DNS of Interfacial Heat and Mass Transfer in Bubble Swarms

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The objective of this work is to develop numerical methods for Direct Numerical Simulation (DNS) of bubbly flows with interfacial transport phenomena (variable surface tension, phase change, heat and mass transfer).
- Bubbly flows with heat and mass transfer are important in natural processes and industrial applications:

Unit-operations in Chemical Engineering: Bubble columns, Chemical and Biochemical Bubble reactors, ...

Assumptions considered in this work:
- **Incompressible** flows of two-phases (or two-fluid) with a clearly differentiated interface.
- **Newtonian** fluids.
- **No coalescence** of the fluid particles (bubbles, droplets).
1. Introduction.

2. Mathematical formulation and numerical methods.

3. Numerical experiments.

Navier-Stokes equations and energy equations\textsuperscript{1,2}

\[ \frac{\partial}{\partial t} \left( \rho_2 \mathbf{v}_2 \right) + \nabla \cdot (\rho_2 \mathbf{v}_2 \mathbf{v}_2) = \nabla \cdot \mathbf{S}_2 + \rho_2 \mathbf{g} \]

\[ \mathbf{S}_2 = -p_2 \mathbf{I} + \mu_2 \left( \nabla \mathbf{v}_2 + (\nabla \mathbf{v}_2)^T \right) \]

\[ \nabla \cdot \mathbf{v}_2 = 0 \]

\[ \frac{\partial}{\partial t} T_2 + \nabla \cdot T_2 \mathbf{v}_2 = \frac{1}{\rho_2 c_{p,2}} \nabla \cdot \lambda_2 \nabla T_2 \]

\[ \frac{\partial}{\partial t} \left( \rho_1 \mathbf{v}_1 \right) + \nabla \cdot (\rho_1 \mathbf{v}_1 \mathbf{v}_1) = \nabla \cdot \mathbf{S}_1 + \rho_1 \mathbf{g} \]

\[ \mathbf{S}_1 = -p_1 \mathbf{I} + \mu_1 \left( \nabla \mathbf{v}_1 + (\nabla \mathbf{v}_1)^T \right) \]

\[ \nabla \cdot \mathbf{v}_1 = 0 \]

\[ \frac{\partial}{\partial t} T_1 + \nabla \cdot T_1 \mathbf{v}_1 = \frac{1}{\rho_1 c_{p,1}} \nabla \cdot \lambda_1 \nabla T_1 \]


Boundary conditions at the interface

\[ \Omega = \Omega_1 \cup \Omega_2 \]

Mass conservation at \( \Gamma \) leads to:
\[ \vec{v}_1 = \vec{v}_2 \]
(no phase change)

No slip B.C.

Momentum balance at \( \Gamma \) leads to:
\[ (\vec{S}_1 - \vec{S}_2) \cdot \vec{n} = \sigma(T) \kappa \vec{n} - \nabla \Gamma \sigma(T) \]

Stress jump B.C. at \( \Gamma \)

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Boundary conditions at the interface

\[ \Omega = \Omega_1 \cup \Omega_2 \]

\[ (c_{p1}, \lambda_1, \rho_1, \mu_1) \]

\[ (c_{p2}, \lambda_2, \rho_2, \mu_2) \]

\[ \Delta V \]

\[ \Delta S \]

Energy balance at \( \Gamma \) leads to:

\[ T_1 = T_2 \]

\[ (\lambda_1 \nabla T_1 - \lambda_2 \nabla T_2) \cdot n = 0 \]

(no phase change)

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Two-phase flow and energy equations: One marker model

\[ \frac{\partial}{\partial t} \rho \mathbf{v} + \nabla \cdot \rho \mathbf{vv} = -\nabla p + \nabla \cdot \mu \left( \nabla \mathbf{v} + (\nabla \mathbf{v})^T \right) \]

\[ + \rho g + (\sigma \kappa \mathbf{n} - \nabla \sigma + \mathbf{n} (\mathbf{n} \cdot \nabla) \sigma) \delta \Gamma \]

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

\[ \frac{\partial}{\partial t} T + \nabla \cdot T \mathbf{v} = \frac{1}{\rho c_p} \nabla \cdot \lambda \nabla T \]

\[ \beta = \beta_1 H_1 + \beta_2 (1 - H_1) \quad \beta = \{\rho, \mu, \lambda, c_p\} \]

\[ \sigma(T) = \sigma_0 + \frac{d \sigma}{dT} (T - T_0) \]

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Interface Capturing: Unstructured level-set method \[1\]

Standard level-set method
[Osher (1988), Sussman (1994)]

\[d(x,t) > 0\]
\[d(x,t) < 0\]

Signed distance function:
\[d(x,t) = \text{sign}(d) \min \{ ||x-x|| \} \ , \text{Eq. (1)}\]

Conservative level-set method
[Olsson and Kreiss (2005)]

\[\Gamma(t) = \{ x | d(x,t) = 0 \}\]
\[\Gamma(t) = \{ x | \phi(x,t) = 0.5 \}\]

Interface profile depends on \(\varepsilon\)
\[\varepsilon = 0.5 h^d\]

Modified level-set function:
\[\phi(x,t) = \frac{1}{2} \left( \tanh \left( \frac{d(x,t)}{2\varepsilon} \right) + 1 \right)\ , \text{Eq. (2)}\]

Geometrical properties of \(\Gamma(t)\):

\[n = \frac{\nabla \phi}{||\nabla \phi||}\quad \text{Eq. (3)}\]

Physical properties, \(\beta = (\rho, \mu, \lambda, \ldots)\)

\[\beta(\phi) = \beta_1 \phi + \beta_2 (1 - \phi)\quad \text{Eq. (4)}\]

\[H_1 = \phi\quad \delta_T = ||\nabla \phi||\quad \text{Eq. (5)}\]

Interface Capturing: Unstructured level-set method [1]

Fig. 1: Advection Eq. 6

Fig. 2: Advection Eq. 6 + Re-Initialization Eq. 7

Advection equation (no phase change) Eq. 5

\[ \frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = 0 \]

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

Advection equation in conservative form, Eq. 6

\[ \frac{\partial \phi}{\partial \tau} + \nabla \cdot \phi \mathbf{v} = 0 \]

Reinitialization equation, Eq. 7

\[ \frac{\partial \phi}{\partial \tau} + \nabla \cdot \phi (1-\phi) \mathbf{n}_{\tau=0} = \nabla \cdot \varepsilon \nabla \phi \]

Coupled volume-of-fluid/level-set method [4]: 1. Interface advection with geometrical VOF-PLIC
2. Surface tension by level-set method

1. Interface advection and geometrical reconstruction: VOF-PLIC method [3].
Indicator function,
\[ f(x, t) = \begin{cases} 
0 & \text{if } x \in \Omega_1 \\
1 & \text{if } x \in \Omega_2 
\end{cases} \]

Indicator function in discretized form,
\[ f_P = \frac{\int_{\Omega_P} f(x, t) dV}{\int_{\Omega_P} dV} \]

Advection equation,
\[ \frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f = 0 \]

PLIC based on Young's reconstruction

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http://dx.doi.org/10.1016/j.compfluid.2015.10.005
2. Distance function reconstruction [4] $\quad$ Surface tension is computed using level-set method (signed distance function)

2.1. Initialize $d(\mathbf{x}, t)$

$$d(\mathbf{x}_P, t) = \begin{cases} 
    d_{\text{max}} & \text{if } f(\mathbf{x}_P, t) \geq 0.5 \\
    -d_{\text{max}} & \text{otherwise}
\end{cases}$$

2.2. Detect a flagged region

2.3. Calculate $|d(\mathbf{x}, t)|$ in the flagged region

$$|d(\mathbf{x}_P, t)| = \min\{d_{P \rightarrow \Pi_1}^{\min}, \ldots, d_{P \rightarrow \Pi_i}^{\min}, \ldots, d_{P \rightarrow \Pi_n}^{\min}\}$$

2.4. Calculate $d(\mathbf{x}, t)$

$$d(\mathbf{x}_P, 0) = \begin{cases} 
    |d(\mathbf{x}_P, t)| & \text{if } f(\mathbf{x}_P, t) \leq 0.5 \\
    -|d(\mathbf{x}_P, t)| & \text{otherwise}
\end{cases}$$

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Interface capturing: multiple marker CLS method $[2, 5]$

\[ \Omega = \Omega_c \cup \Omega_d \]

\[ \Omega_d = \Omega_1 \cup ... \cup \Omega_n \]

(continuous phase)

(disperse phase)

\[ \beta = \{ \rho, \mu, \lambda, c_p \} \]
\[ \beta = \beta_d \phi_d + \beta_c (1 - \phi_d) \]
\[ \phi_d(x, t) = \max \{ \phi_1(x, t), ..., \phi_{n_d-1}(x, t), \phi_{n_d}(x, t) \} \]

Interface advection and reinitialization $[2, 5]$: \[
\begin{align*}
\frac{\partial \phi_i}{\partial t} + \nabla \cdot \phi_i \mathbf{v} &= 0 \\
\frac{\partial \phi_i}{\partial T} + \nabla \cdot \phi_i (1 - \phi_i) \mathbf{n}_i &= \nabla \cdot \varepsilon \nabla \phi_i
\end{align*}\]

for $i = 1, ..., n_d$

Interface geometric properties $[2, 5]$: \[
\begin{align*}
\mathbf{n}_i(\phi_i) &= \frac{\nabla \phi_i}{\|\nabla \phi_i\|} \\
\kappa_i(\phi_i) &= -\nabla \cdot \mathbf{n}_i
\end{align*}\]

for $i = 1, ..., n_d$

Surface tension computed by CSF model (Brackbill et al. 1992). Extension to multiple marker CLS method in $[2, 5]$: \[
\mathbf{f}_\sigma = \sum_{i=1}^{n_d} \left( \sigma(T) \kappa_i \mathbf{n}_i - \nabla \Gamma \sigma \right) \|\nabla \phi_i\| \cdot \\
\Omega_{i+1} \cup \Omega_i
\]

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Numerical methods: Discretization [1, 2]

- Finite-volume method for space discretization [1,2].
- Collocated grid arrangement.

General transport equation, Eq. 1

\[
\int_{V_P} \frac{\partial \psi}{\partial t} dV = \int_{A_P} \left( -\xi G^e(\psi)c + \lambda \nabla \psi \right) \cdot dA + \int_{V_P} S_\psi dV
\]

- Convection
- Compression
- Accumulation
- Diffusion
- Source

\[
\begin{align*}
(p, \nu, \rho, \lambda, c_p, \mu, \phi) & \quad \text{in cell centroids}
\end{align*}
\]

- Gradient at cell \(P\):

\[
(\nabla \psi)_P = (M^T M)^{-1} M^T Y
\]

Least-squares method, Eq. 2

- Diffusion terms: Central-Difference Scheme.
- Convection terms: Novel unstructured flux limiters schemes [1,2].

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Numerical methods: Spatial discretization \([2, 5]\)

- Finite-volume method on collocated grids for space discretization \([1, 2]\).

General transport equation, Eq. 1

\[
\int_{V_p} \frac{\partial \psi}{\partial t} dV = \sum_{f} \Sigma_{f} (\nabla \psi)_f \cdot dA + \int_{V_p} S_{\psi} dV
\]

- Convection
- Compression
- Accumulation
- Diffusion
- Source

\[
\int_{A_p} \lambda \nabla \psi \cdot dA \approx \sum_{f} \Sigma_{f} (\nabla \psi)_f = \sum_{f} \Sigma_{f} ||A_f|| \left( \frac{\psi_f - \psi_p}{||\Delta X_{p-f}||} + (\nabla \psi)_f \cdot \left( \frac{A_f}{||A_f||} - \frac{\Delta X_{p-f}}{||\Delta X_{p-f}||} \right) \right)
\]

- CD scheme
- normal diffusion
- transverse diffusion

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Numerical method: Spatial discretization \([1,2]\)

General transport equation, \textbf{Eq. 1}

\[
\int_{V_P} \frac{\partial \xi \psi}{\partial t} \, dV = \oint_{A_P} \left( -\xi \mathbf{G}^e(\psi) \mathbf{c} + \lambda \nabla \psi \right) \cdot d\mathbf{A} + \int_{V_P} S_\psi \, dV
\]

\textbf{Convection}\hspace{1cm}\textbf{Compression}\hspace{1cm}\textbf{Accumulation}\hspace{1cm}\textbf{Source}\hspace{1cm}\textbf{Diffusion}

Novel and accurate flux-limiter schemes on unstructured meshes \([1,2]\).

\textbf{Node-stencil:}

- \textbf{SUPERBEE (Momentum Eq.)}
- \textbf{SUPERBEE (Energy Eq.)}
- \textbf{SUPERBEE (Advection Eq.)}
- \textbf{CD (Reinit. Eq.)}


Numerical methods: Global algorithm \([1, 2, 6]\)

Global algorithm for two-phase flows with variable surface tension \([1, 2, 6]\):

1. Initialize \(v, T, \kappa, n,\) physical properties.

2. \[\Delta t = 0.1 \min \left( \frac{h}{||v||}, \frac{\rho h^2}{\mu}, \left( \frac{h}{||g||} \right)^{1/2}, \left( \frac{h^3}{4\pi \sigma} \right)^{1/2} \right)\]

3. Interface advection for \(\phi_1, \ldots, \phi_i, \phi_{i+1}, \phi_{nd}\) \([1, 2, 6]\)

4. CLS re-initialization for \(\phi_1, \ldots, \phi_i, \phi_{i+1}, \phi_{nd}\) \([1, 2, 6]\)

5. Calculate the global level-set function, \(\phi_d(x_p, t)\) \([1, 2, 6]\)

6. Update physical properties, interface normals and curvature:
   - \(\kappa(x_p, t), n(x_p, t),\)
   - \(\rho(x_p, t) = \rho(\phi_d), \mu(x_p, t) = \mu(\phi_d), \lambda(x_p, t) = \lambda(\phi_d),\)
   - \(c_p(x_p, t) = c_p(\phi_d).\)

7. Solve momentum equation \([1, 2, 6]\)

   \[\frac{\rho v - \rho^* v^*}{\Delta t} = -C^n + D^n + (\rho - \rho_0) g + \ldots\]

   \[\left( \sum_{i=1}^{n} \sigma(T_i) \kappa_i n_i - \nabla h \sigma(T_i) + n_i (n_i \cdot \nabla h) \sigma(T_i) \right) ||\nabla h||\]

8. Repeat steps 2-7 until to achieve the desired time.

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1 Introduction.
2 Mathematical formulation and numerical methods.
3 Numerical experiments.
4 Conclusions.
Single buoyant bubbles (Validations) [2, 3, 4]

Droplet collision against a fluid interface (Validations) [1]

Hexahedral mesh, 5.98e6 CVs, h = d/30

\[ M = \frac{g d c \rho_c \Delta \rho}{\rho_d^2 \sigma^3} = 8.82 \times 10^{-8} \]

\[ E_o = \frac{g d^2 \Delta \rho_c}{\sigma} = 6.4 \]

\[ \eta_{\rho} = \frac{\rho_c}{\rho_d} = 1.19 \]

\[ \eta_\mu = \frac{\mu_c}{\mu_d} = 0.33 \]

Applications: Gravity-driven bubbly flows \([6, 7]\)

18 bubbles, \(Eo = 3\), \(Mo = 10^{-6}\), \(\eta_\mu = \eta_\rho = \eta_\lambda = 100\). (2086 CPU cores)

- Deformable bubbles do not touch the wall (wall effect).
- Random fluctuations in Reynolds number (Re) of single bubbles.
- Average Reynolds number (Re) of the swarm tends to steady state.
- Predictive simulations: \(Re = Re(Eo, Mo, \text{bubble fraction,} N_b, \text{Conf. Ratio})\).


Falling droplets (Validation) \[8\]

\[ Eo = 6.4, \; Mo = 1.03 \times 10^{-5}, \; \eta_\mu = 0.33, \; \eta_\rho = 1.19, \; CR = 8, \]
\[ (D_\Omega, H_\Omega) = (CR \cdot d, 12d), \; h = d/30 \; (4.4MCVs), \; 256 \; CPU-cores. \]

Falling droplets at $\eta_\mu = 1.0$, $\eta_\rho = 1.2$, $CR = 2$, $(D_\Omega, H_\Omega) = (2d, 10d)$ (square channel), $h = d/40$ ($3.072M$ CVs), $128$ CPU-cores.

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Applications: Falling droplets [8].

Falling droplets at $\eta_\mu = 1.0$, $\eta_\rho = 1.2$, $CR = 2$, $(D_\Omega, H_\Omega) = (2d, 10d)$ (square channels), $h = d/40$ (3.072M CVs), 128 CPU-cores.

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Applications: Falling droplets [8].

Falling droplets at $\eta_{\mu} = 1.0$, $\eta_{\rho} = 1.2$, $CR = 2$, $(D_{\Omega}, H_{\Omega}) = (2d, 10d)$ (square channels), $h = d/40$ (3.072M CVs), 128 CPU-cores.

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Applications: Falling droplets \[8\].

Falling droplets at \(\eta_\mu = 1.0, \eta_\rho = 1.2, CR = 2, (D_\Omega, H_\Omega) = (2d, 10d)\) (square channels), \(h = d/40\) (3.072M CVs), 128 CPU-cores.

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Applications: Falling droplets [8].

Falling droplets at $\eta_\mu = 1.0$, $\eta_\rho = 1.2$, $CR = 2$, $(D_\Omega, H_\Omega) = (2d, 10d)$ (square channels), $h = d/40$ (3.072M CVs), 128 CPU-cores.

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Applications: Falling droplets [8].

Falling droplets at \( \eta_\mu = 1.0, \eta_\rho = 1.2, CR = 2, (D_\Omega, H_\Omega) = (2d, 10d) \) (square channels), \( h = d/40 \) (3.072M CVs), 128 CPU-cores.

Applications: Interaction of 2 falling droplets [8].

2 droplets at $Eo = 2.5$, $Mo = 10^{-7}$, $\eta_\mu = 1.0$, $\eta_\rho = 1.2$, $CR = 4$, $(D_\Omega, H_\Omega) = (4d, 10d)$ (square channels), $h = d/40$ (12.288M CVs), 512 CPU-cores.

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Thermocapillary motion of single droplets ($g=0$) [5]

\[ Ma = \frac{\sigma_T |\nabla T_\infty| d^2 \rho_c \epsilon_c}{4 \mu_c \lambda_c} \]
\[ Re = \frac{\sigma_T |\nabla T_\infty| d^2 \rho_c}{4 \mu_c^2 \epsilon_c} \]
\[ Ca = \frac{\sigma_T |\nabla T_\infty| (d/2)/\mu_c}{2 \sigma_0} \]
\[ t^* = \frac{2 t U_r}{d} \]
\[ V^* = \left( e_y \cdot v_c \right)/U_r \]

<table>
<thead>
<tr>
<th>$Re$</th>
<th>$Ca$</th>
<th>$Ma$</th>
<th>$\eta_p$</th>
<th>$\eta_\mu$</th>
<th>$\eta_\lambda$</th>
<th>$\eta_\epsilon_c$</th>
<th>$U_{YGB}/U_r$</th>
<th>$(U/U_r)_{num}$</th>
</tr>
</thead>
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<tr>
<td>0.066</td>
<td>0.066</td>
<td>0.066</td>
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<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>0.133</td>
<td>0.128</td>
</tr>
</tbody>
</table>

Thermocapillary motion of single droplets (g=0) [5]

Re=5, Ca=0.1, ηρ=ημ=ηcp=ηκ=1.0

\[ Ma = \frac{\sigma T |\nabla T_\infty| d^2 \rho_c c_p, c}{4 \mu_c \lambda_c} \]
\[ Re = \frac{\sigma T |\nabla T_\infty| d^2 \rho_c}{4 \mu_c^2} \]
\[ U_r = \sigma T |\nabla T_\infty| (d/2)/\mu_c \]
\[ t^* = 2 t U_r/d \]
\[ V^* = (e_y \cdot v_c)/U_r \]

Thermocapillary interaction of multiple droplets \((g=0)\)

18 droplets: \(Re=40, Ma=40, Ca=0.04166, \eta_{\rho} = \eta_{\mu} = \eta_{cp} = \eta_{h} = 0.5\)

Mesh: cartesian 240x240x480, \(h=d/40\), 1024 CPU cores
Thermocapillary interaction of multiple droplets ($g=0$)

18 droplets: $Re=40$, $Ma=40$, $Ca=0.04166$, $\eta_\rho=\eta_{\mu}=\eta_{cp}=\eta_\lambda=0.5$

Mesh: cartesian 240x240x480, $h=d/40$
Thermocapillary interaction of multiple droplets ($g=0$)

18 droplets: $Re=40$, $Ma=40$, $Ca=0.04166$, $\eta_r=\eta_\mu=\eta_{cp}=\eta_\lambda=0.5$

Mesh: cartesian $240\times240\times480$, $h=d/40$
Ongoing work: More details in [9]

Mass transfer Coefficient = f(Eo, Mo, Sc, Np, bubble fraction, ...)

Poly-dispersed bubble-swarms  Film boiling

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1. Introduction.
2. Mathematical formulation and numerical methods.
3. Numerical experiments.
Mass conservative interface capturing methods have been introduced for simulation of two-phase flows on 3D unstructured meshes, including surface tension effects. 

A multiple marker interface capturing method has been introduced for simulation of bubble swarms.

These methods have been extensively validated and verified against experiments, analytical and numerical results from the literature.

Current work extends the capabilities of these solvers to interfacial heat and mass transfer, variable surface tension (e.g., Thermocapillary effects).

Future work includes extension of these capabilities to phase-change phenomena and surfactant effects.
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