Unstructured un-split geometrical Volume-of-Fluid methods
- A review

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Abstract

Note: this is an updated preprint of the manuscript accepted for publication in Journal of Computational Physics, DOI: \url{https://doi.org/10.1016/j.jcp.2020.109695}. Please refer to the journal version when citing this work.

Geometrical Volume-of-Fluid (VoF) methods mainly support structured meshes, and only a small number of contributions in the scientific literature report results with unstructured meshes and three spatial dimensions. Unstructured meshes are traditionally used for handling geometrically complex solution domains that are prevalent when simulating problems of industrial relevance. However, three-dimensional geometrical operations are significantly more complex than their two-dimensional counterparts, which is confirmed by the ratio of publications with three-dimensional results on unstructured meshes to publications with two-dimensional results or support for structured meshes. Additionally, unstructured meshes present challenges in serial and parallel computational efficiency, accuracy, implementation complexity, and robustness. Ongoing research is still very active, focusing on different issues: interface positioning in general polyhedra, estimation of interface normal vectors, advection accuracy, and parallel and serial computational efficiency.

This survey tries to give a complete and critical overview of classical, as well as contemporary geometrical VOF methods with concise explanations of the underlying ideas and sub-algorithms, focusing primarily on unstructured meshes and three dimensional calculations. Reviewed methods are listed in historical order and compared in terms of accuracy and computational efficiency.

Keywords: Volume-of-Fluid (VOF), un-split, unstructured mesh, review

1. Introduction

The Volume of Fluid (VOF) method \cite{1,2,3} is widely used to capture interfaces in the numerical simulation of multi-phase flows, owing in part to its many potential advantages: global and local volume conservation, second-order convergence in three dimensions, numerical consistency, numerical stability, robust treatment of interface coalescence and breakup, support for unstructured domain discretization, and a straightforward parallel computation model. These characteristics, however, often remain elusive for many VOF formulations.

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The VOF method approximates the interface with a discrete Heaviside function represented by a volume fraction, i.e. the ratio of the volume occupied by a specific phase in a multi-material computational cell, to the volume of the whole cell. Over the last two decades, different variants of the VOF method have been developed, all of which can be categorized as taking either an algebraic or geometric approach to approximate interface kinematics via an algorithm for advection of volume fractions.

Algebraic VOF methods [4, 5, 6, 7] invoke continuum-based Partial Differential Equation (PDE) discretization schemes for the advection of the volume fraction field. This approach is challenging and can lead to problems, owing to the volume fraction field possessing a large and abrupt change (across the interface) that causes interpolation and subsequently discretization errors, when algebraic advection algorithms are used. The algebraic methods additionally suffer from the loss of numerical consistency caused by artificial diffusion, i.e. the inability to maintain a constant (and not widening) interface width. The loss of consistency likewise leads to the loss in the convergence order. More recent developments of algebraic VOF schemes have alleviated some aforementioned issues, but not all of them.

Geometric VOF methods, instead, rely on geometrical operations to approximate the solution of the volume fraction advection equation. All variants of the geometrical VOF method rely on a cell-by-cell geometrical approximation of the interface, that is reconstructed in multi-material cells by the Piecewise Linear Interface Calculation (PLIC) algorithm. Volume fraction advection is then computed from the geometrical approximation of the interface and cell-faces, cells, or phase-specific material volumes, that are traced along Lagrangian trajectories. This requires additional and complex geometrical operations such as the triangulation and intersection of possibly non-convex self-intersecting polyhedrons with non-planar faces. These geometric approximations enable the advection of the fluid interface in a direction that is independent of the mesh geometry (i.e. the direction of the face-normal vectors), which simultaneously removes mesh-anisotropy errors and introduces support for unstructured meshes. The mesh-anisotropy errors impress the shape of the dual of the cell onto the shape of the advected interface. For example, a sphere advected in the direction of the spatial diagonal on a Cartesian mesh with the algebraic VOF method deforms into an octahedron, because the cell stencil of the algebraic method on a cubic mesh is a dual of a cube - an octahedron. Geometrical reconstruction of the interface and the fluxed phase-specific volumes circumvents the interpolation errors of the algebraic VOF schemes. These geometric approximations are the basis for the second-order convergence, numerical stability and consistency of the geometric VOF methods.

Geometric VOF methods can be further categorized as dimensionally split and un-split. Dimensionally split methods best support structured meshes [11, 12, 13, 14, 15, 16, 17], because they rely on the operator-splitting approach to achieve second-order accuracy, that requires face-normal vectors to be collinear with the coordinate axes (grid lines of the structured mesh). The two main motivations for formulating dimensionally un-split geometric VOF methods are (i) the ability to utilize unstructured meshes for handling geometrically complex solution domains, and (ii) the possibility of increasing the overall solution accuracy by improving the Lagrangian reconstruction of the fluxed phase-specific volume. Dimensionally un-split VOF methods therefore have been and still are very actively investigated.

Algebraic VOF methods solve a linear algebraic system to advect the interface, which is an approach that has a high level of serial and parallel computational efficiency. Geometric VOF methods, on the other hand, rely on different relatively complex explicit geometric sub-algorithms. Local geometrical operations increase the serial computational efficiency of the method. However, geometric
data and calculations follow a moving fluid interface, which can freely leave one parallel process and enter another, easily making a parallel computation imbalanced in terms of the computational load shared by the parallel processes.

The choice of sub-algorithms of the geometric VOF method significantly impacts the solution accuracy. An example PLIC interface is shown in fig. 1 for the standard 3D deformation verification case \[8, 9\] at \(t = 1.5\) s. Two reconstruction algorithms are compared (Youngs \[18\] and simplified Swartz \[10\]), and two triangulation algorithms (barycentric and flux-based \[10\]). The barycentric triangulation uses the centroid of the volume and the triangles from its triangulated boundary to construct tetrahedrons that decompose the volume. The flux-based triangulation relies on the displacement vectors given by the velocity field to decompose the volume into tetrahedrons more accurately. Solutions presented in figs. 1a and 1b are affected for the Youngs reconstruction algorithm by the chosen triangulation. Similarly, comparing figs. 1c and 1d with figs. 1a and 1b the importance in choosing a better reconstruction algorithm is evident, because the more accurate Swartz reconstruction algorithm prevents the artificial breakup of the thin layer.

The effect of the triangulation is barely visible for the simplified Swartz algorithm in figs. 1c and 1d, however the effect is substantial, because it impacts convergence. To emphasize the difference, different gray scale is used in fig. 1e for the simplified Swartz algorithm, using respectively

![Image](image-url)

Figure 1: 3D deformation verification case \[8, 9\] at \(t = 1.5\) s with 64\(^3\) equidistant cubical cells combining reconstruction and flux-volume triangulation algorithms. Results are obtained using the algorithms reported in \[10\].
the barycentric (gray color) and flux-based (black color) triangulation. The convergence-order and absolute accuracy of the standard advection verification cases are primarily affected by the fidelity of the advection in those parts of the interface, where the topological changes occur. The impact of the sub-algorithms is large in fig. 1, even with a prescribed velocity. Therefore, one can safely assume that the choice of sub-algorithms will strongly impact the solution when the velocity results from solving the two-phase Navier-Stokes system.

Improving the sub-algorithms of the geometric VOF method is a topic of ongoing extensive research effort. This survey article tries to give a complete and critical overview of classical as well as contemporary geometrical VOF methods with detailed self-consistent explanations of the underlying ideas and sub-algorithms. The referenced algorithms are systematically categorized and compared in terms of accuracy and computational efficiency. Links to publications used for the comparison are provided, together with brief reviews which are focused on those specific improvements reported in the literature. The aim of this survey article is to provide a solid starting-point for formulation and implementation of dimensionally un-split geometric VOF methods.

2. Geometrical Volume-of-Fluid method

![Figure 2: Multi-material domain.](image)

The core idea of the Volume of Fluid (VOF) method is to capture an evolving interface $\Sigma(t)$ that separates two phases $\Omega^+(t)$ and $\Omega^-(t)$, shown schematically in fig. 2. More precisely, $\Sigma(t)$ is thus defined as the boundary of its adjacent phases, i.e.

$$\Sigma(t) = \partial \Omega^+(t),$$

say, where a given domain $\Omega$ contains two phases $\Omega^+(t)$ and $\Omega^-(t)$, such that

$$\Omega = \Omega^+(t) \cup \Omega^-(t) \cup \Sigma(t).$$

Furthermore, the phases are described by means of phase indicator functions. Thus, for instance,

$$\Omega^+(t) = \{ \mathbf{x} \in \Omega : \chi(t, \mathbf{x}) = 1 \}$$

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with \( \chi(t, \cdot) \) being the (phase) indicator function of \( \Omega^+(t) \), i.e.

\[
\chi(t, x) = \begin{cases} 
1 & x \in \Omega^+(t), \\
0 & x \notin \Omega^+(t).
\end{cases}
\] (4)

This continuum formulation has its discrete analogue, where the Finite Volume method (FVM) is an appropriate discretization approach. In fact, introducing the volume fraction of the phase \(+\) inside a volume \( V \) of magnitude \(|V|\) at time \( t \) as

\[
\alpha(t, V) := \frac{1}{|V|} \int_V \chi(t, x) dV,
\] (5)

it follows that

\[
\alpha(t, V) = \frac{1}{|V|} \int_{V \cap \Omega^+(t)} 1 dV = \frac{|V \cap \Omega^+(t)|}{|V|} = \frac{|V^+(t)|}{|V|},
\] (6)

where \( V^+(t) := V \cap \Omega^+(t) \) is the volume occupied by \( \Omega^+ \) inside the volume \( V \) at time \( t \), which we call the \textit{phase-specific volume}.

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Figure 3: Decomposition of the multi-material solution domain into disjoint subsets \( \{\Omega_k\}_{k \in K} \).

Therefore, eq. (5) defines the volume fraction of phase \( \Omega^+(t) \) inside \( V \), hence \( \alpha \) denotes the \textit{volume of fluid fraction} inside \( V \), if "fluid" refers to the phase labeled by "+". On the discrete level, \( \Omega \) is decomposed into disjoint open sub-volumes (mesh cells, say) \( \Omega_k \) for \( k \in K \), as shown in fig. 3. Given such a decomposition of \( \Omega \) into \( \{\Omega_k\}_{k \in K} \), we define

\[
\alpha_k(t) := \alpha(t, \Omega_k) = \frac{1}{|\Omega_k|} \int_{\Omega_k} \chi(t, x) dV = \frac{|\Omega_k \cap \Omega^+(t)|}{|\Omega_k|} = \frac{|\Omega_k^+(t)|}{|\Omega_k|},
\] (7)

where, equivalently to \( V^+ \) in eq. (6), we call \( \Omega_k^+(t) \) the \textit{phase-specific volume} inside \( \Omega_k \) at time \( t \). Knowledge of \( \{\alpha_k\}_{k \in K} \) directly allows to identify all mesh cells with nonempty intersection with the interface \( \Sigma(t) \), the so-called interface or multi-material cells. Indeed, it holds that

\[
\alpha_k(t) = 0 \iff \Omega_k \subset \Omega^-(t),
\]

\[
\alpha_k(t) \in (0, 1) \iff \Omega_k \cap \Sigma(t) \neq \emptyset,
\]

\[
\alpha_k(t) = 1 \iff \Omega_k \subset \Omega^+(t).
\] (8)
This detection of all interface cells at time \( t \) requires the computation of the indicator function \( \chi \) (or an approximation thereof), for which an evolution equation for \( \chi \) is required. This equation comes from continuum physics and is usually based on the assumption of absence of phase change. In this case, fluid particles cannot cross the interface, i.e. the value of \( \chi \) does not change along a trajectory, viz.

\[
\chi(t, x(t)) \equiv \text{const}
\] (9)

for \( x(\cdot) \) a solution of

\[
\dot{x}(t) = v(t, x(t)),
\] (10)

where \( v \) denotes the velocity field. Note that \( v \) is a two-phase velocity field, hence eq. (10) is an ordinary differential equation (ODE) with discontinuous right-hand side. While, in general, such ODEs can lack solvability or uniqueness, it can be shown that eq. (10) is a well-posed ODE if \( v \) is a physically sound two-phase velocity field even if phase change is allowed [19].

Consequently, the phase indicator \( \chi \) satisfies

\[
\frac{D\chi}{Dt} = 0 \quad \text{(Lagrangian derivative),}
\] (11)

in a certain sense, discussed in more detail below. In an Eulerian form, the basic and well-known transport equation

\[
\partial_t \chi + v \cdot \nabla \chi = 0
\] (12)

for the phase indicator results. Formally, this is the same as the level set equation or, more general, the transport equation for a non-diffusive passive scalar. But in contrast to the level set equation, an interpretation of eq. (12) in a pointwise sense is not useful: at points where \( \chi \) is locally constant, eq. (12) is trivially fulfilled, while, at points where \( \chi \) has a jump discontinuity, eq. (12) can only be valid in a weak sense. Even more, a classical interpretation of eq. (12) in the sense of distributions does not reach far enough. Instead, the theory of functions of bounded variations and related concepts from geometrical measure theory provide an appropriate mathematical framework. Besides derivatives like \( \partial_t \chi \) or \( \nabla \chi \) of the discontinuous indicator function, also nonlinear operations on such quantities are important, such as \( \| \nabla \chi \| \), where \( \| \cdot \| \) denotes the Euclidean norm. In fact, it holds that

\[
\int_V \phi \| \nabla \chi \| dV = \int_{V \cap \Sigma} \phi dS,
\] (13)

i.e. \( \| \nabla \chi \| \) is the Dirac distribution w.r. to \( \Sigma \). Equation (13) is the theoretical basis for numerical approximations of surface quantities like, e.g., surface tension forces. For instance, choosing \( \phi = 1 \) in (13) shows that

\[
|\Sigma \cap V| = \int_{V} \| \nabla \chi \| dV
\] (14)

is the area of the surface \( \Sigma \cap V \) and, mathematically, the right-hand side is the total variation of the Radon measure \( \nabla \chi \). For more information about this subject see, e.g., [20, 21].

Within the VOF method, the discretization of eq. (12) is usually based on the FVM, which is directly related to the integral form of the phase-specific volume balance. This integral form follows by application of the Reynolds transport theorem. Indeed, if \( \Omega_k \subset \Omega \) is a fixed control volume, then

\[
\frac{d}{dt} \int_{\Omega_k} \chi dV = \frac{d}{dt} \int_{\Omega_k \cap \Omega^+(t)} 1 dV = \int_{\Omega_k \cap \Sigma(t)} v \cdot \mathbf{n}^+ dS,
\] (15)
where $v^+ \cdot n^+$ is the speed of normal displacement of $\Sigma(t)$ in the direction of the outer normal $n^+$. Since the standing assumption of no phase change implies
\[ v^+ \cdot n^+ = v^- \cdot n^-, \]
one obtains
\[ \frac{d}{dt} \int_{\Omega_k} \chi dV = \int_{\Omega_k \cap \Sigma(t)} v^+ \cdot n^+ dS. \]
(17)

Note that $n_\Sigma$ is either $n^+$ or $-n^+ (= n^-)$.

\[ \chi(t, \cdot) = 0 \quad \Omega^-(t) \]
\[ \chi(t, \cdot) = 0 \quad \Omega^-(t) \]
\[ \chi(t, \cdot) = 1 \]
\[ \chi(t, \cdot) = 1 \]
\[ \partial V \]
\[ \partial V \]
\[ \partial V(t) \]
\[ \partial V(t_0) \]
\[ \partial V(t_0) \]
\[ \partial V(t_0) \]
\[ \partial V(t_0) \]
\[ \partial V(t_0) \]
\[ \partial V(t_0) \]

(a) Volume $V$ as a fixed control volume, bounded by $\partial V$.
(b) Volume $V(t)$, bounded by $\partial V(t)$, tracked as a co-moving (material) volume with the flow map $\Phi_t$, starting at time $t_0$ with $V(t_0)$.

Figure 4: Fixed control volume $V$ (fig. 4a) versus co-moving (material) volume $V(t)$ (fig. 4b).

From here on, we also assume the flow inside $\Omega^+(t)$ to be incompressible, meaning that $\nabla \cdot v^+ = 0$. Let us note in passing that the transport equation (12) for $\chi$ then, formally, becomes
\[ \partial_t \chi + \nabla \cdot (\chi v^+) = 0. \]
(18)

Employing the divergence theorem with $\nabla \cdot v^+ = 0$, equation (17) implies
\[ \frac{d}{dt} \int_{\Omega_k} \chi dV = - \int_{\partial \Omega_k \cap \Omega^+(t)} v^+ \cdot n^+ dS. \]
(19)

On the right-hand side, the integration runs over the "wetted part" $\partial \Omega_k \cap \Omega^+(t)$ of $\partial \Omega_k$ on which $\chi = 1$ holds, while $\chi = 0$ on the remainder of $\partial \Omega_k$. Therefore, the integral form of the transport equation for $\chi$ in the incompressible case finally reads
\[ \frac{d}{dt} \int_{\Omega_k} \chi dV = - \int_{\partial \Omega_k} \chi v \cdot n dS. \]
(20)
An important variant of eq. (20) employs co-moving (material) volumes. Since we need this concept in a precise manner below, let us recall that for a flow field \( \mathbf{v} : J \times \Omega \rightarrow \mathbb{R}^3 \), \( J = (a,b) \subset \mathbb{R} \), which is continuous in \((t,x)\) and satisfies a local Lipschitz condition w.r. to \( x \), the initial value problems
\[
\dot{x} = \mathbf{v}(t,x(t)), \quad t \in J, \; x(t_0) = x_0
\]  
(21)

have unique local solutions \( x(\cdot; t_0, x_0) \) for every \( t_0 \in J \), \( x_0 \in \Omega \). These solutions exist for all \( t \in J \) if \( \mathbf{v} \) is linearly bounded and satisfies \( \mathbf{v} \cdot n = 0 \) at \( \partial \Omega \). Under the latter impermeability condition, initial values from \( \partial \Omega \) are allowed. While the same result holds for two-phase flows under physically sound assumptions on the jump of \( \mathbf{v}^+ \) at \( \Sigma(t) \) (see [19]), such extensions are not needed here, since we also assume no-slip at \( \Sigma \), i.e.
\[
\mathbf{v}^+ = \mathbf{v}^- = \mathbf{v}^\Sigma,
\]  
(22)

which, together with eq. (16), implies that \( \mathbf{v} \) is continuous at \( \Sigma \) and this, together with the assumed local Lipschitz continuity of \( \mathbf{v}^\pm \) on \( \text{gr}(\Omega^\pm) \), is sufficient.

Now, existence of unique solutions to eq. (21) yields the associated flow map, i.e. the map \( \Phi^t_{t_0} \) defined as
\[
\Phi^t_{t_0}(x_0) := x(t; t_0, x_0),
\]  
(23)

which maps the initial point \( x_0 \) to the point \( x(t) \), where \( x(\cdot) = x(\cdot; t_0, x_0) \) is the solution for the initial condition \( x(t_0) = x_0 \). With this notation, a two-phase co-moving (material) volume \( V(t) \) is given as
\[
V(t) = \Phi^t_{t_0}(V(t_0)) := \{ \Phi^t_{t_0}(x_0) : x_0 \in V(t_0) \}
\]  
(24)

for some initial volume \( V(t_0) \) illustrated in fig. 4b. Under the assumption of no phase change, the phase-specific volume inside \( V(t) \) is also a material volume which, moreover, has constant volume if the velocity field is solenoidal for the respective phase.

At this point it is useful to note that the flow map \( \Phi^s_{t_0} \) also exists for \( s > t \), since the initial value problems have solutions going forward and backward in time. Forward and backward solutions are related by means of time reversal, therefore the backward solution of eq. (21) is the forward solution of the same ODE, but with \(-\mathbf{v}\) instead of \(\mathbf{v}\). Thus, the inverted flow map \( (\Phi^s_{t_0})^{-1} \) is nothing but the flow map to the reversed velocity field \(-\mathbf{v}\), and
\[
\Phi^s_{t_0} \Phi^t_{t_0}(V) = \Phi^s_{t_0} \Phi^t_{t_0}(V) = V.
\]  
(25)

The analogue of eq. (20) for a co-moving volume starting as the cell \( \Omega_k \) at time \( t_0 \) reads as
\[
\frac{d}{dt} \int_{\Phi^t_{t_0}(\Omega_k)} \chi \, dV = 0.
\]  
(26)

Evidently, eq. (26) is equivalent to
\[
|\Phi^t_{t_0}(\Omega_k) \cap \Omega^+(t)| \equiv \text{const.} \quad \text{for } t \in J.
\]  
(27)

Equation (27) is the so-called space (geometric) conservation law, applied to the co-moving volume starting as the cell \( \Omega_k \) at time \( t_0 \), which holds for solenoidal velocity fields \( \nabla \cdot \mathbf{v} = 0 \) inside the phases, and in the absence of phase change. The space conservation law further implies
\[
\alpha(t, \Phi^t_{t_0}(V)) = \frac{|\Phi^t_{t_0}(V) \cap \Omega^+(t)|}{|\Phi^t_{t_0}(V)|} = \frac{|V \cap \Omega^+(t_0)|}{|V|} = \alpha(t_0, V),
\]  
(28)

\[\vdash\]
which is especially relevant for a version of the geometrical VOF method described in section 2.2. Either eq. (20) or eq. (26) represents the core equation of any geometrical VOF method, i.e. a VOF method which employs geometrical calculations for the approximate computation of integrals appearing in the time-integrated form of these relations. Methods covered by this review rely on the geometric approach, where a common challenge is to approximate complicated, non-convex volumes in \( \mathbb{R}^3 \), with non-planar boundaries that arise when integrating eqs. (20) and (26) in time. Of course, one may also try to avoid such complications by replacing the full volume integrals by temporal integrals of volumetric fluxes on the boundary of \( \Omega_k \), or dimensionally (directionally) splitting the evaluation of integrals in eqs. (20) and (26); however, this leads to larger approximation errors.

A completely different approach, leading to the algebraic VOF method relies on the direct discretization of the eq. (15) for \( \lambda \), without aiming at a fully sharp interface representation on the discrete level. However, as outlined in the introduction, this assumption leads to problems with consistency and, therefore, the convergence of the algebraic method. One of the main advantages of the geometric VOF methods is the reduction of numerical diffusion, which significantly reduces the number of interface cells in the interface normal direction.

Discretization of eqs. (20) and (26) leads to two different categories of dimensionally un-split geometrical VOF methods: the flux-based versus the cell-based method. For both methods, \( \Omega \) is decomposed into disjoint \( \Omega_k, k \in K \), such that the definition of \( \alpha_k(t) \) given by eq. (7) applies. The task of both un-split geometrical VOF methods is the following: given a time discretization \( t^0 < t^1 < t^2 < \cdots < t^N \), at each point \( t^n \) in the discretization, given \( \{\alpha_k(t^n)\}_{k \in K} \), compute \( \{\alpha_k(t^{n+1})\}_{k \in K} \) by integrating either eq. (20) or eq. (26) in time over \([t^n, t^{n+1}]\). Details of the temporal integration of eq. (20) and eq. (26) are explained in the following sections.

### 2.1. Flux-based un-split geometrical VOF method

![Figure 5: Calculation of the phase-specific volume \( V_f^{\alpha} \) fluxed through \( S_f \) over time interval \([t^n, t^{n+1}]\) using the flux-based un-split VOF method.](image-url)
By equations (7) and (20),
\[
\frac{d}{dt} \alpha_k(t) = \frac{d}{dt} \frac{1}{|\Omega_k|} \int_{\Omega_k} \chi(t, x) \, dV = -\frac{1}{|\Omega_k|} \int_{\partial\Omega_k} \chi \mathbf{v} \cdot \mathbf{n} \, dS.
\] (29)

Integrating this equation in time over \([t^n, t^{n+1}]\) yields
\[
\alpha_k(t^{n+1}) = \alpha_k(t^n) - \frac{1}{|\Omega_k|} \int_{t^n}^{t^{n+1}} \int_{\alpha_k} \chi \mathbf{v} \cdot \mathbf{n} \, dS \, dt.
\] (30)

Equation (30) is still an exact equation, as no approximations have been applied so far. Notice that eq. (30) has two unknowns: \(\alpha_k\) and \(\chi\). A numerical method based on eq. (30) is termed a dimensionally un-split flux-based geometrical Volume of Fluid method. The un-split flux-based geometrical VOF method utilizes three-dimensional geometrical operations that are not dimensionally split to approximate the integral on the right-hand side of eq. (30). The term \(\int_{t^n}^{t^{n+1}} \int_{\partial\Omega_k} \chi \mathbf{v} \cdot \mathbf{n} \, dS \, dt\) is, in fact, the volume of the phase “+” that is fluxed over the boundary \(\partial\Omega_k\) over the time step from \(t^n\) to \(t^{n+1}\), the so-called fluxed phase-specific volume, shown in fig. \(\text{\ref{fig:fluxed_volume}}\). The boundary \(\partial\Omega_k\) is assumed as piecewise-smooth, composed of smooth surfaces (so-called faces), i.e.
\[
\partial\Omega_k = \bigcup_{f \in F_k} S_f.
\] (31)

Equation (30) can therefore be reformulated as
\[
\alpha_k(t^{n+1}) = \alpha_k(t^n) - \frac{1}{|\Omega_k|} \sum_{f \in F_k} \int_{t^n}^{t^{n+1}} \int_{S_f} \chi \mathbf{v} \cdot \mathbf{n} \, dS \, dt,
\] (32)

where the double integral on the r.h.s. gives the amount of the phase-specific volume, fluxed over the face \(S_f\) during the interval \([t^n, t^{n+1}]\). Introducing the set
\[
V_f^\alpha := \bigcup_{t \in [t^n, t^{n+1}]} \{x : \Phi^n_t(x) \in S_f \cap \Omega^+(t)\} = \bigcup_{t \in [t^n, t^{n+1}]} \Phi^n_t(S_f \cap \Omega^+(t)),
\] (33)
i.e. the part of \(\Omega^+(t)\) which is fluxed over \(S_f\) in \([t^n, t^{n+1}]\), we can rewrite eq. (32) as
\[
\alpha_k(t^{n+1}) = \alpha_k(t^n) - \frac{1}{|\Omega_k|} \sum_{f \in F_k} |V_f^\alpha|.
\] (34)

Equation (34) is still an exact equation. To compute the sets \(V_f^\alpha\), we exploit the flow invariance of \(\Omega^+(\cdot)\) to obtain
\[
V_f^\alpha = \bigcup_{t \in [t^n, t^{n+1}]} \Phi^n_t(S_f) \cap \Phi^n_t(\Omega^+(t)) = \bigcup_{t \in [t^n, t^{n+1}]} \Phi^n_t(S_f) \cap \Omega^+(t^n).
\] (35)

Therefore, if the flux volume across the face \(S_f\) is defined as
\[
V_f = \bigcup_{t \in [t^n, t^{n+1}]} \Phi^n_t(S_f),
\] (36)
$V^\alpha_f$ is expressed using the phase $\Omega^+$, according to

$$V^\alpha_f = V_f \cap \Omega^+(t^n), \quad (37)$$

and inserted back into eq. (34) to solve for $\{\alpha_k(t^{n+1})\}_{k \in K}$. In other words, the fluxed phase-specific volume $V^\alpha_f$, as shown in fig. 3, is computed as an intersection of the volume $V_f$, constructed by tracking $S_f$ backward in time, with the flow map $\Phi$, and the phase $\Omega^+(t^n)$.

It is important to shed some light on the way $V^\alpha_f$ is generally calculated in a discrete setting. The magnitude of the flux volume is given by

$$|V_f| = \int_{t^n}^{t^{n+1}} \int_{S_f} v \cdot n \, dS \, dt. \quad (38)$$

The approximate computation of eq. (38) depends on the chosen equation discretization method, and here we utilize the unstructured FVM. The flux volume $V_f$, given by eq. (36), is also approximated, because of the velocity interpolation and temporal integration used in the approximation of the flow map $\Phi$ in a discrete setting. Approximations used in eq. (36) and eq. (38) are in general very different from each other. Therefore, the flux volume $V_f$ is modified in the geometric VOF method, such that eq. (38) is satisfied. Only if this is achieved, can eq. (37) be used to compute $V^\alpha_f$ and inserted into eq. (34) to solve for $\{\alpha_k(t^{n+1})\}_{k \in K}$, while maintaining volume conservation. Specific approximations, utilized for this purpose by different flux-based geometrical VOF methods, are described in section 4.

2.2. Cell-based un-split geometrical VOF method

The direction in time in which the co-moving volume is tracked distinguishes forward tracking from backward tracking cell-based un-split geometrical VOF methods. Both forward and backward tracking methods utilize geometrical intersections between the images of co-moving volumes and the underlying Eulerian mesh $\{\Omega_l\}_{l \in K}$, in the so-called Eulerian remap step. To help reduce the number of necessary intersections, an intersection stencil of a volume $V$ is defined as the set of all indices of those cells that have a non-empty intersection with $V$, namely

$$C(V) := \{l \in K : V \cap \Omega_l \neq \emptyset\}. \quad (39)$$

For example, the intersection stencil of the forward image of the cell $\Omega_k$ in $\{\Omega_l\}_{l \in K}$ is

$$C(\Phi^{n+1}_l(\Omega_k)) := \{l \in K : \Phi^{n+1}_l(\Omega_k) \cap \Omega_l \neq \emptyset\}. \quad (40)$$

Note that additional indices $l \in K$ must be introduced via eq. (40) because the forward cell image $\Phi^{n+1}_l(\Omega_k)$ generally overlaps with multiple cells from $\{\Omega_l\}_{l \in K}$, and not just its pre-image (the cell $\Omega_k$). Equivalently, forward or backward images of each phase-specific volume $\Omega^+_l(t^n)$ will generally overlap with multiple cells from the mesh $\{\Omega_l\}_{l \in K}$.

2.2.1. Forward tracking

There are two types of forward tracking geometrical VOF methods ([22, 23, 24, 25]) and their main differences are illustrated by fig. 6. The first class of cell-based methods tracks only the phase-specific volume $\Omega^+_l(t^n)$ (fig. 6a), while the second class of methods also tracks the entire cell $\Omega_l$ (fig. 6b).
Figure 6: Computing \{α_k(t^{n+1})\}_{k \in K} by two different forward-tracking methods.

For the first class of methods, phase-specific volumes are tracked forward in time as \( \Phi_i^{n+1}(\Omega_i^{+}(t^n)) \), for \( l \in K \), and distributed over the underlying Eulerian mesh \( \{\Omega_k\}_{k \in K} \) in the Eulerian remapping step to compute \( \{α_k(t^{n+1})\}_{k \in K} \). The volume-conserving flow map conserves the phase-specific volume \( |\Omega_i^{+}(t^n)| \), so we have \( |\Phi_i^{n+1}(\Omega_i^{+}(t^n))| = |\Omega_i^{+}(t^n)| \). In the general case, however, the exact flow map \( \Phi_i^{n+1} \) has to be approximated, which introduces spatial interpolation and temporal integration errors. These errors make it impossible to exactly satisfy the relation \( |\Phi_i^{n+1}(\Omega_i^{+}(t^n))| = |\Omega_i^{+}(t^n)| \), so additional geometrical corrections must be applied to \( \Phi_i^{n+1}(\Omega_i^{+}(t^n)) \) in order to enforce volume conservation.

The Eulerian re-mapping step is used to compute \( \{α_k(t^{n+1})\}_{k \in K} \) from the forward images of phase-specific volumes \( \{\Phi_i^{n+1}(\Omega_i^{+}(t^n))\}_{i \in K} \) (cf. fig. 6a) as

\[
α_k(t^{n+1}) = \frac{1}{|\Omega_k|} \sum_{\ell \in C_{n+1}^+(\Omega_k)} |\Omega_k \cap \Phi_i^{n+1}(\Omega_i^{+}(t^n))|,
\]

where

\[
C_{n+1}^+(\Omega_k) = \{l \in K : \Omega_k \cap \Phi_i^{n+1}(\Omega_i^{+}(t^n)) \neq \emptyset\}
\]

is the intersection stencil of \( \Omega_k \) in \( \{\Phi_i^{n+1}(\Omega_i^{+}(t^n))\}_{i \in K} \). The part of the boundary \( \partial \Omega_i^{+}(t^n) \) that belongs to the interface, \( \Omega_i \cap \Sigma(t^n) \), is approximated, mostly linearly, by the geometrical VOF method (cf. section 3). A computationally efficient calculation of the sum in eq. (41) in a discrete setting is described in section 4.

The second class of forward tracking methods applies the space conservation law given by eq. (27) to the phase-specific volume \( \Omega_i^{+}(t^n) \) and, simultaneously, to the whole cell \( \Omega_i \), given by eq. (28) and
shown in fig. 6b, which leads to

$$|\Phi_t^{n+1}(\Omega_t^+(t^n))| = |\Omega_t^+(t^n)|$$

(43)

and

$$|\Phi_t^{n+1}(\Omega_t)| = |\Omega_t|,$$

(44)

respectively, if the map $\Phi$ is volume-conserving. Equations (43) and (44) yield

$$\alpha(t^{n+1}, \Phi_t^{n+1}(\Omega_t)) = \frac{|\Phi_t^{n+1}(\Omega_t^+(t^n))|}{|\Phi_t^{n+1}(\Omega_t)|} = \frac{|\Omega_t^+(t^n)|}{|\Omega_t|} = \alpha(t^n, \Omega_t) = \alpha(t^n).$$

(45)

Equation (45) states that the volume fraction in the forward cell image $\Phi_t^{n+1}(\Omega_t)$ is the same as the volume fraction of $\Omega_t$. From eq. (7), just like for the previous forward tracking method, we know that

$$\alpha(t^{n+1}) = \frac{|\Omega_t \cap \Omega_t^+(t^{n+1})|}{|\Omega_t|}.$$

(46)

The phase $\Omega_t^+(t^{n+1})$ is a disjoint decomposition of forward phase-specific volume images, i.e.

$$\Omega_t^+(t^{n+1}) = \bigcup_{l \in K} \Phi_t^{n+1}(\Omega_t^+(t^n)).$$

(47)

The final step in evaluating eq. (46) is therefore the computation of $\{\Phi_t^{n+1}(\Omega_t^+(t^n))\}_{l \in K}$, as in the previous method. However, contrary to the first method, $\{\Phi_t^{n+1}(\Omega_t^+(t^n))\}_{l \in K}$ are not calculated using the flow map, as shown in fig. 6a. Instead, $\{\Phi_t^{n+1}(\Omega_t^+(t^n))\}_{l \in K}$ are approximated on the forward image of the whole mesh, $\Phi_l^{n+1}(\{\Omega_t\}_{l \in K})$, using volume fractions on the background Eulerian mesh $\{\Omega_t\}_{l \in K}$, based on eq. (45). Each reconstructed phase-specific volume $\Phi_l^{n+1}(\Omega_t^+(t^n))$ inside the forward image of a cell $\Phi_l^{n+1}(\Omega_t)$ generally overlaps with multiple cells from the background Eulerian mesh $\{\Omega_t\}_{l \in K}$ (cf. fig. 6b), so the $\{\alpha_k(t^{n+1})\}_{k \in K}$ are computed using the Eulerian remapping step given by eq. (41). For example, $\Omega_k^+(t^{n+1})$ is computed on the forward image of the mesh $\Phi_l^{n+1}(\{\Omega_t\}_{l \in K})$ by the PLIC interface reconstruction using $\{\alpha_k(t^n)\}_{k \in K}$ (cf. section 3), and then used to compute $\{\alpha_k(t^{n+1})\}_{k \in K}$ by employing eq. (41). As before, indices $l$ and $k$ are necessary because the forward images of each phase-specific volume overlaps with more than one cell from the background Eulerian mesh.

2.2.2. Backward tracking

Equation (25) is used to express the main idea of backward tracking based on eq. (7), namely

$$\alpha_k(t^{n+1}) = \frac{|\Omega_k \cap \Omega_k^+(t^{n+1})|}{|\Omega_k|} = \frac{|\Phi_l^{n+1}[\Phi_l^{n+1}(\Omega_k) \cap \Omega_l^+(t^n)]|}{|\Omega_k|},$$

(48)

which states that the phase specific volume $\Omega_k^+(t^{n+1})$ can be computed as an intersection of the pre-image of the cell $\Phi_l^{n+1}(\Omega_k)$ (shown schematically in fig. 7a) and $\Omega_l^+(t^n)$. The backward tracking method therefore considers the cell in the Eulerian mesh $\Omega_k$ as a forward image of some pre-image of the cell $\Omega_k$. Because an exact $\Omega_l^+(t)$ is not available, this still leaves the question of approximating
\[ \Phi_{t^{n+1}}(\Omega_k) \cap \Omega^+(t^n) \]. The sub-domain \( \Omega^+(t^n) \) is given in each interface cell \( \Omega_k \) as \( \Omega_k^+(t^n) \), which leads to

\[
\Phi_{t^{n+1}}(\Omega_k) \cap \Omega^+(t^n) = \Phi_{t^{n+1}}(\Omega_k) \cap \bigcup_{l \in \mathcal{C}^+_n(\Phi_{t^{n+1}}(\Omega_k))} \Omega_l^+(t^n),
\]  

(49)

where

\[
\mathcal{C}^+_n(\Phi_{t^{n+1}}(\Omega_k)) = \{ l \in K : \Phi_{t^{n+1}}(\Omega_k) \cap \Omega_l^+(t^n) \neq \emptyset \}
\]  

(50)

is the intersection stencil of the pre-image \( \Phi_{t^{n+1}}(\Omega_k) \) in \( \{ \Omega_l^+(t^n) \}_{l \in K} \). Equation (49) inserted into eq. (48) leads to

\[
\alpha_{k}(t^{n+1}) = \frac{|\Phi_{t^{n+1}}(\Omega_k) \cap \bigcup_{l \in \mathcal{C}^+_n(\Phi_{t^{n+1}}(\Omega_k))} \Omega_l^+(t^n)|}{|\Omega_k|} = \frac{|\bigcup_{l \in \mathcal{C}^+_n(\Phi_{t^{n+1}}(\Omega_k))} \Phi_{t^{n+1}}(\Omega_k) \cap \Omega_l^+(t^n)|}{|\Omega_k|}
\]  

(51)

The intersections \( \Phi_{t^{n+1}}(\Omega_k) \cap \Omega_l^+(t^n) \) are denoted with the darker gray shade in fig. 7 and their union is the phase-specific volume of the phase \( \Omega_l^+(t^n) \) in the pre-image of the cell \( \Omega_k \). Since the volumes \( \Phi_{t^{n+1}}(\Omega_k) \cap \Omega_l^+(t^n) \) form a disjoint decomposition of the phase specific volume in the pre-image of \( \Omega_k \), the union of their forward images is also a union of disjoint sets, which leads to

\[
\alpha_{k}(t^{n+1}) = \frac{1}{|\Omega_k|} \sum_{l \in \mathcal{C}^+_n(\Phi_{t^{n+1}}(\Omega_k))} |\Phi_{t^{n+1}}(\Omega_k) \cap \Omega_l^+(t^n)|.
\]  

(52)
The flow map $\Phi_{n+1}^t$ is volume-conserving, so $|\Phi_{n+1}^t[\Phi_{n+1}^t(\Omega_k) \cap \Omega^n_+]| = |\Phi_{n+1}^t(\Omega_k) \cap \Omega^n_+|$, which leads to the final equation for $\alpha_k(t^{n+1})$, namely

$$\alpha_k(t^{n+1}) = \frac{1}{|\Omega_k|} \sum_{l \in C_+^n(\Phi_{n+1}^t(\Omega_k))} |\Phi_{n+1}^t(\Omega_k) \cap \Omega^n_+|.$$  (53)

Interestingly, once the phase specific volume in the pre-image $\Phi_{n+1}^t(\Omega_k)$ is computed, there is no need to map this volume forward into $\Omega_k$ at $t^{n+1}$: its magnitude is sufficient to compute $\alpha_k(t^{n+1})$. Since the phase specific volume in the pre-image of $\Omega_k$ is a union of intersections, the magnitude of the phase-specific volume is the sum of the magnitudes of these intersections. The backward tracking method therefore performs Eulerian remapping of $\Omega^n_+$ on the pre-image $\Phi_{n+1}^t \Omega_k$ and uses the magnitude of the phase-specific volume in the pre-image to compute $\alpha_k(t^{n+1})$. In the PLIC geometrical VOF method, however, velocity interpolation and temporal integration errors are sources of volume conservation errors in $\Phi$, while the piecewise-linear approximation of $\Omega^n_+(t^n)$ limits the spatial convergence to second order.

### 3. Interface reconstruction

The first implementation of the geometrical VOF method [1] employed the Piecewise Linear Interface Calculation (PLIC), that approximates the interface linearly in each multi-material cell. Later developments such as [2] have simplified the interface approximation to *piecewise constant* Simple Line Interface Calculation (SLIC). A detailed overview of the earliest publications on this topic can be found in [3, page 6, table 1], together with a table summarizing most important contributions. A review of reconstruction algorithms is also available in [26, 15]. A comparison between the order of convergence and relative computational costs for more recent developments is shown in table [1]

PLIC algorithms have prevailed over SLIC algorithms because of their many advantages. A more accurate interface approximation is provided by PLIC algorithms than by SLIC algorithms, resulting in second-order convergent interface advection on structured meshes [12, 27, 16, 28]. The PLIC algorithms enable efficient computations and increased accuracy over a wide span of spatial scales when they support local dynamic Adaptive Mesh Refinement (AMR) [13, 29, 17]. The piecewise planar interface approximation supports the numerical simulation of the transport of insoluble surfactants on the fluid interface [30], which is not possible with the piecewise constant interface approximation given by the SLIC algorithm. The SLIC algorithms generate a substantial amount of *jetsam* (*flotsam*) [15]. Jetsam (flotsam) are elements of the interface that are *artificially separated* and transported with the flow velocity. Noh and Woodward [31] have introduced "jetsam" ("jettisoned goods") and "flotsam" ("floating wreckage") for artificially separated interface elements, according to Kothe et al. [32]. PLIC algorithms based on error minimization can be directly applied to unstructured meshes [22, 33, 23, 34, 35], since they rely on linear traversal of the surrounding cells, without accessing cells in any specific direction. Reconstructing a piecewise linear interface while strictly satisfying conservation of volume requires accurate volume truncation and interface positioning algorithms. The PLIC algorithms do have one general disadvantage: so-called artificial numerical surface tension. It is introduced by the interface reconstruction algorithm in the form of rounding of sharp corners, that occurs during repeated reconstructions of the interface [24, 29]. The advantages of PLIC algorithms make them still the prevailing choice in 3D, compared to still more complex and computationally expensive higher-order interface approximations.
Table 1: PLIC reconstruction algorithms. The convergence order of the reconstruction errors are reported for circular and spherical interfaces. For CIAM and LSF the error convergence order is reported for an ellipse by the authors. Additional citations are listed for those algorithms whose relative costs are not reported in the original publications.

| Algorithm                                      | Convergence | Cost |
|-----------------------------------------------|-------------|------|
| Youngs [13]                                   | 1.0-1.8, [15] | 1    |
| Mosso-Swartz, Mosso et al. [33]               | 2.0         | 3-4  |
| LVIDA, Pilliod and Puckett [26]               | 2.0         |      |
| ELVIDA, Pilliod and Puckett [26]              | 1.9-2.2     | 900  |
| CVNIA, Lioc et al. [34]                       | 2.0         | 50   |
| CLCIR, CBIR, López et al. [37]                | 2.0-2.11    | 3    |
| CIAM, Scardovelli and Zaleski [14]            | 1.0-2.28    | 1    |
| LSF, Scardovelli and Zaleski [14], Aulisa et al. [15] | 2.0         | 1.5  |
| MoF, Dyadechko and Shashkov [22], [38]        | 2.0         | 7    |
| PIR, Mosso et al. [35]                        | 2.0         | 10   |

The Youngs' gradient-based algorithm is taken as the reference for the relative computational cost in all the referenced publications. It is important to note that the algorithm cost does depend on the implementation. However, the costs in [36] are reported on the same software platform, which makes them more objective. The relative costs reported in [26, 14, 34, 37] have been reported on structured Cartesian meshes.

From table 1 it follows that only a sub-set of reconstruction algorithms can be used on unstructured meshes. The main constraint enforced by the algorithms on unstructured meshes is the inability to exercise access to mesh elements in a specific direction, e.g., accessing different face centers by changing their y coordinate. Algorithms that rely on more than the first level of addressing experience a substantial increase in computational complexity on unstructured meshes also in terms of algorithm parallelization using the domain decomposition and message passing parallel programming model. Such computational complexity restrictions should be considered when choosing a PLIC reconstruction algorithm for unstructured meshes. Consequently, if the algorithm’s relative cost reported in table 1 is already high on structured meshes, it can be disregarded as a candidate for unstructured meshes.

To reconstruct the interface in each multi-material cell \( \Omega_k \), the interface normal and position vectors \( (n_k, p_k) \) are computed. The aim of each reconstruction algorithm is to accurately compute those two parameters. At first, \( n_k \) is approximated by the interface orientation algorithm. Then, the interface plane is positioned by the interface positioning algorithm that calculates \( p_k \). In order to achieve second-order convergence in the \( L_1 \) error norm of the volume fraction field for the interface advection, second-order convergence of the interface reconstruction must be ensured. Error convergence of the reconstruction is verified either by some error norm of the difference between the reconstructed and the exact interface normal, or by some error norm of the volume of symmetric difference between the volume bounded by the reconstructed interface, and the volume bounded by the exact interface. In the following sub-sections, a sub-set of the PLIC reconstruction algorithms from table 1 are outlined and categorized into contributions to the interface orientation and
positioning.

3.1. Interface orientation

All interface orientation algorithms rely on the volume fraction field $\alpha$ to approximate $n_k$. Some second-order convergent algorithms rely exclusively on the $\alpha$ field, while others employ additional geometrical calculations to increase convergence.

3.1.1. Youngs’ algorithm

This algorithm, originally developed by Youngs [18], defines $n_k$ as

$$n_k = -\frac{\nabla_k \alpha}{\|\nabla_k \alpha\|}.$$  \hspace{1cm} (54)

The discrete gradient $\nabla_k$ is crucial for maintaining accuracy [39]. On unstructured meshes, the gradient $\nabla_k$ is usually approximated using the unstructured Finite Volume discretization. However, using the FVM for gradient operator discretization is by no means a requirement for the geometrical VOF method - other discretization methods can be used as well. More details on the gradient operator discretization practice on unstructured meshes using unstructured FVM can be found in [10] ch. 2.

Mavriplis [41] has concluded that a wider stencil Inverse Distance Weighted Least Squares Gradient (IDWLSG) approximation delivers accurate results on equidistant hexahedral unstructured meshes. A wider stencil gradient results in a more accurate aerodynamic drag estimation on unstructured meshes and the accuracy and convergence of the Least Squares (LS) gradient deteriorates strongly on unstructured tetrahedral meshes.

Aulisa et al. [15] have proposed a gradient calculation that uses finite differences to compute the components of the volume fraction gradient at cell corners from cell-centered values obtained by averaging finite difference operations. This gradient approximation cannot be applied without modification on unstructured meshes as it relies on accessing cells in a specific direction.

Similar to Mavriplis [41], Aln and Shashkov [36] have proposed a Least Squares (LS) minimization to estimate $\nabla_k \alpha$ on unstructured meshes. However, this minimization differs from the IDWLSG proposed by Mavriplis [41] in the fact that their Linear Least Squares Gradient (LLSG) does not rely on inverse distance weighting. Instead, they have applied a second-order linear approximation of the volume fraction field $\alpha$ using the Taylor series expansion from the centroid $x_k$ of the cell $\Omega_k$:

$$\alpha(x) \approx \alpha_k + \nabla_k \alpha \cdot (x - x_k).$$ \hspace{1cm} (55)

A volume fraction error for the cells in the intersection stencil $C(\Omega_k)$ given by eq. (39) is then defined as

$$\epsilon_{LLSG}(\Omega_k) = \sum_{l \in C(\Omega_k)} \left( \alpha_{l1} - \frac{\int_{\Omega_l} \alpha(x) dV}{|\Omega_l|} \right)^2,$$ \hspace{1cm} (56)

using eq. (55) for $\alpha(x)$. The LS minimization of $\epsilon_{LLSG}$ results in a $3 \times 3$ linear algebraic system that is solved for the 3 components of $\nabla_k \alpha$ in each cell $k$. The LLSG gradient estimation was used for the $\alpha$ field by Garimella et al. [42] for their Arbitrary Lagrangian-Eulerian (ALE) method. On polyhedral unstructured meshes, the explicit construction of a wider gradient stencil as proposed by Mavriplis [41] is redundant because a polyhedral cell is connected to all adjacent cells by its faces.
The only difference between the IDWLSG and LLSG algorithm is the introduction of inverse distance weights in the minimized error functional

\[ \epsilon_{IDWLSG}(\Omega_k) = \sum_{l \in C(\Omega_k)} w_l \left( \alpha_{\Omega_l} - \frac{\int_{\Omega_l} \alpha_l(x) dV}{|\Omega_l|} \right)^2, \]  

(57)

where \( w_l \) is the inversed distance weight given by

\[ w_l = \frac{1}{\sum_{l \in C(\Omega_k)} \frac{1}{\|x_k - x_l\|^p}}. \]

(58)

The weight exponent is set to \( p = 1 \), so adjacent cells have the same influence on the gradient approximation.

Correa et al. [43] compare different gradient operator approximations on unstructured meshes in detail. Their research is aimed at accurate volume rendering in the field of Computer Graphics (CG). Nevertheless, their findings can be directly used for the gradient approximation on unstructured meshes in order to obtain a reasonably accurate initial PLIC interface orientation. The following implications made by Correa et al. [43] should be taken into consideration:

1. Inversed distance based gradient approximations are generally more accurate, especially on unstructured meshes with non-equidistant cells.
2. Inversed distance based methods are more cost effective compared to regression based methods.
3. An increase in the discretization stencil size is important for improving the absolute accuracy of the approximated gradient on hexahedral meshes.

3.1.2. Mosso-Swartz algorithm

The derivation and numerical analysis of the Mosso-Swartz (MS) algorithm was done by Swartz [44] and the algorithmic formulation for unstructured meshes was done by Mosso et al. [33]. For a cell \( \Omega_k \), the initial \( n_k \) is computed using eq. (54). An interface polygon is defined as the intersection between the cell \( \Omega_k \) and the PLIC plane \((p_k, n_k)\), i.e.

\[ Q_k = \{ x \in \Omega_k : (x - p_k) \cdot n_k = 0 \}. \]

(59)

Generally, \( \{\Omega_k\}_{k \in K} \) are volumes bounded by polygons, so the PLIC polygon \( Q_k \) is a set of intersection points between the polygonal boundary of \( \Omega_k \) and the plane \((p_k, n_k)\). The centroid of the interface polygon is, therefore, given as

\[ x_{Q_k} = \frac{1}{|Q_k|} \sum_{q=1}^{|Q_k|} x_q. \]

(60)

We define at this point the interface-cell stencil of a volume \( V \) in the mesh \( \{\Omega_l\}_{l \in K} \) as

\[ C^\alpha(V) = \{ l \in K : V \cap \Omega_l \neq \emptyset \text{ and } 0 < \alpha_l < 1 \}, \]

(61)

i.e. the set of labels of all cells \( \Omega_l \) that have a non-empty intersection with the volume \( V \) and that also have a non-empty intersection with the interface. Using the interface-cell stencil given by
eq. (61), estimated interface normal vectors are computed for each cell $\Omega_k$ from the centroids of interface polygons in the interface-cell stencil $C^\alpha(\Omega_k)$, as

$$N_k = \{n_{k,l} : n_{k,l} \cdot (x_{Q_k} - x_{Q_l}) = 0, \ l \in C^\alpha(\Omega_k), l \neq k\},$$

(62)

To satisfy the orthogonality condition in eq. (62), each estimated normal $n_{k,l}$ is computed as the vector $x_{Q_l} - x_{Q_k}$, rotated $90^\circ$ in the positive direction around the axis $(x_{Q_l} - x_{Q_k}) \times n_k$. The modified interface normal $n_{k}^m$ is obtained iteratively by a least-squares minimization

$$\epsilon_{k}^{MS} = \sum_{l \in C(\Omega_k)} (n_{k}^m - n_{k,l})^2 \rightarrow \min.$$  

(63)

The initial iteration starts with $n_{k}^m = n_k$ as defined for the Youngs algorithm by eq. (54). Once the new interface normal vector $n_{k}^m$ is obtained, the interface is reconstructed, resulting in a new set of interface polygons $Q_k$. To achieve second-order convergence, the steps given by equations 59 to 63 are repeated four times ($m = 1, 2, 3, 4$). Mosso et al. [33] do not provide the motivation for choosing 4 iterations. This has also been discussed by Hernández et al. [45, Table 3.] for the simplified CLCIR method (LLCIR): a single iteration of the Mosso algorithm increases the convergence order on coarser meshes, but is not sufficient to maintain second-order convergence on fine meshes. Dyadechko and Shashkov [23] propose the arithmetic average

$$n_{k}^m = \frac{\sum_{l \in C^\alpha(\Omega_k)} n_{k,l}}{|C^\alpha(\Omega_k)|},$$

(64)

as an alternative way to compute the modified normal, which reduces the computational effort introduced by the four outer iterations, the artificial smoothing of the interface as well as the required mesh resolution. Dyadechko and Shashkov [23] name this modification of the Mosso-Swartz algorithm as the Swartz algorithm.

### 3.1.3. Conservative level contour interface reconstruction

The CLCIR family of algorithms was originally developed by Lópes et al. [37]. Like the modification of the Swartz-Mosso algorithm developed by Dyadechko and Shashkov [23], the CLCIR algorithm relies on estimating the interface normal by performing a local average of the normal vectors from the surrounding interface polygons. The difference between the CLCIR and Swartz-Mosso algorithm variants lies in the way the estimated normal vectors $n_{k,l}$ are computed. CLCIR algorithms rely on an iso-contour reconstruction to compute the estimated normal vectors. To triangulate the iso-contour, a volume-weighted average of volume fractions from surrounding cells is computed at each cell corner-point $x_p$ as

$$\alpha(x_p) = \alpha_p = \frac{\sum_{l \in C(x_p)} \alpha_l |\Omega_l|}{\sum_{l \in C(x_p)} |\Omega_l|},$$

(65)

where

$$C(x_p) = \{k \in K : x_p \in \Omega_k\}$$

(66)

is the point-cell stencil: a set of labels of all cells in $\{\Omega_k\}_{k \in K}$ that contain the cell-corner point $x_p$. From the cell corner-point values defined by 65, an iso-contour (iso-surface) point $x_{pq,\lambda}$ is defined on each cell edge spanned by two cell corner-points $(x_p, x_q)$ according to

$$x_{pq,\lambda} = x_p + s(x_q - x_p), \text{ where } s \in [0, 1], \ \alpha(x_{pq,\lambda}) = \alpha_\lambda$$

(67)

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where $\alpha_\lambda$ is a global iso-value. The parameter $s$ is found using root finding methods if the field used for the iso-contour reconstruction is interpolated with higher-order interpolation methods. López et al. \cite{37} have used a linear approximation of $\alpha$ along the edge, which results in an explicit expression

$$s = \frac{\alpha_\lambda - \alpha_p}{\alpha_q - \alpha_p}, \quad (68)$$

for the $s$ parameter, where $\alpha_p = \alpha(x_p)$, $\alpha_q = \alpha(x_q)$ are given by \cite{65} with $\alpha_\lambda = 0.5$. Once all the edge points with $\alpha_\lambda = 0.5$ have been calculated, the polygonization of the iso-contour is computed by triangulating edge points $x_{pq,\lambda}$ in each cell $c$, while enforcing outward orientation of triangle normal area vectors. The triangulation starts with the calculation of the centroid of the iso-contour in each cell,

$$x_{k,\lambda} = \frac{1}{|E_k|} \sum_{(p,q) \in E_k^b} x_{pq}, \quad (69)$$

where $E_k^b$ is the set of edges of the cell $\Omega_k$, represented by the pairs $(x_p, x_q)$, that contain iso-contour points, because their volume fraction values given by \cite{65} satisfy $\alpha_p < \alpha_\lambda < \alpha_q$, i.e.

$$E_k^b = \{(p,q) : \alpha_p < \alpha_\lambda < \alpha_q\}. \quad (70)$$

The iso-contour centroid $x_{k,\lambda}$ in the cell $\Omega_k$ is subsequently used to compute a triangulation by connecting this centroid with the centroids of neighboring cells from the interface-cell stencil $C^\alpha(\Omega_k)$, into a set of triangles

$$T_k = \{\tau_n = (x_{k,\lambda}, x_{l,\lambda}, x_{m,\lambda}) : l, m \in C^\alpha(\Omega_k), ((x_{l,\lambda} - x_{k,\lambda}) \times (x_{m,\lambda} - x_{k,\lambda})) \cdot n_k > 0\}, \quad (71)$$

where the interface-cell stencil $C^\alpha$ is given by eq. (61). The condition in eq. (71) ensures that the normal of each triangle $\tau_n$, namely

$$n_{\tau_n} := (x_{l,\lambda} - x_{k,\lambda}) \times (x_{m,\lambda} - x_{k,\lambda}), \quad (72)$$

in the triangulation $T_k$ remains oriented in the same direction as the initial PLIC normal $n_k$ given by the Youngs’ algorithm by eq. (54), i.e.

$$n_{\tau_n} \cdot n_k > 0. \quad (73)$$

The normals of the triangles from the triangulation $T_k$ are weighted by the angles at the centroid $x_{k,\lambda}$ to compute the modified interface normal vector

$$n_k^m = \frac{\sum_{n=1}^{\|T_k\|} n_{\tau_n} \beta_n}{\sum_{\tilde{n}=1}^{\|T_k\|} \beta_{\tilde{n}}}. \quad (74)$$

This approximation of the modified interface normal vector is similar to the arithmetic average proposed by Dyadechko and Shashkov \cite{23} in their modification of the Swartz-Mosso algorithm. The corrected normal is used for the interface positioning sub-step of the interface reconstruction algorithm that results in the new interface polygons. López et al. \cite{37} have proposed a repetition of the iso-contour polygonization step as well as a Bézier spline interface approximation to increase the interface orientation accuracy and convergence. Their results \cite{37 tables 1 and 2} do not show

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significant improvements in convergence and absolute accuracy by performing a repeated polygonization step, nor by adding the Bézier triangle patch interpolation (CBIR). The details of the Bézier interface approximation are omitted here and can be found in [37]. The CLCIR method shows a promising and stable second-order of convergence across different mesh densities and is to be considered a good candidate for unstructured meshes, as well as the MS modification proposed by Dyadechko and Shashkov [23], since both methods disregard computationally expensive outer iteration steps.

3.1.4. Linear least squares fit algorithm

The Least Squares Fit (LSF) algorithm was proposed by Scardovelli and Zaleski [14] and extended to 3D by Aulisa et al. [15]. The algorithm starts by an initial estimate of the normal orientation using the Youngs’ algorithm given by eq. (54). The initial $n_k$ is then used to position the interface while upholding the prescribed volume fraction value $\alpha$. A positioned interface plane intersected with the cell $\Omega_k$ results in the interface polygon $Q_k$ given by eq. (59) with the polygon centroid $x_{Q_k}$ given by eq. (60). A second-order convergence is obtained by solving a minimization problem, constructed from the information available in the interface-cell stencil $\mathcal{C}(\Omega_k)$, as follows. A distance between the interface polygon centroid in the current cell $c$ and the centroid in the neighbor cell $n$ is defined as

$$d_{k,l} = \|x_{Q_l} - x_{Q_k}\|_2,$$  \hspace{1cm} (75)

and it is used to compute the average distance to neighboring centroid in the cell $\Omega_k$ as

$$\hat{d}_k = \frac{1}{|\mathcal{C}^{\alpha}(\Omega_k)|} \sum_{l \in \mathcal{C}^{\alpha}(\Omega_k)} d_{k,l},$$  \hspace{1cm} (76)

where $\mathcal{C}^{\alpha}(\Omega_k)$ is given by eq. (61). The individual and the average distance define the variance of the distance as

$$\sigma^2_k = \frac{1}{|\mathcal{C}^{\alpha}(\Omega_k)|(|\mathcal{C}^{\alpha}(\Omega_k)| - 1)} \sum_{l \in \mathcal{C}^{\alpha}(\Omega_k)} (d_{k,l} - \hat{d}_k)^2.$$  \hspace{1cm} (77)

The variance is used to compute the individual weight of each neighboring centroid $x_{Q_l}$ as

$$w_l = \exp \left( -\frac{d^2_{l}}{a\sigma^2_k} \right),$$  \hspace{1cm} (78)

with a free parameter $a$ that Scardovelli and Zaleski [14], Aulisa et al. [15] set to 0.75. The individual weight is then normalized according to

$$w_{l,n} = \frac{w_l}{\sum_l w_l}.$$  \hspace{1cm} (79)

Finally, the weighted distance error

$$\epsilon_{LLSF}^k = \sum_{l \in \mathcal{C}^{\alpha}(\Omega_k)} w_{l,n} \left[ n_k^m \cdot (x_{Q_l} - x_{Q_k}) \right]^2$$  \hspace{1cm} (80)

is minimized. This minimization makes the LSF algorithm similar to the Mosso-Swartz algorithm, in the sense that the $n_k^m$ modified normal is calculated as a result of a least-squares minimization problem. The MS algorithm minimizes the difference between the normal vectors and the LSF
algorithm minimizes the distance to a plane. The error $\epsilon_{LSF}^{k}$ in eq. (80) is minimized with respect to the three components of the corrected interface orientation vector $\mathbf{n}^{k}$, resulting in a $3 \times 3$ linear algebraic equation system that is then solved for the components of $\mathbf{n}^{k}$.

The LSF method ensures a stable second-order convergence for a reconstructed sphere and its absolute accuracy is comparable to CLCIR [37, Table 1]. Table 1 places the LSF algorithm into the class of efficient algorithms with the computational cost that is reported to be only 1.5 times larger than the cost of the Youngs’ algorithm, making LSF an interesting candidate for unstructured meshes.

3.1.5. Moment of fluid algorithm

The Moment of Fluid (MoF) orientation algorithm proposed by Dyadechko and Shashkov [23] relies on the Youngs algorithm for the initial estimate of the interface normal. The second-order convergent improvement of the initial estimate is obtained by minimizing the distance between the reconstructed centroid of the phase-specific volume $x_{k,R}$ and the advected phase centroid $x_{k,A}$, shown schematically in fig. 8.

The reconstructed phase centroid $x_{k,R}$ is computed from the intersection between the positive half-space of the reconstructed interface, and the cell $\Omega_{k}$. The positive half-space of a reconstructed PLIC plane $\mathbf{n}_{k}, \mathbf{p}_{k}$ is defined as

$$H_{k}(t) := \{ \mathbf{x} : \mathbf{n}_{k}(t) \cdot (\mathbf{x} - \mathbf{p}_{k}(t)) \geq 0 \}. \quad (81)$$

The centroid of the phase-specific volume is therefore the centroid of the set

$$R_{k}(t) = H_{k,R}(t) \cap \Omega_{k}, \quad (82)$$

i.e.

$$x_{k,R}(t) = \frac{1}{|R_{k}(t)|} \int_{R_{k}(t)} \mathbf{x} dV. \quad (83)$$

The advected phase volume centroid is initialized as the centroid of the phase-specific volume $\Omega_{k}^{+}$, defined by the initial indicator function $\chi(\cdot, t_{0})$, i.e.

$$x_{k,A}(t_{0}) = \frac{1}{|\Omega_{k}|} \int_{\Omega_{k}} \chi(\cdot, t_{0}) dV. \quad (84)$$
As the interface evolves, phase-specific volumes are contributed from cells in the interface-cell stencil $C^a(\Omega_k)$ into the cell $\Omega_k$ (cf. sections 2.1 and 2.2). Each phase-specific volume has a centroid attributed to it that is additionally tracked along its Lagrangian trajectory. The final advected centroid $x_{k,A}(t)$ is computed as an average of all centroids of phase-specific volumes that were advected into $\Omega_k$ from the candidate cells in $C^a(\Omega_k)$ given by 39. The MoF method is therefore not exclusively a reconstruction method, because it extends the advection of the interface by introducing and tracking centroids of phase-specific volumes. The advection aspect of the MoF advection is addressed in section 4.

In fig. 8, $A_k$ represents the intersection between the input domain and the interface-cell in the initial time step. The error of the initial interface orientation is schematically shown as the shaded region in fig. 8. Assuming the advected phase centroid $x_{k,A}$ is available, the goal of the MoF orientation algorithm is to minimize this shaded region by modifying the direction of the normal vector $n_k$. The difference between the advected and the reconstructed centroid,

$$e_k^{MOF} = \|x_{k,R} - x_{k,A}\|^2,$$

is minimized to compute the corrected interface normal $n_k^A$, resulting in a new advected phase volume centroid $x_{k,A}$. The new volume

$$A_k = \mathcal{H}^A(p_k, n_k^A) \cap \Omega_k,$$

is computed using $\mathcal{H}^A$, the positive halfspace of the PLIC plane passing through $p_k$ with the normal $n_k^A$. Then, the new centroid $x_{k,A}$ can be computed as

$$x_{k,A} = \frac{1}{|A_k|} \int_{A_k} x dV.$$

The MoF orientation algorithm [23, 46, 38] improves the reconstruction in two important ways. The reconstruction procedure is local to the interface cell, making the reconstruction algorithm of the MoF method massively parallel. This does not incur perfect linear scaling however, because the amount of time required by the reconstruction will be linearly proportional to the number of interface cells handled by the parallel process. Not requiring parallel communication for the interface reconstruction is unlike all the aforementioned normal orientation algorithms. Note, however, that the reconstruction does require the centroid to be available and the parallel computation therefore has an additional overhead of both tracing and communicating centroids of phase-specific volumes. Absolute accuracy of the method is much higher than for other orientation methods, making it a better choice for problems where local dynamic refinement is required. Additionally, the centroid-based optimization results in a more accurate automatic nested reconstruction for situations involving more than two phases [38].

3.2. Interface positioning

Whereas reconstruction algorithms differ strongly in the choice of the interface orientation algorithm, the same interface positioning algorithms are shared by many reconstruction algorithms. The aim of a positioning algorithm is to compute the position of the interface plane $p_k$ using a known orientation $n_k$. To achieve this, a piecewise-linear approximation of the interface is used to reformulate the volume fraction as

$$\alpha_k = \alpha_k(n_k, p_k).$$
The interface orientation algorithm provides \( \mathbf{n}_k \), and \( \alpha_k \) is given either by pre-processing or the advection algorithm. Hence, \( p_k \) remains as the only unknown variable in eq. (88). Figure 9 shows the volume fraction as a function of the interface position \( p_k \) along a given orientation vector \( \mathbf{n}_k \). It becomes obvious by inspecting fig. 9 that eq. (88) can be further simplified to a scalar equation

\[
\alpha_k = \alpha_k(x_{\alpha}),
\]

where \( x_{\alpha} \) is the coordinate on the \( \mathbf{n}_k \) axis with respect to an arbitrarily chosen origin \( O_k \). Note that floating-point operations used by the geometrical operations for the positioning are more accurate if a point inside the cell \( \Omega_k \) (e.g. the cell centroid \( x_k \)) is chosen as the origin of the coordinate system, as this reduces the difference between the coordinates of cell corner-points and thus increases the accuracy of floating-point operations \[47\]. To compute the interface position eq. (89) is reformulated as

\[
x_{\alpha} = x_{\alpha}(\alpha_k).
\]

Dyadechko and Shashkov \[23\] have proven that \( \mathbf{n}_k \) and \( \alpha_k \) are sufficient to compute \( x_{\alpha} \) (therefore also \( p_k \)) because the function given by eq. (89) is a strictly monotone function. Currently, there is no function of the form given by eq. (90) that can, given a volume fraction, return an interface position in an arbitrarily shaped cell \( \Omega_k \) without performing some kind of a search: either iterative root finding, or a search for a closed interval that contains \( \alpha_k \) (bracketing interval).

The graphs of \( \alpha_k(\mathbf{n}_k, p_k) \) are shown in figs. 10a to 10c for different primitive cell shapes using the same \( \mathbf{n}_k \). In every case, the function has a diminishing derivative at two positions \( p_k \): the point where the intersection between the half-space defined by the PLIC interface plane and the cell is the complete cell, and another point where the intersection result is an empty set. The diminishing derivative can cause divergence of slope-based numerical methods used to solve eq. (90) for \( p_k \). Note
that there is one special case where the derivative does not diminish: when $n_k$ is collinear with a planar face of $\Omega_k$, which might happen if a planar interface is initialized on a hexahedral mesh.

Several interface positioning algorithms have been developed so far to compute $x_\alpha$. An iterative approach based on the Brent’s method [48] has been used by Rider and Kothe [3]. Equation (90) is evaluated iteratively, starting with an initial guess $x_\alpha^0$, until $x_\alpha$ is computed, such that the prescribed volume fraction $\alpha_k$ is obtained up to a prescribed tolerance. The Brent method [49] is applied because it provides a stable solution to the root finding problem even when subjected to the diminishing function derivative at the endpoints of the interval as shown in fig. 9 schematically and in fig. 10 for actual volume fractions. Rider and Kothe [3] already state that Newton’s iterative method lowers the number of iterations provided an accurate initial starting position for the Brent’s method. In order to better estimate $x_\alpha^0$ in the first step, Rider and Kothe [3] sort the cell points with respect to the projection on $n_k$, defining

$$\mathcal{P}_{k,\Sigma} = (p_1, p_2, \ldots, p_n) \text{ such that } (p_i \cdot n_k) \leq (p_{i+1} \cdot n_k), p_i \text{ is a cell corner-point.}$$

\[\text{(91)}\]
To each $p_i \in P_k$, a volume fraction is assigned as

$$\alpha_{c,i} = \frac{|\Omega_k \cap \mathcal{H}(n_k, p_i)|}{|V_k|},$$

(92)

where $\mathcal{H}$ is a positive half-space at point $p_i$ whose orientation is defined by $n_k$. The cut-out slab is defined as

$$S_{c,i} = \{\Omega_k \cap \mathcal{H}(n_k, p_i) \cap \mathcal{H}(-n_k, p_{i+1}) : i = 1, \ldots, |P_k, \Sigma|\}.$$ (93)

From eqs. (91) and (92), we have

$$\alpha_{c,i} > \alpha_{c,i+1}$$

(94)

and, as a consequence,

$$\exists! S_{c,i} : \alpha_{c,i+1} \leq \alpha_k < \alpha_{c,i} \iff p_k \in S_{c,i}.$$ (95)

A cut-out slab $S_{c,i}$ is then chosen which contains the interface position. At this point, Rider and Kothe [3] apply Brent’s method [48] to locate the interface within the slab.

A semi-analytical approach was extended to arbitrary cell shapes by López and Hernández [50] that sorts the slabs according eq. (93) (similar to Rider and Kothe [3]) and positions the interface within the slab that contains it. Contrary to the algorithm proposed by Rider and Kothe [3], once $S_{c,i}$ is found, an analytical expression is used to compute $p_k$ explicitly. This semi-analytical (bracketing) approach is faster on cubic cells compared to the Brent method used in [3]. Furthermore, López and Hernández [50] state that the sorting and slab calculation step is still computationally the most expensive part of the positioning algorithm.

A simplified iterative approach was proposed by Ahn and Shashkov [46] that also works well with cells of arbitrary shape. Additionally, the average number of iterations for cubic cells is reported in [46] to be smaller than 8 - which is the number of vertices of the cube. This makes the stabilized iterative algorithm comparable to the semi-analytical, even for $\Omega_h$ with hexahedral cells, since the total number of iterations is smaller than for the semi-analytical algorithm where it is necessary to create the cut-out slabs.

Another semi-iterative interface positioning algorithm was proposed by Diot et al. [51] for planar and axis-symmetric convex cells. Their approach is faster than the standard Brent’s iterative method and the algorithm proposed by Dyadechko and Shashkov [23] that relies on the calculation of the interface position $x_\alpha$ within a slab $S_{c,i}$ using interpolation. Table 2 contains results for the axis-symmetric geometry and shows exactly what is to be expected: the average global iteration number for both the method of Dyadechko and Shashkov [23] and Diot et al. [51] are the same, since they both rely on the same sorting and slab calculation steps. However, no reference is made to the stabilized secant/bisection method of Ahn and Shashkov [46], or the method proposed by López and Hernández [50].

Diot and François [52] have extended their 2D and axis-symmetric method [51] to 3D for convex cells of arbitrary shape. Following their work in [51], explicit analytic expressions for computing a volume of 3D slabs $S_{c,i}$ are proposed. Only a comparison with an iterative method based on Brent’s root finding method is provided in the results section of the article. Accuracy and efficiency comparisons with López and Hernández [50], Ahn and Shashkov [46] are not provided.

More recently, López et al. [53] have optimized the bracketing procedure used to calculate the cut-out slabs using linear interpolation of the fill volume, based on signed distances between the cell corner-points and the PLIC interface. Additionally, López et al. [55] have improved the analytical...
expression for the volume calculation in general convex polyhedrons, that additionally increases
the efficiency of interface positioning. Their Coupled Interpolation-Bracketed Analytical Volume
Enforcement (CIBRAVE) is compared [53, fig. 8] with the Brent’s method, Diet and François [52]
and Ahn and Shashkov [46], and shows a significant improvement in terms of the relative CPU
time.

A new iterative positioning algorithm has recently been proposed by [54]. An exact derivative
\( \frac{d\alpha}{dx} (x) \) is computed using the area of the so-called cap polygon, namely

\[
\frac{d\alpha}{dx} = \frac{|\Pi(n_k, p(x)) \cap \Omega_k|}{|\Omega_k|},
\]

(96)

The exact derivative in eq. (96) is used with the Newton method to achieve significantly faster
convergence compared to the Brent’s method or the stabilized secant method of [46]. A cap-polygon
is defined as the intersection between the interface plane \( \Pi(n_k, p(x)) \) and the cell \( \Omega_k \). Its area equals
the derivative of \( \alpha \) with respect to the \( x \)-coordinate of the positioning axis in fig. 9.

Recently, López et al. [55] have proposed an analytical expression for interface positioning in
non-convex polyhedrons. The polyhedron is modeled using a connectivity table that defines each
face as an ordered list of indices from a global set of points. The advantage of the connectivity
table is twofold: the algorithm can be applied to non-convex polyhedrons because the connectivity

table supports disjoint sets and the divergence theorem can be used for the volume calculation. The
divergence theorem increases computational efficiency, as it requires less floating point and memory
operations than tetrahedral decomposition. Connectivity does come with a cost: it significantly
increases the implementation complexity of the algorithm compared to tetrahedral decomposition.
The authors report an increase in computational efficiency in one order of magnitude, compared to
Brent’s method with tetrahedral decomposition. The non-convexity of the polyhedron caused by
the non-planarity of its faces is addressed by triangulation [55, fig. 18].

### 3.3. Reconstruction comparison

The accuracy of the reconstruction can be influenced by the accuracy of the initialization algo-

rithm if the latter is not accurate enough. When using high mesh resolutions, high accuracy of the
initialization must be ensured to avoid the influence of the initialization on the reconstruction and,
subsequently, advection errors.

The volume fraction can be exactly initialized on structured and unstructured meshes for the
spherical interface and it is done approximatively for more complex surfaces [56, 57]. Volume frac-
tions can also be calculated by approximating \( \Omega^+(t) \) with an unstructured mesh, and intersecting
this mesh with the mesh used to approximate the solution domain \( \Omega \) [29]. Furthermore, different
error measures and different verification tests are used to verify the reconstruction algorithm, which
makes it difficult to summarize the results and compare methods. Reconstruction of a circle or a
sphere is a widely used verification case so it is presented in this section as a basis for comparing
reconstruction algorithms. Aulisa et al. [15] have used a sphere of radius \( r = 0.325 \) randomly placed
around the center point \((0.5, 0.5, 0.5)\) in the unit box domain. López et al. [37] have used the same
radius, and have placed the sphere at \((0.525, 0.464, 0.516)\).

Aulisa et al. [15] rely on the numerical quadrature approach to initialize the volume fraction
field for the LSF algorithm. The volume fraction is initialized by reformulating the sharp indicator
function \( \chi(x) \) in a cubic cell as a height function with respect to a face \( S_f \), that is then integrated
as

\[
\alpha_k = \frac{1}{|\Omega_k|} \int_{\Omega_k} \chi(x) \, dV = \frac{1}{|\Omega_k|} \int_{S_f} z^*(x, y) \, dS,
\]

(97)
such that
\[ z^*(x, y) = \min(h, \max(f(x, y) - (k - 1)h, 0)), \tag{98} \]
where \( f(x, y) - z = 0 \) is the surface equation that replaces the sharp phase indicator function \( \chi(x, 0) \), and \( h \) is the length of the cubic cell. Equation (97) is numerically integrated using the Simpson’s quadrature by dividing \( S_f \) into \( 30^2 \) square sub-intervals.

López et al. [37] use a mesh refinement technique for initializing the volume fraction field, originally proposed by Francois et al. [27] and Cummins et al. [58]. A cubic cell is subdivided into octants (quadrants in 2D) in a single refinement level. In total, four refinement levels are used per multi-material cell. In the lowest refinement levels, the interface is approximated linearly and the cell is intersected with the linear interface approximation to compute the volume fraction,
\[ \alpha_k = \frac{1}{|\Omega_k|} \int_{\Omega_k} \chi(x) \, dV = \frac{1}{|\Omega_k|} \sum_{k=1}^{N_s} \frac{|H_k \cap \Omega_k|}{|\Omega_k|}. \tag{99} \]
In eq. (99), \( N_s \) is the number of sub-cells resulting from cell sub-division, \( H_k \) is the halfspace that approximates the interface in the cell \( k \). Table 3 holds reconstruction error values computed as the volume of symmetric difference,
\[ E^1_r = \int_{\Omega_k} |\chi(x) - H_k| \, dV, \tag{100} \]
between the PLIC interface and the exact interface, where \( H_k(x) \) is the positive halfspace given by the PLIC plane (eq. (81)). Equation (100) can be integrated numerically using the exact indicator function as in eq. (97) for hexahedral cells with planar faces.

![Diagram](a) Initialization with mesh-mesh intersection. (b) Volume of symmetric difference.

Figure 11: Error calculation of the MoF method by Ahn and Shashkov [29].

For polyhedral cells, Ahn and Shashkov [36] distribute points uniformly in multi-material cells. The points are then categorized as inside or outside based on the provided geometrical model of the interface, or an explicit indicator function, e.g. a signed distance function. The volume fraction in the multi-material cell is then given as the ratio of the number of inside points and the total number of points in a cell. Later, Ahn and Shashkov [29] use an intersection between two meshes to geometrically calculate the initial centroids and volume fractions for the MoF method. The mesh of the solution domain \( \Omega := \cup_{k \in K} \Omega_k \) is intersected with an unstructured mesh that is used to approximate \( \Omega^+ \). The \( \Omega^+ \) phase is decomposed into disjoint sub-volumes, i.e.
\[ \tilde{\Omega}^+ = \cup_{l \in L} \tilde{\Omega}^+_l. \tag{101} \]
Table 2: Reconstruction error $E^2_r$ computed for a spherical interface by Ahn and Shashkov [36].

| N  | Value types | Youngs  | LVIRA  | MoF    |
|----|-------------|---------|--------|--------|
| 4  | $E^2_r$     | 6.19e-02| 1.53e-01 | 1.43e-02 |
| O  |             | -       | -      | -      |
| 8  | $E^2_r$     | 4.38e-03| 5.35e-03 | 3.64e-03 |
| O  |             | 3.82048 | 4.83813 | 1.97382 |
| 16 | $E^2_r$    | 2.25e-03| 1.34e-03 | 9.43e-04 |
| O  |             | 0.964419| 1.99247 | 1.94884 |
| 32 | $E^2_r$    | 1.11e-03| 3.12e-04 | 2.33e-04 |
| O  |             | 1.012   | 2.10852 | 2.01529 |

Here, $\tilde{\Omega}^+$ denotes an approximation of $\Omega^+$, because the fluid interface ($\Sigma := \partial\Omega^+$) is approximated in $\tilde{\Omega}^+$ as a set of mutually connected polygons. The volume fraction $\alpha_k$ is then calculated using

$$\alpha_k = \frac{|\tilde{\Omega}_k^+|}{|\Omega_k|} = \frac{1}{|\Omega_k|} \sum_{l \in C^+_k(\Omega_k)} |\Omega_k \cap \tilde{\Omega}_l^+|,$$

(102)

since $\tilde{\Omega}_k^+ = \bigcup_{l \in C^+_k(\Omega_k)} \Omega_k \cap \tilde{\Omega}_l^+$. Furthermore,

$$C^+_k(\Omega_k) = \{ l \in K : \Omega_k \cap \tilde{\Omega}_l^+ \neq \emptyset \}$$

(103)

is the intersection stencil of $\Omega_k$ in $\tilde{\Omega}^+$. Calculating $\tilde{\Omega}_l^+$ is therefore important for computing initial $\alpha_k$ by eq. (102), needed for the reconstruction, but also to express the resulting reconstruction error as the volume of symmetric difference

$$E^2_r = \sum_{k \in K} |\tilde{\Omega}_k^+ \cap -\mathcal{H}_k| + |\Omega_k \cap \mathcal{H}_k| - |\tilde{\Omega}_k^+ \cap \mathcal{H}_k|,$$

(104)

where the "−" sign changes the orientation of the halfspace $\mathcal{H}_k$. Contributions to the $E^2_r$ error are illustrated as shaded areas in fig. 11b.

$E^2_r$ errors for a sphere of radius $r = 0.5 - \frac{1}{11}$, positioned at $(0.5 + \frac{1}{11}, 0.5 + \frac{1}{11}, 0.5 + \frac{1}{11})$ are digitized in table 2 from the diagram reported by Ahn and Shashkov [36, fig. 12]. The radius and position of the sphere, as well as the number of mesh elements $N^3$ are different from those used by Aulisa et al. [11] and López et al. [37], so a direct comparison with LSF, CLCIR, CBIR is not possible, even though results in table 2 were generated on unstructured meshes with cubic cells. A comparison between the Youngs’, LSF, CLCIR and CBIR reconstruction algorithms performed by López et al. [37, table 1] is presented here in table 3.

Overall, MoF maintains the best absolute accuracy, with increasing costs, lower than, but comparable to LVIRA for a serial execution on unstructured hexahedral meshes when higher resolution is used [36, table 1]. The LVIRA algorithm, listed in table 1, was used on unstructured meshes by Jofre et al. [59], however the computational efficiency of LVIRA is not reported. To the best of the authors’ knowledge, Ahn and Shashkov [36, table 1] is the only report containing absolute CPU times of the reconstruction algorithm for 3D reconstruction on unstructured meshes. Relative
timings for 3D reconstruction can be found in López et al. [37, table III]. Overall, the (E)LVIRA algorithms require very long execution times. Even though Jofre et al. [59] rely on (E)LVIRA to ensure overall second-order convergence, their work on load balancing of the parallel execution [60] relies on the Youngs’ reconstruction algorithm.

The data summarized in this section is available at http://dx.doi.org/10.25534/tudatalib-162.

4. Volume fraction advection

4.1. Geometric Volume-of-Fluid methods

Early developments of volume fraction advection algorithms have reduced the complexity of geometric operations by adopting a dimensionally split approach. The split advection algorithm solves the volume fraction equation in $D$ steps, where $D$ is the spatial dimension. Volume fraction values are updated once per splitting step, requiring an additional interface approximation (reconstruction) in each of these steps. Computing $D$ interface reconstructions and advection steps per time step in $D$ dimensions increases the computational cost of the dimensionally split approach.

Splitting additionally requires alignment of normal area vectors with coordinate axes and is less volume conservative than the un-split approach. Unstructured meshes do not fulfill this requirement, because, in general, face-normal vectors in an unstructured mesh are not collinear with coordinate axes. A detailed review of dimensionally split algorithms on structured meshes is given by [61], and more details on dimensionally-split algorithms are available in [32, 3, 62, 14, 15]. In their comprehensive review of methods for Direct Numerical Simulations (DNS) of two-phase flows, Scardovelli and Zaleski [62] stated that the dimensionally un-split algorithm ensures better accuracy compared to split algorithm, especially regarding asymmetries in the shape of the advected interface. Here, un-split geometric Volume-of-Fluid advection algorithms are covered in historical order.

In addition to the PLIC interface reconstruction covered in section 3, all flux-based geometric Volume-of-Fluid methods share the same approach for approximatively solving eq. (34). As described in section 3, PLIC reconstruction approximates $\Sigma = \partial \Omega^+ (t^n)$ as a piecewise-planar surface,
i.e. a halfspace $H_k := (p_k(t^n), n_k(t^n))$ in each cell $\Omega_k$ (cf. fig. 12). The phase-specific volume $V_f^\alpha$, fluxed through the face $S_f$ of the cell $\Omega_k$, is approximated using eq. (37),

$$V_f^\alpha = V_f \cap \Omega^+(t^n) \approx \bigcup_{l \in C(S_f)} \tilde{\Omega}_l^+(t^n) \cap V_f.$$  \hspace{1cm} (105)

The volume $V_f$ is computed differently by each geometrical VOF method by approximating the r.h.s. of eq. (36) and

$$C(S_f) = \{ l \in L : S_f \cap \Omega_l \neq \emptyset \},$$  \hspace{1cm} (106)

is the face-cell stencil of the face $S_f$ in $\{ \Omega_k \}_{k \in K}$. Furthermore, the volume $\tilde{\Omega}_l^+(t^n)$ in eq. (105) is approximated using the PLIC halfspace in each cell $\Omega_l$ from $C(S_f)$ as

$$\tilde{\Omega}_l^+(t^n) = \begin{cases} H_l(t^n) \cap \Omega_l & \text{if } 0 < \alpha_l(t^n) < 1, \\ \Omega_l & \text{if } \alpha_l(t^n) = 1, \\ \emptyset & \text{if } \alpha_l(t^n) = 0. \end{cases}$$  \hspace{1cm} (107)

Inserting 107 in 105 and the result into eq. (34), approximatively solves eq. (30) for $\{ \alpha_k(t^{n+1}) \}_{k \in K}$. Available un-split VOF advection algorithms differ in the way they approach the geometrical approximations of $V_f$ and $V_f^\alpha$.

Kothe et al. [32] and later Rider and Kothe [3] proposed a two-dimensional Eulerian flux-based un-split algorithm that uses a constant velocity distribution across an edge (face in 3D) $v_f$ to construct the flux volume $V_f$ and consequently the fluxed phase-specific volume $V_f^\alpha$.

However, they noted that Pilliod and Puckett [26] were the first to develop a directionally un-split multidimensional algorithm ([32, page 3, table 1],[3, page 6, table 1]). The computation of the fluxed phase-specific volumes by the Rider-Kothe Algorithm (RKA) is shown schematically in fig. 12. Compared to using point velocities, the use of constant velocities by the RKA causes an overlap between the flux volumes and subsequently the fluxed phase-specific volumes for two point-adjacent edges, i.e. faces. The overlap is fluxed twice and shown schematically as the shaded triangle in fig. 12. Fluxing the same volume multiple times this way causes overshoots and undershoots. An overshoot is defined for each cell $c$ as

$$\alpha_k^\circ = \max(\alpha_k - 1, 0)$$  \hspace{1cm} (108)

and an undershoot is defined as

$$\alpha_k^\# = \max(-\alpha_k, 0).$$  \hspace{1cm} (109)
If \( \alpha_k^0 = \alpha_k^u = 0, \forall k \in K \), volume fractions \( \{\alpha_k\}_{k \in K} \) are said to be "numerically bounded" and the method is stable. Undershoots and overshoots have been handled in the RKA using explicit conservative redistribution of the volume fraction \( \alpha \). The second-order convergent reconstruction algorithm ELVIRA \[26\] has been used to reconstruct the PLIC interface. Since Rider and Kothe \[3\] have used edge (face) centered velocities to construct the flux volumes, there is no need to correct the geometrical flux volumes for volume conservation. However, this is only true if the edge-centered velocity field upholds the discrete divergence-free condition \( \sum_f F_f = 0 \). Rider and Kothe \[3\] do propose a correction for volume conservation, but for different reasons: they expect the face-centered velocity field to uphold the discrete divergence-free condition only \textit{up to a specified tolerance of a linear solver used to obtain it}. They were aiming at applying their algorithm with velocity fields that result from an approximated solution of the incompressible single-field Navier-Stokes (NS) equation system. In that case, the following correction is necessary:

\[
\partial_t \alpha + \nabla \cdot (\mathbf{v} \alpha) = \alpha \nabla \cdot \mathbf{v}. \tag{110}
\]

However, if \( \mathbf{v}_f \) is exactly divergence-free, no correction for volume conservation is required for the geometrical flux volumes used by the RKA. Using an edge (face) centered velocity simplifies the geometrical form of the geometrical flux volume because it remains convex. Still, the velocity field varies over the edge (face), and the RKA assumes a constant flux velocity over the edge (face). With this assumption, the flux polyhedron can only be non-convex if the face of the control volume is non-convex. The assumption of the constant edge velocity simplifies geometric operations for computing phase volume contributions, especially in three dimensions. The authors proposed two variants of their algorithm: a fully dimensionally un-split algorithm, and the un-split variant constructed from the dimensionally split algorithm. In the latter algorithm, overlaps of phase-specific volumes that appear at cell corners are corrected by additional intersections. In both cases the cell corner velocities are determined from the edge center velocities based on their signs. Rider and Kothe \[3\] have shown that their un-split algorithm is more accurate than the operator split variant.

Mosso et al. \[22\] were the first to propose a cell-based (re-mapping) Lagrangian tracking / Eulerian remapping (LE) method for the dimensionally un-split volume fraction advection that uses a forward projection. They reported a test case involving a translation of a circle on an unstructured irregular hexahedral mesh using a time-periodic and spatially constant velocity field that moves the circle back to the original position. The algorithm shows promising results \[22, figure 5\] in the fact that the shape and the area of the circle are maintained, even on a non-orthogonal unstructured hexahedral mesh.

Mosso et al. \[33\] described the application of their LE method to the problem of a rotating planar and circular interface and the numerical errors that are related to exact, forward Euler, backward Euler and trapezoidal integration of mesh point displacements. They concluded that the use of the trapezoidal integration for the forward projection step of the LE method removes artificial expansion and contraction of the interface. In other words, the trapezoidal integration of point displacements conserves volume - a conclusion that is also drawn later by Chenadec and Pitsch \[25\]. This conclusion is a direct consequence of the fact that the first-order accurate Euler quadrature exhibits artificial error canceling when applied to harmonic functions \[63\].

Harvie and Fletcher \[64\] have proposed the \textit{stream scheme}: a two-dimensional Eulerian flux-based geometrical VOF method that uses a continuous velocity field approximation \textit{within a cell}, and a geometrically reconstructed interface to compute the fluxed phase-specific volumes by approximating the flux volume \( V_f \) as a set of \textit{stream tubes}. The velocity field is given by a streamline...
function formulated as
\[ \Psi(x, y) = \chi_b y x + \chi_x x + \chi_y y, \]  
leading to
\[ \mathbf{v} = \left( \begin{array}{c} \partial_y \Psi \\ -\partial_x \Psi \end{array} \right) = \left( \begin{array}{c} \chi_b x + \chi_y \\ -\chi_b y - \chi_x \end{array} \right). \]  

Given by a stream function, this velocity field is automatically divergence-free. This velocity field is continuous in the face-normal direction, while it is discontinuous in the tangential direction and at cell corner points. Fluxed phase-specific volumes are calculated based on stream tubes given by the velocity field and a discretization of the face in \( N_s \) segments, as shown in fig. [13]. Streamlines define the stream tube of the fluid particle that crosses a face with coordinate \( l \) and width \( w \). The stream tube width is determined by \( N_s \) and the velocity field \( \mathbf{v} \) from the volume conservation law \[64\]. Stream tube geometry is not explicitly approximated. Instead, fluxed phase-specific volumes are integrals of the phase indicator function along the streamline. The PLIC interface approximates the phase indicator function by approximating \( \Omega^+_{k} (t^n) \) from eq. \[7\].

![Figure 13: A schematic representation of the 2D stream scheme \[64\].](image)

The magnitude of the fluxed phase-specific volume is approximated by the stream scheme as
\[ |V^p_f| = \sum_{i=1}^{N_s} |V^p_f(i)| = \sum_{i=1}^{N_s} \int_{L_i} w_i(l) \chi(l) dl, \]  
where \( \chi \) is the parameterized phase indicator function. The accuracy of the stream scheme is comparable to RKA \[3\] for the reversed single vortex test case. A second-order reconstruction algorithm ELVIRA increases the accuracy of the advection. First-order convergent Youngs’ reconstruction algorithm causes errors in handling thin filaments, due to the instabilities in the interface orientation. These instabilities are amplified and cause the interface to break up artificially. The accuracy and computational cost of the stream scheme is highly dependent on \( N_s \). Using \( N_s = 10 \) makes the computational efforts comparable to other dimensionally un-split algorithms. Results also show that the scheme suffers from wisps. Wisps are very small errors in \( \alpha_k \) in cells that should be either completely empty or completely full. Wisps have orders of magnitude lower values than jetsam and flotsam first described by Noh and Woodward \[31\] and later by Rider and Kothe \[3\]. Harvie and Fletcher \[64\] handle wisps by applying a conservative wisp redistribution algorithm that takes into
account the direction of the interface-normal vector. The conservative wisp redistribution algorithm redistributes wisps within the structured 27 cell stencil of a multi-material cell, making it the only point in the stream scheme dependent on the Courant-Friedrichs-Lewy (CFL) condition.

Harvie and Fletcher [65] have proposed the two-dimensional Defined Donating Region (DDR) scheme on Cartesian meshes, that improves volume conservation compared to [3, 64] using unique slopes for the donating regions at cell corners. The DDR scheme constructs defined donating regions shown schematically in fig. 14 for all faces of a cell $c$ whose velocities are directed outward from the cell. The donating regions are intersected with the PLIC interface to compute the fluxed phase-specific volume for each face. Faces $f$, $g$ and $h$ are labeled in fig. 14 to distinguish their respective velocities. The volume of the donating region is a result of the total volume conservation for the cell $c$. The conservation of the total volume for the cell $c$ indirectly introduces the CFL criterion into the scheme. Preventing the characteristic overlap of the flux volumes in the RKA (fig. 12) improves the volume conservation of the DDR scheme together with the correction of the donating region for volume conservation. However, limiting the donating regions to a cell prevents the scheme from fluxing around the corner.

Cerne et al. [39] have analyzed the numerical errors of the geometrical VOF method. They have quantified the reconstruction errors for two-dimensional simulations on structured meshes in the form of reconstruction correctness. They have also described the artificial distortion of the circular interface during translation on coarse meshes. Strongly under-resolved interfaces exhibit artificially high advection velocities. Cerne et al. [39] propose the local dynamic AMR for increasing overall accuracy based on a reconstruction-correctness criterion.

Scardovelli and Zaleski [14] have formalized their 2D Eulerian Implicit - Lagrangian Explicit (EI-LE) method, proposed originally by Aulisa, Manservisi, Scardovelli and Zaleski [66]. The formalization models the steps of the EI-LE scheme using linear maps. Scardovelli and Zaleski [14] extend the original EI-LE scheme as a dimensionally un-split scheme that relies on a single advection and reconstruction step per time step. The scheme still requires the face-normal vectors to be aligned with the coordinate axes, because the method is structured. The EI-LE is the first scheme that reports the absence of wisps and conserves the total area exactly. A result that deserves special attention is the reversed vortex test case [66, figure 10] with no visible wisps in the solution and a reduced geometrical advection error compared to previous methods, including the DDR scheme. The extension of the EI-LE method to unstructured meshes has been suggested by Aulisa, Manservisi, Scardovelli and Zaleski [66], which requires a triangulation of the domain and
a continuous area-preserving linear mapping.

![Schematic representation of the EMFPA scheme](image)

López et al. [67] have combined the volume conservation and numerical boundedness of the DDR method by Harvie and Fletcher [64] and the around-the-corner flux calculation of the RKA method by Rider and Kothe [3] into a new Edge-Matched Flux Polygon Advection (EMFPA) scheme. Shown schematically in fig. 15, the flux volume $V_f$ is defined by the positions of the swept face points $p'_i$ computed as

$$p'_i = p_i + \lambda f s_i,$$

where $\lambda f$ is a face-constant scalar coefficient and $s_i$ is the displacement along the discrete Lagrange trajectory, computed using the Inversed Distance Weighted (IDW) interpolation

$$s_i = \frac{1}{\sum_{f \in C_f(p_i)} w_f} \sum_{f \in C_f(p_i)} w_f v_f^{n+\frac{1}{2}},$$

where

$$C_f(p_i) = \{ f \in F : p_i \in S_f \}$$

is the point-face stencil, the set of indices of those faces $S_f$ of cells $\Omega_k$, which contain $p_i$. The weight $w_f$ in eq. (115) is then defined as

$$w_f = \frac{1}{\|p_i - x_f\|},$$

where $x_f$ is the centroid of the face $S_f$. The face velocity $v_f$ that contributes to the slope is evaluated in an intermediate time step $n + \frac{1}{2} = t + 0.5\delta t$: the velocity field at this time is obtained from a linear interpolation between the current and the next time step, $n$ and $n + 1$, respectively. Using the IDW interpolation to compute the slope $s_i$ of the discrete Lagrange trajectories introduces an interpolation error. On Cartesian equidistant meshes used by López et al. [67], eq. (115) represents an arithmetic average, since all the distances from corner points to face centers are the same. The slope of the discrete Lagrange trajectory influences the overall accuracy of the scheme. The slope $s_i$ and the face-constant parameter $\lambda f$ determine the magnitude of the geometrical flux volume $V_f$ shown as a lightly shaded polygon in fig. 15. Temporal second-order accuracy of $V_f$ is achieved by integrating eq. (38) with a trapezoidal quadrature, namely

$$V_f = \int_t^{t+\delta t} \int_{S_f} v(t) \cdot n \, dS \, dt \approx 0.5\delta t \left( v^n_f + v^{n+1}_f \right) \cdot S_f.$$
Equation (38) must also be exactly satisfied in the discrete sense to ensure volume conservation. This is achieved by introducing a face-constant parameter $\lambda_f$ that scales the flux volume. Calculation of the fluxed phase-specific volumes $V_f^\alpha$ is done geometrically by approximating the solution of eq. (37).

Volume conservation is improved by the EMFPA algorithm proposed by López et al. [67], compared to the original RKA algorithm proposed by Rider and Kothe [3], because of the reduction of the overlap between neighboring flux volumes. However, the face-constant volume conservation adjustment coefficient $\lambda_f$ may cause overshoots and undershoots. López et al. [67] show that their EMFPA algorithm coupled with the Spline Interface Reconstruction (SIR) algorithm results in an overall second-order convergence. They also emphasize the need for a second-order convergent reconstruction algorithm, because of its strong influence on the overall error. They do not quantify errors in volume conservation and numerical stability. The authors mention that some overshoots appear, but only in cells where the slopes $s_i$ are almost orthogonal to $S_f$, in which case a local conservative redistribution algorithm is applied. Additionally, they state that wisps appear, but they do not have an effect on the computational efficiency of the algorithm. The effect of wisps on numerical stability is not addressed.

A dimensionally un-split algorithm proposed by Pilliod and Puckett [26] is based on the work of Bell, Dawson and Shubin [68] and relies on the method of characteristics to integrate the flux volumes in time with either first or second-order accuracy. The scheme is two-dimensional and uses a face-constant velocity for the calculation of the characteristic lines. Unlike the DDR scheme, and similar to the RKA method, this method allows the calculation of the around-the-corner fluxes. Pilliod and Puckett [26] reported volume conservation errors near machine epsilon for a translation of a circle and the rotation slotted disc by Zalesak [4]. Pilliod and Puckett [26] emphasized the importance of using a second-order accurate reconstruction algorithm. Verification cases involving both spatially and temporally varying velocity fields are not presented, as well as the extension to three dimensions.

Dyadechko and Shashkov [23, section 4.1] have relied on the Lagrangian tracking / Eulerian remapping (LE) geometrical VOF method for advecting the volume fraction field in their Moment of Fluid (MoF) method. Cell corner points are traced backward in time to compute ${\{\alpha_k(t^{n+1})\}}_{k\in K}$ using a 4th-order Runge-Kutta (RK) scheme. The method is two-dimensional, and the authors propose the use of bins (Axis-Aligned Bounding Box (AABB)) that simplify the geometry of polygonal cells to increase efficiency when computing phase-specific volumes that contribute to ${\{\alpha_k(t^{n+1})\}}_{k\in K}$. Because the Lagrangian backward tracing does not conserve the volume of the traced cell, Dyadechko and Shashkov [23] rely on a local conservative redistribution for correcting overshoots, undershoots and wisps.

Piecewise Constant Flux Surface Calculation (PCFSC), a three-dimensional extension of the RKA of Rider and Kothe [3] has been proposed by Liovic et al. [34]. The PCFSC algorithm has been developed on structured meshes, but it directly generalizes to unstructured meshes with convex cells. Figure 16 illustrates the PCFSC algorithm. The dimensionally un-split advection is achieved by the flux-based un-split approach, with an important simplification of the flux volume: a single face-centered velocity vector $v_f$ is used to construct the flux volume. A direct consequence of this is a flux volume bounded by planar polygons. Consequentially, triangulation of the flux volume is not necessary, and, if $v_f$ is divergence-free in the discrete sense, the flux volume does not have to be corrected to ensure volume conservation. Flux volumes bounded by planar polygons are additionally more easily intersected. However, as shown in fig. 16, using face-centered velocities $v_f$ and $v_g$ to sweep points of two edge-adjacent faces $f$ and $g$ results in non-unique Lagrange trajectories at
cell-corner points $p_i$, which cause either overlaps or holes between flux volumes along the whole length of an edge, shaded gray in fig. 16. Overlaps and holes between flux volumes cause overshoots, undershoots and wisps in $\{\alpha_k(t^{n+1})\}_{k \in K}$. To suppress these errors, Liovic et al. [34] scale the fluxed phase volume with a scalar coefficient.

Aulisa et al. [15] have extended their EI-LE scheme [66, 14] to support three-dimensional computations on Cartesian meshes. The dimensionally split Eulerian Implicit - Lagrangian Explicit 3D (EILE-3D) and Eulerian Implicit - Lagrangian Explicit 3D Decomposition Simplified (EILE-3DS) schemes conserve mass exactly for sphere translation and rotation test cases. EILE-3DS delivers second-order convergence of the advection errors for the single vortex test case with a decreasing CFL number. Aulisa et al. [15] quantified volume conservation errors for spatially and temporally varying velocity fields. They show that the volume conservation errors of the EILE-3DS method are converging from approximately $1e^{-03}$ to $1e^{-06}$ for their single vortex test case with increased mesh resolution and from $1e^{-04}$ to $1e^{-09}$ for the same test case with $32^3$ volumes and a decreasing CFL number.

Figure 17 illustrates the flux volume calculation of the Face-Matched Flux Polyhedron Advection (FMFPA-3D) advection scheme. The FMFPA-3D scheme constructs a flux volume bounded by planar polygons, like the PCFSC scheme. However, the FMFPA-3D scheme goes one step further than the PCFSC scheme, using a unique velocity at each edge center. Each edge-centered velocity is interpolated from face-centered velocities using faces that share the edge. The faces of the flux volume created by sweeping the edges are planar, because the edge-centered velocity is constant for an edge. However, this does not solve the problem of overlaps or holes between flux volumes, because velocities are not unique at cell corner-points. For example, the edge $e$ with the edge-centered velocity $v_e$ in fig. 17 illustrates this issue: the end-points of this edge are shared with other edges, that have different velocities, so the velocities at cell corners are non-unique. The non-unique velocities cause overlaps or holes for flux volumes at cell corner points, shaded gray in fig. 17 for the edge $e$. Compared to PCFSC (fig. 16), overlaps of the FMFPA-3D are much smaller. The flux volume shown in fig. 17 still needs to be closed by connecting the swept edges of each swept face. The FMFPA-3D scheme closes the flux volume with a plane in order to simplify its geometry by keeping
Hernández et al. have show improved results compared to their 3D implementation of the RKA.

Zhang and Liu have proposed the 2D Polygonal Area Mapping Method (PAM), a 2D LE geometrical VOF method based on Lagrangian tracking and Eulerian remapping, similar to the MoF method. The PAM scheme traces phase-specific volumes forward in time using the flow map and intersects the traced phase-specific volumes with the mesh to compute phase-specific volumes. Tracing points using an RK scheme leads to errors in mass conservation, as velocities evaluated at the material polygon points are not divergence-free. Zhang and Liu do not mention interpolation, so the points seem to be traced using the exact velocity, in which case the errors resulting from velocity interpolation are avoided. After the tracing the material polygons are required to correct material polygons to ensure volume conservation, because the La- range advection is not inherently conserving volume. Topological changes are handled using merging algorithms for polygons. Verification using temporally and spatially varying velocity fields shows that the PAM method is more accurate than EMFPA on structured equidistant meshes. The volume conservation within depends on the mesh resolution. The authors state that the method is overall approximately 20% slower than EMFPA.

Ahn and Shashkov have extended the MoF method proposed by Dyadechko and Shashkov with local dynamic Adaptive Mesh Refinement (AMR) and show an overall second-order convergent solution for a set of standard verification cases, with different levels of local dynamic AMR. Adaptive MoF is implemented in 2D and the same problems in overshoots, undershoots and wisps are dealt with both local and global conservative error redistribution. Ahn et al. have coupled the MoF method with the single-field two-phase NS equation system.

Zhang proposes the Donating Region Approximated by Cubic Splines (DRACS) scheme: a fourth-order accurate representation of the Donating Region (DR). The increase in accuracy is due to flux-volumes having non-linear boundaries approximated with cubic splines. The DRACS scheme uses (E)LVIRA for piecewise linear interface reconstruction, so the fourth-order convergence is only shown for cases where no significant interface deformation occurs (solid body rotation, 2D...
shear with $T = 0.5\,s$). In order to obtain an overall fourth-order accuracy for larger deformations, a higher-order volume conservative interface reconstruction should be used. Zhang [70] motivates the development of the higher-order DRACS method by the need for an accurate curvature calculation required for two-phase flows. Only small interface deformation is presented, so it is not clear if topological changes and strongly deforming interfaces are handled robustly and accurately.

Chenadec and Pitsch [25] have proposed an alternative LE geometrical VOF method that is directly applicable to unstructured meshes with general polyhedral cells. Chenadec and Pitsch [25] name their method Hybrid Lagrangian–Eulerian Method for Multiphase flow (HyLEM) and rely on eq. (26): $\Omega_k$ is considered as a material volume. This idea is interesting because it relies on mesh motion and PLIC reconstruction in order to compute $\{\alpha_k(t^n+1)\}_{k \in K}$, which simplifies somewhat the required intersection in 3D. However, there are at least three difficulties in maintaining volume conservation. First, the condition given by eq. (45) is not upheld without correcting $\Phi_{t^n+1}^t(\Omega_k)$ for volume conservation, because discrete interpolated velocities are used to trace the cell $\Omega_k$ forward in time. Second, the one-to-many relationship required by eq. (41), together with the discontinuities of the PLIC interface at cell faces, may cause volume conservation errors when computing necessary intersections in eq. (41). Third, a 3D calculation will create $\Phi_{t^n+1}^t(\Omega_k)$ as polyhedrons with non-planar faces, so the reconstruction algorithm needs to accommodate this. Chenadec and Pitsch [25] have left the generalization to 3D as future work and have shown for 2D Cartesian meshes that a second-order mass conservation error is achieved using higher-order RK schemes. From numerical experiments, the authors have come to the conclusion that volume conservation errors systematically cancel out when the solutions of forward and backward Lagrangian backtracing are averaged, resulting in a combined forward/backward integration scheme for $\{\alpha_k(t^n+1)\}_{k \in K}$. The effect of systematic cancellation is not surprising because harmonic velocity components are integrated [63]. Chenadec and Pitsch [25] reported third-order accurate volume conservation errors within $[1e-14, 1e-05]$ for the trapezoidal rule for cases with strong interface deformation.

Zhang and Fogelson [71] develop the improved Polygonal Area Mapping Method (iPAM), a fourth-order accurate 2D method that replaces the cubic spline approximation for the nonlinear donating region boundary in the DRACS scheme with multiple piecewise-linear segments. The iPAM has the highest absolute accuracy and convergence-order among all other 2D geometrical VOF methods. However, already the 2D iPAM method is significantly more complex than other geometrical VOF methods. The 2D interface approximation is extended with additional marker points, while coalescence and breakup are handled by directly changing the geometry of the interface, which makes it very similar to the Front Tracking method [72]. Nef polyhedrons are proposed for the extension of iPAM to 3D, for intersections of general polyhedrons [73]. However, the very large number of necessary polyhedron intersections prohibit the use of Nef polyhedrons because of the prohibitive computational costs. iPAM ensures mass conservation by adjusting material polygons using edge manipulation and adding/removing points. The authors state that local volume conservation cannot be fulfilled for some cells (Zhang and Fogelson [71, footnote, page 2370]), however they disregard this issue in favor of the fourth-order convergence of the volume fraction in the $L_1$ norm. The volume (mass) conservation error is not reported for the verification tests. Zhang and Fogelson [71] assume a Lipschitz continuous velocity field in space in their derivation and do not mention interpolation of the velocity field at cell-corner points, a source of an additional error. Still, iPAM delivers a stable higher-order convergence, which makes it an attractive candidate for a possible extension to 3D, especially if the statements regarding its efficiency are confirmed by High Performance Computing (HPC) measurements, and a higher-order numerical method is used for the two-phase Navier-Stokes system.
Marić et al. [4] have used unique velocities at cell-corner points on unstructured meshes using IDW interpolation, together with a Youngs' reconstruction algorithm and an iterative correction of the volumetric flux for volume conservation, similar to EMFPA method [45]. Harvie-Fletcher error redistribution algorithm is used to conservatively correct for overshoots, undershoots, and wisps. Local dynamic Adaptive Mesh Refinement (AMR) increases the accuracy of the advection significantly. Despite the first-order accuracy, the dynamic AMR reduces the error substantially at a small fraction of the overall computational cost, compared to uniform mesh resolution.

Owkes and Desjardins [74] and Jofre et al. [59] have proposed Eulerian flux-based geometrical VOF methods that also rely on unique discrete Lagrange trajectories at cell corner-points. The method proposed by Jofre et al. [59] is directly applicable to unstructured meshes, whereas Owkes and Desjardins [75] state that the extension for unstructured meshes is straightforward. Those two methods share the same correction of the flux volume $V_f$ for volume conservation and the methods of Owkes and Desjardins [75] and Jofre et al. [59] rely on the LVIRA algorithm for the second-order accurate P LIC interface reconstruction. They both show second-order convergent geometrical advection errors, are numerically bounded and volume conservative.

Comminal et al. [76] propose a 2D Cell-wise Conservative Unsplit (CCU) LE scheme. Contrary to [24, 70, 71], where an exact velocity is used at cell corner points, Comminal et al. [76] address the problem of interpolation errors. The CCU method builds upon the ideas proposed in the Geometrical Predictor-Corrector Advection (GPCA) method by Cervone et al. [77]. Higher-order accuracy is used for the vertex displacement integration, and vertex interpolation is second-order accurate (bilinear in GPCA). Comminal et al. [76] show that the overall advection accuracy is influenced mostly by velocity interpolation at cell-corner points and temporal integration of the respective displacements. Compared to PAM and iPAM schemes, CCU is much simpler because it replaces complex explicit manipulation of material polygons with a simple correction of the control volume pre-image for volume conservation similar to the one applied by Owkes and Desjardins [75] and Jofre et al. [59] in 3D. The topological changes of the interface are handled automatically by the interface reconstruction. Of course, the absolute accuracy and convergence of the iPAM and PAM is much higher compared with CCU. However, extending the CCU scheme to 3D on unstructured meshes would involve significantly simpler geometrical operations.

Owkes and Desjardins [78] propose an extension of their earlier method [75], using a staggered solution approach and sub-grid mesh resolution for enhancing mass and momentum conservation. The sub-grid resolution increases the effective resolution of the volume fraction transport of their original scheme in the same way as the dynamic AMR does it in [29] and [74].

Ivey and Moin [79] propose an un-split geometrical VOF method that constructs the flux volume iteratively. The iterative flux volume calculation removes self-intersections, as well as intersections with the neighboring flux volumes. The calculation of the flux volumes can be applied to non-convex star-shaped polyhedral cells. Their Non-Intersecting Flux Polyhedron Advection (NIFPA)-1 scheme has results comparable to those of the Owkes-Desjardins scheme (OD) method [75]. Average CPU times are reported for the construction of the fluxed phase-specific volumes.

Marić et al. [10] propose a flux-aware triangulationable flux volume with non-planar faces (fig. 15). Either an oriented triangulation (fig. 18a), or a centroid triangulation (fig. 18b), are usually used to approximate flux volumes in the un-split geometrical VOF method. The centroid triangulation uses centroids of (generally) non-planar ruled surfaces that bound the flux volume, to decompose the flux volume into tetrahedrons. On the other hand, the oriented triangulation decomposes the ruled surfaces of the flux volume into triangles, either clockwise or counter-clockwise with respect to the normal vector of each ruled surface. Both triangulations generate self-intersections of
(a) Oriented triangulation of a non-convex flux volume $V_f$.

(b) Barycentric triangulation of a non-convex flux volume $V_f$.

(c) Flux-aware triangulation of a non-convex flux volume $V_f$.

(d) A tetrahedron given by the star-point $x'_f$ of $V_f$.

Figure 18: Different triangulations of a non-convex flux volume.

tetrahedrons, even for relatively simple star-shaped non-convex flux volumes, as shown for example in figs. 18a and 18b. The flux-aware triangulation (fig. 18c) correctly decomposes the flux volume $V_f$ into tetrahedrons by calculating a so-called star-point of $V_f$. A star-point of a set is a point with the property that the linear segment between this point and any other point of the set lies inside the set. A star-point of a triangulated $V_f$ is a point that constructs a positive-valued mixed product of the vectors of a tetrahedron constructed from the star-point and any triangle in the triangulation of $\partial V_f$. An example of such a tetrahedron is emphasized in fig. 18d. This tetrahedron is constructed from the star-point that lies on the face $S_f$ ($x'_f$ in fig. 18d), and the triangle given by the edge $(x'_{f,i}, x'_{f,i+1})$ and the centroid $x'_f$ of the mapped face $\Phi^t_n \setminus S_f$. If the mixed product $(x'_f - x'_f) \cdot ((x'_{f,i} - x'_f) \times (x'_{f,i} - x'_f))$ is positive for each triangle in the triangulation of $\partial V_f$, a correct decomposition of the flux volume into tetrahedrons is constructed by the star-point $x'_f$. The tetrahedral decomposition of $V_f$ is then intersected to compute the fluxed phase-specific volume $V^\alpha_f$ in eq. (34). The possibility of both negative and positive contributions to $V^\alpha_f$ caused by $V_f$ having a non-empty intersection with halfspaces $(x_f, S_f), (x_f, -S_f)$ is addressed using local adaptive mesh refinement. Note that the separation of positive and negative contributions substantially decreases computational efficiency. In addition to the flux-aware triangulation, a modification of the Swartz reconstruction algorithm is developed. An extrapolation based on Taylor series from cell centers to cell-corner points with second-order accuracy is proposed for velocities at cell-corner points. A global error redistribution algorithm stabilizes the solution. Compared to contemporary methods, the overall accuracy of the solution is increased by the flux-aware triangulation for verification cases on unstructured hexahedral meshes. Average computational time per time step of the UFVFC-Swartz scheme is similar to the OD method [75].
4.2. Geometric/algebraic Volume-of-Fluid methods

Recently, Volume-of-Fluid methods that reduce the dimensionality in the computation of \( V_f^\alpha \) from three to two dimensions have been introduced. We categorize these methods here as geometric/algebraic methods, to distinguish them from the fully three-dimensional geometric VOF methods. Geometric/algebraic VOF methods approximate the interface either geometrically or implicitly, using an approximation of the phase-indicator function. The reconstructed interface is then used for an algebraic calculation of the fluxed phase-specific volume \( V_f^\alpha \) for solving the reformulated volume fraction equation

\[
\int_{t^n}^{t^{n+1}} \int_{\Omega_h} \partial_t \alpha \, dV \, dt + \sum_f \int_{t^n}^{t^{n+1}} \int_{S_f} \chi(x, t) \mathbf{v} \cdot \mathbf{n} \, dS \, dt = \int_{t^n}^{t^{n+1}} \int_{\Omega_h} \chi(x, t) \nabla \cdot \mathbf{v} \, dV \, dt. \tag{119}
\]

The term on the r.h.s. is a numerical correction given by eq. (110), proposed originally by Rider and Kothe \cite{3}, that can be omitted when the velocity field \( \mathbf{v} \) satisfies the discrete divergence-free condition.

Roenby et al. \cite{80} have proposed the isoAdvector method that calculates \( V_f^\alpha \) as

\[
V_f^\alpha = \int_{t^n}^{t^{n+1}} \int_{S_f} \chi(x, t)(\mathbf{v} \cdot \mathbf{n}) \, dS \, dt = \mathbf{v}_f(t^n) \cdot \mathbf{n}_f \int_{t^n}^{t^{n+1}} \int_{S_f} \chi(x, t) \, dS \, dt + O(\delta t) + O(h^2). \tag{120}
\]

In eq. (120), the velocity \( \mathbf{v}_f(t) \) with which the interface moves across the face \( f \) is formally first-order accurate in time. Velocity \( \mathbf{v}_f \) is the second-order accurate average associated with the centroid of the face \( S_f \) and the final order of accuracy in space depends on the choice of interpolation used for \( \mathbf{v}_f(t) \). Alternatively, Roenby et al. \cite{80} use the approximation \( \mathbf{v}_f \approx \mathbf{n}_f F_f / \| S_f \| \), where \( F_f \) is the volumetric flux over \( S_f \). For polyhedral cells, the unit normal vector of \( S_f \), \( \mathbf{n}_f \), is constant over \( S_f \) and it is computed from a centroid triangulation of the face \( S_f \). Complex three-dimensional calculations are reduced by isoAdvector to two-dimensional calculations, which significantly simplifies geometrical calculations and increases computational efficiency. The core of the isoAdvector scheme is the evaluation of the integral

\[
\int_{t^n}^{t^{n+1}} \int_{S_f} \chi(x, t) \, dS \, dt = \int_{t^n}^{t^{n+1}} A_f(t) \, dt, \tag{121}
\]

where \( A_f(t) \) is the area of the face \( S_f \) that is inside the phase 1 ("wetted" by phase 1) at time \( t \). The isoAdvector schemes relies on a geometric approximation of the interface and polynomial algebraic extrapolation to express \( A_f(t) \). The interface that intersects the face \( S_f \) is approximated with a line, and it defines \( A_f \) at some point in time \( t \). The evolution of \( A_f(t) \) is approximated by computing multiple positions of the interface line by evolving the interface from the downwind cell in space using the cell-centered velocity \( \mathbf{v}_k \), over sub-intervals in the time step \([t^n, t^{n+1}]\) associated with partition points \( t_s \). Using \( A_f(t_s) \), \( A_f(t) \) is extrapolated as a quadratic polynomial, whose exact integral over \( t \) is then used in eq. (120). The reduction of dimensionality and the algebraic extrapolation of \( A_f(t) \) result in a simplification of the scheme, compared to the fully geometrical LE schemes. The correction on the r.h.s. in eq. (120) is not used by the isoAdvector scheme. Recently, Schefuller and Roenby \cite{63} have improved the isoAdvector scheme by introducing a classical PLIC interface whose normal is improved using the Reconstructed Distance Function (RDF) from Cummins et al. \cite{63}: a signed distance is computed at cell centers from the PLIC interface, and the gradient of
the distance field is then used to improve the PLIC normal, iteratively. Results shown by Scheufler and Roenby \[81\] are comparable to contemporary un-split geometrical VOF method at significantly reduced computational costs.

Xie and Xiao \[82\] propose the Tangent of Hyperbola Interface Capturing with Quadratic surface representation and Gaussian Quadrature (THINC/QQ) method. It is based on a multidimensional quadratic polynomial approximation of a diffuse interface, modeled as a hyperbolic tangent function with a user-defined steepness parameter. The THINC/QQ method also approximates the solution of eq. (119) with the r.h.s. term included. The THINC/QQ method relies on a piecewise-quadratic approximation of the interface, while the geometrical LE methods and the isoAdvector scheme rely on a piecewise-linear interface approximation. Like the isoAdvector scheme, the flux across the face $S_f$ is computed in $2D$, relying on the Gauss quadrature of the reconstructed quadratic approximation of the tangent hyperbolic function. THINC/QQ uses a third-order accurate explicit Runge-Kutta scheme for the temporal integration.

The reduction of computational complexity provided by geometric/algebraic methods does come at the cost of a lower overall accuracy and stronger restrictions regarding numerical stability, compared to the fully $3D$ geometric methods, as discussed in the next section. The question remaining for future research is, whether the stability restrictions of the geometric/algebraic schemes can be made less strict and their accuracy increased further in comparison to fully geometrical methods, or if the three-dimensional calculations used by the geometric methods can be made more efficient.

4.3. Advection comparison

Because of the number of reviewed methods, two verification cases are chosen for method comparison: $2D$ shear (single vortex) and $3D$ deformation case. Results available in the literature are mostly directly comparable with each other. The verification of the advection is based on a set of commonly used error measures:

- the volume conservation error
  \[
  E_v = \frac{|\sum_k V_k \alpha_k(t) - \sum_k V_k \alpha_k(t_0)|}{\sum_k V_k \alpha_k(t_0)}, \quad (122)
  \]

- the geometrical (shape) error
  \[
  E_g = \sum_k V_k |\alpha_k(t) - \alpha^e_k|, \quad (123)
  \]

- the normalized variant of the shape error
  \[
  E_n = \frac{\sum_k V_k |\alpha_k(t) - \alpha^e_k|}{\sum_k V_k \alpha^e_k}, \quad (124)
  \]

- and the numerical boundedness (stability) error
  \[
  E_b = \max_k \max((\alpha_k - 1), 0), \max_k ((0 - \alpha_k), 0)). \quad (125)
  \]

For those publications that have defined the used CPU architecture and measured absolute CPU times, an average CPU time used per time-step by the VOF method ($T_e$) is used for comparison. One should note that a direct comparison of algorithms on different CPU architectures is difficult, as a change in the architecture may cause a substantial change in the computational efficiency of
most algorithms. Additionally, performance measurements should be reported in absolute units with sufficient statistical information (an average value does not suffice), performed on a dedicated computing node (to avoid the influence of the operating system), with disabled CPU scaling, and using compiler optimizations that are otherwise used for productive computations. Although using different CPU architectures may strongly impact performance measurements, differences in orders of magnitude cannot be justified by the difference in CPU architecture, especially when relatively similar CPU architectures are used.

Verification tests for the interface advection must be carefully selected because the velocity functions used in the literature are all compositions of harmonic functions. Temporal integration of such functions with the first-order accurate Euler quadrature is prone to artificial error cancellation, resulting in an artificial second-order convergence.

### 4.3.1. 2D shear (single vortex)

The 2D shear verification case was introduced originally by R. J. Leveque. The test consists of a circular interface of radius \( r = 0.15 \), with the center \( c = (0.5, 0.75, 0) \). An explicitly prescribed velocity \( \mathbf{v}(\mathbf{x}, t) = \mathbf{v}(u_x(t), u_y(t), 0) \) is given as

\[
\begin{align*}
    u_x(t) &= \sin(2\pi y) \sin^2(\pi x) \cos \left( \frac{\pi t}{T} \right), \\
    u_y(t) &= -\sin(2\pi x) \sin^2(\pi y) \cos \left( \frac{\pi t}{T} \right),
\end{align*}
\]

in a unit square solution domain with \( CFL = 1 \). Results of the 2D shear case have recently been summarized for contemporary methods by Comminal et al. and their table is extended in table by additional results that were obtained for the same mesh resolutions.

The 2D shear results of the isoAdvector were computed with resolutions alternative to those reported in the literature, using [100\(^2\), 200\(^2\), 400\(^2\)] cubical volumes, so they cannot be directly summarized in table. Additionally \( CFL = 0.5 \) instead of 1 was used. Volume conservation error \( E_v \) is reported near machine tolerance, and numerical boundedness error \( E_b \) is within \([1 \times 10^{-6}, 1 \times 10^{-7}]\). The \( E_n \) advection errors of the isoAdvector scheme are \( E_n = [4.7 e^{-02}, 1.2 e^{-02}, 2.3 e^{-03}] \), scaled with the area of the circular interface to \( E_g = [3.32 e^{-03}, 8.48 e^{-04}, 1.63 e^{-04}] \), with respective convergence orders (1.96, 2.38). Therefore, the isoAdvector shows second order convergence for \( CFL = 0.5 \) for the 2D shear case with shape and numerical boundedness errors that are somewhat worse than those reported for the most recent fully geometrical LE method. Reported total CPU time used for the verification cases of [13, 60, 314] seconds confirms the computational efficiency of this geometric/algebraic VOF method. The isoAdvector-plicRDF by Scheufler and Roenby diverges with \( CFL = 1 \), but recovers second-order convergence at \( CFL = 0.5 \) [81, table 3], cf. table. The isoAdvector-plicRDF method delivers better results than THINC/QQ using a higher \( CFL = 0.5 \) condition. Reported execution times of the isoAdvector-plicRDF are significantly smaller than for other LE un-split geometrical VoF methods.

The \( E_g \) errors reported for the THINC/QQ method are approximately two times higher than \( E_g \) errors computed by the most recent geometrical LE methods. Xie and Xiao report the numerical boundedness error \( E_b \) only for the circle translation verification case. \( E_b \) is reported
within $\approx 1e-8, \approx 1e-7$ for $CFL = 0.2$ and $\approx 1e-7, \approx 1e-2$ for $CFL = 0.8$ for different values of the interface thickness parameter $\beta$.

| T     | Method                  | $E_g$ (32) | $E_g$ (64) | $O$ (32) | $E_g$ (128) | $O$ (64) | $E_g$ (256) | $O$ (128) |
|-------|-------------------------|------------|------------|----------|-------------|----------|-------------|----------|
| 0.5   | RK [31]                 | 7.29e-4    | 1.42e-4    | 2.36     | 3.90e-5     | 1.86     | -           | -        |
|       | RK [31]                 | 7.29e-4    | 1.42e-4    | 2.36     | 3.90e-5     | 1.86     | -           | -        |
|       | Stream [63]             | 5.51e-4    | 1.19e-4    | 2.32     | 3.38e-5     | 1.71     | -           | -        |
|       | EMFPA-SIR [67]          | 4.45e-4    | 7.99e-5    | 2.48     | 2.04e-5     | 1.97     | -           | -        |
|       | UFVFC-Swartz [10]       | 6.56e-4    | 9.89e-5    | 2.73     | 2.29e-5     | 2.11     | 4.38e-6     | 2.39     |
|       | MZ [35]                 | 4.68e-4    | 6.91e-5    | 2.76     | 2.07e-5     | 1.74     | -           | -        |
|       | GPCA [77]               | 4.12e-4    | 7.32e-5    | 2.41     | 1.93e-5     | 1.93     | -           | -        |
|       | OD [75]                 | -          | -          | -        | -           | -        | -           | -        |
|       | NIFPA-1 [79]            | -          | -          | -        | -           | -        | -           | -        |
|       | CCU [76]                | 3.20e-4    | 7.68e-5    | 2.06     | 1.32e-5     | 2.54     | 2.45e-6     | 2.43     |
|       | iPAM ($h_L = 0.1h$) [71]| 4.07e-5    | 4.96e-6    | 3.04     | 5.86e-7     | 3.08     | -           | -        |
| 2.0   | RK [31]                 | 2.36e-3    | 5.85e-4    | 2.01     | 1.31e-4     | 2.16     | -           | -        |
|       | Stream [63]             | 2.37e-3    | 5.65e-4    | 2.07     | 1.32e-4     | 2.10     | -           | -        |
|       | EMFPA-SIR [67]          | 2.14e-3    | 5.39e-4    | 1.99     | 1.29e-4     | 2.06     | -           | -        |
|       | MZ [35]                 | 2.11e-3    | 5.28e-4    | 2.00     | 1.28e-4     | 2.05     | -           | -        |
|       | GPCA [77]               | 2.18e-3    | 5.32e-4    | 2.05     | 1.29e-4     | 2.03     | -           | -        |
|       | CCU [76]                | 1.86e-3    | 4.18e-4    | 2.15     | 9.62e-5     | 2.12     | 1.97e-5     | 2.29     |
|       | iPAM ($h_L = 0.1h$) [71]| 8.34e-5    | 1.05e-5    | 2.99     | 1.37e-6     | 2.94     | -           | -        |
| 8.0   | THINC/QQ ($CFL=0.15$)   | 6.70e-2    | 1.52e-2    | 1.98     | 3.06e-3     | 2.27     | -           | -        |
|       | isoAdvvector-plicRDF ($CFL=0.5$) [51]| - | 1.26e-02 | 2.27 | 2.61e-03 | 2.19 | 5.71e-4 | 2.44 |
|       | NIFPA-1 [79]            | -          | 1.14e-2    | -        | 2.68e-3     | 2.01     | 5.37e-04    | 2.32     |
|       | RK [31]                 | 4.78e-2    | 6.96e-3    | 2.78     | 1.44e-3     | 2.27     | -           | -        |
|       | Stream [63]             | 3.72e-2    | 6.79e-3    | 2.45     | 1.18e-3     | 2.52     | -           | -        |
|       | EMFPA-SIR [67]          | 3.77e-2    | 6.58e-3    | 2.52     | 1.07e-3     | 2.62     | 2.35e-4     | 2.19     |
|       | MZ [35]                 | 5.42e-2    | 7.85e-3    | 2.79     | 1.05e-3     | 2.90     | -           | -        |
|       | GPCA [77]               | -          | -          | -        | 1.17e-3     | -        | -           | -        |
|       | OD [75]                 | -          | 7.58e-3    | -        | 1.88e-3     | 2.01     | 4.04e-4     | 2.22     |
|       | UFVFC-Swartz [10]       | 3.78e-2    | 5.74e-3    | 2.72     | 1.45e-3     | 1.98     | 3.77e-4     | 1.95     |
|       | OD-S [76]               | -          | 1.04e-2    | 2.95     | 1.344e-3    | 1.94     | 3.50e-4     | 2.22     |
|       | CCU [76]                | 3.81e-2    | 4.58e-3    | 3.06     | 1.00e-3     | 2.20     | 1.78e-4     | 2.59     |
|       | AMR-MoF [29]            | 2.33e-2    | 3.15e-3    | 2.88     | 5.04e-4     | 2.64     | -           | -        |
|       | iPAM ($h_L = 0.1h$) [71]| 6.21e-4    | 7.85e-5    | 2.99     | 9.89e-6     | 2.99     | -           | -        |

Table 4: $E_g$ errors of the 2D shear (single vortex case) with $CFL = 1$, with $N^2$ square volumes, with $(N)$ given in the first row of the table.

Geometrical LE VOF methods are stable for $CFL \leq 1$, and show volume conservation and numerical stability (boundedness) errors near machine tolerance, while $CFL = 0.15$ was used by Xie and Xiao [82] for the 2D shear case. As the $CFL$ condition determines the temporal accuracy, this makes it difficult to perform a direct comparison with other LE methods. One might argue that the $CFL$ magnitudes are much smaller when the advection scheme is coupled to the NS system, as the time steps become restricted by physical stability parameters. Then, $E_b \approx 1e-07$ for $CFL = 0.2$ would allow stable simulations of multiphase problems with large density ratios with THINC/QQ. Still, as volume conservation and numerical stability errors, as well as CPU times, are not reported
for 2D shear and 3D deformation cases, it is difficult to fully compare the THINC/QQ to standard geometrical LE VOF methods.

Absolute computational times expressed either per time step, or as total execution time for the verification case, are not reported for many methods, making them difficult to compare in terms of computational efficiency. CPU time is often omitted with a claim that the interface advection usually takes up only a fraction of the computational time compared to the pressure-velocity coupling algorithm. With the geometrical component added to any LE scheme, this might not be true, depending on the cost of 3D geometrical operations. Average CPU time per time step required for the interface advection has been reported in [74, 75, 78, 10] and total computational times were reported in [29, 71, 80]. The CPU times reported by Zhang and Fogelson [71] for the iPAM scheme with $h_L = 0.1h$ were [984, 4172, 16709] for meshes with $[32^2, 64^2, 128^2]$ cells, with a reported third-order convergence as listed in table 4.

Overall, for the 2D shear case, the iPAM, AMR-MoF, CCU and GPCA methods result in by far the best absolute error values compared to other methods. An interesting fact is that two of those methods are cell-based LE methods, that avoid the construction and correction of flux polyhedrons and approach the problem of Eulerian re-mapping on the basis of cell pre-images. Cell-based methods decompose images of polyhedral (polygonal) cells into tetrahedrons (triangles) more easily, compared to the flux-based methods that require complex tetrahedral decomposition of flux volumes $V_f$. Higher-order interpolation of the vertex displacements proposed first for the GPCA and then for CCU method is an additional factor that improves accuracy. Apart from iPAM with its sub-grid interface resolution, AMR-MoF and Unsplit Face-Vertex Flux Calculation (UFVFC)-Swartz, other geometrical LE methods rely on one or the other variant of the ELVIRA reconstruction algorithm. Total errors in simulations with many interface cells are influenced substantially by the reconstruction error and for those cases, the MoF reconstruction still delivers the most accurate results for the 2D shear case.

### 4.3.2. 3D deformation

The 3D deformation case was used by Enright et al. [8] for the Particle Level Set (PLS) method and it was originally proposed by Smolarkiewicz [9]. It has subsequently been used by many authors to verify the geometrical VOF method as well. The 3D shear verification consists of a sphere with radius $r = 0.15$, centered at $(0.35, 0.35, 0.35)$, and the velocity given by

$$\mathbf{v}(\mathbf{x}, t) = \begin{pmatrix}
2\sin(2\pi y) \sin(\pi x)^2 \sin(2\pi z) \cos \left(\frac{\pi t}{T}\right) \\
-\sin(2\pi x) \sin(\pi y)^2 \sin(2\pi z) \cos \left(\frac{\pi t}{T}\right) \\
-\sin(2\pi x) \sin(2\pi y) \sin(\pi z)^2 \cos \left(\frac{\pi t}{T}\right)
\end{pmatrix}, \quad (128)$$

where $T = 3$ and $CFL = 0.5$. 

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| CFL=0.5 | N           | $E_v$  | $E_b$  | $E_g$  | $O(E_g)$ | $T_v$ | $T_r$ |
|--------|-------------|--------|--------|--------|----------|-------|-------|
| isoAdvector-plicRDF [81] | 32 | $CFL_\Sigma = 0.5$ | 1.08e-16 | 2.12e-14 | 8.36e-3 | - 0.058 | 0.049 |
| THINC/QQ [82] | 32 | $CFL = 0.25$ | - | - | 7.96e-3 | 1.46 | - | - |
| Jofre et al. [79] | 32 | - | - | 6.92e-3 | - | - | - |
| Owkes et al. [75] | 32 | 2.79e-15 | 2.34e-17 | 6.98e-3 | 1.73 | 0.78 | - |
| PCFSC-CVTNA [34] | 32 | - | - | 6.91e-3 | 1.58 | - | - |
| FMFPA-3D-CLCIR [37] | 32 | $CFL = 1.0$ | - | - | 6.85e-3 | 1.53 | - | - |
| NIFPA-1 [79] | 33 | - | - | 6.71e-3 | 1.58 | - | - |
| FMFPA-3D-CBIR [37] | 32 | $CFL = 1.0$ | - | - | 6.64e-3 | 1.67 | - | - |
| UFVFC-Swartz [10] | 32 | 2.46e-15 | 0.0 | 5.86e-3 | 1.91 | 0.69 | 0.14 |
| Owkes et al. [78] | 32 (64) | - | - | 5.86e-3 | 1.91 | 0.69 | 0.14 |
| isoAdvector-plicRDF [81] | 64 | $CFL_\Sigma = 0.5$ | 9.75e-16 | 6.41e-14 | 3.25e-3 | 1.36 | 0.15 | 0.13 |
| isoAdvector [80] | 64 | - | - | 3.00e-3 | 2.31 | - | - |
| THINC/QQ [82] | 64 | $CFL = 0.25$ | - | - | 2.89e-3 | 1.67 | - | - |
| Jofre et al. [79] | 64 | - | - | 2.43e-3 | 1.51 | - | - |
| FMFPA-3D-CLCIR [37] | 64 | $CFL = 1.0$ | - | - | 2.38e-3 | 2.47 | - | - |
| Owkes et al. [75] | 64 | 1.675e-14 | 2.752e-17 | 2.10e-3 | 1.89 | 2.85 | - |
| NIFPA-1 [79] | 65 | - | - | 2.24e-3 | 2.16 | - | - |
| FMFPA-3D-CBIR [37] | 64 | $CFL = 1.0$ | - | - | 2.09e-3 | 2.57 | - | - |
| PCFSC-CVTNA [34] | 64 | - | - | 1.99e-3 | 2.69 | - | - |
| UFVFC-Swartz [10] | 64 | 6.01e-15 | 0.0 | 1.56e-3 | 2.34 | 2.81 | 0.51 |
| Owkes et al. [78] | 64 (128) | 6.01e-14 | 1.11e-16 | 5.68e-4 | 2.05 | 9.799 | - |
| THINC/QQ [82] | 128 | $CFL = 0.25$ | - | - | 9.05e-4 | - | - | - |
| isoAdvector-plicRDF [81] | 128 | $CFL_\Sigma = 0.5$ | 3.705e-15 | 1.1e-15 | 6.57e-4 | 2.31 | 0.52 | 0.39 |
| isoAdvector [80] | 128 | 1.20e-12 | 1.1e-7 | 6.04e-4 | 2.33 | - | - |
| Jofre et al. [79] | 128 | - | - | 6.37e-4 | - | - | - |
| Owkes et al. [75] | 128 | 1.68e-14 | 2.75e-17 | 5.63e-4 | - | 12.2 | - |
| NIFPA-1 [79] | 129 | - | - | 4.99e-4 | 1.89 | - | - |
| FMFPA-3D-CLCIR [37] | 128 | $CFL = 1.0$ | - | - | 4.31e-4 | 2.47 | - | - |
| PCFSC-CVTNA [34] | 128 | - | - | 3.09e-4 | 2.14 | - | - |
| FMFPA-3D-CBIR [37] | 128 | $CFL = 1.0$ | - | - | 3.52e-4 | 2.59 | - | - |
| UFVFC-Swartz [10] | 128 | 1.56e-14 | 0.0 | 3.08e-4 | - | 12.00 | 2.37 |
| Owkes et al. [78] | 128 (256) | 9.33e-14 | 3.33e-20 | 1.37e-4 | 1.51 | 26.636 | - |
| isoAdvector [80] | 256 | 9.40e-9 | 1.1e-10 | 1.20e-4 | - | - | - |
| isoAdvector-plicRDF [81] | 256 | $CFL_\Sigma = 0.5$ | 2.030e-14 | 2.366e-16 | 9.54e-5 | 2.78 | 2.63 | 1.67 |

Table 5: Advection error $E_g$ comparison for the 3D deformation case with $T = 3$ and $\max_\Omega(CFL) = 0.5$ and $N^3$ cubical volumes. Bracketed $N$ values represent the double sub-grid scale resolution used for the advection by Owkes and Desjardins [78]. For cases with $CFL \neq 0.5$, used $CFL$ value is added, and $CFL_\Sigma$ is the $CFL$ condition applied for interface cells $0 < \alpha_k < 1$.

The difficulty in developing dimensionally un-split LE VOF methods in three-dimensions is
reflected in the small number of methods with actual three-dimensional results (cf. tables 4 and 5). Volume conservation and numerical boundedness errors are often not reported in the literature, as well as performance measurements in absolute CPU time, which complicates a direct method comparison.

The most accurate is the Owkes-Desjardins Sub-resolution (OD-S) because its volume fraction advection uses local dynamic mesh refinement. The differences between OD-S and UFVFC-Swartz are based on different interface reconstruction algorithms (ELVIRA and simplified Swartz, respectively), different interpolation of cell-corner velocities, and different temporal integration. Double mesh resolution for the OD-S given by local mesh refinement doubles the average CPU time per time-step, confirming the linear complexity in terms of the number of mixed cells.

The benefits of adding the Cubic Bézier Interface Reconstruction (CBIR) reconstruction step to the Face-Matched Flux Polyhedron Advection (FMFPA-3D) scheme by Hernández et al. [45], López et al. [37] can be seen in table 5. The absolute error values are decreased somewhat by the CBIR step, leading to a slightly increased convergence order. However, as CPU times are not reported, it is difficult to know whether this improvement increases computational costs significantly. Additionally, the errors of the FMFPA-3D-(CLCIR,CBIR) combinations are sorted with respect to their magnitudes in table 5, ignoring the fact that CFL = 1 was used by López et al. [37], Hernández et al. [45].

A second-order accurate temporal integration method will already resolve the temporal derivative of the velocity functions given by eqs. (127) and (128) very accurately, because of the low frequency in the cosine temporal term. Because of this, the reconstruction error has a stronger influence in the 3D deformation case, so using higher CFL numbers reduces the absolute error magnitude. A comparison between FMFPA-3D and other methods is based on the same CFL numbers by López et al. [37], Hernández et al. [45].

CFL = 0.25 was used for the THINC/QQ method by Xie and Xiao [82], and no $E_v, E_b, T_e$ is reported for the 3D deformation case, which somewhat complicates direct comparison. Considering the aforementioned temporal integration resolution, the third-order Runge-Kutta scheme used in THINC/QQ certainly resolves the temporal derivative with sufficient accuracy, and the use of the smaller CFL number might be related to the stability limits of the higher-order flux reconstruction. Absolute error magnitudes of the THINC/QQ are approximately two times larger than the errors reported by the most recent geometrical LE VOF methods.

Roenby et al. [80] report $E_v, E_b$ errors as well as the total CPU time. The results of the isoAdvector scheme are worse than those of THINC/QQ scheme on coarser mesh resolutions, and better than THINC/QQ on finer mesh resolutions, but still twice as large than the error magnitudes reported for other contemporary geometrical LE schemes. However, CPU times reported for the isoAdvector in Roenby et al. [80] show significant improvement in computational efficiency compared to geometrical LE schemes. The isoAdvector-plicRDF method by Schuenfl and Roenby [81] delivers similar results to LE geometrical VoF methods on coarser mesh resolutions, but is on average two times less accurate on finer mesh resolutions. This is compensated with higher computational efficiency compared to other methods. Note that the results of isoAdvector-plicRDF are computed for the 3D deformation case in table 5 for max(CFL$_\Sigma$), the maximal CFL condition at the interface and not for the whole domain, which somewhat complicates a direct comparison.

Data and tables summarized in this section are available at http://dx.doi.org/10.25534/tudatalib-162.
5. Conclusions

The presented review of numerous methods used for the reconstruction of the PLIC interface and the advection of the volume fraction field outlined in sections 3 and 4 shows that the LE geometrical VOF methods are actively being researched. Main obstacles in developing accurate, robust and efficient geometrical VOF methods in 3D with support for unstructured meshes are the complex geometrical operations required for handling non-convex geometrical objects with non-planar faces, as well as the increase in computational complexity caused by the unstructured mesh topology. Although an extension of a geometrical VOF method to support 3D computation on unstructured meshes is often claimed to be straightforward, the number of publications that actually do report results on 3D unstructured meshes shows that this is not the case.

It seems that a direct comparison of methods based solely on the data available in the literature is often not possible. Interface reconstruction methods are very difficult to compare, as different error measures, initialization methods and validation cases are employed. The advection tests seem to be more standardized. However, different initialization algorithms that may play a role on fine mesh resolutions, different CFL values, and different mesh resolutions are often used for the advection as well. Normalized time units are often used to report performance measurements, without providing the absolute CPU time used for the normalization, making it difficult to compare the methods directly.

Reducing the dimensionality of geometrical calculations by the isoAvector and THINC/QQ schemes is an exciting approach because it significantly reduces the complexity and computational costs of the geometrical VOF methods while keeping the errors comparable with other contemporary methods. Reduction of computational costs is especially relevant for unstructured meshes, where a significant computational overhead is introduced by 3D intersections when calculating fluxed phase-specific volumes. Convergence does seem to be better with lower CFL numbers for the isoAdvector and THINC/QQ methods, as those methods avoid the calculation of the around-the-corner flux, and they have a reduced Lagrangean aspect of the calculation compared to fully un-split methods. However, hydrodynamic stability criteria imposed by surface-tension forces are often imposing much stricter time steps than the CFL criterion, at least in the context of two-phase DNS.

Benefits of higher order of accuracy to the interpolation of velocity at cell-corner points and temporal integration is confirmed by 2D results of the cell-based LE geometrical VOF methods: AMR-MoF [29], GPCA [77] and CCU [70]. The highest accuracy shown in 2D by the iPAM method [71] and AMR-MoF [29] and in 3D by the OD-S method [78] shows the effect on the absolute error magnitude caused by adding sub-grid scale resolution and additional advection information to interface (iPAM, and MoF, respectively) or to the volume fraction advection (OD-S).

Conversely to increasing the order of accuracy, reduced geometrical complexity of the geometrical algebraic VOF methods coupled with dynamic AMR might, in our opinion, present an effective way to achieve accurate, robust, and efficient solutions for an extensive range of two-phase DNS problems, as simpler algorithms are more straightforward to develop and implement in a scientific software, and are likely to have better parallel computational efficiency. Similarly, the high level of accuracy of three-dimensional geometric VOF methods [75, 59, 78, 79, 10] motivates a further development of computationally efficient three-dimensional geometric calculations.

6. Acknowledgements

Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – project id 26519115 – SFB 1194, sub-projects B01 and Z-INF.
Calculations for this research were conducted on the Lichtenberg high performance computer of the TU Darmstadt.

The first author is grateful for the fruitful discussions with his colleague, Dr.-Ing. Dirk Gründing, that have helped to improve the sections 2.1 and 2.2 of the manuscript.

The authors extend their gratitude to Dr. Christopher B. Ivey for the tabular result data of the NIFPA-1 method.
References

1. DeBar RB. Fundamentals of the KRAKEN code. *Tech Rep* 1974;:UCID–17366.

2. Hirt CW, Nichols BD. Volume of fluid (VOF) method for the dynamics of free boundaries. *J Comput Phys* 1981;39(1):201–25. doi:10.1016/0021-9991(81)90145-5

3. Rider WJ, Kothe DB. Reconstructing Volume Tracking. *J Comput Phys* 1998;141(2):112–52. doi:10.1006/jcph.1998.5906

4. Zalesak ST. Fully multidimensional flux-corrected transport algorithms for fluids. *J Comput Phys* 1979;31(3):335–62. doi:10.1016/0021-9991(79)90051-2

5. Ubbink O, Issa R. A method for capturing sharp fluid interfaces on arbitrary meshes. *J Comput Phys* 1999;153(1):26–50.

6. Muzaferrisa S. A two-fluid navier-stokes solver to simulate water entry. In: *Proceedings of 22nd symposium on naval architecture, 1999*. National Academy Press; 1999:638–51.

7. Wacławczyk T, Koronowicz T. Comparison of cicsam and hric high-resolution schemes for interface capturing. *Journal of theoretical and applied mechanics* 2008;46:325–45.

8. Enright D, Fedkiw RP, Ferziger J, Mitchell I. A Hybrid Particle Level Set Method for Improved Interface Capturing; vol. 183. 2002. ISBN 0001401106. doi:10.1006/jcph.2002.7166

9. Smolarkiewicz P. The multi-dimensional Crowley advection scheme. 1982. doi:10.1175/1520-0493(1982)110<1968:TMDCAS>2.0.CO;2

10. Marić T, Marschall H, Bothe D. An enhanced un-split face-vertex flux-based VoF method. *J Comput Phys* 2018;doi:10.1016/j.jcp.2018.03.048

11. Scardovelli R, Zaleski S. Analytical Relations Connecting Linear Interfaces and Volume Fractions in Rectangular Grids. *J Comput Phys* 2000;164(1):228–37. doi:10.1006/jcph.2000.6567

12. Renardy Y, Renardy M. PROST: A Parabolic Reconstruction of Surface Tension for the Volume-of-Fluid Method. *J Comput Phys* 2002;183(2):400–21. doi:10.1006/jcph.2002.7190

13. Popinet S. Gerris: A tree-based adaptive solver for the incompressible Euler equations in complex geometries. *J Comput Phys* 2003;190(2):572–600. doi:10.1016/S0021-9991(03)00298-5

14. Scardovelli R, Zaleski S. Interface reconstruction with least-square fit and split Eulerian-Lagrangian advection. *Int J Numer Methods Fluids* 2003;41(3):251–74. doi:10.1002/fld.431

15. Aulisa E, Manservisi S, Scardovelli R, Zaleski S. Interface reconstruction with least-squares fit and split advection in three-dimensional Cartesian geometry. *J Comput Phys* 2007;225(2):2301–19. doi:10.1016/j.jcp.2007.03.015

16. Popinet S. An accurate adaptive solver for surface-tension-driven interfacial flows. *J Comput Phys* 2009;228(16):5838–66. doi:10.1016/j.jcp.2009.04.042
17. Agbaglah G, Delaux S, Fuster D, Hoepffner J, Josserand C, Popinet S, Ray P, Scardovelli R, Zaleski S. Simulation parallèle adaptative octree d’écoulements multiphasiques par suivi d’interface de type volume de fluide. 2011. doi:10.1016/j.crme.2010.12.006

18. Youngs D. Time-Dependent Multi-material Flow with Large Fluid Distortion. Numer Methods Fluid Dyn 1982;273–85.

19. Bothe D. On moving hypersurfaces and the discontinuous ODE-system associated with two-phase flows. Nonlinearity (in press) 2020; doi:10.1088/1361-6544/ab987d.

20. Giusti E, Williams GH. Minimal surfaces and functions of bounded variation; vol. 2. Springer; 1984.

21. Evans L. Measure theory and fine properties of functions. Routledge; 2018.

22. Mosso S, Swartz B, Kothe D, Ferrell R. A Parallel, Volume-Tracking Algorithm for Unstructured Meshes. In: Schiano P, Ecer A, Periaux J, Satofuka N, eds. Parallel Comput. Dyn. Algorithms Results Using Adv. Comput. MAY; Capri, Italy. ISBN 9780444823274; 1996:368–75. doi:10.1016/B978-044482327-4/50113-3.

23. Dyadechko V, Shashkov M. Moment-of-fluid interface reconstruction. Math Model Anal 2005;836:1–41. doi:10.1016/j.cma.2009.08.009.

24. Zhang Q, Liu PLF. A new interface tracking method: The polygonal area mapping method. J Comput Phys 2008;227(8):4063–88. doi:10.1016/j.jcp.2007.12.014.

25. Chenadec VL, Pitsch H. A 3D unsplit Forward/Backward Volume-of-Fluid approach and coupling to the level set method. J Comput Phys 2013;233(1):10–33. doi:10.1016/j.jcp.2012.07.019.

26. Pilliod JE, Puckett EG. Second-order accurate volume-of-fluid algorithms for tracking material interfaces. J Comput Phys 2004;199(2):465–502. doi:10.1016/j.jcp.2003.12.023.

27. Francois MM, Cummins SJ, Dendy ED, Kothe DB, Sicilian JM, Williams MW. A balanced-force algorithm for continuous and sharp interfacial surface tension models within a volume tracking framework. J Comput Phys 2006;213(1):141–73. doi:10.1016/j.jcp.2005.08.004.

28. Owkes M, Desjardins O. A mesh-decoupled height function method for computing interface curvature. J Comput Phys 2015;281:285–300. doi:10.1016/j.jcp.2014.10.036.

29. Ahn HT, Shashkov M. Adaptive moment-of-fluid method. J Comput Phys 2009;228(8):2792–821. doi:10.1016/j.jcp.2008.12.031.

30. James AJ, Lowengrub J. A surfactant-conserving volume-of-fluid method for interfacial flows with insoluble surfactant. 2004. doi:10.1016/j.jcp.2004.06.013.

31. Noh WF, Woodward PR. SLIC (Simple Line Interface Calculation) method. Proc Fifth Int Conf Numer Methods Fluid Dyn June 28–July 2, 1976 Twente Univ Enschede 1976::330–40. doi:10.1007/3-540-08004-X_336.

32. Kothe DDB, Rider WW, Mosso SS, Brock JJ. Volume tracking of interfaces having surface tension in two and three dimensions. Aiaa 96-0859 1996;25. doi:10.2514/6.1996-859.
33. Mosso SJ, Swartz BK, Kothe DB, Clancy SP. Recent enhancements of volume tracking algorithms for irregular grids. *Los Alamos Natl Lab, Los Alamos, NM, LA_UR_96.277* 1996;:20–3. doi:10.1016/j.compfluid.2005.09.003

34. Liovic P, Rudman M, Liow JL, Lakehal D, Kothe D. A 3D unsplit-advection volume tracking algorithm with planarity-preserving interface reconstruction. *Comput Fluids* 2006;35(10):1011–32. doi:10.1016/j.compfluid.2005.09.003

35. Mosso S, Garasi C, Drake R. A smoothed two- and three-dimensional interface reconstruction method. *Comput Vis Sci* 2008;12(7):365–81. doi:10.1007/s00791-008-0108-y

36. Ahn HT, Shashkov M. Multi-material interface reconstruction on generalized polyhedral meshes. *J Comput Phys* 2007;226(2):2096–132. doi:10.1016/j.jcp.2005.09.003

37. López J, Zanzi C, Gomez P, Faura F, Hernández J. A new volume of fluid method in three dimensions—Part II: Piecewise-planar interface reconstruction with cubic-Bezier fit. *Int J Numer Methods Fluids* 2008;14(14):4427–36. doi:10.1158/1078-0432.CCR-08-0458.

38. Dyadechko V, Shashkov M. Reconstruction of multi-material interfaces from moment data. *J Comput Phys* 2008;227(11):5361–84. doi:10.1016/j.jcp.2007.12.029

39. Cerne G, Petelin S, Tiselj I. Numerical errors of the volume-of-fluid interface tracking algorithm. *Int J Numer Methods Fluids* 2002;38(November 2000):329–50. doi:10.1002/fld.228

40. Moukalled F, Mangani L, Darwish M. The finite volume method in computational fluid dynamics. *An Advanced Introduction with OpenFOAM and Matlab* 2016:3–8.

41. Mavriplis DJ. Revisiting the Least-Squares Procedure for Gradient Reconstruction on Unstructured Meshes. *16th AIAA Comput Fluid Dyn Conf* 2003; NASA CR–2003doi:10.2514/6.2003-3986

42. Garimella R, Kucharik M, Shashkov M. An efficient linearity and bound preserving conservative interpolation (remapping) on polyhedral meshes. *Comput Fluids* 2007;36(2):224–37. doi:10.1016/j.compfluid.2006.01.014

43. Correa CD, Hero R, Ma KL. A comparison of gradient estimation methods for volume rendering on unstructured meshes. *IEEE Trans Vis Comput Graph* 2011;17(3):305–19. doi:10.1109/TVCG.2009.105

44. Swartz B. The second-order sharpening of blurred smooth borders. *Math Comput* 1989;52(186):675. doi:10.1090/S0025-5718-1989-0983313-8

45. Hernández J, López J, Gomez P, Zanzi C, Faura F. A new volume of fluid method in three dimensions—Part I: Multidimensional advection method with face-matched flux polyhedra. *Int J Numer Methods Fluids* 2008;58(8):601–29. doi:10.1002/fld.1776

46. Ahn HT, Shashkov M. Geometric algorithms for 3D interface reconstruction. In: *Proc. 16th Int. Meshing Roundtable, IMR 2007*. ISBN 9783540751021; 2008:405–22. doi:10.1007/978-3-540-75103-8_23

47. Shewchuk JR. Lecture Notes on Geometric Robustness. 2013:1–95.

48. Brent RP. Algorithms for minimization without derivatives. Dover Publications; 2013.
49. Brent RP. An algorithm with guaranteed convergence for finding a zero of a function. 1971. doi:10.1093/comjnl/14.4.422

50. López J, Hernández J. Analytical and geometrical tools for 3D volume of fluid methods in general grids. J Comput Phys 2008;227(12):5939–48. doi:10.1016/j.jcp.2008.03.010

51. Diot S, François MM, Dendy ED. An interface reconstruction method based on analytical formulae for 2D planar and axisymmetric arbitrary convex cells. J Comput Phys 2014;275:53–64. doi:10.1016/j.jcp.2014.06.060

52. Diot S, François MM. An interface reconstruction method based on an analytical formula for 3D arbitrary convex cells. J Comput Phys 2016;305:63–74. doi:10.1016/j.jcp.2015.10.011

53. López J, Hernández J, Gómez P, Faura F. A new volume conservation enforcement method for PLIC reconstruction in general convex grids. J Comput Phys 2016;316:338–59. URL: http://dx.doi.org/10.1016/j.jcp.2016.04.018
doi:10.1016/j.jcp.2016.04.018

54. Chen X, Zhang X. A predicted-Newton’s method for solving the interface positioning equation in the MoF method on general polyhedrons. J Comput Phys 2019;384:60–76. URL: https://doi.org/10.1016/j.jcp.2018.12.038
doi:10.1016/j.jcp.2018.12.038

55. López J, Hernández J, Gómez P, Faura F. Non-convex analytical and geometrical tools for volume truncation, initialization and conservation enforcement in VOF methods. J Comput Phys 2019;392:666–93. URL: https://doi.org/10.1016/j.jcp.2019.04.055
doi:10.1016/j.jcp.2019.04.055

56. Kromer J, Bothe D. Highly accurate computation of volume fractions using differential geometry. J Comput Phys 2019;396(July):761–84. URL: https://doi.org/10.1016/j.jcp.2019.07.005
doi:10.1016/j.jcp.2019.07.005

57. Jones BW, Malan AG, Ilangakoon NA. The initialisation of volume fractions for unstructured grids using implicit surface definitions. Comput Fluids 2019;179:194–205. URL: https://doi.org/10.1016/j.compfluid.2018.10.021
doi:10.1016/j.compfluid.2018.10.021

58. Cummins SJ, Francois MM, Kothe DB. Estimating curvature from volume fractions. Comput Struct 2005;83(6-7):425–34. doi:10.1016/j.compstruc.2004.08.017

59. Jofre L, Lehmkuhl O, Castro J, Oliva A. A 3-D Volume-of-Fluid advection method based on cell-vertex velocities for unstructured meshes. Comput Fluids 2014;94:14–29. doi:10.1016/j.compfluid.2014.02.001

60. Jofre L, Borrell R, Lehmkuhl O, Oliva A. Parallel load balancing strategy for Volume-of-Fluid methods on 3-D unstructured meshes. J Comput Phys 2015;282:269–88. doi:10.1016/j.jcp.2014.11.009

61. Tryggvason G, Scardovelli R, Zaleski S. Direct Numerical Simulations of Gas–Liquid Multiphase Flows. Cambridge University Press; 2011. ISBN 978-0-521-78240-1.

62. Scardovelli R, Zaleski S. Direct Numerical Simulation of Free-Surface and Interfacial Flow. Annu Rev Fluid Mech 1999;31(1):567–603. doi:10.1146/annurev.fluid.31.1.567

54
63. Weideman JAC. Numerical integration of periodic functions: A few examples. *The American mathematical monthly* 2002;109(1):21–36.

64. Harvie DJ, Fletcher DF. A New Volume of Fluid Advection Algorithm: The Stream Scheme. *J Comput Phys* 2000;162(1):1–32. doi:10.1006/jcph.2000.6510

65. Harvie DJE, Fletcher DF. A new volume of fluid advection algorithm: The defined dominating region scheme. *Int J Numer Methods Fluids* 2001;35(2):151–72. doi:10.1002/1097-0363(20010130)35:2<151::AID-FLD87>3.0.CO;2-4

66. Aulisa E, Manservisi S, Scardovelli R, Zaleski S. A geometrical area-preserving Volume-of-Fluid advection method. *J Comput Phys* 2003;192(1):355–64. doi:10.1016/j.jcp.2003.07.003

67. López J, Hernández J, Gómez P, Faura F. A volume of fluid method based on multidimensional advection and spline interface reconstruction. *J Comput Phys* 2004;195(2):718–42. doi:10.1016/j.jcp.2003.10.030

68. Bell JB, Dawson CN, Shubin GR. An unsplit, higher order godunov method for scalar conservation laws in multiple dimensions. *J Comput Phys* 1988;74(1):1–24. doi:10.1016/0021-9991(88)90065-4

69. Ahn HT, Shashkov M, Christon MA. The moment-of-fluid method in action. *Commun Numer Methods Eng* 2009;25(10):1099–18. doi:10.1002/cnm.1135

70. Zhang Q. On a Family of Unsplit Advection Algorithms for Volume-of-Fluid Methods. *SIAM J Numer Anal* 2013;51(5):2822–50. doi:10.1137/120978882

71. Zhang Q, Fogelson A. Fourth-Order Interface Tracking in Two Dimensions via an Improved Polygonal Area Mapping Method. *SIAM J Sci Comput* 2014;36(5):2369–400. doi:10.1137/140951886

72. Tryggvason G, Bunner B, Esmaeeli A, Juric D, Al-Rawahi N, Tauber W, Han J, Nas S, Jan YJ. A front-tracking method for the computations of multiphase flow. *J Comput Phys* 2001;169(2):708–59. doi:10.1006/jcph.2001.6726

73. Hachenberger P, Kettner L, Melhorn K. Boolean operations on 3D selective Nef complexes: Data structure, algorithms, optimized implementation and experiments. *Computational Geometry* 2007;38:64–99. doi:10.1016/j.comgeo.2006.11.009

74. Marić T, Marschall H, Bothe D. voFoam - A geometrical volume of fluid algorithm on arbitrary unstructured meshes with local dynamic adaptive mesh refinement using OpenFOAM. *arXiv preprint arXiv:13053417* 2013.

75. Owkes M, Desjardins O. A computational framework for conservative, three-dimensional, unsplit, geometric transport with application to the volume-of-fluid (VOF) method. *J Comput Phys* 2014;270:587–612. doi:10.1016/j.jcp.2014.04.022

76. Comminal R, Spangenberg J, Hattel JH. Cellwise conservative unsplit advection for the volume of fluid method. *J Comput Phys* 2015;283:582–608.
77. Cervone A, Manservisi S, Scardovelli R, Zaleski S. A geometrical predictor–corrector advection scheme and its application to the volume fraction function. *J Comput Phys* 2009;228(2):406–19.

78. Owkes M, Desjardins O. A mass and momentum conserving unsplit semi-Lagrangian framework for simulating multiphase flows. *J Comput Phys* 2017;332:21–46. doi:10.1016/j.jcp.2016.11.046

79. Ivey CB, Moin P. Conservative and bounded volume-of-fluid advection on unstructured grids. *J Comput Phys* 2017;350:387–419. doi:10.1016/j.jcp.2017.08.054

80. Roenby J, Bredmose H, Jasak H. A Computational Method for Sharp Interface Advection. *RSoc Open Sci* 2016;3(11). doi:10.1098/rsos.160405

81. Scheufler H, Roenby J. Accurate and efficient surface reconstruction from volume fraction data on general meshes. *J Comput Phys* 2019;383:1–23. doi:10.1016/j.jcp.2019.01.009 arXiv:1801.05382.

82. Xie B, Xiao F. Toward efficient and accurate interface capturing on arbitrary hybrid unstructured grids: The THINC method with quadratic surface representation and Gaussian quadrature. *J Comput Phys* 2017;349:415–40. doi:10.1016/j.jcp.2017.08.028

83. Hoefler T, Belli R. Scientific benchmarking of parallel computing systems 2015;:1–12doi:10.1145/2807591.2807644.

84. R. J. Leveque . High-resolution conservative algorithms for incompressible flow. *SIAM J Numer Anal* 1996;33(2):627–. doi:10.1137/0733033

85. Mencinger J, Zun I. A PLIC-VOF method suited for adaptive moving grids. *J Comput Phys* 2011;230(3):644–63. doi:10.1016/j.jcp.2010.10.010