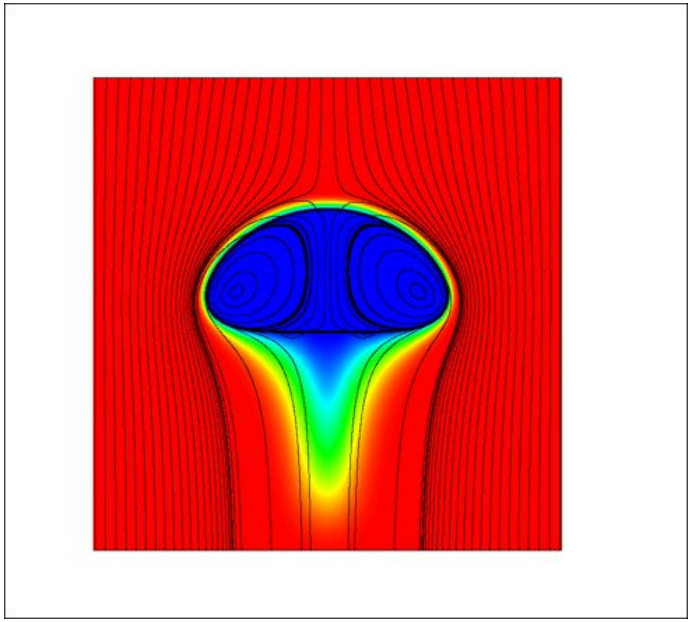
Direct Numerical Simulation of Two-Phase Flows with phase change



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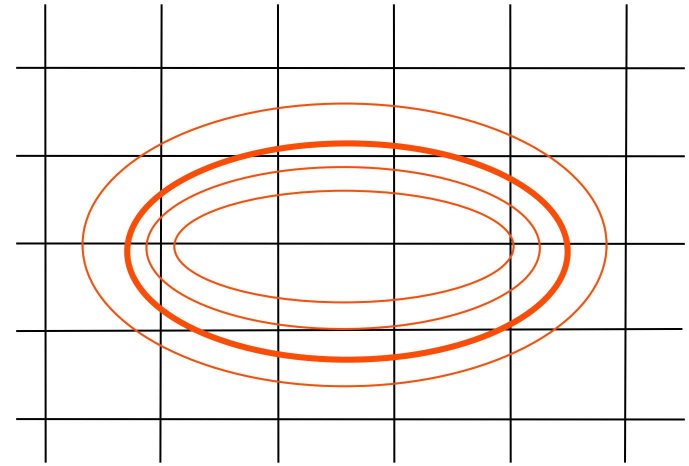
1. Level Set Method



ϕ : signed distance function

$\phi < 0$ Gas phase

$\phi = 0$ Liquid-gas interface

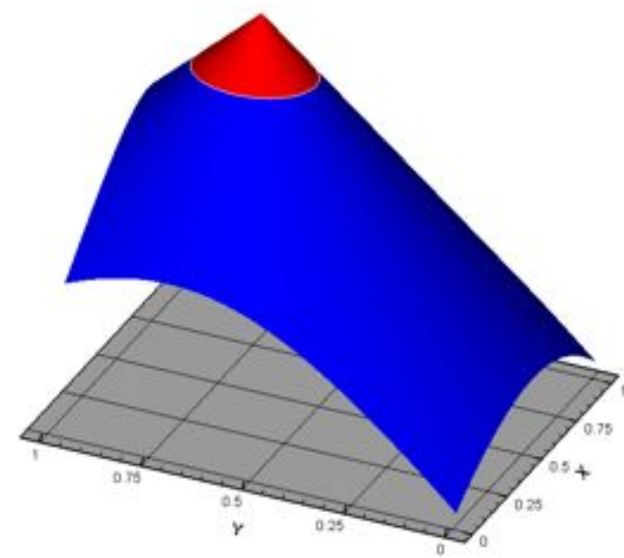
$\phi > 0$ Liquid phase

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 & al, JCP 1994)



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

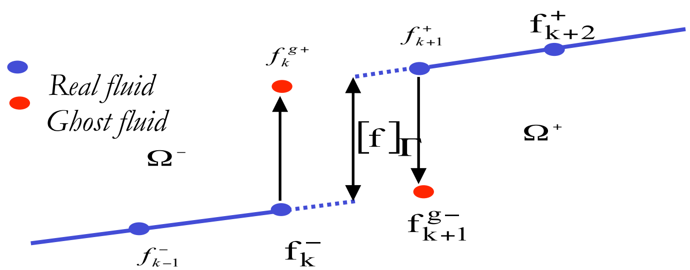
Numerical schemes : Runge-Kutta 2 or 3 and fifth order WENO-Z

2. The Ghost Fluid Method : a Sharp Interface Method

Ghost Fluid Method (Fedkiw & 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 & al, JCP 2000)

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

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

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

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

3. Conservation laws and jump conditions

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

- 4. Ghost Fluid Thermal Solver for Boiling GFTSB (Gibou & al, JCP 2007, Tanguy & 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).
- Contact angle set at 50°.

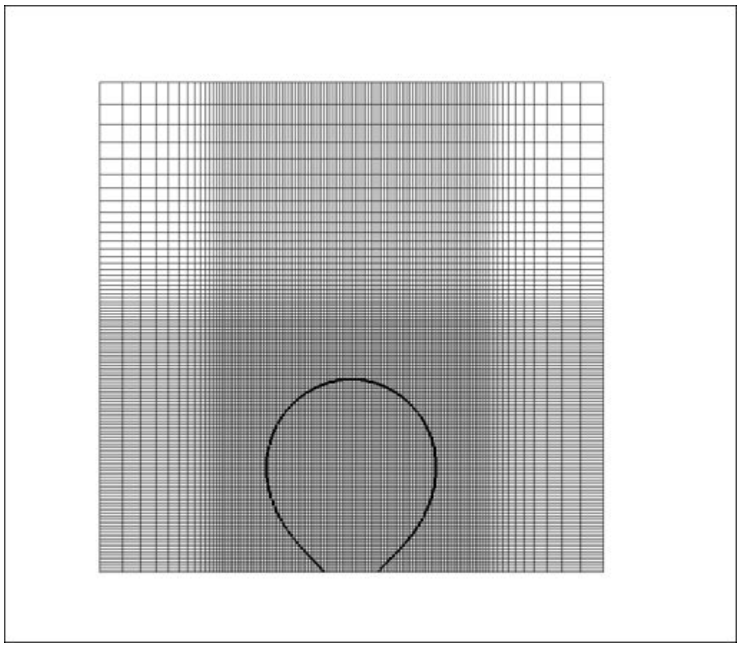
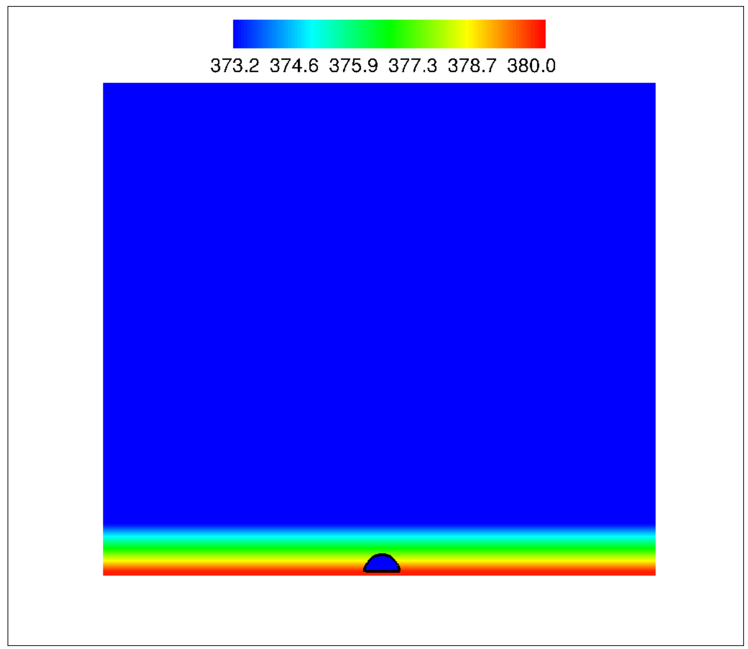
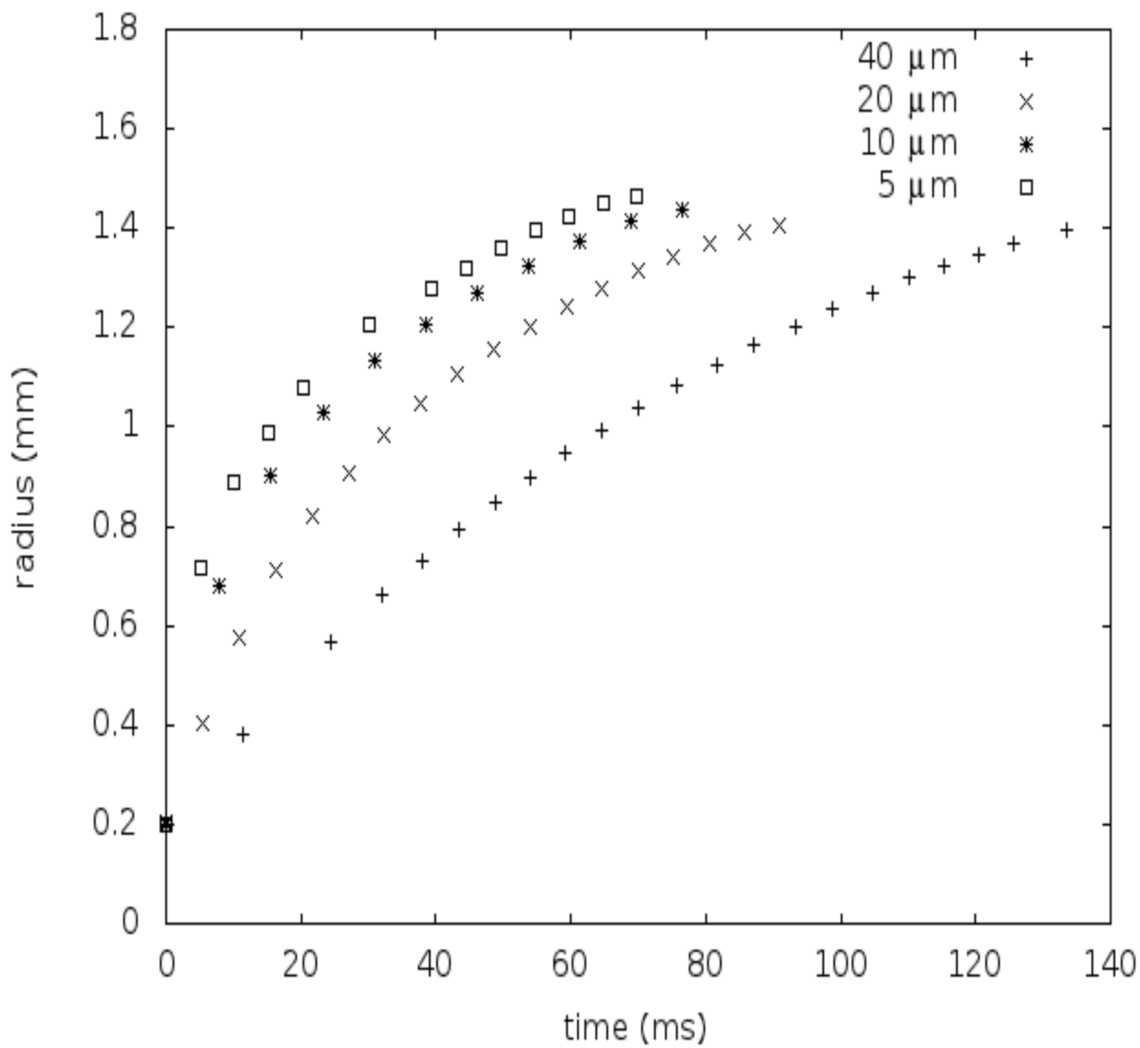


Figure : Example of a Non-uniform axisymetric mesh



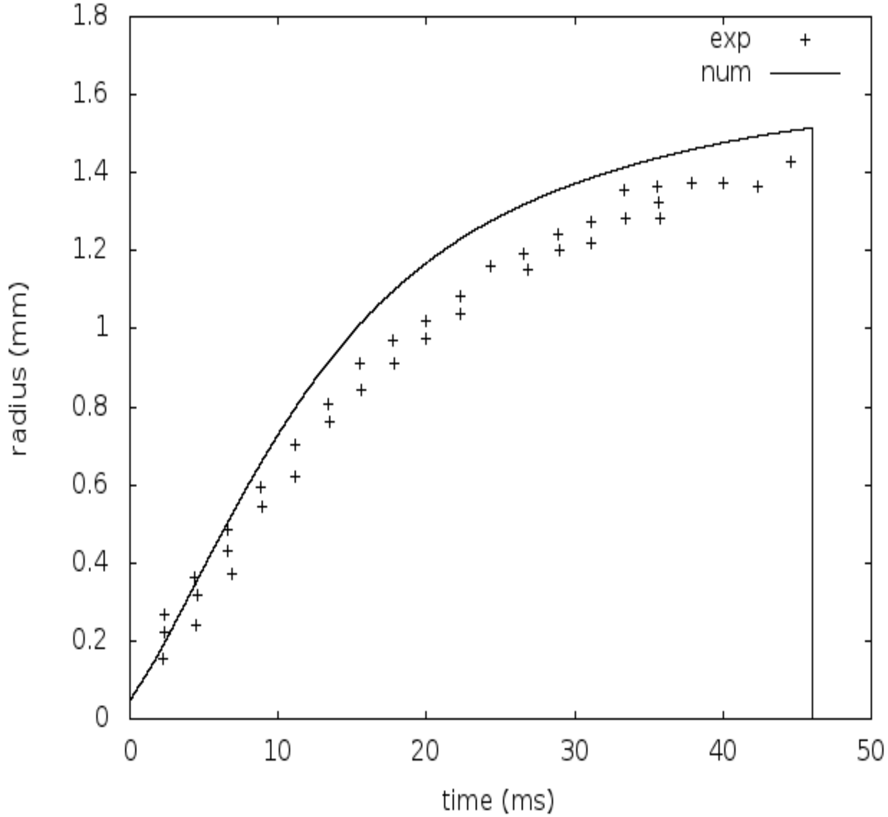
6. Nucleate Boiling : spatial convergence



Grid sensitivity study on the bubble radius

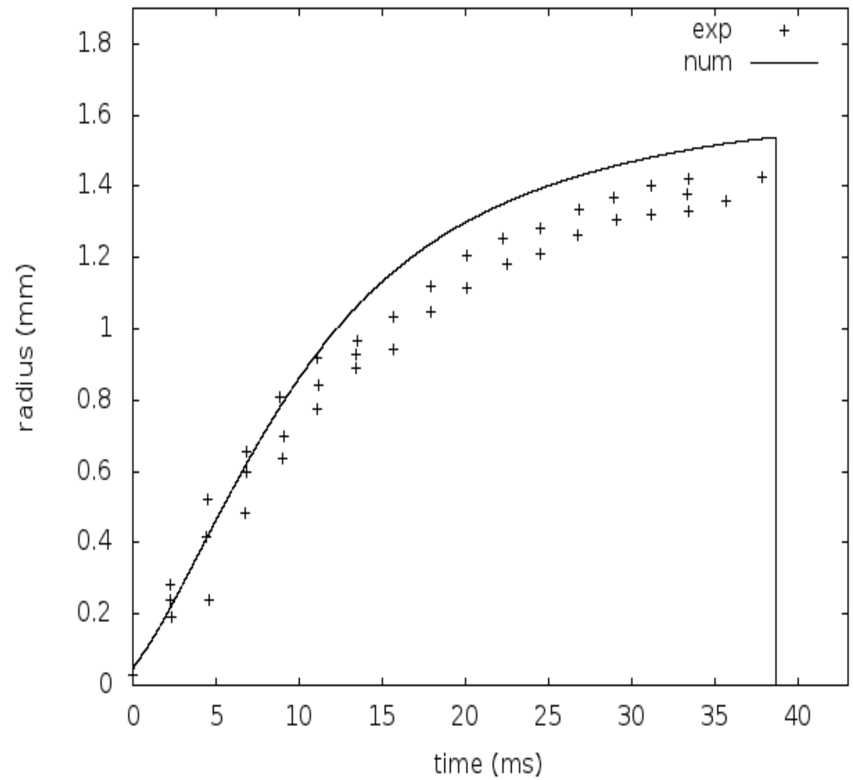
7. Nucleate Boiling : Comparisons between simulations and experimental results

ΔT=7 K



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

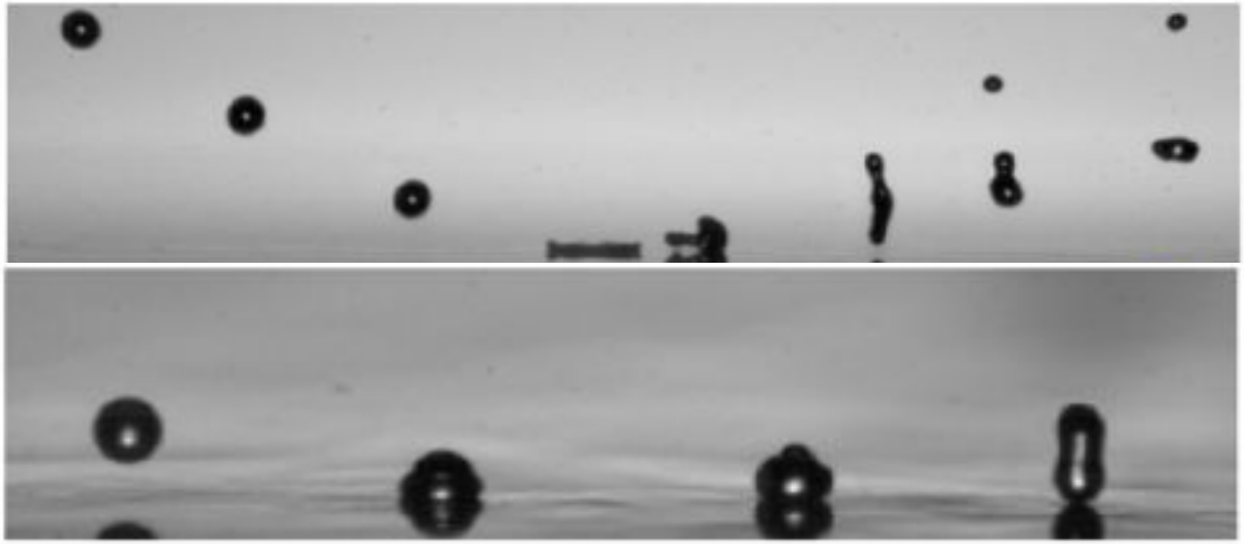
ΔT=8 K



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

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

8. 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

9. Ghost Fluid Thermal Solver for Evaporation (Tanguy & al, 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

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

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

- 10. Ghost Fluid Thermal Solver for Boiling and Evaporation GFTSBE (Rueda Villegas & al, Submitted JCP)

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

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

$$T\Big|_\Gamma = \frac{L_{vap} M_1 T_{sat}}{L_{vap} M_1 - R T_{sat} ln\left(\frac{P_1|_\Gamma}{P_0}\right)}$$
$$P_1\Big|_\Gamma = \frac{-Y_1|_\Gamma P_0 M_2}{(M_1 - M_2) Y_1|_\Gamma - M_1}$$

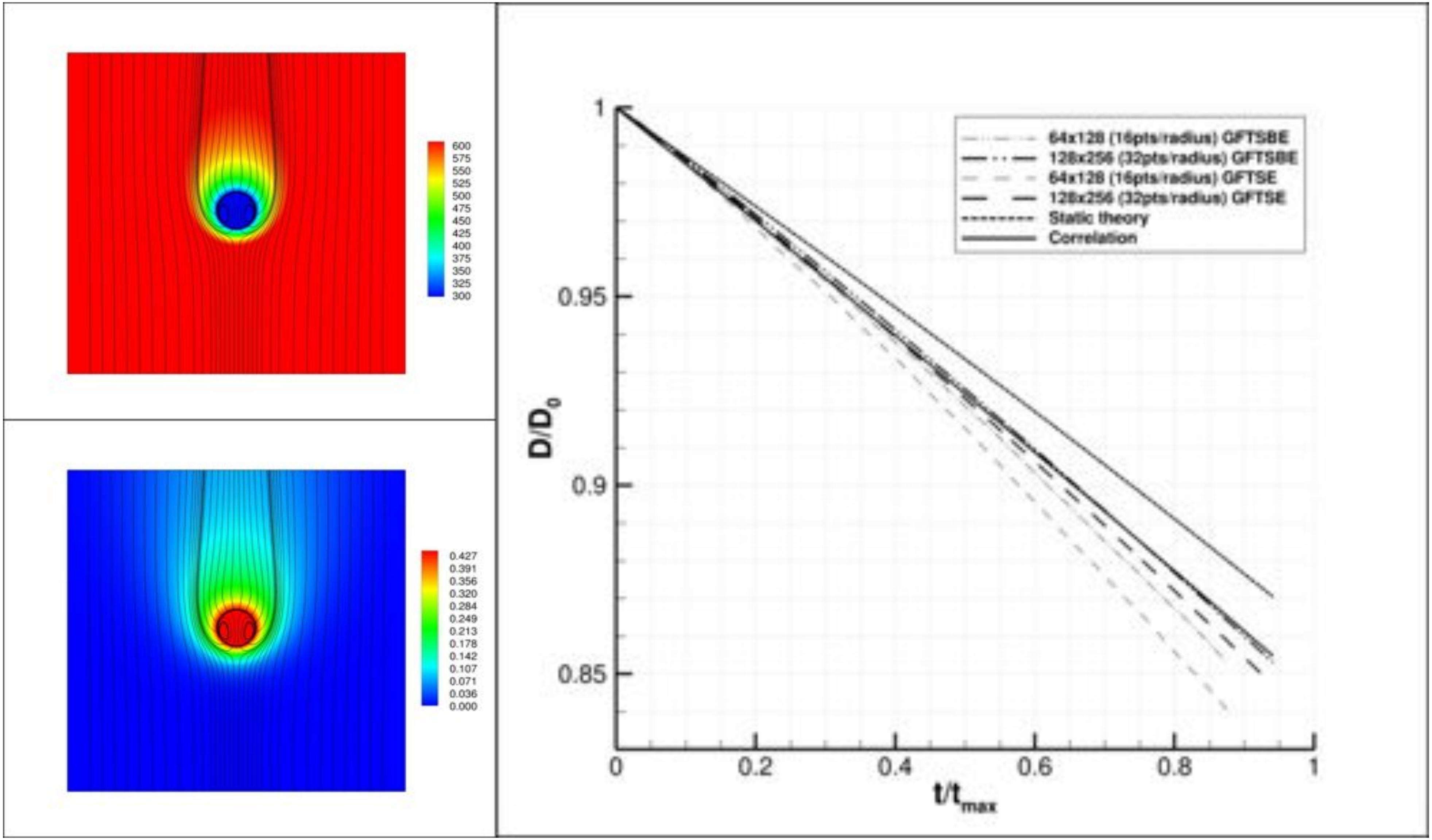
Step 2 : Compute the phase change mass flow rate from the thermal flux jump condition

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

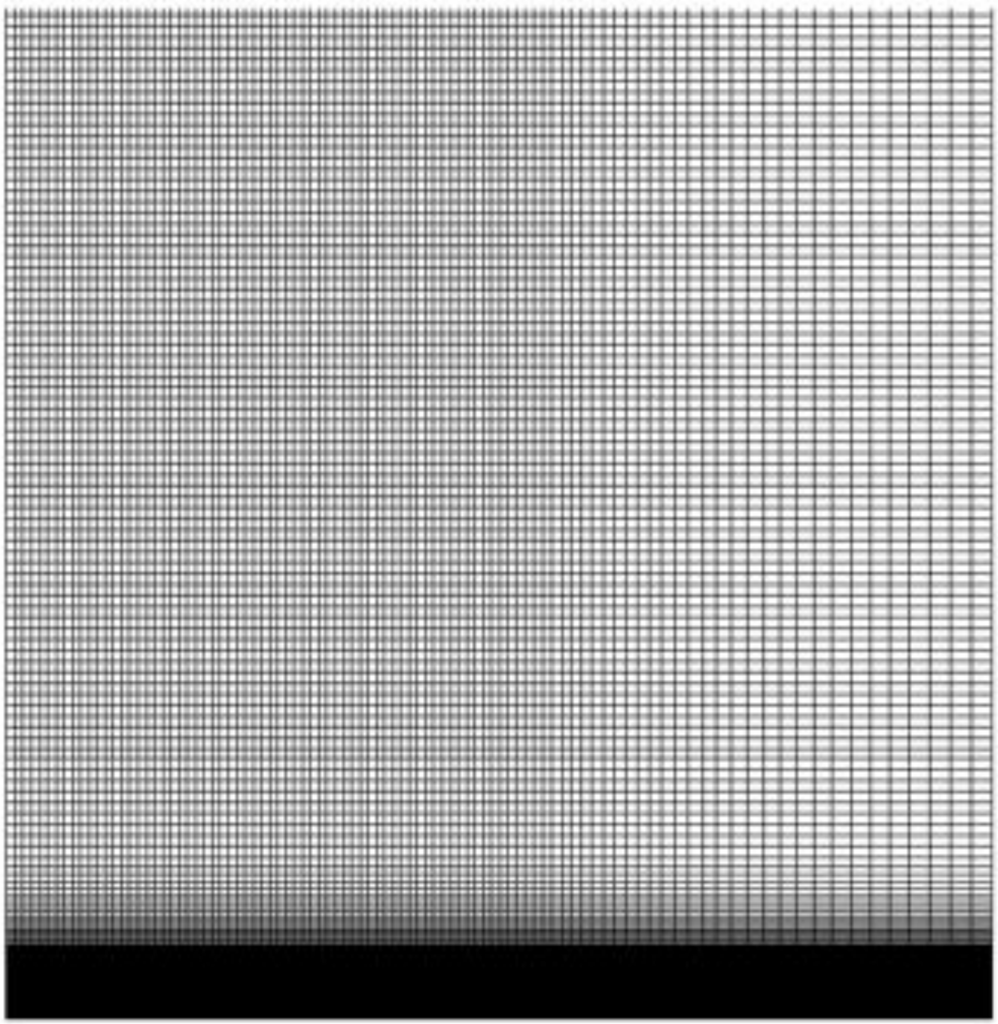
Step 3 : update the mass fraction field in the gas phase with a prescribed robin boundary condition at the interface

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

11. Moving droplet evaporation



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



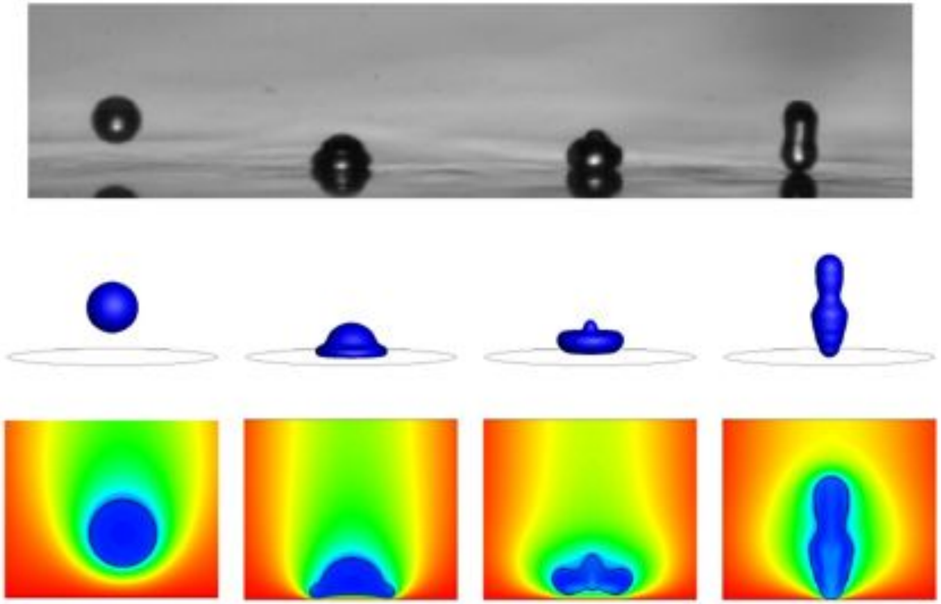
Implicit temporal discretizationf for all the diffusion terms

- 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

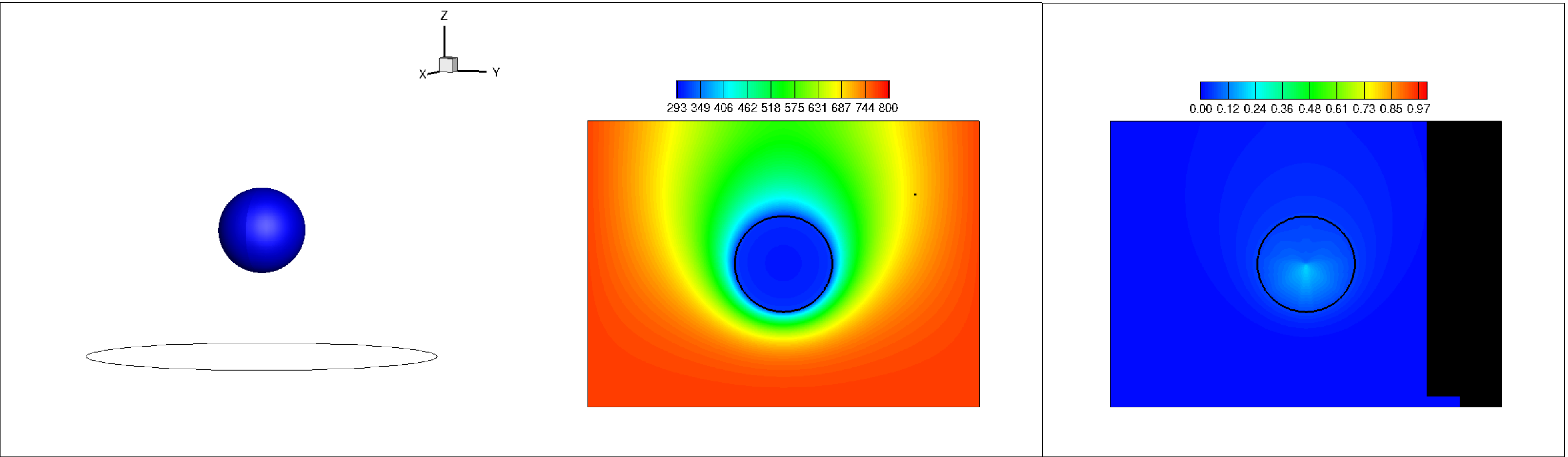
13. Comparisons of simulations with experimental data : We = 7.5



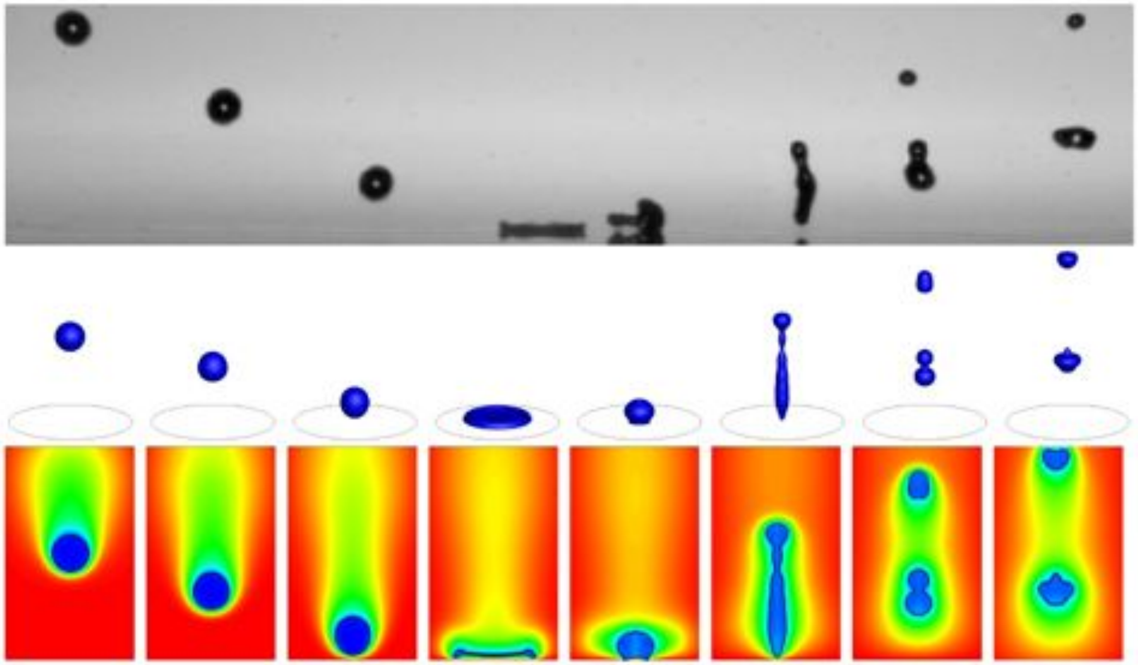
Water droplet
Tw = 823 K

2D axisymetric simulations

Experiments from
Dunand, Lemoine & Castanet
Experiments in Fluids 2013



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



Water droplet
Tw = 823 K

2D axisymetric simulations

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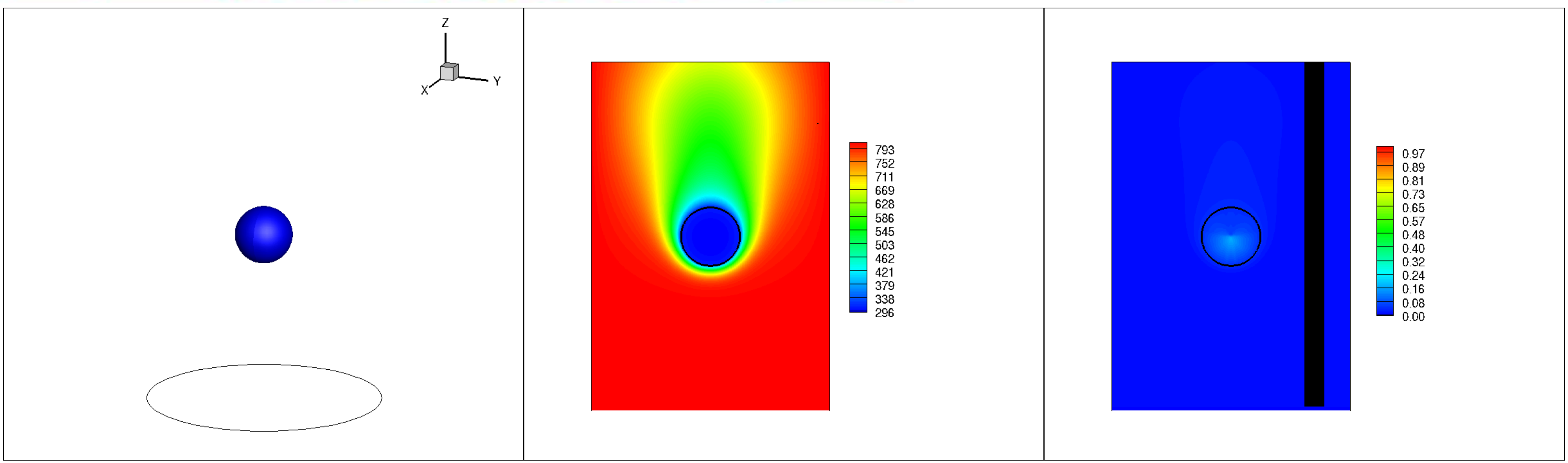
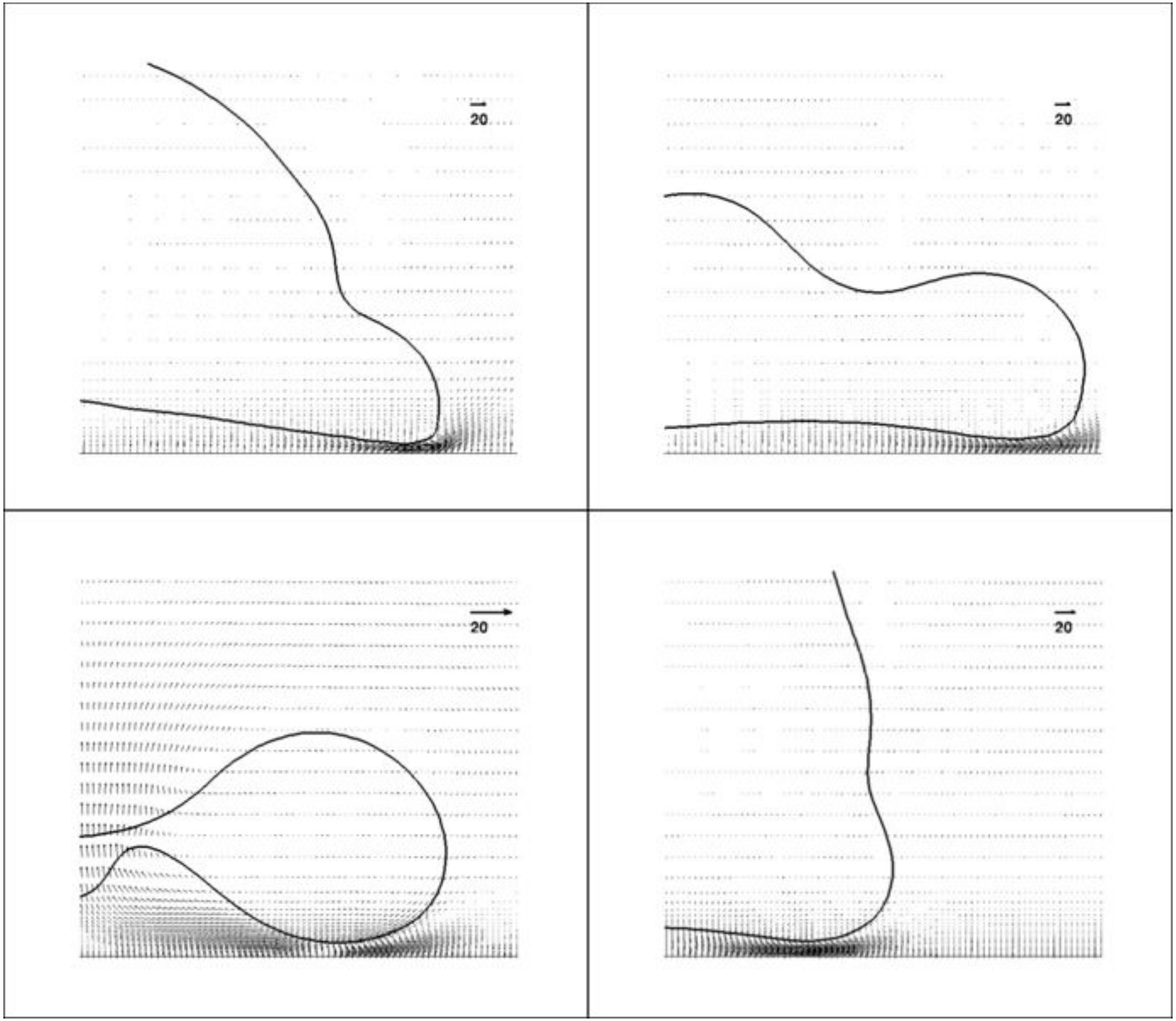
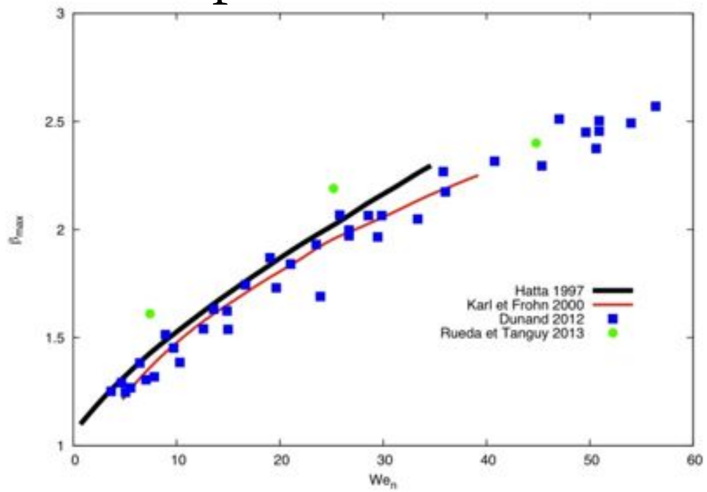


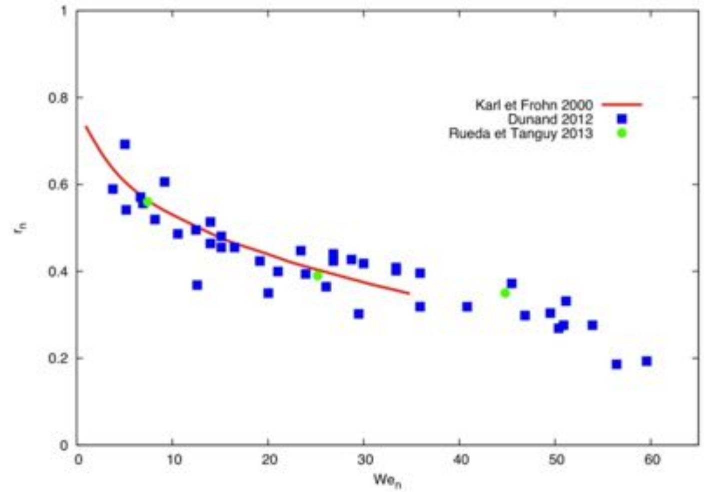
- 15. Velocity field snapshots in the vapor layer



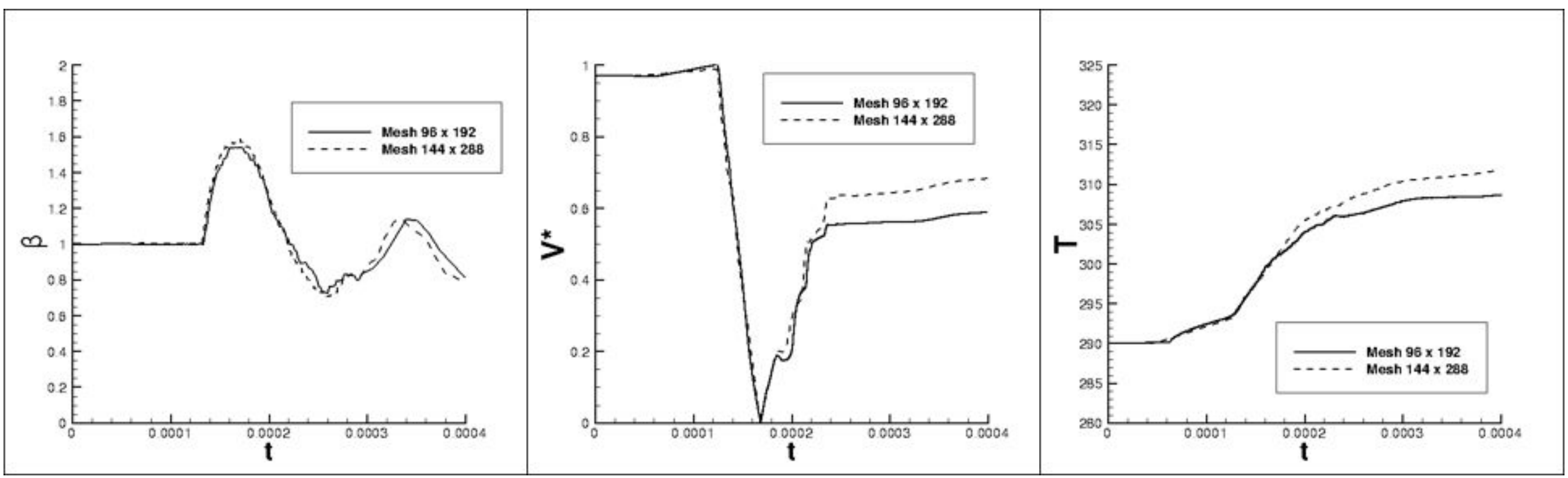
■ 16. Quantitative Comparisons and grid sensitivity studies Quantitative Comparisons and



Maximum spreading diameter vs incident Weber Number



Restitution coefficient vs incident Weber Number



17. Perspectives

Heat transfer at the interface wall

- Nucleate Boiling (Perfectly wetting liquid and higher Jakob number)
- Evaporation of a sessile droplet with a contact line (Marangoni Convection)
- Multi-bubbles nucleate boiling

Turbulence and phase change

- Evaporation of droplets in a turbulent flow (PhD thesis Romain Alis)
- Interaction of a turbulent superheated vapor with a liquid pool (PhD thesis Elena Roxana-Popescu)
- Condensation of droplets on a cold plate (Postdoctoral study Mathieu Lepilliez)