

# Numerical study of a high order 3D FEM-Level Set approach for immiscible flow simulation

Stefan Turek, Otto Mierka, Shuren Hysing and Dmitri Kuzmin

**Abstract** Numerical simulation of incompressible multiphase flows with immiscible fluids is still a challenging field, particularly for 3D configurations undergoing complex topological changes. In this paper, we discuss a 3D FEM approach with a high-order Stokes elements ( $Q_2/P_1$ ) for velocity and pressure on general hexahedral meshes. A discontinuous Galerkin approach with piecewise linear polynomials (dG(1)) is used to treat the Level Set function. The developed methodology allows the application of special redistancing algorithms which do not change the position of the interface. We explain the corresponding FEM techniques for treating the advection steps and surface tension effects, and validate the corresponding 3D code with respect to both numerical test cases and experimental data. The corresponding applications describe the classical rising bubble problem for various parameters and the generation of droplets from a viscous liquid jet in a coflowing surrounding fluid. Both of these applications can be used for rigorous benchmarking of 3D multiphase flow simulations.

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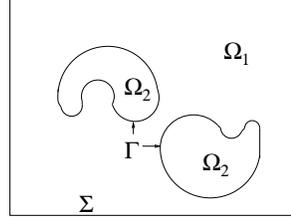
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## 1 INTRODUCTION

Multiphase flow problems are very important in many applications, and performing accurate, robust and efficient numerical simulations of them has been the object of numerous research and simulation projects for many years.

One of the main challenges for the underlying numerical methods is that the position of the moving interface between two fluids is unknown and must be determined as a part of the boundary value problem which should be solved. If we assume a domain  $\Omega$  with two immiscible fluids, then the time dependent subdomains  $\Omega_1(t)$  and  $\Omega_2(t)$  are bounded by an external boundary  $\Sigma$  and a dynamic interior boundary or interface  $\Gamma(t)$  which might consist of several components (see Figure 1).



**Fig. 1** Sketch of the complete domain  $\Omega = \Omega_1 \cup \Gamma \cup \Omega_2$ .

Then, the usual model for laminar (multiphase) flow is described by the incompressible Navier-Stokes equations

$$\begin{aligned} \rho(\mathbf{x}) \left[ \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right] - \nabla \cdot (\mu(\mathbf{x}) [\nabla \mathbf{u} + (\nabla \mathbf{u})^T]) + \nabla p = \rho(\mathbf{x}) \mathbf{g} + \mathbf{f}_\Gamma(\sigma) \quad (1) \\ \nabla \cdot \mathbf{u} = 0 \quad \text{in} \quad \Omega = \Omega_1 \cup \Gamma \cup \Omega_2 \quad (2) \end{aligned}$$

which contain an additional force term  $\mathbf{f}_\Gamma(\sigma)$  due to the surface tension  $\sigma$  at the free interface  $\Gamma$ . Here, the density  $\rho$  as well as the viscosity  $\mu$  are variable and discontinuous, that is

$$\rho(\mathbf{x}, t) = \begin{cases} \rho_1, & \forall \mathbf{x} \in \Omega_1(t) \\ \rho_2, & \forall \mathbf{x} \in \Omega_2(t) \end{cases}, \quad \mu(\mathbf{x}, t) = \begin{cases} \mu_1, & \forall \mathbf{x} \in \Omega_1(t) \\ \mu_2, & \forall \mathbf{x} \in \Omega_2(t) \end{cases} \quad (3)$$

which significantly influences the velocity  $\mathbf{u}$  as well as the pressure  $p$ .

This contribution describes the numerical analysis and application of a new Level Set approach in the framework of the Finite Element Method (FEM) for such multiphase flow problems. For this reason the open-source CFD package FEATFLOW ([www.featflow.de](http://www.featflow.de)) was utilized and extended with the corresponding newly created Level Set module such that the existing methodology of the FEATFLOW approach, namely flexible, high order FEM discretization schemes in space and time with flux correction [37] and edge-oriented stabilization techniques [63], unstructured meshes with adaptive grid deformation, efficient Newton-Multigrid solvers and parallelization based on domain decomposition could be directly exploited.

The outline of the paper is as follows: After a short description in section 2 of the state-of-the-art regarding interface tracking and capturing methods,

particularly for Level Set approaches, we describe in section 3 the chosen solution technique which is based on a discrete projection method [61, 62] for the Navier-Stokes equations, the Level Set advection equation and the corresponding reinitialization procedure. Moreover, the discretization aspects regarding the incompressible Navier-Stokes equations using the Crank-Nicolson method and the  $Q_2/P_1$  element pair are discussed in section 3, too, whereas the details of the employed Discontinuous Galerkin FEM approach with  $P_1$  elements for the Level Set equation can be found in section 4. Section 5 presents several numerical results which first of all evaluate the grid independent behaviour of the developed CFD solver. Furthermore, based on corresponding experimental and computational studies, we propose and discuss new benchmark configurations for prototypical 3D multiphase flows which can be used for ‘simple’ validation and evaluation of multiphase flow CFD codes without the necessity of complex postprocessing operations. Finally, the results are summarized in section 6 where an outlook is provided for more complex 3D multiphase flow problems.

## 2 MATHEMATICAL MODEL

The free interface  $\Gamma$  is constantly being deformed and moved so that its position has to be treated as an unknown and determined in every time step. Depending on the technique for the representation of the interface, one can distinguish between *front tracking* and *front capturing* approaches which can be realized on fixed as well as dynamic moving meshes. For an overview of existing numerical approaches and their classification we recommend references [55] and [58]. The “natural” front tracking approach [2],[24],[44],[66] is based on an explicit tracing of the dynamic interface between the two phases. Here, in the case of Lagrangian finite element methods [28], the underlying mesh has to be constantly adapted to the free interface so that the grid points move with the interface. More flexibility is promised by the *Arbitrary Lagrangian Eulerian* (ALE) formulation [5],[6],[9],[20],[22] and [52] which is based on local grid adaptation and which provides excellent results in the case of moderate deformations (for instance for small waves at the free surface). Moreover, there are many more techniques of fictitious domain and Chimera type which allow the highly accurate tracking of the dynamic interfaces via overlapping surface meshes [29]. However, such front tracking methods do not allow large deformations of the free interfaces or even topological changes such as drop formation and bubble breakup or coalescence, which typically lead to highly distorted meshes. Moreover, the computational costs regarding the implementation and also CPU timings are often very large for complex 3D simulations.

In contrast to such Lagrangian methods, Eulerian front capturing methods are much more robust and flexible. They are applicable even to free inter-

face problems with significant topology changes (breakup of bubbles, fragmentation, coalescence, etc.). Based on the early Marker-and-Cell method of Harlow and Welch [68], the implicit reconstruction of the interface is based on an indicator function  $\phi(\mathbf{x}, t)$  which contains the information about the corresponding subdomain for the point  $\mathbf{x}$  at time  $t$ . The distribution in the complete domain  $\Omega$  can then be calculated via the scalar transport equation

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0 \quad (4)$$

so that the exact position of the free interface  $\Gamma(\phi)$  at any time can be reconstructed from  $\phi$  with the help of postprocessing techniques. One of the most well known methods is the Volume-of-Fluid (VOF) method [1, 45] in which case the indicator function  $\phi$  can be interpreted as volume fraction which should have the discrete values 0 or 1 depending on the location of  $\mathbf{x}$ :

$$\phi(\mathbf{x}, t) = \begin{cases} 1, & \forall \mathbf{x} \in \Omega_1(t) \\ 0, & \forall \mathbf{x} \in \Omega_2(t) \end{cases} \quad (5)$$

The numerical drawback of this approach is that artificial diffusion smears out the (originally) discontinuous indicator function which arises from the solution of the discretized advection problems resulting in a boundary layer with  $0 < \phi < 1$ . Therefore, numerical schemes and locally adapted meshes have to be designed to address this boundary layer as thin as possible so that the corresponding error for reconstructing the free interface is reduced. Moreover, due to the steep gradients and the discontinuity of the indicator function, standard Galerkin schemes lead to unphysical oscillations which significantly deteriorate the accuracy or even lead to unphysical over- and undershoots. As conclusion, the development of corresponding high-order monotone discretization schemes in combination with unstructured, locally refined meshes still belongs to the numerical challenges one has to solve.

As a successful alternative, the Level Set approach [46],[47],[56] has been established which represents the interface as zero isoline of a continuous indicator function  $\phi$  which should be close to the distance with respect to the free interface

$$\phi(\mathbf{x}, t) = \begin{cases} \text{dist}(\mathbf{x}, \Gamma), & \forall \mathbf{x} \in \Omega_1(t) \\ -\text{dist}(\mathbf{x}, \Gamma), & \forall \mathbf{x} \in \Omega_2(t) \end{cases} \quad (6)$$

so that  $\Gamma(t) = \{\mathbf{x} \in \Omega \mid \phi(\mathbf{x}, t) = 0\}$  holds. In contrast to the VOF approach,  $\phi$  as a distance function is smooth and allows the calculation of a globally defined normal vector  $\mathbf{n}$  towards the interface  $\Gamma$  and of the corresponding curvature via

$$\mathbf{n} = \frac{\nabla \phi}{|\nabla \phi|}, \quad \kappa = -\nabla \cdot \mathbf{n} = -\nabla \cdot \left( \frac{\nabla \phi}{|\nabla \phi|} \right). \quad (7)$$

Here, special FEM techniques for gradient recovery can be used which allow highly accurate approximations of normals and curvature [58] which are necessary for the direct evaluation of the surface tension force  $\mathbf{f}_\Gamma = \kappa\sigma\delta(\phi)\mathbf{n}$ , with  $\delta(\phi)$  denoting the corresponding Dirac Delta function. Hence, the development and implementation of a typical Level Set approach consists of performing the following sequence of tasks:

- Discretization of the Level Set transport problem (4)
- Reinitialisation, resp., redistancing of the Level Set function.
- Additional correction so that mass and volume is preserved (if necessary).
- Calculation of normal vector fields (and curvature if needed) based on  $\phi$ .
- Evaluation of the discontinuous fluid parameters  $\rho(\phi)$ ,  $\mu(\phi)$ , and of  $\mathbf{f}_\Gamma$ , with or without reconstruction of  $\Gamma$ .

The above sequence of tasks involves a myriad of different possibilities and choices which inevitably lead to numerous differing solution approaches. This is evident from the rich collection of publications on Level Set methods which also demonstrates the high potential of these methods for a wide range of applications (see for instance the books by Osher [46] and Sethian [56]). However, the resulting quality of the solutions mainly depends on the underlying numerical and computational approaches, and one has to acknowledge the fact that most of existing Level Set codes are still based on finite differences on uniform Cartesian meshes which is easy to implement. The drawback is that the computational cost typically is quite high since uniform mesh refinement has to be performed to resolve the necessary scales, particularly near the fluidic interfaces, but also due to complicated geometries with small-scale structures. Unstructured meshes are particularly well suited for such approaches which leads us to finite volume and finite element discretization methods which are the most prominent candidates for unstructured simulation approaches. Examples for corresponding approaches in the framework of VOF and Level Set methods can be found in [3],[9],[11],[19],[33],[41],[43],[53]. In many approaches, for example in the *Interface Proximity Adaption Method* of Barth and Sethian [3], the mesh is locally refined near the interface which also is quite easy to find if  $\phi$  is a distance function [41]. Although finite element methods together with locally refined grids seem to possess a very advantageous behaviour for simulation of multiphase flow problems with free interfaces, most existing Level Set codes are still based on finite differences. It is only during the last ten years that FEM codes have been successfully applied for these special CFD problems ([49],[54],[57]; see also [18],[26],[43],[50],[58],[60]). However, there is still a huge potential for improvement if ‘*optimal*’ modern discretization and solution techniques shall be adapted to the special characteristics of FEM-Level Set methods. In constructing a modern Level Set solver it is important to focus on unstructured meshes with local grid refinement strategies for highly nonstationary multiphase flow simulations, and make detailed studies for higher numerical stability. Additionally, stable and accurate discretization of the convective terms

(for instance, VOF and Phase-Field methods show very steep gradients near the interface, similarly as Level Set approaches without redistancing), robust treatment of large density differences, and the handling of large surface tension  $\sigma$  also require special attention.

Summarizing the properties of FEM-Level Set techniques for multiphase flow problems, we can conclude the following (potentially) advantageous behaviour in comparison to interface tracking methods as well as VOF and Phase-Field approaches which motivates our recent and future work for the combination of FEM and Level Set methods:

- If the Level Set function satisfies the distance property, it is smooth so that even on highly uniform meshes qualitatively good results can be obtained. Local refinement around the interface will help to improve the accuracy, but in contrast to VOF and Phase-Field methods, which may lead to smeared interfaces due to numerical diffusion or to unphysical oscillations due to steep gradients, adaptive meshes are not necessary.
- Accurate FEM discretizations of higher order can be adapted to the special characteristics of Level Set functions, that means higher smoothness because of the distance function properties.
- Accurate representations of the interface are provided, without explicit description, but even for complex geometrical changes, which is important for handling the surface tension term.
- Auxiliary quantities like normal vectors and curvature are provided, even globally, which is particularly advantageous for the Continuous Surface Force (CSF) [8] approach.

On the other hand, there are still several problems with Level Set approaches (and some of them are also valid for VOF and Phase-Field methods) which are numerically challenging and which are in the focus of our recent and also planned research activities:

- The standard Level Set formulation is not conservative which may lead to mass loss.
- Since reinitialisation is necessary to preserve the distance property, often highly expensive computational operations might be necessary, for instance via solving globally the Eikonal equation, or redistancing is based on ‘cheaper’ methods which however change the position and shape of the interface, leading again to mass loss.
- Due to the standard explicit treatment of surface tension, the time step size is restricted by the *capillary time step restriction*, that means the necessary time steps depend by purely numerical reasons on the size of surface tension and on the local mesh size.

In the following sections, we first of all describe the overall solution technique which is based on a discrete projection method which is followed by a discussion of the FEM discretization details, particularly regarding the Discontinuous Galerkin approach for treating the Level Set equation.

### 3 DISCRETE PROJECTION METHODS FOR NAVIER-STOKES EQUATIONS

In this section, we briefly review the ‘Discrete Projection method’ as a special variant of Multilevel Pressure Schur Complement (MPSC) approaches for the solution of incompressible flow problems, and we combine it with FEM discretization techniques. We will explain some characteristics of high-resolution FEM schemes as applied to incompressible flow problems and discuss the computational details regarding the efficient numerical solution of the resulting nonlinear and linear algebraic systems. Furthermore, we will discuss the coupling mechanisms between the ‘basic’ flow model (standard Navier-Stokes equations for velocity and pressure) and the scalar transport equations for the Level Set indicator function in our multiphase flow solver.

#### 3.1 Discretization techniques

For a better illustration, we consider first of all numerical solution techniques for the (single phase) incompressible Navier-Stokes equations,

$$\begin{aligned} \mathbf{u}_t - \nu \Delta \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p_\rho &= \mathbf{f} \\ \nabla \cdot \mathbf{u} &= 0, \quad \text{in } \Omega \times (0, T] \quad \text{with } p_\rho = \frac{p}{\rho} \quad \text{and } \nu = \frac{\mu}{\rho} \end{aligned} \quad (8)$$

for given force  $\mathbf{f}$  which might contain the surface tension. Moreover, boundary values are prescribed on the boundary  $\partial\Omega$  as well as an initial condition at  $t = 0$ . Solving this problem numerically is still a considerable task in the case of long time calculations and high Reynolds numbers, particularly in 3D and also in 2D if the time dynamics is complex. The common solution approach is a separate discretization in space and time. We first (semi-) discretize in time by one of the usual methods known from the treatment of ordinary differential equations, such as the Forward or Backward Euler-, the Crank-Nicolson- or Fractional-Step- $\theta$ -scheme, or others, and obtain a sequence of generalized stationary Navier-Stokes problems.

**Basic  $\theta$ -scheme:**

Given  $\mathbf{u}^n$  and  $\Delta t = t_{n+1} - t_n$ , then solve for  $\mathbf{u} = \mathbf{u}^{n+1}$  and  $p_\rho = p_\rho^{n+1}$

$$\frac{\mathbf{u} - \mathbf{u}^n}{\Delta t} + \theta[-\nu \Delta \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u}] + \nabla p_\rho = \mathbf{g}^{n+1} \quad , \quad \nabla \cdot \mathbf{u} = 0 \quad , \quad \text{in } \Omega \quad (9)$$

with right hand side  $\mathbf{g}^{n+1} := \theta \mathbf{f}^{n+1} + (1-\theta) \mathbf{f}^n - (1-\theta)[- \nu \Delta \mathbf{u}^n + \mathbf{u}^n \cdot \nabla \mathbf{u}^n]$ .

In the following simulations, the parameter  $\theta$  is chosen as  $\theta = 1/2$ , representing the Crank-Nicolson-scheme which is of second order. Alternatively, the Fractional-Step- $\theta$ -scheme [65] which uses three different values for  $\theta$  and for the time step  $\Delta t$  at each time level, is another excellent candidate with slightly better robustness properties.

For the spatial discretization, we choose a finite element approach which is based on a suitable variational formulation. On the finite mesh  $\mathcal{T}_h$  (3D hexahedral elements in our case) covering the domain  $\Omega$  with local mesh size  $h$ , one defines polynomial trial functions for velocity and pressure. These spaces  $H_h$  and  $L_h$  should lead to numerically stable approximations as  $h \rightarrow 0$ , i.e., they should satisfy the so-called *inf-sup* (LBB) condition [23]

$$\min_{q_h \in L_h} \max_{\mathbf{v}_h \in H_h} \frac{(q_h, \nabla \cdot \mathbf{v}_h)}{\|q_h\|_0 \|\nabla \mathbf{v}_h\|_0} \geq \gamma > 0 \quad (10)$$

with a mesh-independent constant  $\gamma$ . While the original FEATFLOW solvers are based on *rotated multilinear* nonconforming finite element functions for the velocity and piecewise constant pressure approximations, we recently extended the complete solver package to higher order Stokes elements, namely conforming triquadratic ansatz functions for the velocity and linear pressure approximations ( $Q_2/P_1$ ), which belongs to the ‘best’ finite element pairs for laminar incompressible flow due to their accuracy and robustness. Since so far most of our numerical simulations have been performed for small up to moderate Reynolds numbers, the (nonlinear) convective operator was discretized using standard stabilization techniques only. Currently, we use edge-, resp., face-oriented FEM stabilization techniques [63] which can be easily realized for higher order ansatz functions, too. Here, special jump terms of the gradient of the solution as well as of the test function have to be included into the weak formulation which leads to a consistent stabilization, for stationary as well as nonstationary configurations. It is planned to apply this technique in the case of higher Reynolds number flows, too, which will be a subject of our further studies for such multiphase flow problems. For an overview regarding such special FEM stabilization techniques, we refer to [48, 63] and particularly to [12] which contains corresponding results for the  $Q_2/P_1$  approach, too.

### 3.2 Solution techniques

Using the same notation  $\mathbf{u}$  and  $p_\rho$  also for the coefficient vectors in the representation of the approximate solution, the discretized Navier-Stokes equations may be written as a coupled (nonlinear) algebraic system of the form:

Given  $\mathbf{u}^n$  and  $\mathbf{f}$ , compute  $\mathbf{u} = \mathbf{u}^{n+1}$  and  $p_\rho = p_\rho^{n+1}$  by solving

$$A\mathbf{u} + \Delta t B p_\rho = \mathbf{g} \quad , \quad B^T \mathbf{u} = 0, \quad \text{where} \quad (11)$$

$$\mathbf{g} = [M - \theta_1 \Delta t N(\mathbf{u}^n)]\mathbf{u}^n + \theta_2 \Delta t \mathbf{f}^{n+1} + \theta_3 \Delta t \mathbf{f}^n. \quad (12)$$

Here and in the following, we use the more compact form for the diffusive and advective part

$$N(\mathbf{v})\mathbf{u} := -\nu \Delta \mathbf{u} + \mathbf{v} \cdot \nabla \mathbf{u} \quad (13)$$

while  $M$  is the (lumped) mass matrix [67],  $B$  is the discrete gradient operator, and  $-B^T$  is the associated divergence operator. Furthermore,

$$A\mathbf{u} = [M - \theta \Delta t N(\mathbf{u})]\mathbf{u}, \quad N(\mathbf{u}) = K(\mathbf{u}) + \nu L, \quad (14)$$

where  $L$  is the discrete Laplacian and  $K(\mathbf{u})$  is the nonlinear transport operator incorporating a certain amount of artificial diffusion due to some appropriate FEM stabilization as described before. The solution of nonlinear algebraic systems like (11) is a rather difficult task and many aspects, namely the treatment of the nonlinearity and of the incompressibility as well as the outer control of the couplings, need to be taken into account. Consequently, this leads to a great variety of incompressible flow solvers which are closely related to one another but exhibit considerable differences in terms of their stability, convergence, and efficiency. The Multilevel Pressure Schur Complement (MPSC) approach outlined below makes it possible to put many existing solution techniques into a common framework and to combine their advantages so as to obtain better run-time characteristics.

The fully discretized Navier-Stokes equations (11) as well as the linear subproblems to be solved within the outer iteration loop for a fixed-point defect correction or, with a similar structure, for a Newton-like method admit the following representation

$$\begin{bmatrix} A & \Delta t B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ p_\rho \end{bmatrix} = \begin{bmatrix} \mathbf{g} \\ 0 \end{bmatrix}. \quad (15)$$

In general, we have  $A = M + \beta N(\mathbf{u})$ , with  $\beta = -\theta \Delta t$  for time-dependent problems. If the operator  $A$  is nonsingular, the velocity can be formally expressed as

$$\mathbf{u} = A^{-1}(\mathbf{g} - \Delta t B p_\rho) \quad (16)$$

and plugged into the discretized continuity equation

$$B^T \mathbf{u} = 0 \quad (17)$$

which gives a scalar *Schur complement* equation for the pressure only

$$B^T A^{-1} B p_\rho = \frac{1}{\Delta t} B^T A^{-1} \mathbf{g}. \quad (18)$$

Thus, the coupled system (15) can be handled as follows

1. Solve the Pressure Schur Complement (PSC) equation (18) for  $p_\rho$ .
2. Substitute  $p_\rho$  into relation (16) and compute the velocity  $\mathbf{u}$ .

It is worth mentioning that the matrix  $A^{-1}$  is full and should not be assembled explicitly. Instead, an auxiliary problem is to be solved by a direct method or by inner iterations. For instance, the velocity update (16) is equivalent to the solution of the discretized momentum equation  $A\mathbf{u} = \mathbf{g} - \Delta t B p_\rho$ . Likewise, the matrix  $S := B^T A^{-1} B$  is never generated in practice. Doing so would be prohibitively expensive in terms of CPU time and memory requirements. It is instructive to consider a preconditioned Richardson method which yields the following **basic iteration** for the PSC equation

$$p_\rho^{(l+1)} = p_\rho^{(l)} - C^{-1} \left[ S p_\rho^{(l)} - \frac{1}{\Delta t} B^T A^{-1} \mathbf{g} \right], \quad l = 0, \dots, L-1. \quad (19)$$

Here,  $C$  has to be chosen as suitable preconditioner to  $S$  but being easier to ‘invert’ in an iterative way. The number of PSC cycles  $L$  can be fixed or chosen adaptively so as to achieve a prescribed tolerance for the residual. The basic idea behind the family of global MPSC schemes is the construction of globally defined additive preconditioners for the Schur complement operator  $S = B^T A^{-1} B$ . Recall that the matrix  $A$  has the following structure

$$A := M + \beta K(\mathbf{u}) + \gamma L, \quad (20)$$

where  $\beta = -\theta \Delta t$  and  $\gamma = \nu \beta$ . Unfortunately, even today it is still a very challenging task to construct a matrix  $\tilde{A}$  and a preconditioner  $C = B^T \tilde{A}^{-1} B$  that would be a sufficiently good approximation to all three components of  $A$  and  $S$ , respectively; particularly for the convective part with  $K(\mathbf{u})$ . Therefore, one may start with developing individual preconditioners for the reactive ( $M$ ) and diffusive ( $L$ ) part, while the convective ( $K$ ) part is neglected by applying this special kind of operator splitting. In our case, the Reynolds numbers in the considered flow configurations are so far quite small, so that this approach can be justified, particularly if small time steps are used to resolve to complex dynamical behaviour. Therefore, the (lumped) mass matrix  $M$  proves to be a reasonable approximation to the complete operator  $A$ , so that our basic iteration (19) for the pressure Schur complement equation

$$p_\rho^{(l+1)} = p_\rho^{(l)} + [B^T M^{-1} B]^{-1} \frac{1}{\Delta t} B^T A^{-1} \left[ \mathbf{g} - \Delta t B p_\rho^{(l)} \right] \quad (21)$$

can be interpreted and implemented as a *discrete projection scheme*, if  $L = 1$ , such as those proposed in [14],[25]. Here, the important step is that for the chosen Stokes element pair,  $Q_2/P_1$ , the matrix  $P := B^T M^{-1} B$  can be explicitly built up relatively easily even in a domain decomposition framework due to the chosen discontinuous pressure. Then, the main algorithmic steps are as follows [61]:

1. Solve the ‘viscous Burgers’ equation for  $\tilde{\mathbf{u}}$

$$A\tilde{\mathbf{u}} = \mathbf{g} - \Delta t B p_\rho^{(l)}.$$

2. Solve the discrete ‘Pressure-Poisson’ problem

$$Pq_\rho = \frac{1}{\Delta t} B^T \tilde{\mathbf{u}}.$$

3. Correct the pressure and the velocity

$$p_\rho^{(l+1)} = p_\rho^{(l)} + q_\rho, \quad \mathbf{u} = \tilde{\mathbf{u}} - \Delta t M^{-1} B q_\rho$$

In essence, the right-hand side of the momentum equation is assembled using the old pressure iterate and the intermediate velocity  $\tilde{\mathbf{u}}$  is projected onto the subspace of solenoidal functions so as to satisfy the constraint  $B^T \mathbf{u} = 0$ . Moreover, the matrix  $P$  corresponds to a mixed discretization of the Laplacian operator [25] so that this method is a discrete analogue of the classical projection schemes derived by Chorin ( $p_\rho^{(0)} = 0$ ) and Van Kan ( $p_\rho^{(0)} = p_\rho(t_n)$ ) via operator splitting for the continuous problem.

Next, we apply this special operator-splitting approach to the full multiphase flow system with a discontinuous density  $\rho(\phi)$  and viscosity  $\mu(\phi)$  distribution, that means

$$\begin{aligned} \rho(\phi) \left[ \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right] - \nabla \cdot (\mu(\phi) [\nabla \mathbf{u} + (\nabla \mathbf{u})^T]) + \nabla p = \\ = \rho(\phi) \mathbf{g} + \mathbf{f}_{\Gamma, \sigma}(\phi) \end{aligned} \quad (22)$$

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0, \quad \nabla \cdot \mathbf{u} = 0. \quad (23)$$

After discretization in space and time, we obtain again a system of nonlinear algebraic equations which can be written in matrix form as follows

$$A_u(\mathbf{u}^{n+1}, \phi^{n+1}) \mathbf{u}^{n+1} + \Delta t F(\phi^{n+1}) + \Delta t B p^{n+1} = \mathbf{g}_u, \quad (24)$$

$$A_\phi(\mathbf{u}^{n+1}) \phi^{n+1} = g_\phi, \quad B^T \mathbf{u}^{n+1} = 0. \quad (25)$$

Note that equation (24) in contrast to (11) and (14) is multiplied with  $\rho(\phi)$ , which gives rise to the modified operators  $M_\rho$ ,  $K_\rho(\mathbf{u})$  and  $L_\mu$ . Here and below the superscript  $n+1$  refers to the time level, while subscripts identify the origin of discrete operators ( $u$  for the momentum equation and  $\phi$  for the Level Set equation); moreover,  $\rho$  and  $\mu$  are evaluated w.r.t. the old time level  $t^n$  which makes this formulation semi-implicit. Note that we have the freedom of using different finite element approximations and discretization schemes for the velocity  $\mathbf{u}$  and indicator function  $\phi$ , and the discrete problem (24)–(25) can be solved again in the framework of the discrete projection method. For

relatively small time steps, this strategy works very well, and simulation software can be developed in a modular way making use of optimized multigrid solvers. Consequently, in the simplest case (just one outer iteration per time step), the sequence of algorithmic steps to be performed is as follows:

1. Compute  $\tilde{\mathbf{u}}$  from the momentum equation
 
$$A_u(\tilde{\mathbf{u}}, \phi^n)\tilde{\mathbf{u}} = \mathbf{g}_u - \Delta t F(\phi^n) - \Delta t B p^n.$$
2. Solve the discrete Pressure-Poisson problem
 
$$P_\rho q = \frac{1}{\Delta t} B^T \tilde{\mathbf{u}} \text{ with } P_\rho := B^T M_\rho^{-1} B$$
3. Correct the pressure and the velocity
 
$$p^{n+1} = p^n + q, \quad \mathbf{u}^{n+1} = \tilde{\mathbf{u}} - \Delta t M_\rho^{-1} B q.$$
4. Solve the Level Set equation for  $\phi$ 

$$A_\phi(\mathbf{u}^{n+1})\phi^{n+1} = g_\phi.$$

Due to the nonlinearity of the discretized convective terms, resp., of the reinitialisation step, iterative defect correction or Newton-like methods, resp., corrections via redistancing, must be invoked in steps 1 and 4. However, due to the assumed relatively small time steps, such nonlinear iteration methods are not critical for the complete flow simulation.

## 4 THE FEM-LEVEL SET-dG(1) APPROACH

Our chosen Level Set approach is based on a first order Discontinuous Galerkin discretization in space, dG(1)-FEM, that means on piecewise linear polynomials. In the following, we will discuss the corresponding techniques for the discretization of the advection equation, for the treatment of the surface tension force and for the reinitialisation procedure.

### 4.1 *Discontinuous Galerkin upwinding for the Level Set approach*

There are several ways to approximate and solve Discontinuous Galerkin approximations for the Level Set function  $\phi$  [13],[18],[39],[44]. The general form of the Level Set transport equation involving the normal front velocity

can for instance be solved directly by using a Runge-Kutta dG-formulation for the Hamilton-Jacobi equations [30, 38]. The starting point to introduce our discretization of the Level Set transport equation is as follows

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0 \quad (26)$$

with a given velocity field  $\mathbf{u}$ . In our case  $\mathbf{u}$  is taken as the convective velocity from the Navier-Stokes solver and must accordingly be updated in each time step. We have  $\mathbf{u} \cdot \mathbf{n} = u_n$ , where  $\mathbf{n}$  is the unit normal to the interface  $\Gamma$  according to (7). The Level Set equation (26) can thus be rewritten as

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\mathbf{u}\phi) = \phi \nabla \cdot \mathbf{u}. \quad (27)$$

The reformulated Level Set equation above is simply a linear convection or advection equation in conservative formulation with a source term on the right hand side. We continue to rewriting it in weak form by introducing a triangulation,  $\mathcal{M}_h$ , of the domain  $\Omega$  where  $\mathcal{E}$  is an element  $\mathcal{E} \in \mathcal{M}_h$ . We are thus seeking an approximated solution in the following space

$$V_h = \{v_h \in L^\infty(\Omega) : v_h|_{\mathcal{E}} \in V_h(\mathcal{E}), \forall \mathcal{E} \in \mathcal{M}_h\}.$$

Here,  $V_h(\mathcal{E})$  denotes the local discrete test and trial spaces. The corresponding derivation follows by multiplying equation (26) by a suitably chosen test function after which partial integration over each element  $\mathcal{E}$  is performed. If the trial solution space is accordingly discretized as  $\phi_h \in V_h(\mathcal{E})$  this results in:

$$\int_{\mathcal{E}} v_h \frac{\partial \phi_h}{\partial t} dx = \int_{\mathcal{E}} \phi_h \mathbf{u} \cdot \nabla v_h dx - \int_{\partial \mathcal{E}} v_h \phi_h \mathbf{u} \cdot \mathbf{n}_{\mathcal{E}} ds + \int_{\mathcal{E}} v_h \phi_h \nabla \cdot \mathbf{u} dx, \quad (28)$$

$$\forall v_h \in V_h(\mathcal{E}),$$

where  $\mathbf{n}_{\mathcal{E}}$  is the outward pointing unit normal belonging to element  $\mathcal{E}$ . The fluxes on the internal boundaries are twofold defined since the underlying test and trial spaces are discontinuous. This is handled by replacing the outer flux in the last term of the right-hand side of equation (28) with a numerically upwinded flux, that is

$$\int_{\mathcal{E}} v_h \frac{\partial \phi_h}{\partial t} dx = \int_{\mathcal{E}} \phi_h \nabla \cdot (\mathbf{u}v_h) dx - \int_{\partial \mathcal{E}} v_h \phi_h^{up} \mathbf{u} \cdot \mathbf{n}_{\mathcal{E}} ds, \quad \forall v_h \in V_h(\mathcal{E}). \quad (29)$$

The upwinding flux is calculated as

$$\phi^{up} = \phi^- \text{ if } \mathbf{u} \cdot \mathbf{n}_{\mathcal{E}} \geq 0, \text{ and } \phi^+ \text{ otherwise}$$

where  $\phi^-$  and  $\phi^+$  are defined as

$$\phi^- = \lim_{\epsilon \rightarrow 0^-} \phi(\mathbf{x} + \epsilon \mathbf{n}_\epsilon, t)$$

$$\phi^+ = \lim_{\epsilon \rightarrow 0^+} \phi(\mathbf{x} + \epsilon \mathbf{n}_\epsilon, t).$$

In other words this means that  $\phi^{up}$  is the value of  $\phi$  taken from an upwind element at an element interface.

In our approach, equation (29) is discretized in space by firstly constructing the triangulation  $\mathcal{M}_h$  by subdivision in hexahedral elements  $\mathcal{E}$ . Furthermore both the test and trial function spaces,  $v_h$  and  $\phi_h$ , are constructed by employing linear 1st order polynomial basis functions on each element  $\mathcal{E}$ , the so-called dG(1) approach. These basis functions are completely determined by interior nodes of the element and are thus discontinuous at inter-element edges. Moreover, the discretization in time utilizes as before the standard 2nd order Crank-Nicolson scheme as described for instance in [62].

## 4.2 Treatment of surface tension effects

Surface tension effects are taken into account through the following force balance at the interface  $\Gamma$

$$[\mathbf{u}]|_\Gamma = 0, \quad [-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)]|_\Gamma \cdot \mathbf{n} = \sigma\kappa\mathbf{n}$$

where  $\mathbf{n}$  is the unit normal at the interface pointing into  $\Omega_1$ ,  $[\mathbf{A}]|_\Gamma = \mathbf{A}|_{\Omega_1 \cap \Gamma} - \mathbf{A}|_{\Omega_2 \cap \Gamma}$  denotes the jump of a quantity  $\mathbf{A}$  across the interface,  $\sigma$  is the surface tension coefficient, and  $\kappa$  is the curvature of the interface  $\Gamma$ . The first condition implies continuity of the velocity across the interface, whereas the second describes the force balance on  $\Gamma$ . Two strategies are often used to handle the curvature term, either to rewrite it as a volume force, that means

$$\mathbf{f}_{st} = \sigma\kappa\mathbf{n}\delta(\Gamma, \mathbf{x})$$

where  $\delta(\Gamma, \mathbf{x})$  is the Dirac delta function localizing the surface tension forces to the interface, or to introduce the Laplace-Beltrami operator  $\Delta_\Gamma$  on the interface, that means:

$$\kappa\mathbf{n} = \Delta_\Gamma \text{id}$$

and integrating the corresponding term in the weak formulation of the problem by parts [5, 20]. In the case of our current explicit treatment we get

$$(\mathbf{f}_{st}, \mathbf{v}) = \int_{\Gamma^n} \sigma\kappa^n \mathbf{n}^n \cdot \mathbf{v} d\Gamma \quad (30)$$

where the superscript  $n$  denotes the previous time level. The extension of the surface integrals into volumetric ones can be obtained by the indicated incorporation of the Dirac Delta function  $\delta = \delta(\Gamma, \mathbf{x})$ , which has the value  $\infty$

at the location of the interface,  $\phi = 0$ , and zero elsewhere, that means:

$$(\mathbf{f}_{st}, \mathbf{v}) = \int_{\Omega} \sigma \kappa^n \mathbf{n}^n \cdot \mathbf{v} \delta(\Gamma^n) dx \quad (31)$$

According to the applied CSF approach we approximate the Dirac Delta function  $\delta$  by a continuous regularized one, which is a smooth function in the vicinity  $\epsilon$  of the interface:

$$\delta(\phi) = \begin{cases} \phi < 0 & \max(0, \frac{1}{\epsilon} + \frac{1}{\epsilon^2} \phi) \\ \phi \geq 0 & \max(0, \frac{1}{\epsilon} - \frac{1}{\epsilon^2} \phi) \end{cases} \quad (32)$$

Since the interface normal  $\mathbf{n}^n$  and curvature  $\kappa^n$  are higher order derivatives of the Level Set function  $\phi^n$ , their distributions can be obtained by a combination of appropriate projection and gradient recovery techniques. Accordingly, the continuous (piecewise trilinear) interface normal  $\mathbf{n}_{Q_1}^n$  is obtained by  $L_2$ -projection (and normalization) from the piecewise discontinuous  $P_1$  space into the continuous  $Q_1$  space. Finally, the continuous approximation  $\kappa_{Q_1}^n$  of the curvature  $\kappa^n$  is reconstructed via  $L_2$ -projection, too,

$$\int_{\Omega} \kappa_{Q_1}^n w dx = - \int_{\Omega} w \nabla \cdot \mathbf{n}_{Q_1}^n dx, \quad (33)$$

where  $w$  denotes the test functions from the conforming trilinear  $Q_1$  space.

One of the remaining challenging problems is the *capillary time step restriction* which couples the time step size with the (local) mesh size  $h$  and  $1/\sigma$  leading to very high computational cost due to such strict stability constraints. Beside the classical work by Bänsch, who developed a semi-implicit approach for front tracking, the FEM-Level Set approach by Hysing [32] is one of the very few attempts for interface capturing methods, which is in the focus of our future research on 3D multiphase flow problems. Very recently, there was published an alternative method by Sussmann [59] which contains a survey on this problem and existing solution strategies. However, it still has to be stated that the combination of adaptive Level Set or VOF methods on locally adapted meshes shows severe numerical problems if configurations with large surface tension shall be simulated in an accurate, robust and efficient way. And, moreover, the challenges further increase for non-Newtonian multiphase fluids, for instance for Power Law models ('shear thinning' [15]) or for viscoelastic fluids [69] which even for single-phase flows lead to huge problems for large Weissenberg numbers. Nevertheless, we are convinced that the described FEM-Level Set techniques have the potential to solve these challenging problems in future.

As a final comment, in the framework of variational formulations, the corresponding volume integral can be reduced to a boundary integral which serves as natural boundary condition at the free interface [51],[58]. Moreover,

if partial integration of the *Laplace-Beltrami* operator is applied in tangential direction of the interface [5],[6],[16],[21],[27],[40] then the calculation of second derivatives of  $\phi$  for the curvature can be omitted which can be used for very efficient evaluations of the surface tension force in combination with Level Set functions satisfying the distance property. This is in contrast to the usual finite difference approaches which require a less accurate *Continuum Surface Force* (CSF) approximation of the (singular) Delta function [8]. The above mentioned alternative treatment of the surface tension force term is in the scope of our forthcoming studies.

### 4.3 Reinitialization procedure for LS-dG(1)

For the accurate calculation of the normal vector and curvature, as defined in (7), and hence for the accurate position and shape of the dynamic interface, one has to take care that  $\phi$  satisfies - at least near the interface  $\Gamma$  - the distance property which typically is achieved via appropriate postprocessing of a given numerical approximation  $\tilde{\phi}$ . Since the direct *reinitialisation*  $\phi_i := \text{sign}(\tilde{\phi}_i)\text{dist}(\mathbf{x}_i, \Gamma)$  is very expensive, one way to do the corresponding corrections is to solve the so-called Eikonal equation  $|\nabla\phi| = 1$  [31],[36] with boundary conditions  $\phi = 0$  on  $\Gamma = \{\mathbf{x} \in \Omega \mid \tilde{\phi}(\mathbf{x}) = 0\}$ . Typical methods are based on *fast marching* [56] or *fast sweeping* [70], while another approach is based on pseudo-timestepping for this nonlinear equation which leads to a Hamilton-Jacobi PDE:

$$\frac{\partial\phi}{\partial\tau} = \text{sign}(\tilde{\phi})(1 - |\nabla\phi|), \quad \phi|_{\tau=0} = \tilde{\phi} \quad (34)$$

Corresponding numerical approaches exploit that this problem can be written as a (nonlinear) transport equation

$$\frac{\partial\phi}{\partial\tau} + \mathbf{w} \cdot \nabla\phi = \text{sign}(\tilde{\phi}), \quad \text{with } \mathbf{w} = \text{sign}(\tilde{\phi}) \frac{\nabla\phi}{|\nabla\phi|}. \quad (35)$$

By stability reasons, the (discontinuous) sign function is typically replaced by a smoothed approximation which may lead to loss of accuracy and shift of the free interface. In the framework of FEM, the *interface local projection* of Parolini [50] helps, particularly for piecewise linear functions leading to a constant gradient vector, which combines the advantages of direct and PDE-based reinitialisation. Then, the correction of  $\tilde{\phi}$  mostly consists of 3 steps:

1. In mesh cells which contain the free boundary  $\Gamma$ , an exact reconstruction via (piecewise constant) gradient is applied.
2. Use a  $L_2$  projection to obtain a best approximation of  $\phi$  near  $\Gamma$ .

3. Outside of the ‘surface domain’  $\Omega_{\text{int}}$ , solve equation (35) using the already calculated values of  $\phi$  at the boundary of  $\Omega_{\text{int}}$  as Dirichlet boundary conditions.

According to our implementation, the reinitialization of the Level Set distribution is based on the advantages offered by the Discontinuous Galerkin Finite Element Method dG(1). This particularly means that we perform segregated reinitialization procedures on different groups of elements. The identified groups are as follows:

- elements intersected by the interface, we denote them by  $\mathcal{E} \subset \mathcal{M}^0$
- few layers of elements in positive direction ( $\phi > 0$ ) from the interface,  $\mathcal{E} \subset \mathcal{M}^+$
- few layers of elements in negative direction ( $\phi < 0$ ) from the interface,  $\mathcal{E} \subset \mathcal{M}^-$
- the rest of the domain, these are the elements  $\mathcal{E} \subset \mathcal{M}^\infty$

Such a segregated approach enables us to get rid of the discontinuity that the sign function  $S(\phi)$  exhibits at elements intersected by the interface. Moreover, it reduces the computational overhead since the PDEs are computed in a reduced computational domain only. Summarizing, the developed algorithm for the reinitialization is as follows

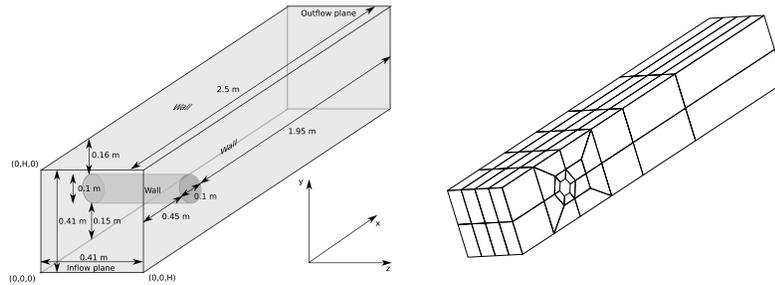
1. Direct reinitialization for  $\mathcal{E} \subset \mathcal{M}^0$ :  $\phi^n \xrightarrow{|\nabla\phi|=1} \phi^{n+1}$
2. PDE based solution for  $\mathcal{E} \subset \mathcal{M}^+$  with  $\frac{\partial\phi}{\partial\tau} + \mathbf{n} \cdot \nabla\phi = +1$
3. PDE based solution for  $\mathcal{E} \subset \mathcal{M}^-$  with  $\frac{\partial\phi}{\partial\tau} - \mathbf{n} \cdot \nabla\phi = -1$
4. Prescription of far field values for  $\mathcal{E} \subset \mathcal{M}^\infty$ :  $\phi_{\text{RI}}^{n+1} = \phi^\infty$

where  $\mathbf{n} := \mathbf{n}^n = \frac{\nabla\phi^n}{|\nabla\phi^n|}$ . The coupling between the individual groups of elements is achieved by imposing of boundary conditions from  $\mathcal{E} \subset \mathcal{M}^0$  for the PDE based reinitialization which is treated via the Fictitious Boundary Method approach [42]. One has to keep in mind that the discontinuous sign function does not cause a problem in the 2nd and 3rd step since the discontinuity has been treated already in step 1. Additionally, the Level Set function can be corrected due to mass loss which typically is performed by adding an appropriate constant  $c_\phi$  so that the total volume of both phases remains constant [58]. Moreover, further improvements can be obtained via high order discretization and grid adaptivity [13] which is subject of ongoing research.

## 5 NUMERICAL SIMULATIONS

This section contains several numerical studies for validating and evaluating the methodology described in the previous sections.

### 5.1 Single phase flow around a cylinder



**Fig. 2** Geometry and coarse mesh for the ‘Flow around cylinder’ benchmark.

The first incompressible flow problem to be dealt with, particularly to demonstrate the accuracy of the high-order  $Q_2/P_1$  approach, is the well-known benchmark *Flow around cylinder* developed in 1995 for the priority research program “Flow simulation on high-performance computers” under the auspices of DFG, the German Research Association [64]. This project was intended to facilitate the evaluation of various numerical algorithms for the incompressible Navier-Stokes equations in the laminar flow regime. A quantitative comparison of simulation results is possible on the basis of relevant flow characteristics such as pressure values as well as drag and lift coefficients, for which sufficiently accurate reference values are available (see also: [www.featflow.de/en/benchmarks/ff\\_benchmarks.html](http://www.featflow.de/en/benchmarks/ff_benchmarks.html)).

Here, we consider the steady incompressible flow around a cylinder with circular cross-section. An in-depth description of the geometrical details and boundary conditions can be found in reference [4] and [64] which contain all relevant information regarding this benchmark configuration. The flow at  $Re = 20$  is actually dominated by diffusion and could be simulated by the standard Galerkin method without any extra stabilization. The corresponding results are shown in Table 1 and demonstrate the high quality of the  $Q_2/P_1$  approach compared to quasi-reference values from the literature [7],[35].

**Table 1** Mesh convergence results (levels 2 to 6) in terms of drag, lift and pressure difference for the ‘DFG Flow around cylinder problem’ at  $Re = 20$ . Comparison of our results with reference results [7],[35].  $\Delta P$  refers to the pressure difference (front/back) on the cylinder and  $C_D$  and  $C_L$  are the normalized ( $\frac{1}{2}\rho U_{\text{mean}}^2 L_{\text{cyl}} D_{\text{cyl}}$ ) drag and lift coefficients.

Level	$\Delta P$	$C_D$	$C_L$	NEL	NDOF( $\mathbf{u}, p$ )
2	0.171956	6.01954	0.012316	768	21,560
3	0.171553	6.13973	0.009569	6,144	199,200
4	0.171156	6.17433	0.009381	49,152	1,482,816
5	0.171031	6.18261	0.009387	393,216	11,432,064
6	0.171022	6.18465	0.009397	3,145,728	89,760,016
Authors		Reference values			
Braack [7]	0.171007	6.18533	0.009401	1,000,000	40,000,000
John [35]	0.170779	6.18533	0.009401	2,000,000	55,000,000

## 5.2 Two-phase flow of a rising bubble

The rising bubble configurations described in this section were chosen as the ones established by the numerical studies of van Sint Annaland et al. [1] in order to validate the implementation of our Level Set approach. According to the mentioned studies the cases B, C and D were analysed which result in a considerable deformation of the initial bubble. The ratios of physical properties ( $\rho_g : \rho_l$  and  $\mu_g : \mu_l$ ) of the present phases were set to (1 : 100). The ratios of bubble diameter,  $d_b$ , with respect to the domain sizes,  $a_x, a_y, a_z$ , were  $(d_b : a_x : a_y : a_z) = (3 : 10 : 10 : 20)$ . The values of interfacial tension coefficient  $\sigma_{gl}$  and gravitational acceleration  $g_z$  for the simulations were set based on the characteristic Eötvös and Morton numbers defined as in [10]:

$$\text{Mo} = \frac{g_z \mu_l^4 \Delta \rho_{gl}}{\rho_l^2 \sigma_{gl}}, \quad \text{Eo} = \frac{g_z \Delta \rho_{gl} d_b^2}{\sigma_{gl}} \quad (36)$$

As a result of the given settings the bubbles deform to a final shape and they reach an equilibrium rising velocity,  $v_\infty$ , characterized by the Reynolds number defined as in [10]:

$$\text{Re} = \frac{\rho_l v_\infty d_b}{\mu_l} \quad (37)$$

Since the Level Set approach by its nature does not preserve mass of the individual phases certain mass correction techniques were incorporated to prevent artificial ‘mass transformation’ from one phase to the other. To this end we adopted a simple but efficient method proposed by Smolianski [58] which elevates the levelset function at every timestep with a limited constant  $\min(d_\varepsilon, \max(-d_\varepsilon, c_\phi))$ , where  $d_\varepsilon$  is related to the characteristic element size and  $c_\phi$  is a value enforcing absolute mass conservation. According to our

experience setting  $d_\varepsilon$  to 3% of the characteristic element size already prevents the occurrence of permanent mass loss.

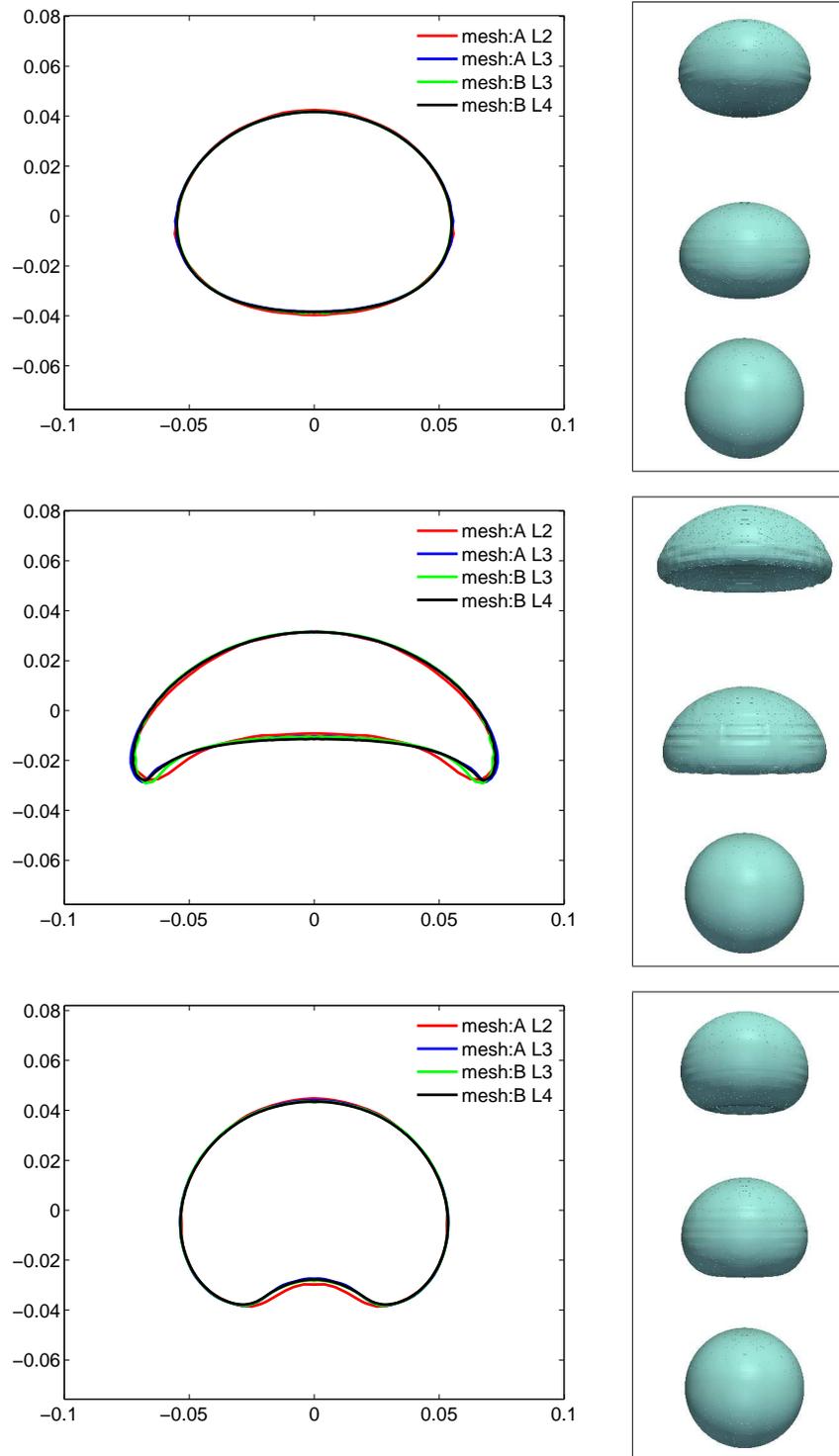
In order to achieve mesh independent simulation results in terms of bubble shape and terminal rising velocity we performed the simulations on two sets of meshes of two consequent levels of refinements (mesh A with refinement level 2, 3 and mesh B refinement level 3, 4). As it can be seen from Fig. 3, which displays the equilibrium bubble shapes centered with respect to their center of mass, the bubble shapes converge fairly well with increasing mesh resolution, especially in case B and D. The terminal rise velocities compared with the empirical predictions of Grace [10] and numerical predictions of van Sint Annaland [1] are given in Tab. 2. Despite the mesh independent properties of the obtained results the comparison of the terminal rise velocities shows a weaker correlation of our results with the empirical predictions of Grace than it was the case in van Sint Annaland’s computational studies. This contradiction leaves behind the challenges for further numerical analysis, possibly leading to a benchmark problem to which other researchers will also be welcome to contribute, like as it happened for the well known 2D rising bubble problem [34].

**Table 2** Resulting Reynolds numbers obtained for the different configurations. Subscripts E, S stand for empirical and simulational reference values from Grace [10] and van Sint Annaland [1], respectively. The last four values refer to our simulation results obtained on mesh A and B and on refinement levels 2, 3 and 4.

Case	Shape	Mo	Eo	Re <sub>E</sub>	Re <sub>S</sub>	Re <sub>mAl2</sub>	Re <sub>mAl3</sub>	Re <sub>mBl3</sub>	Re <sub>mBl4</sub>
B	Ellipsoidal	0.100	9.71	4.6	4.3	5.50	5.50	5.60	5.60
C	Skirted	0.971	97.1	20.0	18.0	17.7	18.0	18.0	18.0
D	Dimpled	1000	97.1	1.5	1.7	2.00	2.03	2.03	2.03

### 5.3 Droplet dripping simulation

The corresponding experimental setup involves a two phase problem consisting of glucose-water mixture (as continuous phase) and silicon oil (as dispersed phase). The measurements are restricted to the so called dripping mode. This mode is characterized by relatively low volumetric flowrates and by the fact that the droplets are generated in the near vicinity of the capillary so that the stream length is comparable with the size of the generated droplets. Since the temperature is kept at a constant value during the whole experiment all physical properties of the present phases are constant. The experimental measurements were realized (by the group of Prof. Walzel, BCI, TU Dortmund) to obtain statistically averaged quantities such as droplet



**Fig. 3** Left: Cutplanes of continuous reconstructions of the interphase for the equilibrium bubble shapes. Right: Time evolution of the bubble shapes (from bottom to top). The cases are organized as: Top - case B -  $Eo=9.71$ ,  $Mo=0.1$ ; Middle - case C -  $Eo=97.1$ ,  $Mo=0.971$ ; Bottom - case D -  $Eo=97.1$ ,  $Mo=1000$ .

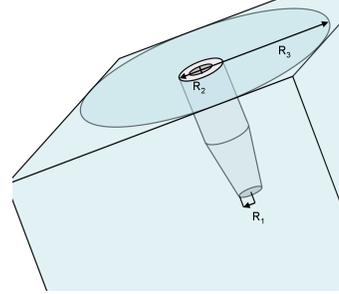
size, droplet generation frequency and stream length. These experimentally measured quantities are compared with our subsequent simulation results.

The basic units used to define the derived quantities are the following ones:

$$\begin{aligned} [\text{length}] &= dm, \\ [\text{time}] &= s, \\ [\text{mass}] &= kg \end{aligned}$$

The list of physical quantities is as follows:

$$\begin{aligned} g_z &= -9.81 m s^{-2} = -98.1 dm s^{-2} \\ \sigma &= 0.034 N m^{-1} = 0.034 kg s^{-2} \\ \rho_C &= 1340 kg m^{-3} = 1.34 kg dm^{-3} \\ \rho_D &= 970 kg m^{-3} = 0.97 kg dm^{-3} \\ \mu &= \mu_C = \mu_D = 500 mPa s = 0.050 kg dm s^{-1} \end{aligned}$$



Sketch of the benchmark domain

The list of geometrical parameters reads:

$$\begin{aligned} [\text{domain size}] &= [-0.15 : 0.15] \times [-0.15 : 0.15] \times [0.0 : 1.2] dm^3 \\ [\text{inner capillary radius}] &= R_1 = 0.015 dm \\ [\text{outer capillary radius}] &= R_2 = 0.030 dm \\ [\text{primary phase inflow radius}] &= R_3 = 0.15 dm \end{aligned}$$

The boundary conditions imposed on the inflow velocity are the following:

$$w = \begin{cases} a_2(R_1 - r)(R_1 + r) & \text{if } 0 < r < R_1 \quad (\text{Dispersed phase}) \\ a_1(R_3 - r)(r - R_2) & \text{if } R_2 < r < R_3 \quad (\text{Continuous phase}) \\ 0 & \text{otherwise} \end{cases}$$

The parameters  $a_1$  and  $a_2$  are defined to achieve the required volumetric flowrates:

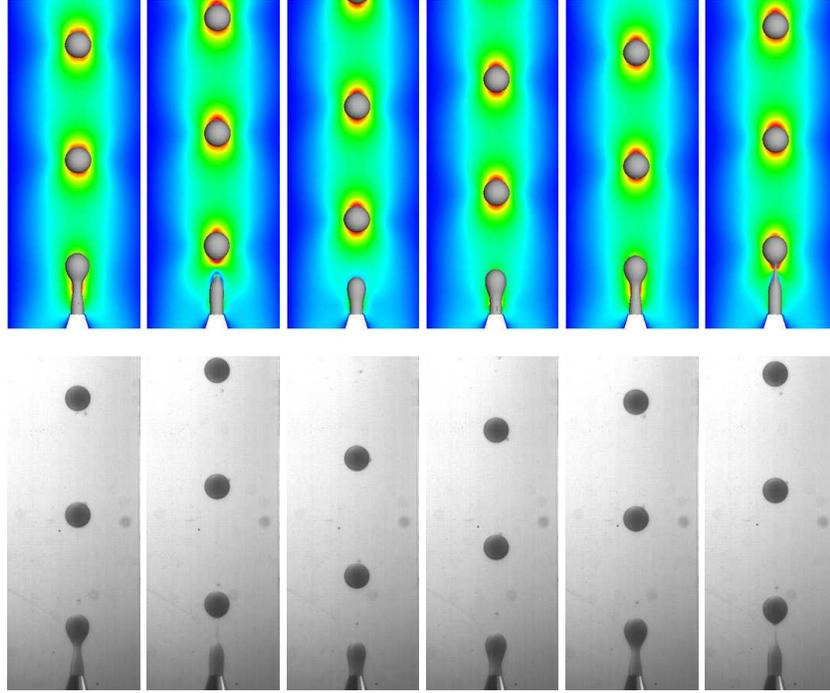
$$\begin{aligned} \dot{V}_C &= \int_{R_2}^{R_3} (2\pi r a_1 (R_3 - r)(r - R_2)) dr = \\ &= -2\pi a_1 \left[ \frac{r^4}{4} - (R_2 + R_3) \frac{r^3}{3} + R_2 R_3 \frac{r^2}{2} \right]_{R_2}^{R_3} = \frac{\pi a_1}{6} (R_2 + R_3) (R_3 - R_2)^3. \\ \dot{V}_D &= \int_0^{R_1} (2\pi r a_2 (R_1 - r)(R_1 + r)) dr = 2\pi a_2 \left[ \frac{R_1^2 r^2}{2} - \frac{r^4}{4} \right]_0^{R_1} = \frac{\pi a_2}{2} R_1^4. \end{aligned}$$

The volumetric flowrates for the simulations are set to:

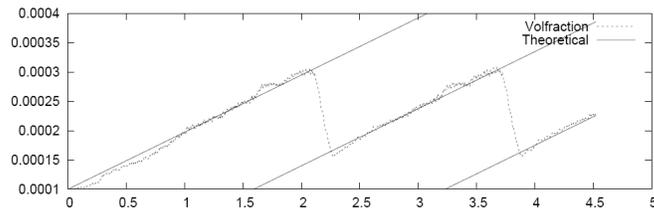
$$\dot{V}_C = 99.04 \text{ ml min}^{-1} = 99.04 \text{ cm}^3 \text{ min}^{-1} = 99.04 \frac{10^{-3} \text{ dm}^3}{60 \text{ s}} = 1.65 \cdot 10^{-3} \text{ dm}^3 \text{ s}^{-1},$$

$$\dot{V}_D = 3.64 \text{ ml min}^{-1} = 3.64 \text{ cm}^3 \text{ min}^{-1} = 3.64 \frac{10^{-3} \text{ dm}^3}{60 \text{ s}} = 6.07 \cdot 10^{-5} \text{ dm}^3 \text{ s}^{-1},$$

which is guaranteed by setting  $a_1 = 10.14 \text{ dm}^{-1} \text{ s}^{-1}$  and  $a_2 = 763.7 \text{ dm}^{-1} \text{ s}^{-1}$ .



**Fig. 4** Sequence of one droplet separation compared with experimental measurements.



**Fig. 5** Evolution of the volume of the secondary phase. Theoretical lines are characterized by the slope  $q = 6.07 \cdot 10^{-5} \text{ dm}^3 \text{ s}^{-1}$ .

The resulting process leads to a pseudo-steady state, where the droplet separation happens according to the so called dripping mode. The frequency

of the given mode is  $f = 0.60 \text{ Hz}$  (cca  $0.58 \text{ Hz}^{\text{exp}}$ ), which produces droplets of size  $d = 0.058 \text{ dm}$  (cca  $0.062 \text{ dm}^{\text{exp}}$ ). The maximum stream length during the process is  $L = 0.102 \text{ dm}$  (cca  $0.122 \text{ dm}^{\text{exp}}$ ). The snapshots of one full droplet generation compared with experimental measurements are given in Fig. 4. The time evolution of the volume of the secondary phase is given in Fig. 5. As it can be seen, the increase of the volume of the dispersed phase follows the theoretically expected trend in a reasonable way despite of the fact that the mass correction technique (previously described in section 5.2) was not activated.

## 6 SUMMARY

In this contribution, we have shown that the realization of a new FEM-Level Set approach in the framework of Discontinuous Galerkin Finite Elements together with special PDE based reinitialization techniques leads to very efficient simulation tools for modelling multiphase flow problems. The implemented parallel 3D multiphase flow solver has been validated in the case of the rising bubble and for the droplet dripping problem. Detailed description of these problems together with the obtained results – which are accurate and in fairly good agreement with the corresponding empirical data – are left in form of a benchmark proposal for the engineering community.

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