Numerical investigation of two-fluid flows by FreeFem++

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Background and objective

Viscous two-phase flows covers a lot of interesting phenomena in fluid dynamics. For example

- Rising bubble
- Droplet impact
- Dam breaking phenomena, etc....

These phenomena are formulated by free boundary value problem of the Navier-Stokes equations. In particular, we are interested in deformation of the interface between two fluids.

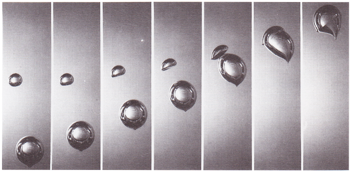


Fig. Interaction of two rising bubbles from "*A Gallery of Fluid Motion*" (2003).

Objective

- Numerical simulation of viscous incompressible two-phase flows by FreeFEM++
- We mainly consider rising bubble problem in 2D, because there are a lot of related results. In particular, Hysing *et al.* (2009) proposed a **quantitative benchmark problem**.
  (But, we do not rely on any specialties of 2D).

Governing equations (1)

The Navier-Stokes equations

- $\Omega \subset \mathbb{R}^2$: bounded domain with boundary $\partial\Omega$.
- $\Omega = \Omega_1(t) \cup \Gamma(t) \cup \Omega_2(t)$.
  - Fluid j occupies $\Omega_j(t)$ $(j = 1, 2)$. Density and viscosity of fluid j are $\rho_j > 0$ and $\nu_j > 0$ (const.). In this talk, $\rho_1 > \rho_2$ is assumed.
  - $\Gamma(t) = \partial\Omega_1(t) \cap \partial\Omega_2(t)$ is the interface between two fluids.
  - $\Omega_1(t) \cap \Omega_2(t) = \emptyset$ (immiscible flow).

The Navier-Stokes equations

$$\rho(\partial_t \boldsymbol{u} + \boldsymbol{u} \cdot \nabla \boldsymbol{u}) = \operatorname{div}(2\nu\mathbb{D}(\boldsymbol{u}) - p\mathbb{I}) + \boldsymbol{F}, \quad t > 0, \boldsymbol{x} \in \Omega, \tag{1a}$$

$$\operatorname{div} \boldsymbol{u} = 0, \quad t > 0, \boldsymbol{x} \in \Omega. \tag{1b}$$

$\boldsymbol{u} = (u_1(t, \boldsymbol{x}), u_2(t, \boldsymbol{x}))$: velocity, $p = p(t, x)$: pressure (unknown variables).
$\boldsymbol{F} = \boldsymbol{f}_{\text{gravity}} = (0, -\rho g)$, $g > 0$ is gravitational acceleration (const.).
$\mathbb{I}$: 2×2 unit matrix.

$$\mathbb{D}(\boldsymbol{u}) = \frac{1}{2}(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^\top) = \frac{1}{2}(\partial_j u_i + \partial_i u_j)_{i,j=1,2}, \qquad (\rho, \nu) = \begin{cases} (\rho_1, \nu_1), & \boldsymbol{x} \in \Omega_1(t), \\ (\rho_2, \nu_2), & \boldsymbol{x} \in \Omega_2(t). \end{cases} \tag{1c}$$

Governing equations (2)

Conditions on the interface $\Gamma(t)$

On the interface $\Gamma(t)$, the surface tension is taken into account.

Conditions on the interface $\Gamma(t)$

$$[\boldsymbol{u}]|_{\Gamma(t)} = \boldsymbol{0}, \quad [2\nu\mathbb{D}(\boldsymbol{u}) - p\mathbb{I}]|_{\Gamma(t)} \cdot \boldsymbol{n}|_{\Gamma(t)} = \sigma\kappa\boldsymbol{n}|_{\Gamma(t)} \tag{1d}$$

- $\sigma > 0$: surface tension constant
- $\kappa = \kappa(t, \boldsymbol{x})$: curvature of the interface
- $\boldsymbol{n}|_{\Gamma(t)}$: unit normal at the interface $\Gamma(t)$ pointing into $\Omega_1(t)$.
- $[\bullet]_\Gamma = \bullet|_{\Omega_1(t)\cap\Gamma(t)} - \bullet|_{\Omega_2(t)\cap\Gamma(t)}$: jump of quantity "$\bullet$".

(1d) implies

- Velocity continuously across the interface $\Gamma(t)$
- Surface tension balances the jump of the normal stress.

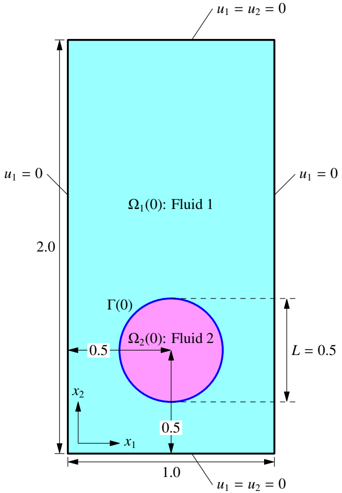
In addition to (1a)–(1d), boundary condition for $\boldsymbol{u}$ on $\partial\Omega$ and initial conditions: $\boldsymbol{u}|_{t=0}$ and $\Gamma(0)$ are required.

Rising bubble problem (1)

Domain / Parameters / Initial Conditions

As a typical example of interfacial flows, we consider rising bubble problem. We use the same settings of Test Case 2 in Hysing *et al.* (2009).

- $\Omega = (0,1) \times (0,2)$
- On Top/Bottom wall: $\boldsymbol{u} = \boldsymbol{0}$ (non-slip B.C.)
- On Left/Right wall: $u_1 = 0$ (free-slip B.C.)
- Initial velocity: $\boldsymbol{u}|_{t=0} = \boldsymbol{0}$
  buoyancy generates the motion of fluid
- $\Gamma(0) = \{\boldsymbol{x} \in \Omega \,|\, (x_1 - 0.5)^2 + (x_2 - 0.5)^2 = 0.25^2\}$
- $\sigma = 1.96$
- $(\rho_1, \nu_1) = (1000.0, 10.0)$,
  $(\rho_2, \nu_2) = (1.0, 0.1)$, $g = 0.98$
  - Reynolds number $\mathcal{R} = \dfrac{\rho_1 U_g L}{\nu_1} = 35.0$
  - Eötvös number $\mathcal{E} = \dfrac{\rho_1 U_g^2 L}{\sigma} = 125.0$
    $r_0 = 0.25,\ L = 2r_0,\ U_g = \sqrt{2 g r_0}$



Rising bubble problem (2)

Related Results

There are a lot of related results. For example...

- Sussman, Smereka & Osher (1994): Finite difference & level set method. Reinitialization of level set function with hyperbolic PDE was proposed.
- Tabata (2007): FEM based energy stable approximation.
- Hysing *et al*. (2009): Quantitative benchmark problem for rising bubble was proposed. Results by three different groups were presented. FEM+Levelset/FEM+ALE
- Doyeux *et al*. (2013): The same benchmark problem by French group FEM+Levelset (Feel++).
- Gross & Reusken (2010): Text book of numerical methods for two-phase incompressible flows

To capture the interface $\Gamma(t)$, we are due to level set method introduced by Osher & Sethian (1988).

Level set function

Let ϕ be signed distance function:

$$\phi(t,\boldsymbol{x}) = \begin{cases} \operatorname{dist}(\boldsymbol{x},\Gamma(t)), & \boldsymbol{x} \in \Omega_1(t), \\ 0, & \boldsymbol{x} \in \Gamma(t), \\ -\operatorname{dist}(\boldsymbol{x},\Gamma(t)), & \boldsymbol{x} \in \Omega_2(t). \end{cases}$$

ϕ is called level set function.
ϕ must satisfy $|\nabla\phi| = 1$ a.e. $\boldsymbol{x} \in \Omega$.

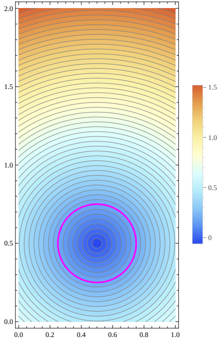


Fig. Density plot of $\phi(0,\boldsymbol{x})$ and its zero level set

By using ϕ, the interface $\Gamma(t)$ is represented as

$$\Gamma(t) = \{\boldsymbol{x} \in \Omega \,|\, \phi(t,\boldsymbol{x}) = 0\}, \quad t \geqq 0. \tag{2}$$

In our case,

$$\phi(0,\boldsymbol{x}) = \sqrt{(x_1-0.5)^2 + (x_2-0.5)^2} - 0.25\,.$$

Level set method (2)

Level set formulations (1)

$\boxed{\Omega \textbf{ and } (\rho, \nu)}$

$$\Omega = \begin{cases} \Omega_1(t), & \phi > 0, \\ \Gamma(t), & \phi = 0, \\ \Omega_2(t), & \phi < 0, \end{cases} \qquad (\rho, \nu) = \begin{cases} (\rho_1, \nu_1), & \phi > 0, \\ (\rho_2, \nu_2), & \phi < 0. \end{cases} \tag{3}$$

Let $H(\phi)$ be the Heviside function so that

$$H(\phi) = \begin{cases} 1, & \phi \geqq 0, \\ 0, & \phi < 0. \end{cases}$$

Then ρ and ν are given by

$$\rho(\phi) = \rho_1 H(\phi) + \rho_2(1 - H(\phi)),$$
$$\nu(\phi) = \nu_1 H(\phi) + \nu_2(1 - H(\phi)).$$

Level set method (3)

Level set formulation (2)

Surface tension

By using level set function ϕ, surface tension force is converted into volume force of the form

$$\boldsymbol{f}_{\mathrm{ST}} = \sigma\kappa\boldsymbol{n}|_{\Gamma(t)}\delta(\phi) \tag{4}$$

Here $\delta(\phi)$ is Dirac's delta whose support is the zero level set of ϕ.
Normal vector on $\Gamma(t)$ and the curvature κ are given by

$$\boldsymbol{n}|_{\Gamma(t)} = \left.\frac{\nabla\phi}{|\nabla\phi|}\right|_{\phi=0}, \qquad \kappa(t) = -\operatorname{div}\boldsymbol{n}|_{\Gamma(t)} = -\operatorname{div}\left.\frac{\nabla\phi}{|\nabla\phi|}\right|_{\phi=0} \tag{5}$$

Deformation of interface

In level set method, the deformation of interface is described by motion of zero level set of $\phi(t,\boldsymbol{x})$. $\phi(t,\boldsymbol{x})$ is driven by the transport equation.

$$\partial_t\phi + \boldsymbol{u}\cdot\nabla\phi = 0$$

Level set method (4)

Resulting problem

The resulting problem is coupled system of the Navier-Stokes equations and transport equation.

Resulting problem

$$\rho(\phi)(\partial_t \boldsymbol{u} + \boldsymbol{u} \cdot \nabla \boldsymbol{u}) = \operatorname{div}(2\nu(\phi)\mathbb{D}(\boldsymbol{u}) - p\mathbb{I}) + \boldsymbol{f}_{\mathsf{ST}} + \boldsymbol{f}_{\mathsf{gravity}}, \tag{6a}$$

$$\operatorname{div} \boldsymbol{u} = 0, \tag{6b}$$

$$\partial_t \phi + \boldsymbol{u} \cdot \nabla \phi = 0 \tag{6c}$$

$$\boldsymbol{u}(0, \boldsymbol{x}) = \boldsymbol{u}_0(\boldsymbol{x}) \equiv (0, 0), \tag{6d}$$

$$\phi(0, \boldsymbol{x}) = \phi_0(\boldsymbol{x}) = \sqrt{(x_1 - 0.5)^2 + (x_2 - 0.5)^2 - 0.25^2} \tag{6e}$$

$$\oplus \text{ boundary condition for } \boldsymbol{u} \text{ on } \partial\Omega. \tag{6f}$$

Here

$$\boldsymbol{f}_{\mathsf{ST}} = \sigma\kappa\boldsymbol{n}|_{\Gamma(t)}\delta(\phi), \tag{6g}$$

$$\boldsymbol{f}_{\mathsf{gravity}} = (0, -\rho(\phi)g) \tag{6h}$$

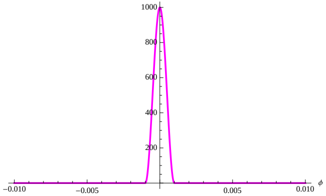
Numerical approximation (1)

Approximation of $\delta(\phi)$ and $H(\phi)$

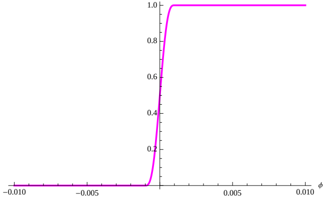
In numerical computation, we need approximations of $\delta(\phi)$ and $H(\phi)$ as continuous functions.

$$\delta(\phi) \approx \delta_\varepsilon(\phi) = \begin{cases} \dfrac{1}{2\varepsilon}\left(1 + \cos\left(\dfrac{\pi\phi}{\varepsilon}\right)\right), & |\phi| < \varepsilon, \\ 0, & |\phi| \geqq \varepsilon. \end{cases}$$

$$H(\phi) \approx H_\varepsilon(\phi) = \begin{cases} 1, & \phi \geqq \varepsilon, \\ \dfrac{1}{2} + \dfrac{1}{2}\left(\dfrac{\phi}{\varepsilon} + \dfrac{1}{\pi}\sin\left(\dfrac{\pi\phi}{\varepsilon}\right)\right), & |\phi| < \varepsilon, \\ 0, & \phi \leqq -\varepsilon. \end{cases}$$



(a) $\delta_\varepsilon(\phi)$ with $\varepsilon = 10^{-3}$



(b) $H_\varepsilon(\phi)$ with $\varepsilon = 10^{-3}$

Remark

- $\delta_\varepsilon(\phi)$ and $H_\varepsilon(\phi)$ are continuous function of ϕ
- ε is determined by mesh sizes near $\Gamma(t)$
- In FreeFem++, we can use numerical levelset.
  - `int1d(Th,levelset=phi){...}`

Numerical approximation (2)

Weak form and Full-discretized problem

Finite element spaces

- $\mathbf{V}_h \subset H^1(\Omega)^2, \Pi_h \subset L^2_0(\Omega) = \left\{p \in L^2(\Omega) \mid \int_\Omega p\, d\boldsymbol{x} = 0\right\}, X_h \subset L^2(\Omega)$
- Find solution $(\boldsymbol{u}_h, p_h, \phi_h) \in \mathbf{V}_h \times \Pi_h \times X_h$
  - $\mathbf{V}_h \times \Pi_h$: Hood-Taylor (P2/P1-elements)
  - X_h: P1-element

Weak formulation of full discretized problem

$$
\begin{aligned}
&\frac{1}{\tau}\left(\rho_\varepsilon(\phi_h^n)\boldsymbol{u}_h^{n+1}, \boldsymbol{v}_h\right) + (2\nu_\varepsilon(\phi_h^n)\mathbb{D}(\boldsymbol{u}_h^{n+1}), \mathbb{D}(\boldsymbol{v}_h)) \\
&\qquad - (p_h^{n+1}, \operatorname{div} \boldsymbol{v}_h) = \frac{1}{\tau}(\boldsymbol{u}_h^n \circ \boldsymbol{X}^n) + (\boldsymbol{F}(\phi_h^n), \boldsymbol{v}_h) + \text{b.d.t.}, \quad \forall \boldsymbol{v}_h \in \mathbf{V}_h, && \text{(7a)} \\
&(\operatorname{div} \boldsymbol{u}_h^{n+1} + \alpha p_h^{n+1}, q_h) = 0, \quad \forall q_h \in \Pi_h, && \text{(7b)} \\
&\phi_h^{n+1} = \tau \phi_h^n \circ \boldsymbol{X}^n && \text{(7c)}
\end{aligned}
$$

Reinitialization (1)

What is reinitialization ?

- The level set function ϕ is required to keep $|\nabla\phi(t,\boldsymbol{x})| = 1$ a.e.$\boldsymbol{x} \in \Omega$ for any $t \geqq 0$, because ϕ is signed distance function.
- However, in numerical computation with level set method, $|\nabla\phi_h^n|$ loses such a property as time goes by.
- Since $\partial_t \phi + \boldsymbol{u} \cdot \nabla\phi = 0$ is nonlinear hyperbolic PDE, we require some stabilized technique to solve the transport equation. e.g., Characteristic method, SUPG, etc...

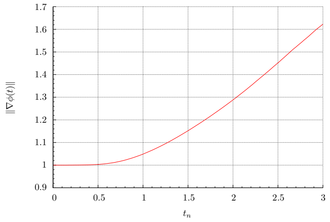


Fig. Time sequence of $\|\nabla\phi_h^n\|$ of a numerical computation without any reinitialization for ϕ

We need to recover $|\nabla\phi_h| = 1$. The prodecure to recover such a property of ϕ_h is called Reinitialization.

In this talk, we use PDE based reinitializations.

- R.I. by hyperbolic PDE (Sussmann *et al.* (1994))
- R.I. by elliptic PDE (Basting & Kuzmin (2013)).

Reinitialization (2)

R.I. with nonlinear elliptic PDE

Recently Basing & Kuzmin (2013) introduced R.I. with nonlinear elliptic PDE as follows.

R.I. with nonlinear elliptic PDE, Basting & Kuzmin (2013)

Let $\phi(t, \boldsymbol{x})$ be a function which is required to recover $|\nabla\phi| = 1$ and $\psi = \psi(\boldsymbol{x}; t)$ be solution to the following variational problem.

$$((1 - 1/|\nabla\psi|)\nabla\psi, \nabla\phi)_\Omega + \beta\langle\psi, \varphi\rangle_{\{\phi=0\}} = 0, \quad \forall\varphi \in C^\infty(\Omega), \tag{ERI}$$

where $\beta \gg 1$ is parameter of penalization. Then $\psi(\boldsymbol{x}; t)$ may have the same zero level set of ϕ and may become signed distance function.

Remark

- Find fixed point by successive approximation. Rate of convergence is better than hyperbolic PDE based R.I..
- It is very easy to implement in finite element method.
- Mathematical justification is not verified (but it works well).

Benchmark Values (1)

Centroid / Center of mass

In order to estimate our numerical results with Hysing *et al.* (2009), we introduce some benchmark values.

Centroid vector / Center of mass

$$\boldsymbol{X}_c(t) = (X_{c,1}(t), X_{c,2}(t)), \quad X_{c,j}(t) = \frac{1}{|\Omega_2(t)|}\int_{\Omega_2(t)} x_j \, d\boldsymbol{x}$$

- $X_{c,1}$: axi-symmetricity of bubble
- $X_{c,2}$: vertical location of center of mass

Since $\Omega_2(t) = \{\boldsymbol{x} \in \Omega \mid \phi(t,\boldsymbol{x}) < 0\}$, the centroid vector is reformulated as follow.

$$X_{c,j}(t) = \frac{\displaystyle\int_\Omega x_j \mathbb{1}_{\{\phi<0\}}(\boldsymbol{x}) \, d\boldsymbol{x}}{\displaystyle\int_\Omega \mathbb{1}_{\{\phi<0\}}(\boldsymbol{x}) \, dx}.$$

$\mathbb{1}_D$ is the indicator function on D.

Benchmark Values (2)

Circularity

The degree of circularity $\chi = \chi(t)$ is defined as

$$\chi(t) = \frac{P_a(t)}{P_b(t)} = \frac{\text{perimeter of area-equivalent circle}}{\text{Perimeter of bubble}}$$

Here P_a is the perimeter of a circle with diameter d_a, i.e., $P_a = \pi d_a$, such a circle has area equal to that of bubble with perimeter P_b.

Remark

- Volume of bubble is preserved $\Longrightarrow P_a \equiv \pi r_0^2$ (constant, in our case $r_0 = 0.25$).
- By the level set function ϕ and approximation of Dirac's delta $\delta_\varepsilon(\phi)$, P_b is given and approximated by

$$P_b = \oint_{\{\phi=0\}} d\sigma \approx \int_\Omega \delta_\varepsilon(\phi)\, d\boldsymbol{x}$$

Benchmark Values (3)

Mean velocity in Bubble / Rise velocity

Mean Velocity in Bubble

$$\boldsymbol{U}_c(t) = (U_{c,1}(t), U_{c,2}(t)), \quad U_{c,j}(t) = \frac{1}{|\Omega_2(t)|} \int_{\Omega_2(t)} u_j(t, \boldsymbol{x})\, d\boldsymbol{x}$$

- $U_{c,1}$ denotes axi-symmetricity of motion in bubble
- $U_{c,2}$ is so called rise velocity

Similar manner as in centroid vector,

$$U_{c,j}(t) = \frac{\displaystyle\int_{\Omega} \mathbb{1}_{\{\phi(t,\boldsymbol{x})<0\}} u_j(t, \boldsymbol{x})\, d\boldsymbol{x}}{\displaystyle\int_{\Omega} \mathbb{1}_{\{\phi(t,\boldsymbol{x})<0\}}\, d\boldsymbol{x}}$$

Benchmark Values (4)

$\|\nabla\phi(t)\|$ and $|\Omega_2(t)|$

In Hysing *et al.* (2009), $\boldsymbol{X}_c(t), \chi(t), \boldsymbol{U}_c(t)$ are used for their benchmark problem (in particular, $X_{c,2}(t), \chi(t), U_{c,2}(t)$ are used.)
In addition to these benchmark values, we also observe $\|\nabla\phi\|$ and $|\Omega_2(t)|$ for checking $|\nabla\phi_h^n| = 1$ and mass-preservation of fluid 2 in our computation.

$\boxed{\|\nabla\phi(t)\|}$

In order to check the level set function satisfies $|\nabla\phi| = 1$ for a.e. $\boldsymbol{x} \in \Omega$ in our numerical computation, we observe L^1 mean value of $|\nabla\phi|$.

$$\|\nabla\phi(t)\| := \frac{1}{|\Omega|}\int_\Omega |\nabla\phi(t,\boldsymbol{x})|\, d\boldsymbol{x}$$

If $|\nabla\phi| \equiv 1$ for any $\boldsymbol{x} \in \Omega$, $\|\nabla\phi(t)\| \equiv 1$ for all t.

Volume of fluid 2

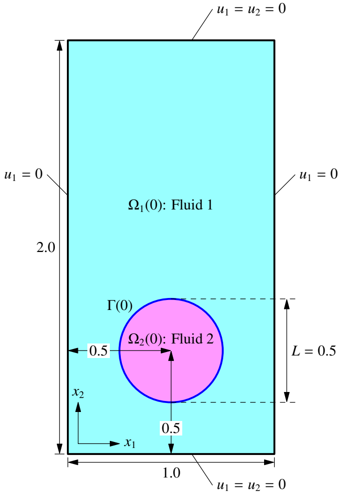
$$|\Omega_2(t)| = \int_{\Omega_2(t)} d\boldsymbol{x} = \int_\Omega \mathbb{1}_{\{\phi<0\}}\, d\boldsymbol{x}.$$

This value is used in benchmark values of Hysing *et al.* (2009).

Numerical experiments (1)

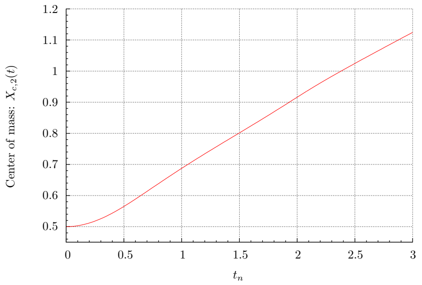
Parameters / Settings of Benchmark problem

- $\Omega = (0,1) \times (0,2)$
- On Top/Bottom wall: $\boldsymbol{u} = \boldsymbol{0}$ (non-slip B.C.)
- On Left/Right wall: $u_1 = 0$ (free-slip B.C.)
- Initial velocity: $\boldsymbol{u}|_{t=0} = \boldsymbol{0}$
- $\phi(0, \boldsymbol{x}) = \sqrt{(x_1 - 0.5)^2 + (x_2 - 0.5)^2} - 0.25.$
- $(\rho_1, \nu_1) = (1000.0, 10.0)$,
  $(\rho_2, \nu_2) = (1.0, 0.1), g = 0.98, \sigma = 1.96$
- Temporal step size: $\tau = 10^{-3}$
- Computational mesh at each time step is refined by adaptive mesh.
  In particular, a lot of mesh points are taken near the interface.

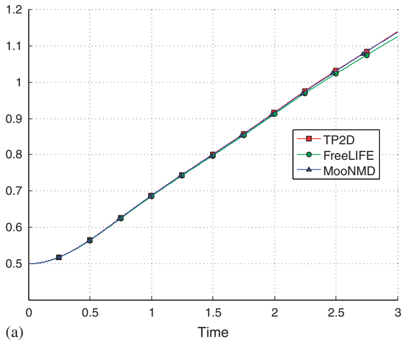


Numerical experiments (2)

Quantitative benchmark: Centroid $X_{c,2}(t)$



(a) Our numerical computation



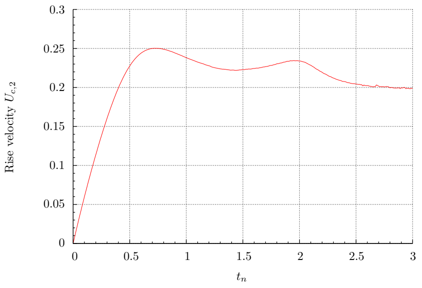
(b) Results of Hysing *et al.*(2009)

Fig. Time sequence of $X_{c,2}(t_n)$

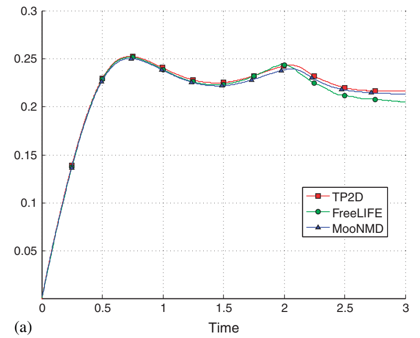
TP2D: TU Dortmund / FreeLIFE: EPFL Lausanne / MooNMD: Univ. Magdeburg

Numerical experiments (3)

Quantitative benchmark: Rise-velocity



(a) Our numerical computation

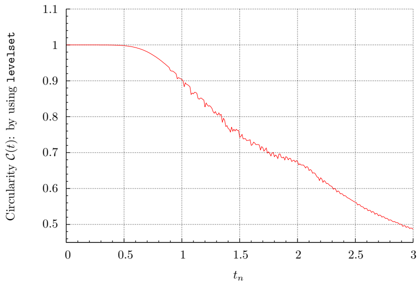


(b) Results of Hysing *et al.*(2009)

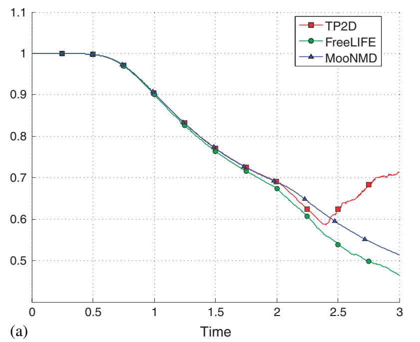
Fig. Time sequence of rise velocity $U_{c,2}(t_n)$

Numerical experiments (4)

Quantitative benchmark: Circularity



(a) Our numerical computation



(b) Results of Hysing *et al.* (2009)

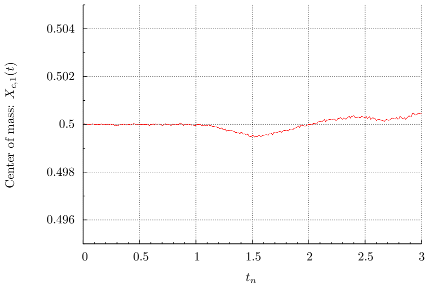
Fig. Time sequence of circularity

- By the above three benchmark values, our result is similar to that of FreeLIFE (EPFL Lausanne).

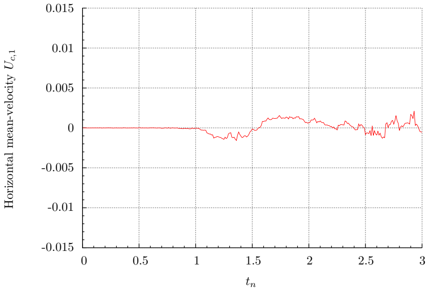
Numerical experiments (5)

Quantitative benchmark: Symmetricity

Using $X_{c,1}(t)$ and $U_{c,1}(t)$, we observe symmetricity of the motion of bubble.



(a) Time sequence of $X_{c,1}(t_n)$ which is the first component of centroid vector $\boldsymbol{X}_c(t_n)$.
Time-Average: $\overline{X_{c,1}} = 0.499992787.$
$X_{c,1}(0) - \overline{X_{c,1}} = 7.21 \times 10^{-6} > 0$

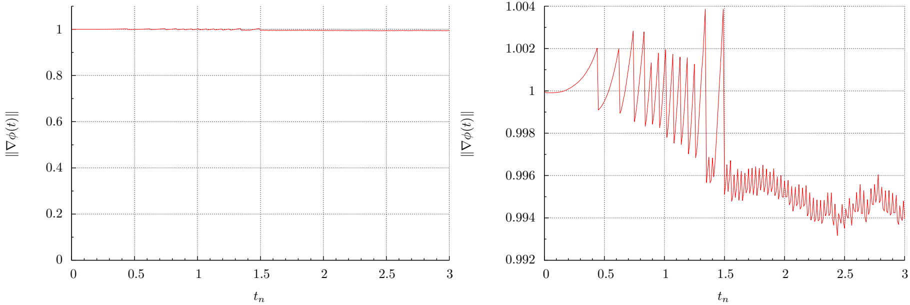


(b) Time sequence of $U_{c,1}(t_n)$ which is the first component of mean velocity $\boldsymbol{U}_c(t_n)$.
Time-Average: $\overline{U_{c,1}} = 8.75 \times 10^{-5} > 0$

Fig. Time sequence of $X_{c,1}(t_n)$ and $U_{c,1}(t_n)$

Numerical experiments (6)

Quantitative benchmark: $\|\nabla \phi_h^n\|$



(a) Time sequence of $\|\nabla \phi_h^n\|$ (macroview) (b) Time sequence of $\|\nabla \phi_h^n\|$ (microview)

Fig. Time sequence of $\|\nabla \phi_h^n\|$.

- **Time-average**: $\overline{\|\nabla \phi_h\|} = 0.997385$, $1 - \overline{\|\nabla \phi_h\|} = 0.002615$
- $\|\nabla \phi_h(3.0)\| = 0.993951$, $1 - \|\nabla \phi_h(3.0)\| = 0.006049$

Numerical experiments (7)

Quantitative benchmark: Volume of bubble

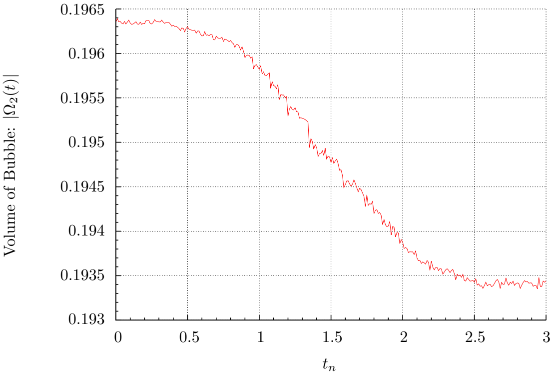


Fig. Time sequence of $|\Omega_2(t_n)|$ (macroview)

- $|\Omega_2(0.0)| = \pi r_0^2 \approx 0.19635$ (initial value)
- $|\Omega_2(3.0)| = 0.193442$
- In our computation, 1.5% of fluid 2 was lost.

Thank you for your attention.