermal Solver for Boiling and Evaporation GFTSBE (L. Rueda Villegas, R. Alis, M. Lepilliez, S. Tanguy, JCP 2016)

Step 1 : Update separately the temperature field in the liquid phase with a prescribed non-uniform Dirichlet boundary condition at the interface

$$\rho_l Cp_l T_l^{n+1} - \Delta t \nabla \cdot \left(k_l \nabla T_l^{n+1}\right) = \rho_l Cp_l \left(T_l^n - \Delta t \vec{V}_l^n \cdot \nabla T_l^n\right) \qquad if\, \phi > 0$$

$$\rho_g Cp_g T_g^{n+1} - \Delta t \nabla \cdot \left(k_g \nabla T_g\right) = \rho_g Cp_g \left(T_g^n - \Delta t \vec{V}_g^n \cdot \nabla T_g^n\right) \qquad if\, \phi < 0$$

$$T\big|_\Gamma = \frac{L_{vap} M_1 T_{sat}}{L_{vap} M_1 - R T_{sat} ln\left(\frac{P_1|_\Gamma}{P_0}\right)}$$

$$P_1\big|_\Gamma = \frac{-Y_1|_\Gamma P_0 M_2}{(M_1 - M_2) Y_1|_\Gamma - M_1}$$

Step 2 : Compute the phase change mass flow rate from the thermal flux jump condition

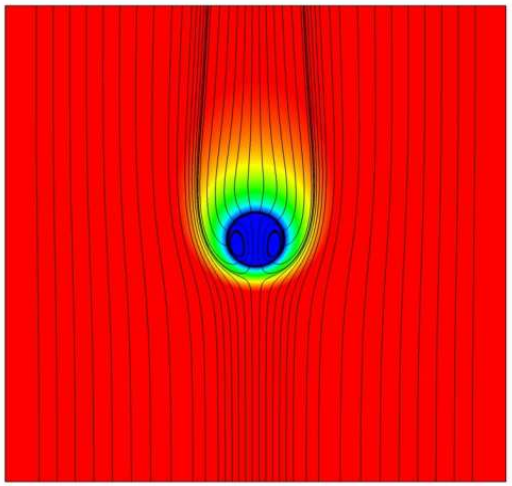
$$\dot{m} = \frac{[k \nabla T \cdot \vec{n}]_\Gamma}{L_{vap}}$$

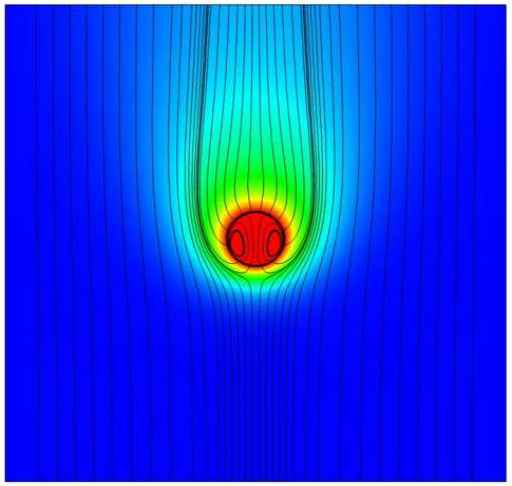
Step 3 : update the mass fraction field in the gas phase with a prescribed robin boundary condition at the interface

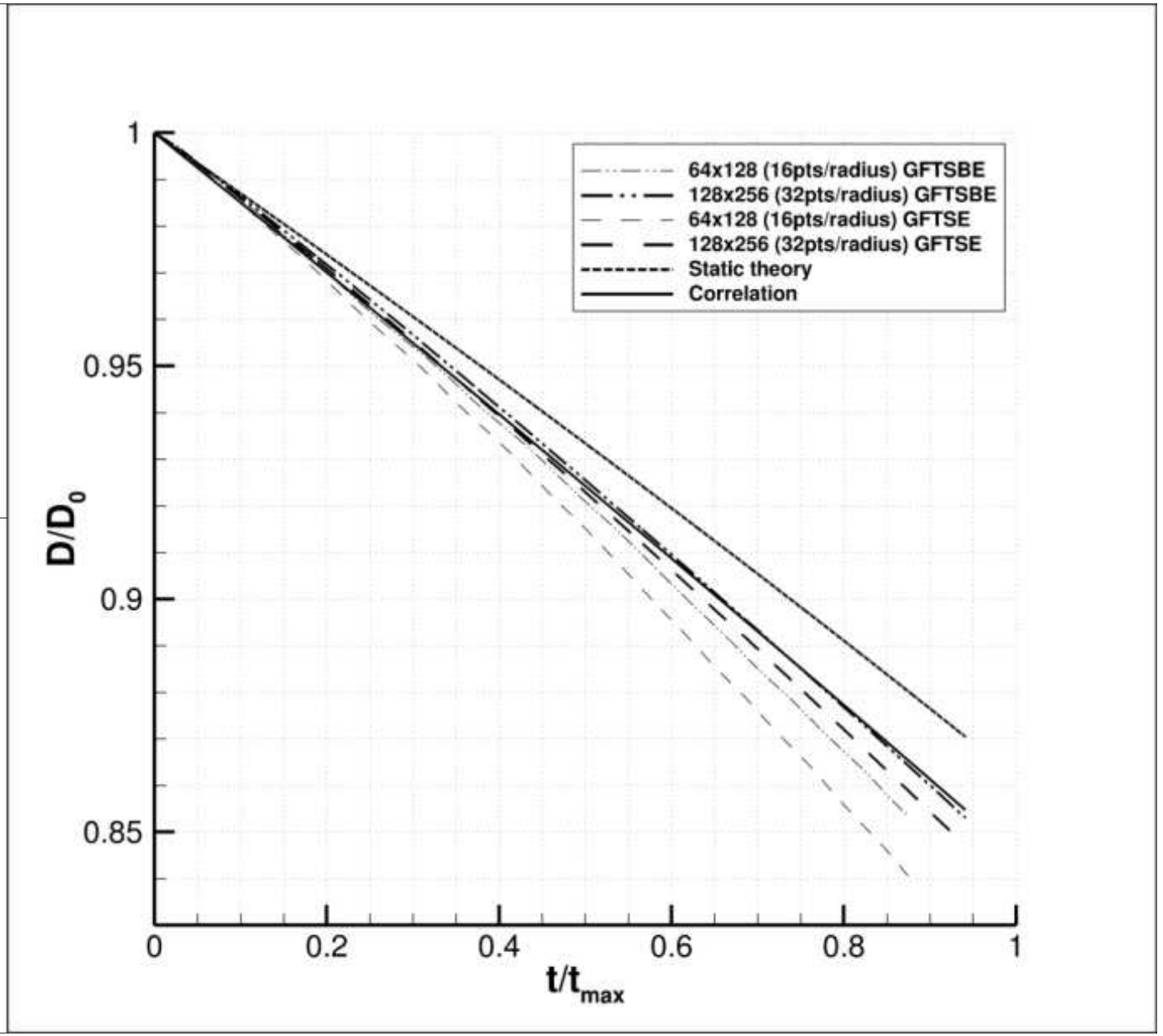
$$\rho_g Y_1^{n+1} - \Delta t \nabla \cdot \left(\rho_g D_m \nabla Y_1^{n+1}\right) = \rho_g \left(Y_1^n - \Delta t \vec{V}_g^n \cdot \nabla Y_1^n\right) \qquad if\, \phi < 0$$

$$\dot{m} Y_1|_\Gamma + \rho_g D_m \nabla Y_1 \cdot \vec{n}|_\Gamma = \dot{m}$$

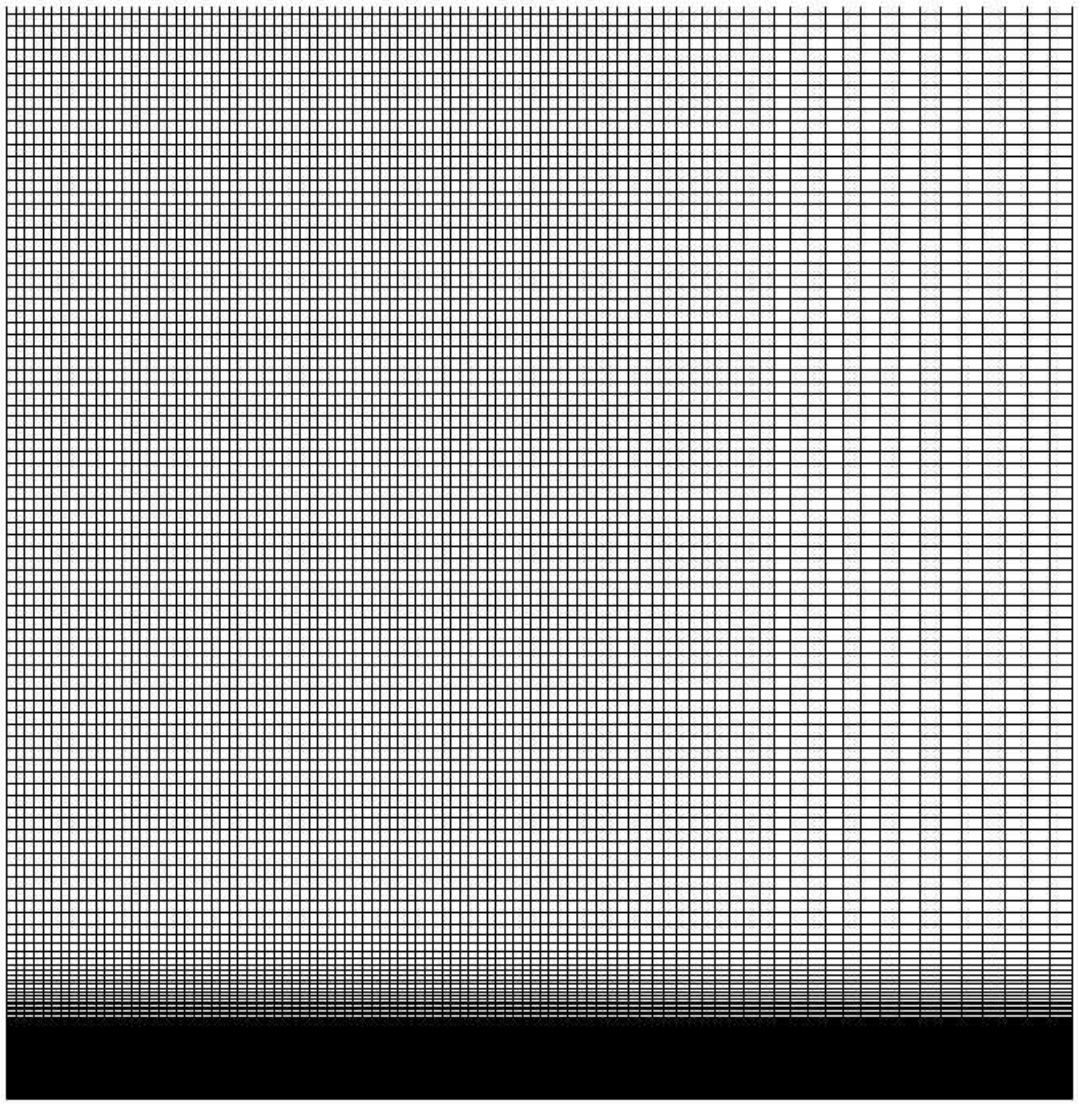
13. Moving droplet evaporation







- 14. Very refined grids to capture the formation of the thin vapor layer



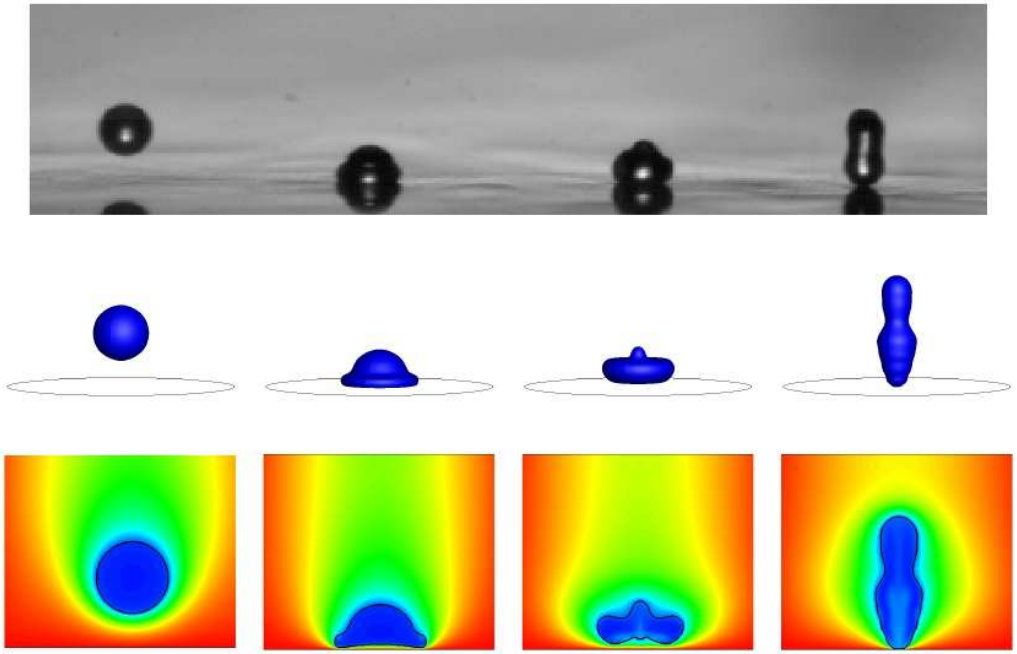
Implicit temporal discretizationf for all the diffusion terms

- 1 linear system to solve for pressure
- 2 linear systems to solve the 2 velocity component
- 1 linear system to solve liquid temperature
- 1 linear system to solve the gas temperature
- 1 linear system to solve the mass fraction field
- 1 linear system to compute a ghost field for Pressure

- 7 linear systems at each time step

All these linear systems are symmetric definite positive and can be solved with standard black box tool

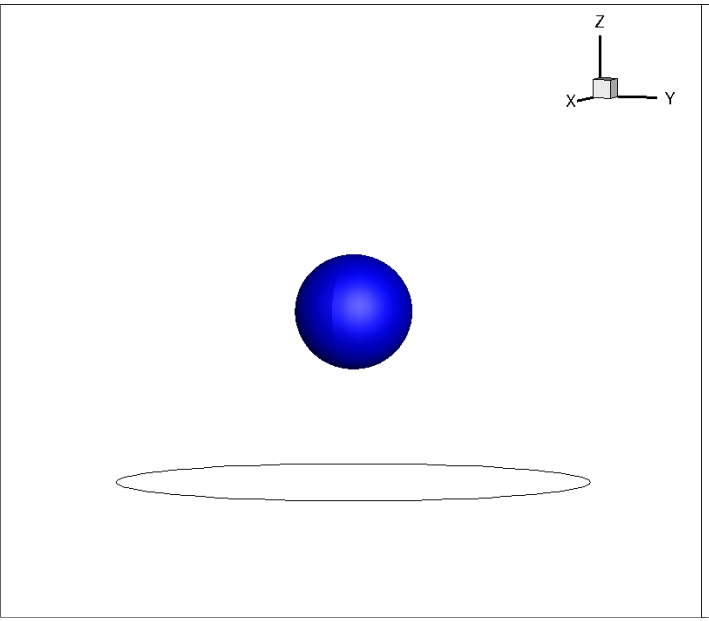
15. Comparisons of simulations with experimental data : We = 7.5

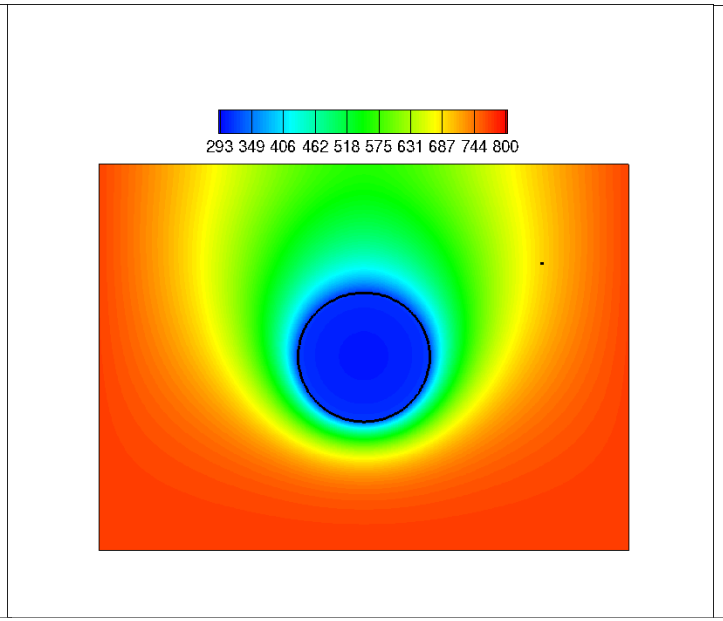


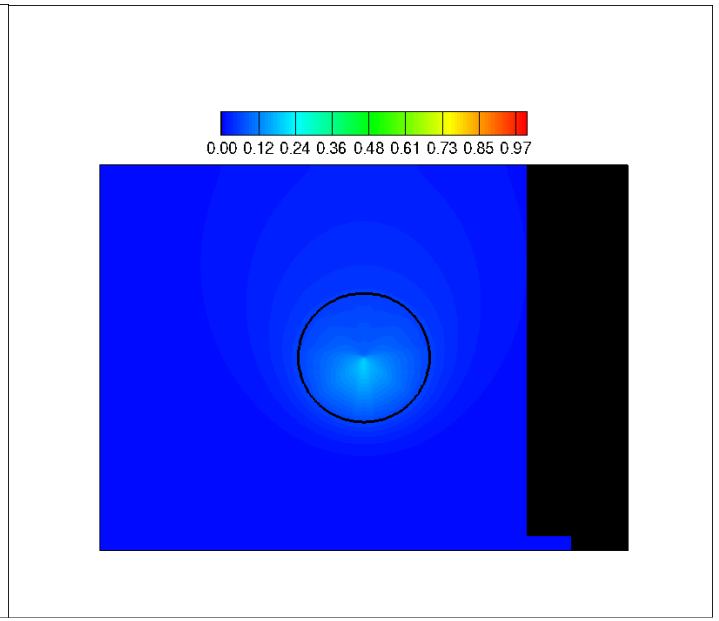
Water droplet
Tw = 823 K

2D axisymetric simulations

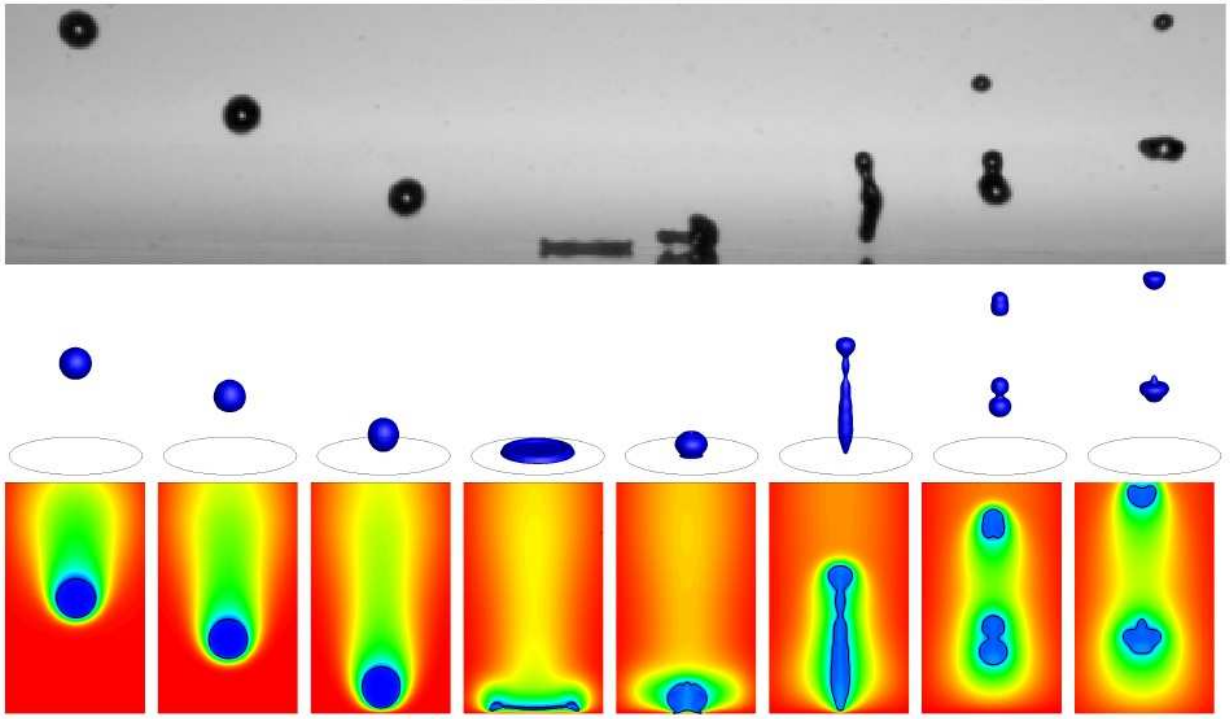
Experiments from
Dunand, Lemoine & Castanet
Experiments in Fluids 2013







16. Comparisons of simulations with experimental data : We = 45



Water droplet
Tw = 823 K

2D axisymetric simulations

Experiments from
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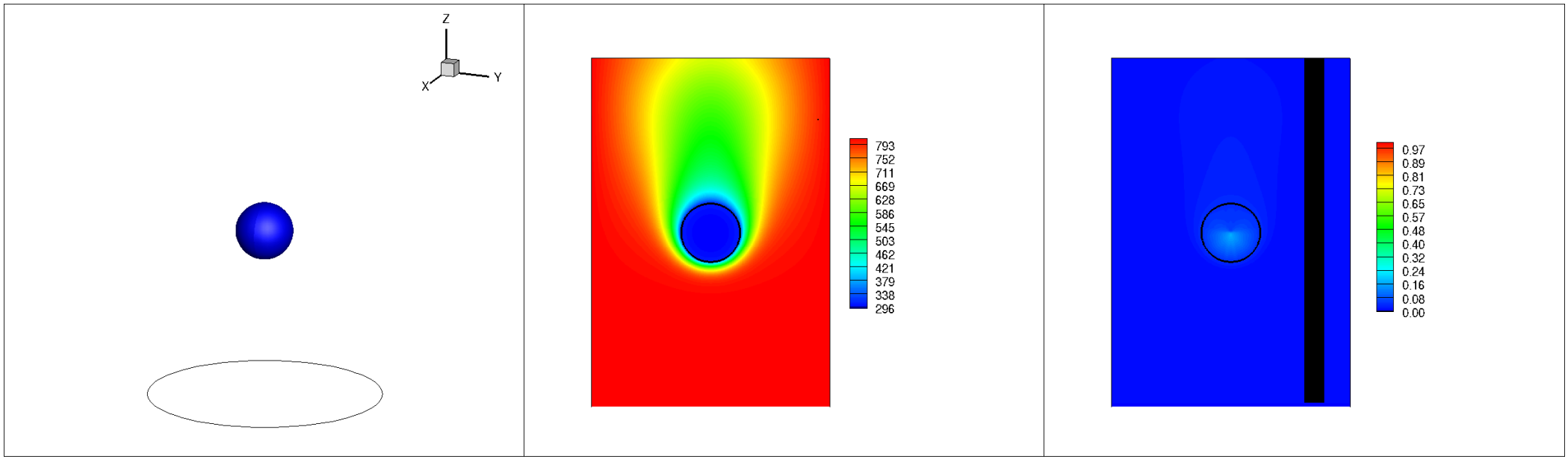
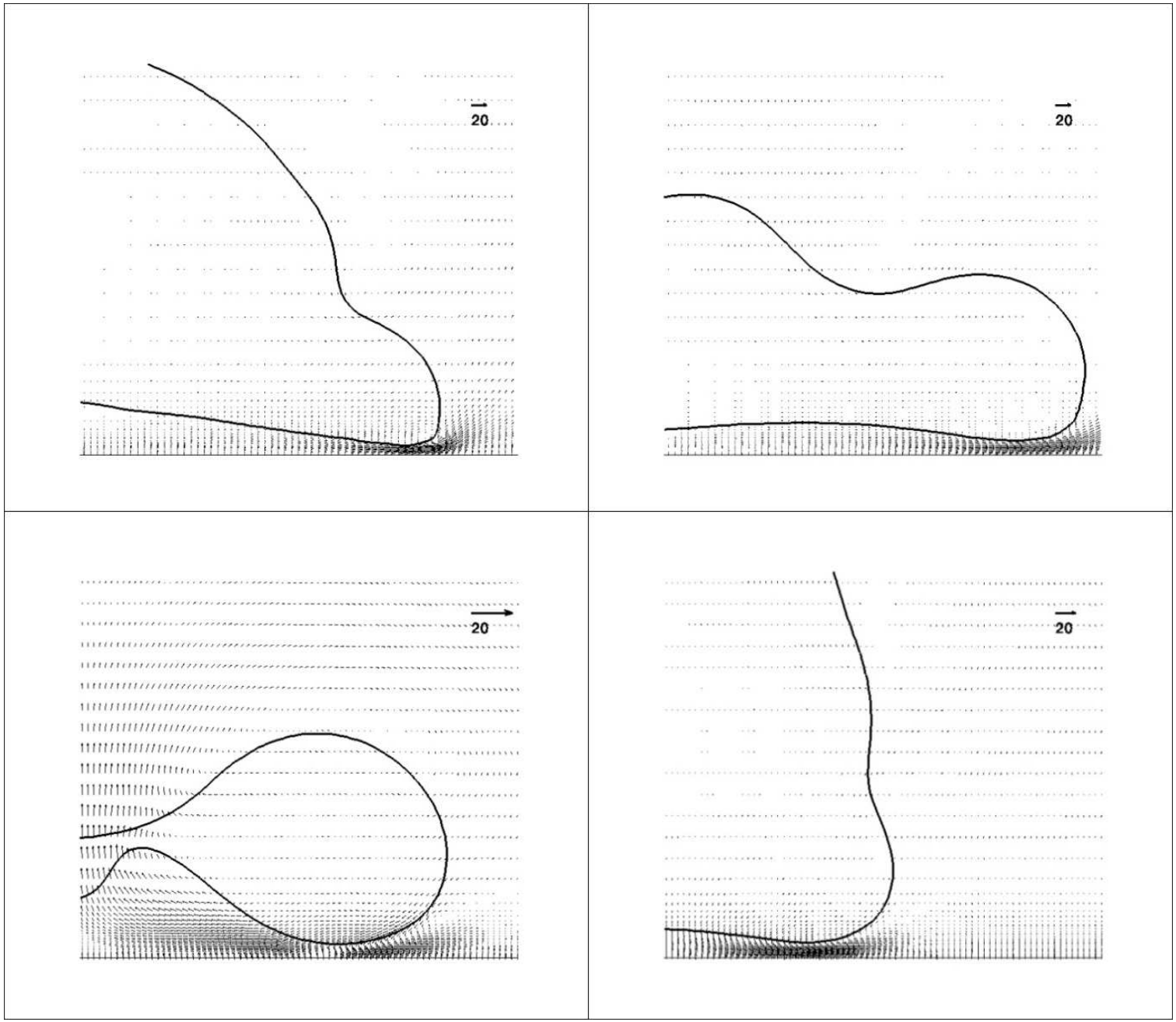
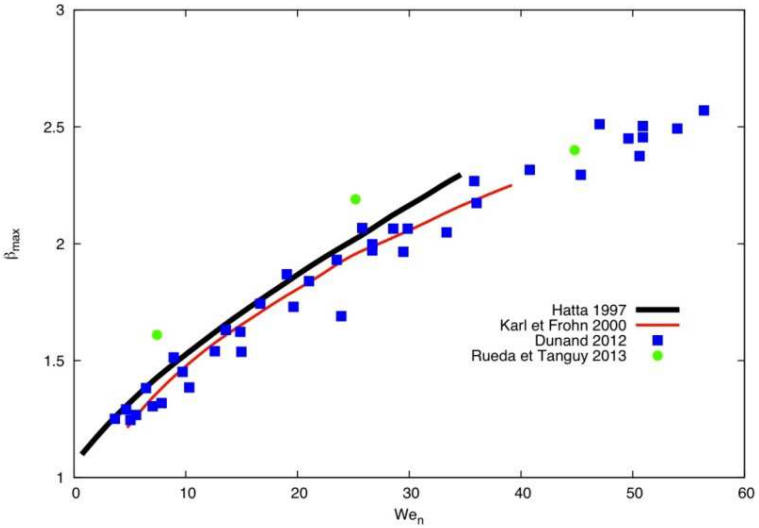


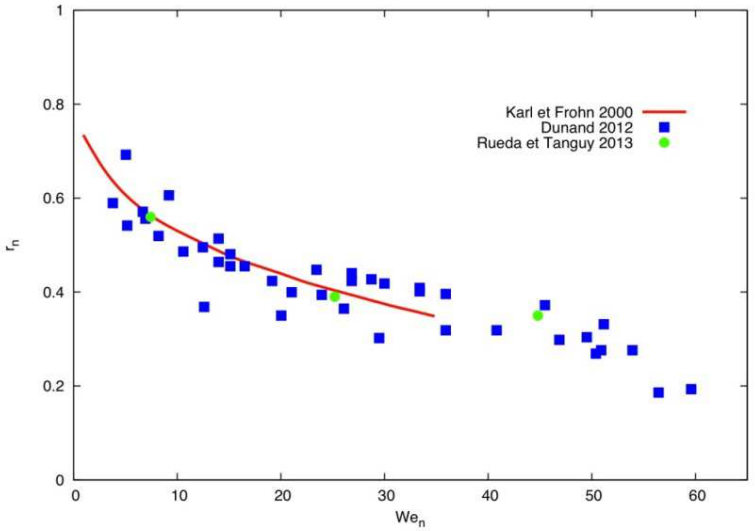
- 17. Velocity field snapshots in the vapor layer



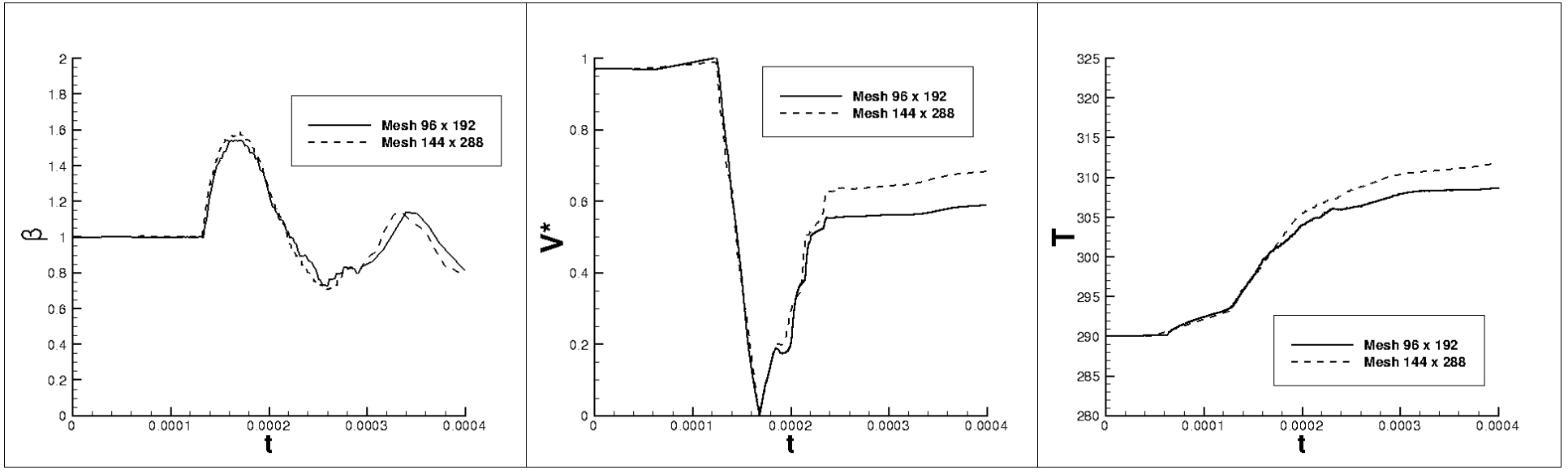
- 18. Quantitative Comparisons and grid sensitivity studies (L. Rueda Villegas, S. Tanguy, G. Castanet, O. Caballina, F. Lemoine, IJHMT 2017)



Maximum spreading diameter vs incident Weber Number

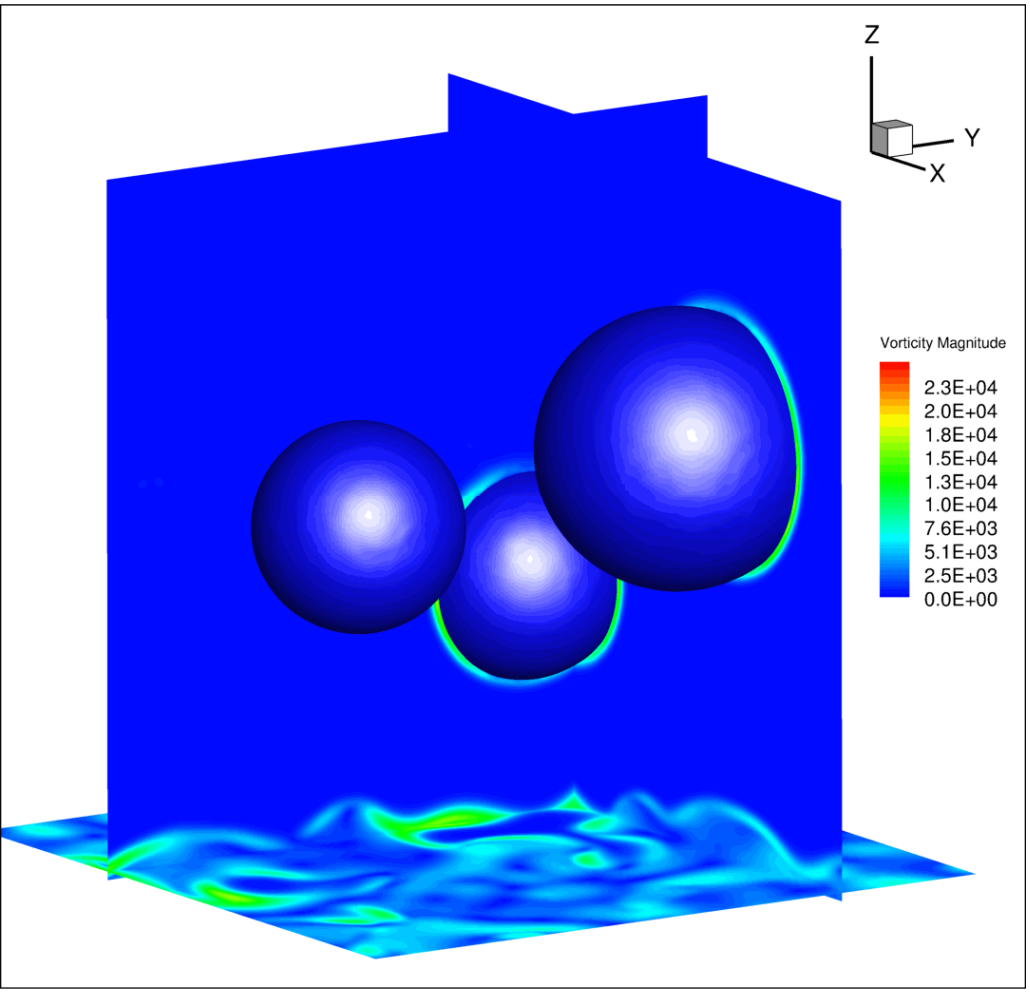


Restitution coefficient vs incident Weber Number



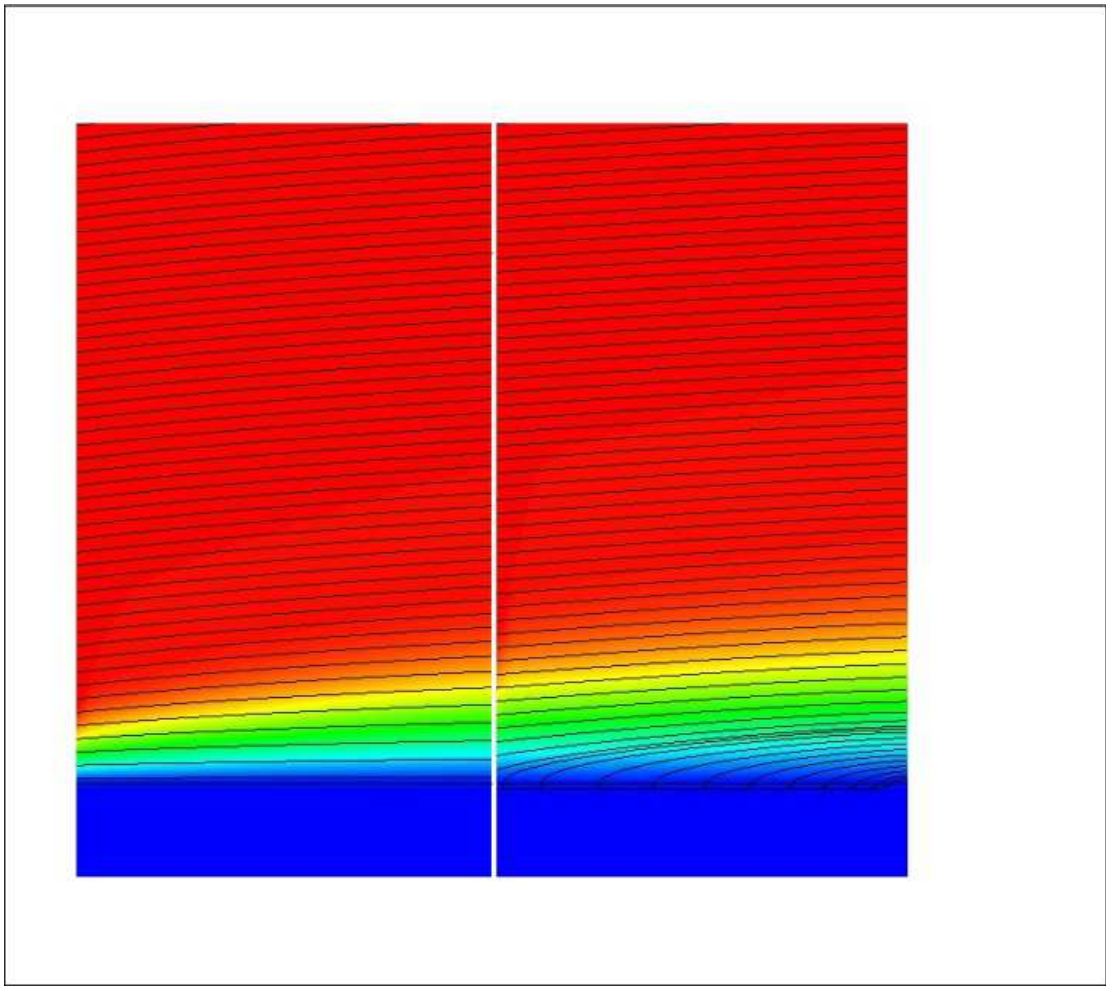
19. Perspectives: interaction phase change/external flow

Droplets in a turbulent flow
(Work in progress PhD Thesis R. Alis)



Parallel simulation on a 256 x 256 x 256 grid
with a Black Box MultiGrid solver
for solving linear systems

Liquid pool sheared by a superheated vapor flow
(Work in progress PhD Thesis E. R. Popescu



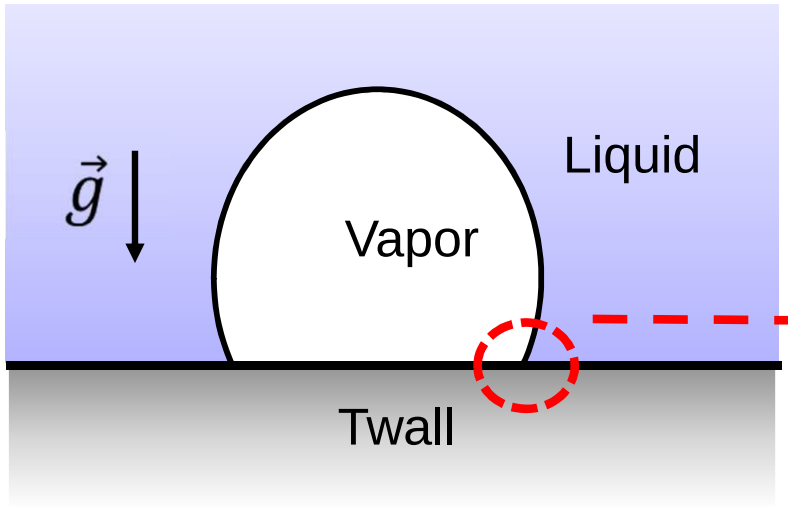
2D Simulation on a 1024 x 1024 grid
with a Black Box MultiGrid solver
for solving linear systems

- 20. Thanks for funding Institutes

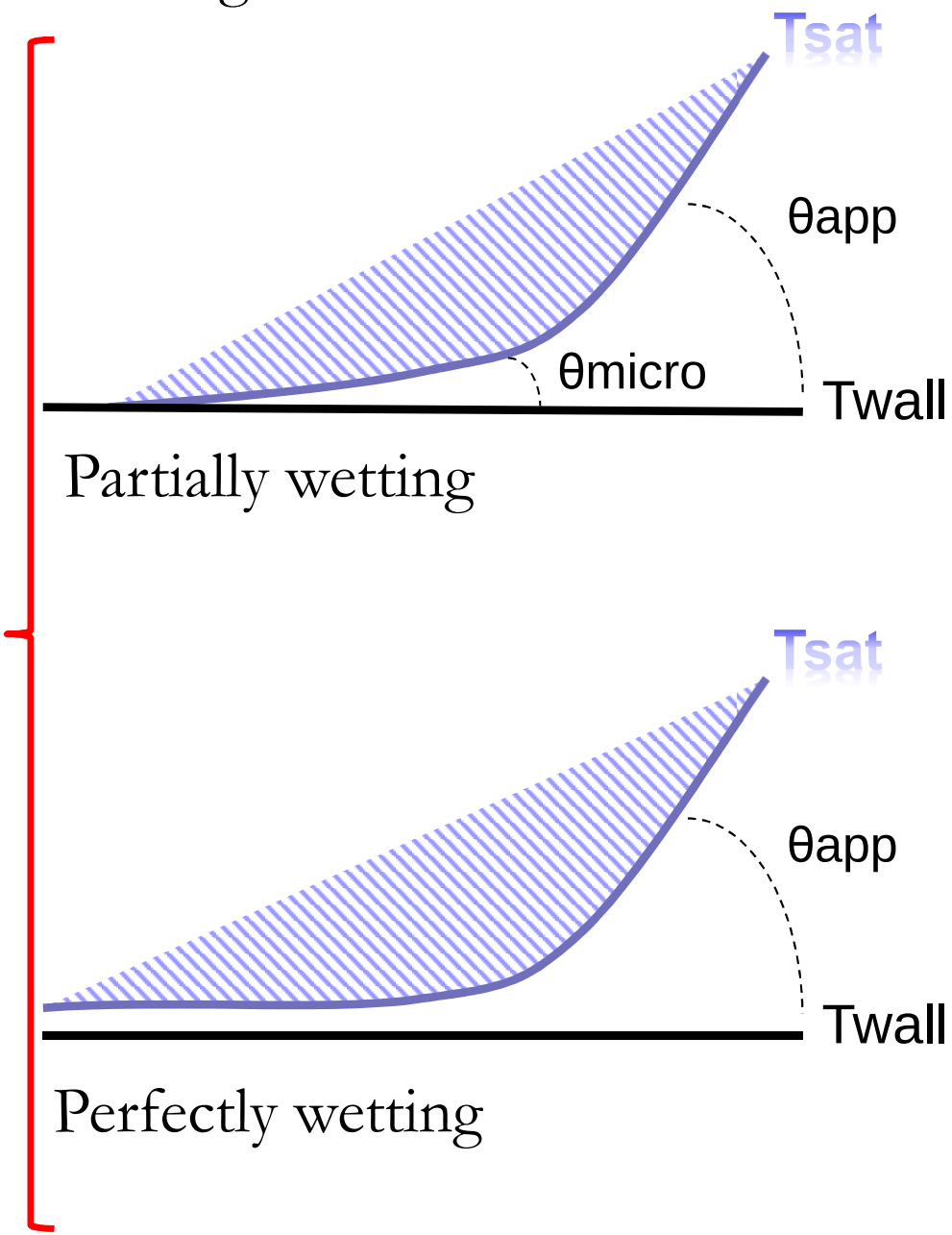
- ANR for the financial support of L. Rueda Villegas PhD thesis on « the Direct Numerical Simulation of Leidenfrost effect » in the framework of the IDHEAS Project

- CNES for supporting the Phd Thesis of Michaël Sagan and the postdoc of Grégory Huber on « the Direct Numerical Simulation of Nucleate Boiling »

- Nucleate Boiling : Micro region or not micro region ?

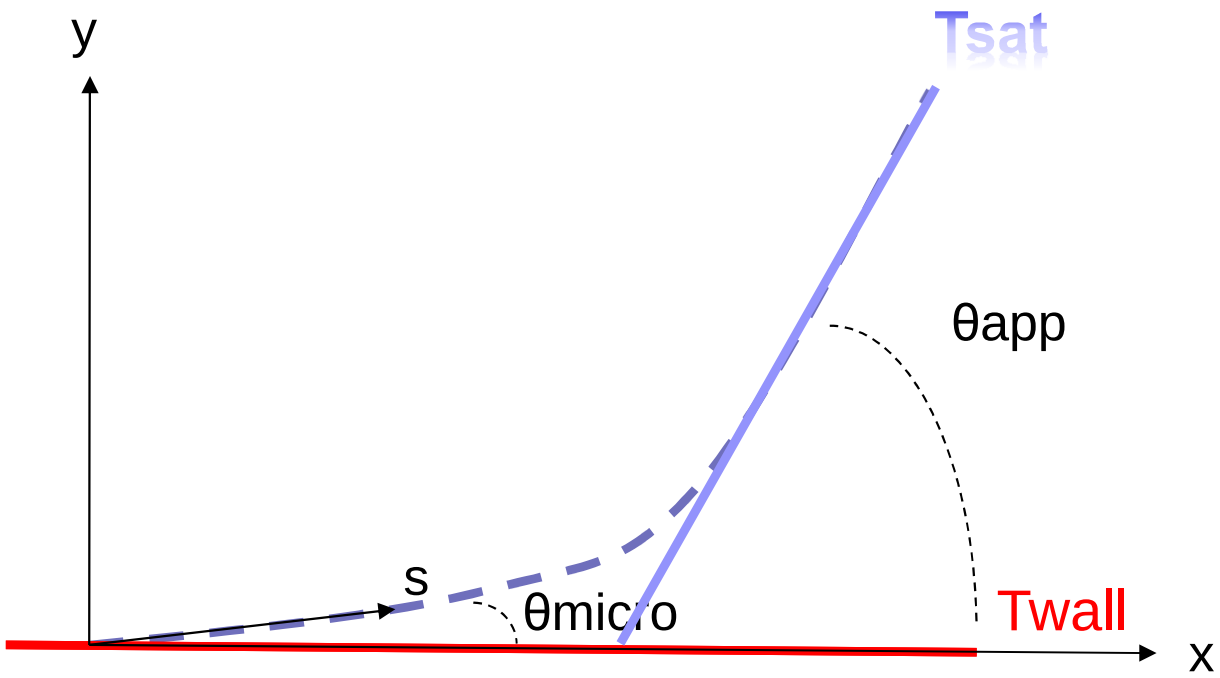


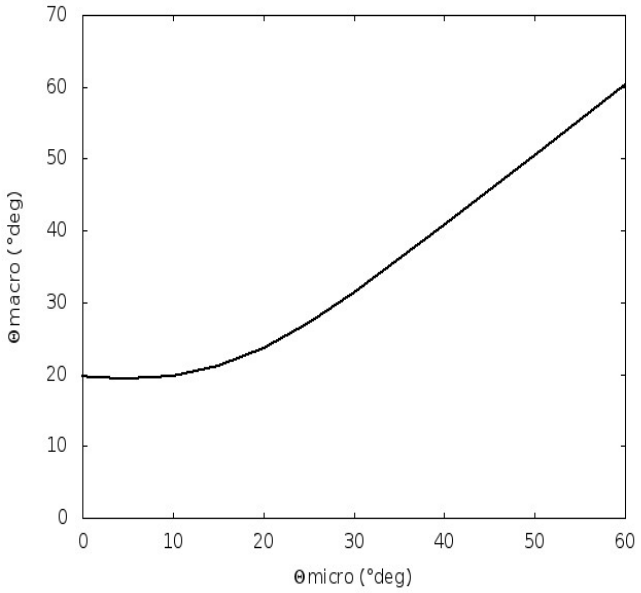
$\Delta T = Twall - Tsat = 7\ K$

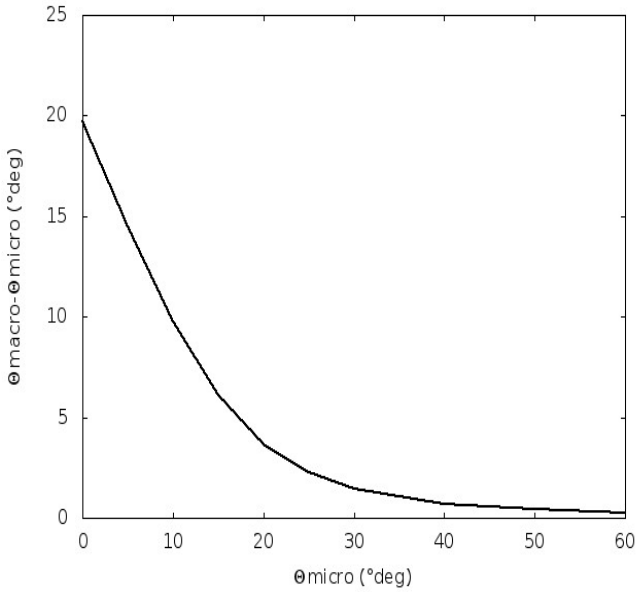


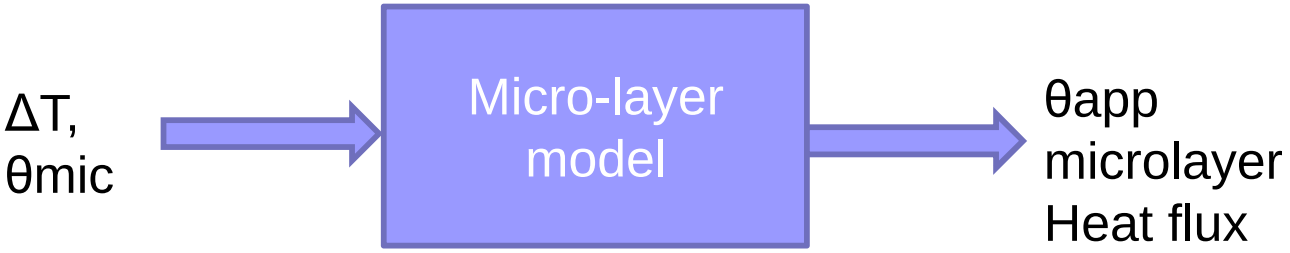
Micro layer description

- Nucleate Boiling : Micro region or not micro region ?









$$\Delta T = 7K, \theta_{app} = 50° \Leftrightarrow \theta_{mic} = 49{,}66°$$