Schriftenreihe aus dem Institut für Strömungsmechanik

Herausgeber
J. Fröhlich, R. Mailach

Institut für Strömungsmechanik
Technische Universität Dresden
D-01062 Dresden

Band 39

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A modelling approach for deformable gas bubbles

TUDpress
2023

Die vorliegende Arbeit wurde am 12. Januar 2022 an der Fakultät Maschinenwesen der Technischen Universität Dresden als Dissertation eingereicht und am 2. August 2023 erfolgreich verteidigt.

This work was submitted as a PhD thesis to the Faculty of Mechanical Science and Engineering of TU Dresden on 12 January 2022 and successfully defended on 2 August 2023.

Gutachter | Reviewers
1. Prof. Dr.-Ing. habil. Jochen Fröhlich, TU Dresden
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Bibliografische Information der Deutschen Nationalbibliothek
Die Deutsche Nationalbibliothek verzeichnet diese Publikation in der Deutschen Nationalbibliografie; detaillierte bibliografische Daten sind im Internet über http://dnb.d-nb.de abrufbar.

Bibliographic information published by the Deutsche Nationalbibliothek
The Deutsche Nationalbibliothek lists this publication in the Deutsche Nationalbibliografie; detailed bibliographic data are available in the Internet at http://dnb.d-nb.de.

ISBN 978-3-95908-637-0

bei Thelem Universitätsverlag
und Buchhandlung GmbH & Co. KG
Dresden und München
www.tudpress.de

Gesetzt vom Autor. | Typeset by the author.
Printed in Germany.

Technische Universität Dresden
Institute of Fluid Mechanics
2023

A modelling approach for deformable gas bubbles

A thesis submitted to the Faculty of Mechanical Engineering of the Technische Universität Dresden in partial fulfilment of the requirements for the degree of Doctor of Engineering Sciences (Dr.-Ing.)

by

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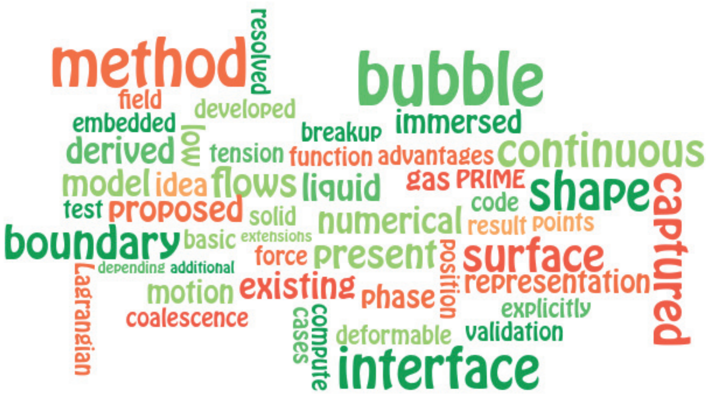
Date of submission: 12 January 2022

May you never outgrow bubbles.

Author unknown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Acknowledgements

First of all, I would like to appreciate the willingness of the members of our society to invest in scientific work. I am glad that I was given the opportunity to contribute as a researcher at the Institute of Fluid Mechanics at Technische Universität Dresden.

Most of my thanks go to my doctoral supervisor *Prof. Dr.-Ing. habil. Jochen Fröhlich*, without whom not a single word or result of this thesis would have been possible. Dear Mr Fröhlich, you have opened the door to a field of activity that I never want to close again. Your wealth of ideas, your enthusiasm and your confidence were necessary conditions for this work. When I saw only trees, you helped me to see the wood again or vice-versa.

Furthermore, I would like to thank the whole staff of the chair. Against all odds, every single colleague was so helpful and friendly that some of them have become real friends of mine. Special thanks go to *Silvio Tschisgale*, *Denis Koschichow*, *Ramandeep Jain*, *Bernhard Ott*, *Bastian Löhrer*, *Ronja May*, *Thomas Hafemann*, *Matthias Joppa*, *Tobias Hanisch*, *Claudia Liersch*, *Annette Roewer* and *Frank Rüdiger*, to mention only the first names of a long list.

Finally, I would like to thank my whole patchwork family, including my sister, and of course my beloved partner *Nora*. They have always supported me without ever asking for anything in return and have at all times given me the freedom to nurture my curiosity, which is a great privilege.

Abstract

The present work contributes to the field of numerical simulation of multiphase flows with a focus on gas bubbles in liquids. The general difficulty in modelling multiphase flows is to handle the interfaces. An interface can exist between solid, liquid and gaseous phases. Position and shape of the interface are captured with very different accuracy or are even neglected, depending on the selected method. If captured, it can be captured implicitly or explicitly, with the latter providing the most realistic picture. The immersed boundary code PRIME allows the explicit capture of phase boundaries of the solid-liquid and solid-gaseous type. The present work contributes to a third boundary type, the interface between gas and liquid as it appears in bubbly flows. This is a challenge due to the deformability of the bubbles. The **basic idea** is two-fold: first, the interface motion and the interfacial forces are derived from the Navier-Stokes equations, allowing a Lagrangian specification of the surface motion and the surface loads. Second, based on these equations of motion, the bubble shape is captured via a non-local parametric representation. Thus, the bubble is explicitly known as a continuous object. This is an essential difference to conventional methods, where it is common to define the surface position via marker points or, implicitly, by an indicator function. Through this continuous, Lagrangian representation, the bubble can change position and shape and is coupled locally with the fluid field depending on its location. **Advantages** are the preservation of the efficiency of the immersed boundary method, the robustness of the shape even on a coarse grid, the simple calculation of the surface tension, the exact preservation of the bubble volume, the advantageous collision behaviour with solid walls as well as the controllability of coalescence and breakup. Further advantages result from post-processing, because shape parameters can be derived without any problems. Building on preliminary work, an alternative approach for resolved bubble modelling is thus available, allowing more advanced numerical predictions in the future.

Zusammenfassung

Die vorliegende Arbeit leistet einen Beitrag im Bereich der numerischen Simulation von Mehrphasenströmungen mit Schwerpunkt auf Gasblasen in Flüssigkeiten. Die generelle Schwierigkeit bei der Modellierung von Mehrphasenströmungen besteht im Umgang mit der Phasengrenze. Diese kann zwischen festen, flüssigen und gasförmigen Phasen bestehen. Lage und Form der Phasengrenze werden je nach Methode mit sehr unterschiedlicher Genauigkeit erfasst oder gar vernachlässigt. Falls sie erfasst wird, kann sie implizit oder explizit erfasst werden, wobei letzteres das realistischste Bild liefert. Der Immersed-Boundary-Code PRIME gestattet die explizite Erfassung der Phasengrenzen vom Typ fest-flüssig und fest-gasförmig. Die vorliegende Arbeit treibt die Erweiterung auf den Phasengrenzentypus gasförmig-flüssig voran, wie er in blasenbeladenen Strömungen auftritt. Dies ist aufgrund der Deformierbarkeit der Gasblasen eine Herausforderung. Die **Grundidee** ist zweigeteilt: Erstens wird die Bewegung der Blasenoberfläche aus den Standardgleichungen derart hergeleitet, dass sie eine Lagrangesche Betrachtungsweise der Bewegung und der Kräfte ermöglicht, ohne dass die Strömung im Blaseninneren abgebildet werden muss. Nachdem diese Bewegungsgleichung bekannt ist, erfolgt zweitens die Erfassung der Blasenform über eine nicht-lokale parametrische Repräsentation. Damit ist die Blase explizit als kontinuierliches Objekt bekannt. Dies ist ein wesentlicher Unterschied zu herkömmlichen Methoden, bei denen die Lage der Phasengrenze über Oberflächenpunkte definiert wird oder aus einer Indikatorfunktion rekonstruiert werden muss. Durch diese kontinuierliche, Lagrangesche Repräsentation kann die Blase Position und Form verändern und wird je nach Aufenthaltsort lokal mit dem Fluidfeld gekoppelt. **Vorteile** sind der Erhalt der Effizienz der Immersed-Boundary-Methode, die Robustheit der Form auch auf grobem Gitter, die einfache Berechnung der Oberflächenspannung, der exakte Erhalt des Blasenvolumens, das vorteilhafte Kollisionsverhalten mit festen Wänden sowie die Kontrollierbarkeit von Koaleszenz und Breakup. Weitere Vorteile ergeben sich beim Post-Processing, denn Formparameter können problemlos abgeleitet werden. Aufbauend auf Vorarbeiten ist damit ein alternatives Verfahren zur aufgelösten Blasenmodellierung verfügbar, was weitergehende numerische Vorhersagen ermöglicht.

Contents

1 Introduction

1.1 Relevance of modelling bubbly flows

Bubbles accompany our everyday lives from childhood, which is why they seem so familiar to us. But as usual, a closer inspection reveals the true complexity and what first seemed so simple is suddenly difficult or impossible to predict. And the quality of our predictions has always been a good measure of our understanding.

Nature knows many applications for bubbly flows. Water spiders use air bubbles to build up an underwater oxygen supply, humpback whales trap krill with bubble-nets, star-nosed moles can track their prey because air bubbles transport the smell, and there are countless other examples (Langley, 2020). Among these, at least the whales demonstrate a certain degree of predictive ability and understanding.

Figure 1.1: *Air bubbles in water.*

The phenomena observed in bubbly flows are numerous. A bubble may grow, deform, collide, burst or coalesce. And when two bubbles *kiss and tumble* (Vélez-Cordero et al., 2011) it is close to a real love story. Typically, a rising bubble may trigger trailing vortices which in turn affect the bubble shape and its behaviour. The interaction with surrounding fluid can be very strong and may lead to contrary effects. Bubbles often accelerate the liquid or, quite the opposite, slow it down. They may generate turbulence - or dampen it. Bubbles are both fascinating in themselves and even of industrial relevance, for example in pipes (Nakoryakov et al., 1996; Krepper et al., 2005) or bubble columns (Shu et al., 2019). However, they are difficult to predict, particularly when they change their shapes.

Countless experimental and analytical studies have been undertaken to identify the underlying mechanisms needed to predict bubbly flows with deformable bubbles. Many of them have found their way into the classic text book of Clift et al. (1978), which has served as a good starting point for decades. Since then, numerous other experiments have been conducted (Tomiyama et al., 2002a,b; Hosokawa et al., 2002; Aoyama et al., 2016). However, each measurement technique is limited to certain quantities so that the overall picture cannot be revealed by experimentalists only.

Numerical simulations of deformable bubbles have proven to be a valuable complement. Here, a lot of progress has been made since Unverdi and Tryggvason (1992) presented their pioneering numerical results on deformable bubbles, for example methods like those described in Feng and Bolotnov (2017); Cifani et al. (2018). But our predictive abilities are still unsatisfactory. For example, huge numbers of cells are needed, increasing with the bubble's Reynolds number (Esmaeeli and Tryggvason, 2005). Even though the tremendous growth of high performance computing is making large simulations more and more affordable, the computational cost is definitely still one important limiting factor for our predictions. However, not the only one. There are phenomena which cannot be predicted at all until including some empirical knowledge.

Each method involves a trade-off between the following criteria:

- suitability for physical problem class and physical system of interest
- accuracy (determined by validation)
- robustness
  - numerical stability
  - low sensitivity of results
- efficiency (computational cost)

For a method to be useful at all, each of the four criteria must be met to at least some degree. Whether these criteria are well balanced can only be judged with respect to the quantities of interest.

The concluding remarks in *Struggle with computational bubble dynamics* (Tomiyama, 1998) still apply today:

> *"Even after almost ten years struggle with Computational Bubble Dynamcis, we are still not satisfied with our current status [...] what is important for us is to make the best of the advantages of each method and not to discard a method only for its temporal shortcomings."*

It is questionable whether an optimal method exists. Any progress towards more sophisticated methods is appreciated. Fortunately, not all ideas have been exploited yet: It turns out that a novel numerical method for deformable gas bubbles can be derived, rethinking the work of Schwarz et al. (2016). The resulting method can be seen as a building block for a general framework which is suitable to predict flow scenarios with rigid particles, flexible structures, and deformable bubbles.

1.2 Research goal and structure of the thesis

The goal is to propose a **novel numerical method for deformable gas bubbles** in liquid. The main requirements for the method are:

- Each bubble surface is resolved and of variable shape.
- To be suitable for bubble swarms, the method is required to give reasonable results even for comparatively poor spatial and temporal resolution.

The idea of the method can be summarised as follows:

- Each bubble surface is considered as an *embedded boundary*. This allows to derive a local bubble force field, which is only non-zero at the bubble surface's location.
- Each bubble surface is represented as *global continuous parametrisation*. The idea is taken from Schwarz et al. (2016) and developed further.

The method is developed in four steps:

Chapter 1 This is the present chapter. The following section defines the physical **system of interest** as a bubbly flow with deformable gas bubbles with constant material properties. An overview on **existing methods** for this kind of flow is given, clarifying the novelty of the current approach.

Chapter 2 The **fundamentals** of two-phase flow are recalled in condensed form to the extent needed. This is necessary to understand the assumptions in the consecutive derivation steps precisely.

Chapter 3 The **basic idea** is elaborated and the **equations of motion** for the embedded interface are derived.

Chapter 4 The **complete method** is obtained combining the equations of motion from the previous chapter with the continuous representation of the bubble shape by spherical harmonic functions.

Once the basic method is fully described, it is tested and extended:

Chapter 5 The **testing** phase. Selected verification and validation cases are presented.

Chapter 6 Some bubble phenomena, like breakup or coalescence, cannot be covered by the proposed method naturally and require sub-models. Some **extensions** for the present method are proposed and demonstrated.

Chapter 7 Strengths and limitations of the method. Possible improvements and **conclusions**.

1.3 Physical system of interest

The following physical assumptions are made and valid throughout the present work, unless stated otherwise:

- The flow is viscous, Newtonian, and incompressible.
- There is no phase change. Temperature changes are negligible.
- The domain is filled with liquid containing a certain number of bubbles.
- Liquid density ρ_ℓ and liquid viscosity μ_ℓ are constant.

Moreover, the following gas bubble assumptions are made:

- A bubble is defined as fluid particle with comparatively low density and viscosity ratios, i.e. with $\rho_g \ll \rho_\ell$ and $\mu_g \ll \mu_\ell$.
- Density and viscosity are constant within each bubble.
- The surface tension coefficient is constant for each bubble.
- Each bubble can have different material properties.

As a consequence, the method developed throughout this work is *not* designed to model heavy fluid particles with dominant inner friction, i.e. it is *not* designed to predict droplet behaviour.

1.4 Methodical classification

A brief overview of existing numerical methods for flows with deformable bubbles is provided. For this purpose, a property-based classification is sought first. More general methodical classifications are available (Loth, 2010). The present method is already taken into account.

Classification. Each method can be characterised by certain modelling decisions, which are recalled first. Each decision has far-reaching consequences in terms of applicability to specific problems, accuracy and computational time.

First, one has to decide whether the **interface** should be **resolved or not resolved**. Hence a method can be classified as

- I) interface-resolving (zero-thickness or diffuse), or
- ¬I) not interface-resolving.

States in between are conceivable, but not discussed here. A method is considered as interface-resolving, if it contains the position of the interface and a directional information for each adjacent phase. Some methods include a diffuse interface representation, others are based on a zero-thickness representation of the interface. Interface-resolving methods with zero-thickness representation of the interface are more accurate, but significantly more expensive which is why they are seldom applied to large problems.

Secondly, one has to decide about the **physical model**. This implies a decision on the scales to be modelled. A fluid can be considered as

1. an ensemble of particles, or
2. a continuum.

This decision is closely connected to the third decision, the equations to solve, i.e. the **mathematical model**. The most common equations are:

- $\mathrm{NSE_n}$) n-phase Navier-Stokes equations (n-field or one-field formulation, see Sec. 2)
- $\mathrm{NSE_\alpha}$) phase-averaged Navier-Stokes equations
- $\mathrm{NSE_1}$) single-phase Navier-Stokes equations coupled with additional equations of motion
- PFE) Phase field equations
- BE) Boltzmann equation

If the interface is resolved (I), a fourth decision must be made. One has to decide about the **interface storage location**. There are mainly three options:

- IV) The interface location is not stored explicitly (*volume methods*).
- IS) The interface location is stored explicitly (*surface methods*).
- IA) The interface location is stored as a subset of the fluid mesh (*aligned mesh methods*).

The idea to distinguish volume and surface methods goes back to Yeoh and Tu (2019). Volume methods typically base on a globally defined indicator function or volume markers. In both cases, separate effort must be made to determine the interface position.

Surface methods realise the interface either

ISD) discretely (usually by a set of surface points with or without connectivity) or

ISC) continuously (as an analytic function).

Remark 1. The terms *interface-resolving* and *phase-resolving* are not equivalent. Free surface flows, for example, are usually modelled *interface-resolving*, but not fully *phase-resolving* as the gas phase is neglected.

Remark 2. Note that the terms *volume methods* and *surface methods* are not equivalent to *Eulerian methods* and *Lagrangian methods*. The first two describe the interface storage location, whereas the last two refer to the frame of reference (spatially fixed or attached to the moving material, respectively). In principle, volume methods based on a Lagrangian description are conceivable. This applies analogously to the surface methods which are not necessarily Lagrangian methods. Eulerian surface methods are conceivable.

Remark 3. The terms *interface tracking* and *interface capturing* are also common in literature. They are not always used consistently, but in the majority of cases they are defined as synonyms for *surface methods* (IS) and *volume methods* (IV), respectively.

Existing methods. Further properties can be identified to distinguish existing approaches. However, the above should suffice for the current purpose. The most common method which does not resolve the interface (¬I) is the so called Euler-Euler method based on NSE_α. The most common methods which does resolve the interface (I) is the volume of fluid method purely based on volume fraction transport (NSE_n-IV). If extended by a reconstruction algorithm, a surface representation is available (NSE_n-IV+S). The classical level-set method (NSE_n-IV) can be extended to a particle level-set method (NSE_n-ISD). The front-tracking method (NSE_n-ISD) is a further example. An overview on the interface-resolving methods for bubbly flows is given in Tab. 1.1, together with relevant references. Note that the focus is on bubbles in viscous fluids, which is why methods like the boundary element method reported in Zhang and Liu (2015) are not included. Note that the overview in Tab. 1.1 is incomplete and that the methods often cannot be sharply distinguished from each other.

Present method. In the present work, a method of type NSE_1-ISC is proposed, based on solving the one-phase Navier-Stokes equations, representing the interface explicitly in a continuous manner (illustrated in Fig. 3.1). The proposed method is already included in the overview in Tab. 1.1 for guidance, although the details will be explained later. From a certain perspective, the present method borrows elements from immersed boundary methods, immersed interface methods, front-tracking methods and even ghost-cell methods. To the best of the author's knowledge, there is no method of this type yet.

Table 1.1: *Common interface-resolving methods for deformable bubbles in viscous fluid, including the method proposed.*

physical model	**equations**	interface storage location: volume: aligned fluid grid	interface storage location: volume: indicator function	interface storage location: volume: ↳ volume fraction	interface storage location: volume: ↳ signed-distance	interface storage location: volume: volume markers	interface storage location: surface: surface markers	interface storage location: surface: local parametrisation[a]	interface storage location: surface: global parametrisation	**name of the method**	**references**	properties: inner flow field computed	properties: bubble volume conserved	properties: indicator function computed
bubble as liquid phase	two-phase NSE	✓								GIM	Scardovelli and Zaleski (1999); Loth (2010)	✓	✓	
			✓	✓						VOF	Hirt and Nichols (1981), Roenby et al. (2016)	✓	(✓)	✓
						✓				MAC	Welch et al. (1965); McKee et al. (2008)	✓	(✓)	
			✓		✓					LS	Sussman et al. (1994); Balcázar et al. (2015)	✓	(✓)	✓
			✓	✓						PLS	Shimada et al. (2008)	✓	(✓)	✓
			✓	✓	✓					CLSVOF	Sussman et al. (2007); Kwakkel et al. (2013)	✓	(✓)	✓
							✓			FT	Unverdi and Tryggvason (1992); Roghair et al. (2016)	✓	(✓)	✓
							✓			IIM	Li and Lai (2001); Lee and LeVeque (2003)	✓	(✓)	✓
							✓			GCM	Dadone and Grossman (2004)	✓	(✓)	✓
							✓			CC	Ye et al. (2001)	✓	(✓)	✓
bubble as embedded boundary	single-phase NSE + interfacial forces								✓	IBUB[b]	present work		✓	
bubble as rigid body undergoing deformations	single-phase NSE + equations for translation, rot., deformation								✓	IBM	Schwarz et al. (2016)		✓	✓
liquid, particles, free energy	NSE and others					✓[c]				SPH	Hu and Adams (2006); Szewc et al. (2013)	✓	(✓)	
			✓							LBM	Amaya-Bower and Lee (2010)	✓	(✓)	✓
			✓							PFM	Badalassi et al. (2003)	✓	(✓)	✓

Abbreviations: GIM *grid interface methods* | VOF *volume-of-fluid method* | MAC *marker-and-cell method* | LS *level-set method* | PLS *particle-level-set method* | CLSVOF *coupled level-set/volume-of-fluid method* | FT *front-tracking method* | IIM *immersed interface method* | GCM *ghost-cell method* | SPH *smoothed-particle hydrodynamics* | IBUB *immersed bubble interface method*[b] | LBM *lattice Boltzmann method* | PF *phase-field method*

[a] Some methods use splines or similar local parametrisations to improve the interface transport, but the interface position itself is stored somewhere else. [b] Provisional name. [c] Particles occupy a certain volume.