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

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1. Level Set Method

$\phi$ : signed distance function

$\phi < 0$  Gas phase

$\phi = 0$  Liquid-gas interface

$\phi > 0$  Liquid phase

Convection equation :  \[ \frac{\partial \phi}{\partial t} + V \cdot \nabla \phi = 0 \]
(Osher & Sethian, JCP 1989)

Redistance equation :  \[ \frac{\partial d}{\partial \tau} = \text{sign}(\phi)(1 - |\nabla d|) \]
(Sussman et al, JCP 1994)

Geometrical properties :  \[
\begin{aligned}
|\nabla \phi| &= 1 \\
\kappa(\phi) &= -\nabla \cdot n
\end{aligned}
\]

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

<table>
<thead>
<tr>
<th>Conservation law</th>
<th>Jump conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \nabla \cdot \vec{V} = 0 )</td>
<td>( [\vec{V}]_r = \dot{m} \left[ \frac{1}{\rho} \right]_r \vec{n} )</td>
</tr>
<tr>
<td>( \rho \frac{D\vec{V}}{Dt} = -\nabla p + \nabla \cdot (2\mu \nabla \vec{v}) + \rho \vec{g} )</td>
<td>( [p]_r = \sigma \kappa + 2 \left[ \frac{\rho \vec{V}_n}{\rho} \right]_r - \dot{m}^2 \left[ \frac{1}{\rho} \right]_r )</td>
</tr>
<tr>
<td>( \rho C_p \frac{DT}{Dt} = \nabla \cdot (k \nabla T) )</td>
<td>( [k \nabla T \cdot \vec{n}]<em>r = \dot{m} \left( L</em>{vap} + (C_{pliq} - C_{pvap})(T_{sat} - T) \right) )</td>
</tr>
<tr>
<td>( \rho \frac{DY_1}{Dt} = \nabla \cdot (\rho D_m \nabla Y_1) )</td>
<td>( [\rho D_m \nabla Y_1 \cdot \vec{n}]_r = -\dot{m} [Y_1]_r )</td>
</tr>
</tbody>
</table>
Step 1: Update the temperature field in the liquid phase with a prescribed uniform Dirichlet boundary condition at the interface

\[ \rho_l C_p l T_l^{n+1} - \Delta t \nabla \cdot (k_l \nabla T_l^n) = \rho_l C_p l \left( T_l^n - \Delta t \bar{V}_l^n \cdot \nabla T_l^n \right) \quad \text{if } \phi > 0 \]

\[ T|_{\Gamma} = T_{\text{sat}} \]

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

\[ \rho_g C_p g T_g^{n+1} - \Delta t \nabla \cdot (k_g \nabla T_g) = \rho_g C_p g \left( T_g^n - \Delta t \bar{V}_g^n \cdot \nabla T_g^n \right) \quad \text{if } \phi < 0 \]

\[ T|_{\Gamma} = T_{\text{sat}} \]

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

\[ \dot{m} = \frac{[k \nabla T \cdot \vec{n}]_{\Gamma}}{L_{\text{vap}}} \]
5. Nucleate Boiling: numerical simulation

- 2D axisymmetric non-uniform mesh.
- Wall thermal conduction.
- Initial thermal boundary layer (Kays and Crawford, 1980).

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

- $Ja = 21$ ($\Delta T=7$ K), $\theta_{app} = 50^\circ$, $\rho_{liq}/\rho_{vap} = 1604$

Figure: Example of a Non-uniform axisymmetric mesh
6. Nucleate Boiling: spatial convergence

Grid sensitivity study on the bubble radius
7. Nucleate Boiling: Comparisons between simulations and experimental results

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

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

\[ R_{Fritz} = 0.104\theta \sqrt{\frac{\sigma}{g(\rho_l - \rho_v)}}. \]

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

\[ \alpha = 0.00219 \text{ and } n = 1.43 \]

Variation of the dimensionless departure radius with the Jakob number

10. Leidenfrost droplets: evaporation and boiling

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

\[
\rho_g Y_1^{n+1} - \Delta t \nabla \cdot \left( \rho_g D_m \nabla Y_1^{n+1} \right) = \rho_g \left( Y_1^n - \Delta t \bar{V}_g \cdot \nabla Y_1^n \right) \quad \text{if } \phi < 0
\]

\[
Y_1 \bigg|_I = \frac{P_1 |_{I} M_1}{P_1 |_{I} M_1 + (P_0 - P_1 |_{I}) M_2}
\]

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

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

\[
\dot{m} = \frac{\rho_g D_m \nabla Y_1 \cdot \vec{n} |_{I}}{1 - Y_1 |_{I}}
\]

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

\[
\rho C_p T^{n+1} - \Delta t \nabla \cdot \left( k \nabla T^{n+1} \right) = \rho C_p \left( T^n - \Delta t B \left( \bar{V}^n, T^n \right) \right)
\]

\[
[k \nabla T \cdot \vec{n}] |_{I} = \dot{m} \left( L_{vap} + (C_{pliq} - C_{pvap}) (T_{sat} - T |_{I}) \right)
\]
Step 1: Update separately the temperature field in the liquid phase with a prescribed non-uniform Dirichlet boundary condition at the interface

\[
\rho_l C_p l T_l^{n+1} - \Delta t \nabla \cdot (k_l \nabla T_l^{n+1}) = \rho_l C_p l \left( T_l^n - \Delta t \nabla \bar{V}_l^n \cdot \nabla T_l^n \right) \quad \text{if } \phi > 0
\]

\[
\rho_g C_p g T_g^{n+1} - \Delta t \nabla \cdot (k_g \nabla T_g) = \rho_g C_p g \left( T_g^n - \Delta t \nabla \bar{V}_g^n \cdot \nabla T_g^n \right) \quad \text{if } \phi < 0
\]

\[
T\bigg|_\Gamma = \frac{L_{vap} M_1 T_{sat}}{L_{vap} M_1 - RT_{sat} \ln \left( \frac{P_1|_\Gamma}{P_0} \right)}
\]

\[
P_1\bigg|_\Gamma = \frac{-Y_1|_\Gamma P_0 M_2}{(M_1 - M_2)Y_1|_\Gamma - M_1}
\]

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

\[
\rho_g Y_1^{n+1} - \Delta t \nabla \cdot \left( \rho_g D_m \nabla Y_1^{n+1} \right) = \rho_g \left( Y_1^n - \Delta t \nabla \bar{V}_g^n \cdot \nabla Y_1^n \right) \quad \text{if } \phi < 0
\]

\[
\dot{m} Y_1|_\Gamma + \rho_g D_m \nabla Y_1 \cdot \vec{n}|_\Gamma = \dot{m}
\]
13. Moving droplet evaporation
Implicit temporal discretization 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 axisymmetric simulations

Experiments from
Dunand, Lemoine & Castanet
Experiments in Fluids 2013
16. Comparisons of simulations with experimental data: \( \text{We} = 45 \)

Water droplet
\( \text{Tw} = 823 \text{ K} \)

2D axisymmetric simulations

Experiments from Dunand, Lemoine & Castanet
Experiments in Fluids 2013
17. Velocity field snapshots in the vapor layer

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)

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

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

2D Simulation on a 1024 x 1024 grid
with a Black Box MultiGrid solver
for solving linear systems
20. Thanks for funding Institutes

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Nucleate Boiling: Micro region or not micro region?

\[ \Delta T = T_{\text{wall}} - T_{\text{sat}} = 7 \text{ K} \]
Nucleate Boiling: Micro region or not micro region?

\[ \Delta T = 7 \, K, \, \theta_{app} = 50^\circ \iff \theta_{mic} = 49.66^\circ \]