Efficient three-material PLIC interface positioning on unstructured polyhedral meshes

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Abstract

This paper introduces an efficient algorithm for the sequential positioning (also referred to as nested dissection) of two planar interfaces in an arbitrary polyhedron, such that, after each truncation, the respectively remaining polyhedron admits a prescribed volume. This task, among others, is frequently encountered in the numerical simulation of three-phase flows when resorting to the geometric Volume-of-Fluid (VoF) method [7]. For two-phase flows, the recent work of Kromer and Bothe [8] addresses the positioning of a single plane by combining an implicit bracketing of the sought position with up to third-order derivatives of the volume fraction. An analogous application of their highly efficient root-finding scheme to three-material configurations requires computing the volume of a twice truncated arbitrary polyhedron. The present manuscript achieves this by recursive application of the GAUSSIAN divergence theorem in appropriate form, which allows to compute the volume as a sum of quantities associated to the faces of the original polyhedron. With a suitable choice of the coordinate origin, accounting for the sequential character of the truncation, the volume parametrization becomes co-moving with respect to the planes. This eliminates the necessity to establish topological connectivity and tetrahedron decomposition after each truncation. After a detailed mathematical description of the concept, we conduct a series of carefully designed numerical experiments to assess the performance in terms of polyhedron truncations. The high efficiency of the two-phase positioning persists for sequential application, thereby being robust with respect to the input data and possible intersection topologies. In comparison to an existing decomposition-based approach, the number of truncations was reduced by up to an order of magnitude, further highlighting the superiority of the divergence-based volume computation. The increase in performance is highly beneficial not only for single core application, but also for an embedded application within a parallelized flow solver, as load imbalance can be reduced significantly. In view of an integration into existing numerical schemes, the proposed algorithm, besides its applicability to unstructured meshes, is self-contained, i.e. it requires no external decomposition libraries.

Keywords— Piecewise Linear Interface Calculation (PLIC), interface reconstruction, Volume-of-Fluid (VoF), unstructured grids, multi-material, triple-line

1 Introduction

Multiphase flows play an important role in nature, science and technology, ranging from processes in clouds where droplets interact with already frozen particles to groundwater predictions where porous media are present. Like the examples indicate, not only two, but often three interacting phases are of relevance. One-field approaches like the Volume-of-Fluid method (VoF) by Hirt and Nichols [7] have the advantage that only one set of conservation equations has to be solved, leading to a significant reduction in the computational effort. For multi-material
flow simulations in the context of the geometric VoF method, the approximate reconstruction of the interfaces, separating the respective phases, plays a key role in avoiding numerical diffusion and preserving a sharp interface. In the **Piecewise Linear Interface Calculation** (PLIC), every computational cell may contain a plane for each pair of phases. As can be seen in figure 1, the numerical simulation of three-phase interaction features a spectrum of different topologies. At the contact line, the involved interfaces must form a prescribed contact angle. Besides the contact line, a three-phase cell may also contain a thin film, i.e. with a thickness smaller than the cell size. Especially for small contact angles, thin films may extend to regions far away from the contact line, thereby entrapping small portions of the third phase. In terms of topological classification, non-wetted, fully wetted and partially wetted (i.e., with a contact line) cells can be distinguished. Prior to the reconstruction, however, the belonging to the aforementioned classes is unknown. With an intentionally coarse resolution, facilitating the visual identification of the individual PLIC planes, figure 2 illustrates some time instants of a prototypical collision process, where the interfaces are subject to highly dynamic deformation.

**Figure 1:** Topological interface configurations of three-phase fluid flows on a Cartesian grid.

**Figure 2:** Direct numerical simulation of a liquid droplet (red) colliding with solid sphere (blue) in an ambient gas. Orange planes indicate the interface in cells where all three phases are present. The simulation was performed with FS3D \[6\] with a constant static contact angle \( \theta = 179^\circ \) and a preliminary version of the topology capturing PLIC orientation algorithm \[14\] on an intentionally coarse grid to distinguish the depicted interfaces.

Figure 3 gathers possible configurations for three phases. In particular for unstructured meshes with non-convex cells, obtaining the position of a single plane with both accuracy and efficiency poses a challenging task: firstly, because truncating a polyhedron may result in a variety of topologically different sub-polyhedra, and, secondly, because the truncated volume must match the prescribed value by translating the plane along its normal. Obviously, the task becomes considerably more demanding in the presence of more than one plane.

In essence, there are three conceptually distinct components of multi-material interface reconstruction: **material ordering**, **(normal) orientation** and **positioning**, where the latter can be further decomposed into scalar root-finding and volume computation of truncated polyhedra. We extend the work of Kromer and Bothe \[8\] to the sequential PLIC positioning problem in three spatial dimensions, where we assume the material order and the respective normals to be given. Due to its high practical relevance, we exclusively consider the **three material** case.

**Figure 3** illustrates the common approaches that can be found in the literature. The **onion-skin** approach consists of a sequential, but otherwise independent positioning of all planes in the polyhedron: with \( N \) pairs...
Figure 3: Different algorithms for multi-material reconstruction: onion-skin with layer structure (leftmost) and
unphysical domain overlap (second), nested dissection (third) and power-diagram with generators \( g_i \) and weights
\( \omega_i \) (fourth). Note that, with corresponding normals and volume fractions, the nested dissection redistributes
the domain overlap produced by the onion-layer scheme (purple, hatched).

of volume fractions and normals \( \{\alpha^*, n^*_\Gamma\}_{i=1}^N \), the \( n \)-th plane is positioned such that its negative halfspace
truncates from the polyhedron \( P \) a sub-polyhedron \( P_n \), whose volume accumulates the volumes of all prede-
cessors, i.e.
\[
|P_n| = |P| \sum_{i=1}^n \alpha^*_i.
\]
The simplicity in concept and implementation complexity, however, also bears
some disadvantages: for some configurations of input-data, an unphysical overlap of the reconstructed phase
domains may occur. The **nested dissection** overcomes this unphysical artifact by positioning the \( n \)-th plane
in a polyhedron truncated by its \( n - 1 \) predecessors. The **power-diagram** method introduces an additional
degree of freedom, by allowing for kinks of the respective planes. In methods of this class, the positioning relies
on weighted **Voronoi** diagrams and smoothing the resulting interfaces; cf., e.g., Schofield et al. [18, 19] and see
the rightmost panel in figure 3 First, so-called generators \( g_i \) are computed by solving a least-squares problem
in a rectangular domain containing the cell under consideration. With those generators \( g_i \) fixed in space, the
weights \( \omega_i \) are adjusted such that the induced volume fractions match the prescribed ones. However, to the
best of our knowledge, all methods of this class were published for two spatial dimensions, and the complexity
of the volume computation can be expected to increase strongly in three spatial dimensions. Indeed, Schofield
et al. [19] indicate that the aforementioned smoothing becomes considerably more involved in three spatial
dimensions. Also, it is not clear whether a triple-line exists for all configurations of input data. In fact, the
authors of the present manuscript could not find a general proof for the existence of solutions in two spatial
dimensions.

Literature shows that multiple numerical studies on three-phase flow employ VoF with PLIC. Thus an im-
provement of the performance of the PLIC positioning for this situations is of high relevance to improve overall
performance as well as lower the load imbalance in parallelized codes. A few examples for three-phase flow
simulations with different applications are the following: Patel et al. [11] simulate an idealized pore structure
formed by spheres filled with oil which is flooded with water. Baggio and Weigand [3] studied the impact
on a structured surface. Both with VoF in a **Cartesian** grid, thus multiple cells exist in the computational
domain, where three phases occur. Those examples are both employing a stationary solid phase. Reitzle et al.
[15] modelled the solidification process of water, where moving three-phase cells are present shortly before the
droplet is fully frozen. For the simulation of phenomena in clouds for weather prediction, also the interaction of
an already frozen with a supercooled droplet is of interest, thus a situation where multiple moving three-phase
cells are present. Another situation, in which a three-component reconstruction with a contact line is necessary,
is the collision of immiscible liquids, where also two deforming and moving VoF fields are present in a gaseous
continuous phase, forming contact lines [14].
1.1 Literature review

Due to the inherent difference in mathematical and implementation complexity, the literature contributions are reviewed based on the spatial dimension.

1.1.1 Two spatial dimensions

For Cartesian meshes, Choi and Bussmann [5] introduce an approach to reconstructing a three-material cell that accurately estimates interface normals, determines the position of a triple point if it exists, and exactly conserves mass. Employing an onion-skin type approach, they require the sequence of reconstruction to be determined, where the first interface normal is computed by the method of Youngs [21]. The second normal is reconstructed such that the volume fractions induced by the corresponding plane $\Gamma_2$ best approximate (in a least-squares sense) those in the neighborhood of $P$. Schofield et al. [19] propose a second-order accurate material-order-independent interface reconstruction technique, based on the work of Schofield et al. [18], where no topology for the material regions is assumed a priori. They employ a weighted Voronoi diagram (called power diagram) to simultaneously approximate the phase-centroids of all materials, which are then used to determine the respective normals; cf. figure 3. By iteratively adjusting the weights of the point generators associated to the materials in a cell, the interfaces are positioned to match the respective volume fractions. Schofield et al. [19] investigate equidistant Cartesian meshes and report that, in a qualitative sense, the reconstructed multi-material interfaces outperform gradient-based methods; cf. their fig. 11. However, they also find that for cells with high aspect ratios, this can [...] give poor results for multimaterial cells. Schofield and Christon [17] conduct a series of numerical tests for the aforementioned algorithm. Anderson et al. [2] reconstruct the interfaces in Cartesian cells by a combination of subdivision (between 125 and 1000 per cell) and probabilistic reordering by simulated annealing, based on the volume fraction data of the neighboring cells. While, for the cases investigated, the reconstructed interfaces are qualitatively superior to those obtained by PLIC, the huge computational effort, induced by the subdivision, renders their algorithm impractical. Based on the neighboring normals, Caboussat et al. [4] employ a minimization procedure for the reconstruction of a triple point.

1.1.2 Three spatial dimensions

Ahn and Shashkov [1] introduce a recursive algorithm for nested dissection based on tetrahedron decomposition, which is applicable to convex and non-convex polyhedra $P$. However, for the latter to be accessible for their tetrahedron decomposition scheme, the weighted sum of the vertices needs to be a star-point of $P$. Their fig. 6 (bottom right) nicely illustrates that the computational effort of this strategy grows very quickly; cf. figure 4.

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A star-point $x$ of a polyhedron is any point $x \in P$ such that $x + \lambda(y - x) \in P \forall (\lambda, y) \in [0, 1] \times P$, i.e. the line connecting $x$ with any other point $y \in P$ must be entirely contained in $P$. For weakly non-convex polyhedra, the weighted sum of the vertices can be assumed to be a star-point. However, care has to be taken in general.

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Figure 4: Nested dissection algorithm of Ahn and Shashkov [1] with triangular decomposition.
Pathak and Raessi [12] introduce a comprehensive algorithm for the interface reconstruction, covering both normal reconstruction from volume fractions and positioning of the PLIC interfaces, where the latter part of their algorithm resorts to a combination of decomposition and BRENT’s method. While Pathak and Raessi [12] report above first-order convergence for the computed normals, they do not provide any performance measures for their positioning algorithm.

Objectives

In one form or another, all the literature contributions employ extraction of topological connectivity and decomposition. While this may be feasible for simple cells, e.g., tetrahedra and cuboids, the computational effort becomes huge for general non-convex polyhedra; cf. figure 4. As stated in Kromer and Bothe [8], the computational costs can be alleviated by a proper parametrization of the truncated volume. In principle, a three-phase positioning for a sequential PLIC algorithm can be achieved by a combination of two subsequent positioning steps inside different polyhedra, which can be each performed similar to a positioning of a single plane in an unstructured grid. However, the fact that the truncated polyhedron shares multiple faces with the original one becomes huge for general non-convex polyhedra; cf. figure 4. As stated in Kromer and Bothe [8], the computational costs can be alleviated by a proper parametrization of the truncated volume. In principle, a three-phase positioning for a sequential PLIC algorithm can be achieved by a combination of two subsequent positioning steps inside different polyhedra, which can be each performed similar to a positioning of a single plane in an unstructured grid. However, the fact that the truncated polyhedron shares multiple faces with the original one can be exploited to reduce the computational effort. The present work harnesses this knowledge.

Before we formulate the problem under consideration in subsection 1.3, the upcoming subsection 1.2 introduces the employed notation along with the relevant quantities.

1.2 Notation

Let $P \subset \mathbb{R}^3$ be an arbitrary polyhedron whose boundary $\partial P = \bigcup F_k$ is composed of $N_F$ planar polygonal faces $F_k$ with outer normal $n_k^F$. While the faces may be non-convex, we assume that the respective boundary $\partial F_k$ admits no self-intersection. Each face consists of the vertices $x_{k,m}$ ($m = 1 \ldots N_k^F$), which are ordered counter-clockwise with respect to $n_k^F$. To the edges $E_{k,m} = \text{conv} \left( x_{k,m}, x_{k,m+1} \right)$, we assign the outer co-normal $N_{k,m}$ with $\langle n_k^F, N_{k,m} \rangle = 0$. Note that, with a counter-clockwise orientation of the vertices, $N_{k,m}$ can be computed by normalizing $(x_{k,m+1} - x_{k,m}) \times n_k^F$. Throughout this work, the subscript $k$ ($m$) always refers to the faces (edges/vertices). For better readability, the respective summation limits, i.e. the number of faces and edges/vertices on a face, are suppressed. Also, for notational convenience, the indices $m$ are assumed to be periodic, i.e. $x_{k,N_k^F+1} = x_{k,1}$.

Let $n_{\Gamma_1}$ and $n_{\Gamma_2}$ be the primary (subscript 1) and secondary (subscript 2) unit normals. With some arbitrary but spatially fixed common origin $x_{\Gamma,0}$, the associated signed distances $s$ (primary) and $t$ (secondary), respectively, define a family of planes

$$\Gamma_1(s) = \{ x \in \mathbb{R}^3 : \phi_{\Gamma_1}(x) = s \} \quad \text{and} \quad \Gamma_2(t) = \{ x \in \mathbb{R}^3 : \phi_{\Gamma_2}(x) = t \} \quad \text{with} \quad \phi_{\Gamma_1}(x) = \langle x - x_{\Gamma,0}, n_{\Gamma_1} \rangle, \tag{1}$$

together with their associated negative and positive halfspaces

$$H^-(u) := \{ x \in \mathbb{R}^3 : \phi_{\Gamma_1}(x) \leq u \} \quad \text{and} \quad H^+(u) := \{ x \in \mathbb{R}^3 : \phi_{\Gamma_1}(x) \geq u \}.$$

Assuming, for the moment, that $\langle n_{\Gamma_1}, n_{\Gamma_2} \rangle \neq 1$, the line of intersection of the planes, say, $\Psi := \Gamma_1(s) \cap \Gamma_2(t)$, can be parametrized as

$$\Psi(u; s, t) = y_0(s) + t\tau_\Psi + u\mu_\Psi. \tag{2}$$

Planarity is required for the application of the Gaussian divergence theorem, i.e. non-planar polygonal faces must be decomposed accordingly.
with \[ y_0(s) = x_{\Gamma,0} + s \frac{n_{\Gamma_1} - (n_{\Gamma_1},n_{\Gamma_2})n_{\Gamma_2}}{1 - (n_{\Gamma_1},n_{\Gamma_2})^2}, \quad \tau_\Psi = \frac{n_{\Gamma_2} - (n_{\Gamma_1},n_{\Gamma_2})n_{\Gamma_1}}{1 - (n_{\Gamma_1},n_{\Gamma_2})^2} \quad \text{and} \quad \mu_\Psi = \frac{n_{\Gamma_1} \times n_{\Gamma_2}}{1 - (n_{\Gamma_1},n_{\Gamma_2})^2}. \] Equation \(^2\) can be understood as follows: the signed distances of the planes, i.e. \(s\) and \(t\), determine the plane intersection \(\Psi\), while \(u\) varies along \(\Psi\). The advantage of this choice of \(\tau_\Psi\) and \(\mu_\Psi\) will become clear below.

### 1.3 Problem formulation

For a given polyhedron \(P\) with center \(x_{\Gamma,0}\), two pairs \(\{n_{\Gamma},\alpha_1^*\}\) of unit normals \(n_{\Gamma}\) and volume fractions \(0 < \alpha_1^* < 1\) and \(0 < \alpha_2^* < 1 - \alpha_1^*\) (both of which refer to the original volume \(|P|\)), solve the following problems:

**primary positioning:** Find the primary signed distance \(s^*\) such that \(|P \cap H_1^{-}(s^*)| = \alpha_1^*|P|\), i.e. such that the plane \(\Gamma_1(s^*)\) truncates from \(P\) a sub-polyhedron with volume \(\alpha_1^*|P|\). Let \(P^\text{cut} := P \cap H_1^{-}(s^*)\) denote the remaining sub-polyhedron with volume \((1 - \alpha_1^*)|P|\), within which the secondary plane is positioned.

**secondary positioning:** Find the secondary signed distance \(t^*\) such that \(|P^\text{cut} \cap H_2^{-}(t^*)| = \alpha_2^*|P^\text{cut}|\), i.e. such that the secondary plane \(\Gamma_2\) truncates from the remnant polyhedron \(P^\text{cut}\) a sub-polyhedron with volume \(\alpha_2^*|P| = \frac{\alpha_1^*}{1 - \alpha_1^*}|P^\text{cut}|\).

Figure 5 illustrates the procedure and some of the quantities for a cuboid.

Figure 5: Illustration of sequential truncation for a cuboid: After positioning the primary plane \(\Gamma_1\), one obtains the truncated polyhedron \(P^\text{cut}\) (center), within which the secondary plane \(\Gamma_2\) is positioned. In this specific instance, the triple line \(\Psi\) intersects the faces \(F_4\) and \(F_5\).

Let \(X\) and \(X^\text{cut}\), respectively, be the set of vertices of the original \((P)\) and truncated \((P^\text{cut})\) polyhedron. The associated signed distances

\[
\hat{S} = \{ (x - x_{\Gamma,0},n_{\Gamma_1}) : x \in X \} \quad \text{and} \quad \hat{S}^\text{cut} = \{ (x - x_{\Gamma,0},n_{\Gamma_2}) : x \in X^\text{cut} \}
\]

correspond to the values of \(s\) for which the planes \(\Gamma_1\) and \(\Gamma_2\) pass through a vertex (single or multiple). Let the unique elements \(s_i\) of \(\hat{S}\) be arranged in ascending order \((s_i < s_{i+1})\) and define mutually disjoint so-called brackets \(B_i := (s_i,s_{i+1})\) with \(B_1 := [s_1,s_2]\), where the notation analogously applies to \(\hat{S}^\text{cut}\); cf. figure 6 for an illustration in two spatial dimensions.

Within each bracket, the volume of a truncated polyhedron can be parametrized by a cubic polynomial in \(s\) and \(t\), respectively. Note that, globally, i.e. on \(\bigcup B_i\) and \(\bigcup B_i^\text{cut}\), the volume is strictly monotonous and at least continuous\(^\text{3}\). The target brackets \(B^*\) and \(B^\text{cut,*}\), respectively, contain the sought roots \(s^*\) and \(t^*\).

\(^\text{3}\)An in-depth analysis of the regularity can be found in \([8, \text{note 2.1}]\)
The positioning problem comprises two conceptually distinct subtasks: the efficient **computation of the volume** of truncated polyhedra as well as the **root-finding** of the scalar volume function. The present paper resorts to the root-finding algorithm of Kromer and Bothe [8], which was shown to be very efficient for several classes of polyhedra and an extensive set of combinations of volume fractions and normals; cf. appendix A for a description. The necessary adaptation of the volume computation will be the subject of the remainder: section 2 outlines the general mathematical strategy for sequential truncation, while section 3 provides the details for the numerical treatment. Before that, however, it is instructive to consider the possible configurations of the input data \( \{n_\Gamma, \alpha^*\} \).

**Topological configurations.** The sequential positioning may encounter different configurations, which are illustrated in figure 7 from left to right:

- **triple:** In a triple configuration, the intersection \( \Psi \) of the planes is partially contained within the convex hull of the cell, i.e. \( \Psi \cap \text{conv} (P) \neq \emptyset \). Note that, for non-convex polyhedra, this does not necessarily correspond to a "physical" triple line, since \( \Psi \cap P \) may be empty; cf. the right panel in figure 10.

- **fully wetted:** As the name suggests, a configuration of this type features a primary plane whose intersection with the polyhedron is fully contained in the negative halfspace of the secondary plane, i.e. \( (\Gamma_1 \cap P) \subset H^-_2 \).

- **fully wetted (parallel degenerate), \( \langle n_{\Gamma_1}, n_{\Gamma_2} \rangle = 1 \):** The planes \( \Gamma_1 \) and \( \Gamma_2 \) are aligned, implying that the negative halfspace of \( \Gamma_1 \) is a subset of the negative halfspace of \( \Gamma_2 \). Thus, the secondary positioning problem corresponds to a translated version of the first one, i.e. \( \{\alpha_2^*, n_{\Gamma_2}^*, P^{\text{cut}}\} \equiv \{\alpha_1^* + \alpha_2^*, n_{\Gamma_2}, P\} \), both of which can be solved independently.

- **non-wetted:** If the negative halfspaces of \( \Gamma_1 \) and \( \Gamma_2 \) do not overlap in the polyhedron, i.e. if \( (H^-_1 \cap H^-_2) \cap P = \emptyset \), the configuration is denoted non-wetted.

- **anti-parallel:**
non-wetted (anti-parallel degenerate, \( \langle n_{\Gamma_1}, n_{\Gamma_2} \rangle = -1 \)): The negative half-spaces of \( \Gamma_1 \) and \( \Gamma_2 \) do no overlap at all, implying that the primary truncation of the polyhedron \( P \) does not affect the secondary truncation. Thus, \( \{ \alpha_2^*, n_{\Gamma_2}, P_{\text{cut}} \} \equiv \{ \alpha_1^*, n_{\Gamma_1}, P \} \), and one may solve \( \{ \alpha_1^*, n_{\Gamma_1}, P \} \) and \( \{ \alpha_2^*, n_{\Gamma_2}, P \} \) independently.

Note that the aforementioned degenerations, which significantly reduce the problem complexity, can be assessed from the input data. Accordingly, the remainder of this paper focuses on the non-degenerate cases, i.e. \(|n_{\Gamma_1}, n_{\Gamma_2}| < 1\). In other words, in what follows, the primary and secondary plane are assumed to admit a non-empty intersection \( \Psi = \Gamma_1 \cap \Gamma_2 \).

**Remark 1.1 (Ambiguity of degeneration).** It is worth noting that the above definition of degeneration is not unique. As can be seen in the rightmost panel in figure 7, a parallel orientation, i.e. \( \langle n_{\Gamma_1}, n_{\Gamma_2} \rangle = 1 \), is not a necessary condition for \( \{ \alpha_2^*, n_{\Gamma_2}, P_{\text{cut}} \} \equiv \{ \alpha_1^*, \alpha_2^*, n_{\Gamma_2}, P \} \). In fact, one requires \( (\Gamma_1 \cap P) \subset (P_{\text{cut}} \cap H_{\Gamma_2}^{-}) \) for a fully wetted configuration, which may correspond to any \( \langle n_{\Gamma_1}, n_{\Gamma_2} \rangle \in [-1, 1] \). While such a more general definition obviously reduces the computational effort, its robust detection based on the input data becomes considerably involved, especially for non-convex polyhedra.

## 2 Volume computation for twice truncated polyhedra

For the sequential truncation of an arbitrary polyhedron, the efficient computation of the volume introduced in Kroner and Bothe \[8\] requires some conceptual adaptation. However, the analytical considerations concerning the regularity directly apply to the sequential truncation. Hence, instead of reproducing them here, the interested reader is referred to \[8, subsection 2.1\]. By application of the Gaussian divergence theorem, the volume of a truncated polyhedron \( P \) with outer unit normal \( n_P \in \{ n_F^\tau \} \) can be expressed as

\[
|H_{\Gamma_1}^{-} \cap P| = \int_{H_{\Gamma_1}^{-} \cap P} 1 dx = \frac{1}{3} \int_{\partial(H_{\Gamma_1}^{-} \cap P)} \langle x - x_T, n_P \rangle d\sigma \\
= \frac{1}{3} \left( \sum_k \langle x_k^\tau - x_T, n_k^\tau \rangle |H_{\Gamma_1}^{-} \cap F_k| + \langle x_{\Gamma,0} - x_T, n_{\Gamma_1} \rangle + s \right) |\Gamma_1 \cap P|,
\]

i.e. as a sum of face-based quantities, each of which is a binary product of the immersed area and the signed distance to an arbitrary but common origin \( x_T \). For a single truncation, one of the boundary segments is located on the truncating plane, namely \( \Gamma_1 \cap P \). Its contribution to eq. \[5\] becomes zero if one chooses any origin \( x_T \) coplanar to \( \Gamma_1 \), i.e. \( \langle x_T - x_{\Gamma,0}, n_{\Gamma_1} \rangle + s = 0 \). In the two-dimensional sketch in the center panel of figure \[8\] this corresponds to translating the point marked by \( \bullet \) along the dashed line. Analogous to eq. \[5\], the volume of a sequentially truncated polyhedron reads

\[
|H_{\Gamma_2}^{-} \cap P_{\text{cut}}| = \frac{1}{3} \left( \sum_k \langle x_k^\tau - x_T, n_k^\tau \rangle |H_{\Gamma_2}^{-} \cap H_{\Gamma_1}^+ \cap F_k| \right. \\
+ \left. \langle x_{\Gamma,0} - x_T, n_{\Gamma_1} \rangle + s \right) |\Gamma_1 \cap H_{\Gamma_2}^{-} \cap P| + \langle x_{\Gamma,0} - x_T, n_{\Gamma_2} \rangle + t \right) |\Gamma_2 \cap P_{\text{cut}}|,
\]

where the boundary contains two segments \( \Gamma_1 \cap H_{\Gamma_2}^{-} \cap P \) and \( \Gamma_2 \cap P_{\text{cut}} \), respectively located on the truncating planes. In order to eliminate both contributions to eq. \[6\], \( x_T \) needs to be coplanar to both \( \Gamma_1(s) \) and \( \Gamma_2(t) \),
corresponding to \( \langle \mathbf{x}_T - \mathbf{x}_{T,0}, \mathbf{n}_{T_i} \rangle + s = 0 \) and \( \langle \mathbf{x}_T - \mathbf{x}_{T,0}, \mathbf{n}_{T_i} \rangle + t = 0 \). Thus, the origin \( \mathbf{x}_T \) looses one tangential degree of freedom, i.e. it can only be translated along the intersection \( \Psi = \Gamma_1 \cap \Gamma_2 \). In the two-dimensional sketch in the rightmost panel of figure 8, the line of intersection \( \Psi \) degenerates to a point (●).

Figure 8: Computation of the area of face \( F_k \) immersed in the negative halfspace of the primary (blue) and secondary (red) plane. The bold lines (center/right) indicate the boundary segments with non-zero contribution to eqs. (5) and (6), respectively, assuming the depicted origins \( x_{0,k} \) (●/●). For the primary truncation (center), the last constraint in eq. (8) drops out, implying that \( \mathbf{x}_{0,k} \) can be translated along the dashed line. In the presence of a secondary plane (right), however, the choice of \( x_{0,k} \) which simultaneously eliminates the plane contributions is unique.

**Immersed face area.** Let \( F_k^\text{cut} := \mathcal{H}^+ \cap F_k \). By recursive application of the Gaussian divergence theorem, the secondary immersed area \( |\mathcal{H}_2^+ \cap F_k^\text{cut}| \) on face \( F_k \) becomes

\[
|\mathcal{H}_2^\text{cut} \cap F_k^\text{cut}| = \frac{1}{2} \sum_{m} \langle x_{k,m}^F - x_{0,k}, N_{k,m} \rangle |\mathcal{H}_2^+ \cap \mathcal{H}_2^- \cap E_{k,m}|
\]

\[
+ \frac{1}{2} \left( y_{\Gamma_1,k} - x_{0,k}, \frac{n_{\Gamma_1} - \langle n_{\Gamma_1}, n_{k}^F \rangle n_{k}^F}{1 - \langle n_{\Gamma_1}, n_{k}^F \rangle^2} \right) |\Gamma_1 \cap \mathcal{H}_2^- \cap F_k|
\]

\[
+ \frac{1}{2} \left( y_{\Gamma_2,k} - x_{0,k}, \frac{n_{\Gamma_2} - \langle n_{\Gamma_2}, n_{k}^F \rangle n_{k}^F}{1 - \langle n_{\Gamma_2}, n_{k}^F \rangle^2} \right) |\Gamma_2 \cap F_k^\text{cut}|
\]

(7)

with arbitrary points \( y_{\Gamma_i,k} \) coplanar to both \( F_k \) and \( \Gamma_i \) (●/● in figure 8 illustrate some candidates). In order to eliminate the last two contributions in eq. (7), after some manipulations, one finds that the origin \( x_{0,k} \) associated to the face \( F_k \) is subject to three scalar constraints:

\[
\begin{align*}
\langle x_{0,k} - x_{k,1}^F, n_{k}^F \rangle & = 0 \quad (\text{coplanar to } F_k), \\
\langle x_{0,k} - x_{T,0}, n_{\Gamma_1} \rangle & = s \quad (\text{coplanar to } \Gamma_1(s)), \\
\langle x_{0,k} - x_{T,0}, n_{\Gamma_2} \rangle & = t \quad (\text{coplanar to } \Gamma_2(t)),
\end{align*}
\]

(8)

 corresponding to a unique choice; cf. the right panel in figure 8 for an illustration.

**Remark 2.1** (Multiple truncation). A secondary implication of eq. (5) is that the Gaussian divergence theorem cannot be employed to generalize this concept for positioning more than two planes sequentially, since the choice of \( x_{0,k} \in \mathbb{R}^3 \) would be subject to more than three constraints. For a multi-material application, with, say, \( M \) different materials, the topological connectivity of the truncated polyhedron must be re-established \( \lceil \frac{M-1}{2} \rceil \) times.
The upcoming section 3 derives the computational details of the strategy outlined above.

3 Computational details

The robust treatment of intersections requires a hierarchically consistent evaluation of the topological properties of vertices \( \{ x_{F,k,m} \} \) and edges \( \{ E_{k,m} \} \). With respect to the orientable hypersurface \( \Gamma_i \), described by the level-set function given in eq. (1), the logical status \( \mathcal{S}_i \) of any vertex is either interior (\( \mathcal{S}_i = -1 \)), intersected (\( \mathcal{S}_i = 0 \)) or exterior (\( \mathcal{S}_i = 1 \)). The hierarchically superior entity is an edge \( E \), whose status is an injective function of the status of its associated vertices \( \{ \nu_u, \nu_v \} \).

Table 1: Edge status as function of the status of the associated vertices; cf. note 3.1.

| \( \mathcal{S}_i(\nu_u) \) | exterior | interior | intersected | exterior | interior | intersected |
|-----------------|----------|----------|-------------|----------|----------|-------------|
| 1               | -1       | ±1       | -1          | 0        | 0        | 0           |
| \( \mathcal{S}_i(\nu_v) \) | 1       | -1       | ±1          | 0        | 1        | -1          |
| \( \mathcal{S}_i(E) \) | 1       | -1       | 0           | 2        | -2       | 3           |

An edge with at least one of its vertices located on \( \Gamma_i \) becomes degenerate, where the type of degeneration depends on the status of the remaining vertex; cf. table 1.

Note 3.1 (Floating point operations). For the purpose of numerical robustness, the status assignment employs a tubular neighborhood of thickness \( 2\epsilon_{\text{zero}} \) around \( \Gamma_i \), corresponding to the interval \((-\epsilon_{\text{zero}}, \epsilon_{\text{zero}})\). One obtains the logical status (with respect to the plane \( \Gamma_i \)) of a vertex \( x \) as

\[
\mathcal{S}_i(x) := \begin{cases} 
0 & \text{if } |\phi_{\Gamma_i}(x)| < \epsilon_{\text{zero}}, \\
\text{sign} \left( \phi_{\Gamma_i}(x) \right) & \text{if } |\phi_{\Gamma_i}(x)| \geq \epsilon_{\text{zero}}.
\end{cases}
\]

Thus, any point whose absolute distance to \( \Gamma_i \) falls below \( \epsilon_{\text{zero}} \) is considered to be on \( \Gamma_i \). Note that the choice of an appropriate tolerance strongly depends on the absolute value of the characteristic length of the polyhedron \( \mathcal{P} \). Throughout this work, we let \( \epsilon_{\text{zero}} := 10^{-14} \). In fact, all zero-comparisons are implemented in this way.

As outlined in section 2, we employ the Gaussian divergence theorem to compute the volume of the intersection of a polyhedron \( \mathcal{P} \) and the negative halfspace of a plane \( \Gamma_1 \) by

\[
\alpha_1(s) = \frac{1}{|\mathcal{P}|} \sum_k (\langle x_{F,k,1} - x_{\Gamma,0}, n_k \rangle + s\langle n_{\Gamma_1}, n_k \rangle) A_k^{\text{primary}}(s),
\]

where, for the reader’s convenience, we write \( A_k^{\text{primary}} := |\mathcal{H}_1 \cap F_k| \); cf. eq. (5). After finding the signed distance \( s^* \) corresponding to \( \alpha_1^* \), one obtains a truncated polyhedron \( \mathcal{P}^{\text{cut}}(s^*) := \mathcal{H}_1^+ \cap \mathcal{P} \). For the present application, we choose a representation in terms of truncated faces \( F_k^{\text{cut}} := \mathcal{H}_1^+ \cap F_k \), each of which corresponds to a list of truncated edges \( E_{k,m}^{\text{cut}} := \mathcal{H}_1^+ \cap E_{k,m} \); cf. figure 9 and note 3.2 for details. Note that, due to the intended application of the Gaussian divergence theorem, the truncated edges do not need to form a closed polygon. However, this presupposes the choice of a specific origin \( x_{0,k}(t; s^*) \) introduced in section 2 which we shall derive in what follows.
Note 3.2 (Truncated faces $F_{k}^{\text{cut}}$). The truncated edges $E_{k,m}^{\text{cut}}$ are obtained based on the logical status (cf. table 1) of the vertices $\{x_{k,m}^{\mathcal{F}}, x_{k,m+1}^{\mathcal{F}}\}$ of the original edge $E_{k,m}$:

$$E_{k,m}^{\text{cut}} := \begin{cases} \emptyset & \text{if the edge } E_{k,m} \text{ is } \Gamma_{1}\text{-interior, i.e. } \mathcal{G}(E_{k,m}) = -1, \\ E_{k,m} & \text{if the edge } E_{k,m} \text{ is } \Gamma_{1}\text{-exterior, i.e. } \mathcal{G}(E_{k,m}) = 1, \\ \text{conv} \left( x_{k,m}^{\mathcal{F}}, \hat{x}(s^{*}) \right) & \text{if the edge is intersected (} \mathcal{G}(E_{k,m}) = 0 \text{) and } \mathcal{G}(x_{k,m}^{\mathcal{F}}) = 1, \\ \text{conv} \left( \hat{x}(s^{*}), x_{k,m+1}^{\mathcal{F}} \right) & \text{if the edge is intersected (} \mathcal{G}(E_{k,m}) = 0 \text{) and } \mathcal{G}(x_{k,m}^{\mathcal{F}}) = -1, \end{cases}$$

(10)

where the intersection of the edge $E_{k,m}$ with the (primary) plane $\Gamma_{1}$ contains precisely the point

$$\hat{x}(s^{*}) = x_{k,m}^{\mathcal{F}} + \frac{s^{*} + (x_{\Gamma,0}^{\mathcal{F}} - x_{k,m}^{\mathcal{F}}, n_{\Gamma_{1}}^{\mathcal{F}})}{\langle x_{k,m+1}^{\mathcal{F}} - x_{k,m}^{\mathcal{F}}, n_{\Gamma_{1}}^{\mathcal{F}} \rangle} (x_{k,m+1}^{\mathcal{F}} - x_{k,m}^{\mathcal{F}}).$$

(11)

Equation (11) can be understood as follows: interior (exterior) edges are discarded (copied), while the $\Gamma_{1}$-interior vertex ($\mathcal{G}= -1$) of an intersected edge is replaced by the intersection with $\Gamma_{1}$. Figure 9 provides an illustration.

In analogy to the truncation of the original polyhedron $\mathcal{P}$, the secondary volume fraction is obtained by application of the GAUSSIAN divergence theorem to the truncated polyhedron $\mathcal{P}^{\text{cut}}$, i.e.

$$\alpha_{2}(t; \mathcal{P}^{\text{cut}}(s^{*})) = \frac{|\mathcal{H}_{2}^{\mathcal{F}}(t) \cap \mathcal{P}^{\text{cut}}(s^{*})|}{|\mathcal{P}|} = \frac{1}{2|\mathcal{P}|} \sum_{k} \Gamma_{0,k}^{V} + t \Gamma_{1,k}^{V} A_{k}(t; s^{*}),$$

(12)

where $A_{k} := |\mathcal{H}_{2}^{\mathcal{F}} \cap \mathcal{H}_{1}^{\mathcal{F}} \cap \mathcal{F}_{k}|$; cf. figure 8. Using the definitions from 1.2 the volume coefficients read

$$\gamma_{0,k}^{V} := \langle x_{k,1}^{\mathcal{F}}, y_{0}(s^{*}), n_{k}^{\mathcal{F}} \rangle \quad \text{and} \quad \gamma_{1,k}^{V} := \langle \tau_{\mathcal{F}}, n_{k}^{\mathcal{F}} \rangle.$$  

(13)

For ease of notation, we drop the asterisk for the primary signed distance for the remainder of this paper.

Note 3.3 (Rescaling). For reasons of numerical robustness, the secondary volume fraction in eq. (12) refers to the volume of the truncated polyhedron, i.e. $0 \leq \alpha_{2} \leq 1$. Thus, the target secondary volume fraction must be rescaled accordingly, i.e. $\alpha_{2}^{*}$ becomes $\frac{\alpha_{2}^{*}}{1 - \alpha_{1}^{*}}$. 

---

Figure 9: Original face $F_{k}$ (left) and associated truncation $F_{k}^{\text{cut}}$ (right; cf. note 3.2), defined as a list of truncated edges $E_{k,m}^{\text{cut}}$. The $\circ$ and $\blacksquare$ indicate the vertices of the original polygon and the intersections with $\Gamma_{1}$, respectively. Note that the edges $E_{k,m}^{\text{cut}}$ do not form a closed polygon, since the boundary segments located on the primary plane $\Gamma_{1}$ (dashed) are not contained.
3.1 The computation of the immersed area $A_k$

As stated in eq. (7), the computation of the immersed area exploits the Gaussian divergence theorem, i.e.

$$A_k = \frac{1}{2} \sum_m \langle x_{k,m} - x_{0,k}, N_{k,m} \rangle |E_{k,m}|. \quad (14)$$

For $\langle \mu, n_k^F \rangle \neq 0$, the origin $x_{0,k}$ is the unique intersection of $\Psi$ with the plane containing the face $F_k$, namely

$$x_{0,k}(t; s) = y_0(t) - \frac{\langle y_0(t) - x_{k,m}, n_k^F \rangle}{\langle \mu, n_k^F \rangle} \mu + t \left( \frac{\langle \tau, n_k^F \rangle}{\langle \mu, n_k^F \rangle} \mu \right) =: y_0(t) + t \tau_{\Psi,k}, \quad (15)$$

where eq. (3) contains the definition of the involved quantities. In general, the intersection will not be located in the convex hull of the face $F_k$, i.e. $x_{0,k} \notin \text{conv}(F_k)$; cf. figure [8].

Note 3.4 (Robustness). While $x_{0,k} \notin F_k$ poses no challenge in theory, a naive numerical evaluation suffers from severe loss of precision. To see why this is the case, let $h$ be the characteristic length associated to the face (e.g., the largest edge length, i.e. $h := \max_{m} |E_{k,m}|$) and assume the intersection of the planes $\Psi$ to be almost parallel to the face $F_k$, say, $|\langle \mu, n_k^F \rangle| = \epsilon$ with $\epsilon \ll 1$. Then, one obtains $\sup_m \{\langle x_{k,m} - x_{0,k}, N_{k,m} \rangle\} = O(\epsilon^{-1})$, whereas $\inf_m \{\langle x_{k,m} - x_{0,k}, N_{k,m} \rangle\} = O(h)$, i.e. the summands in eq. (14) admit values which may differ by several orders of magnitude. To circumvent this obstacle, the computation of the area must take into account the intersection topology of the respective face $F_k$.

We introduce the coefficients

$$\gamma_{0,k,m}^A = \begin{cases} \langle x_{k,m} - y_0(t), N_{k,m} \rangle & \text{if } t \in [t_{k}^{\Psi,-}, t_{k}^{\Psi,+}], \\ \langle x_{k,m}, N_{k,m} \rangle + \frac{\langle x_{k,m} - x_{0,k}, n_{k}^F \rangle}{1 - \langle n_{k}^F, n_{G_2} \rangle^2} \langle N_{k,m}, n_{G_2} \rangle & \text{if } t \notin [t_{k}^{\Psi,-}, t_{k}^{\Psi,+}], \end{cases} \quad (16)$$

where, by replacing $n_{G_2}$ with $n_{G_1}$, it can be seen that the second case in the above equation corresponds to a choice of $x_{0,k}$ analogous to the primary plane truncation; cf. Kromer and Bothe [8, eq. (19)]. Then, the secondary immersed area can be cast as

$$A_k = \frac{1}{2} \sum_m \gamma_{0,k,m}^A (s) + \tau_{1,k,m}(s) \begin{cases} \ell(E_{k,m}; t) & \text{if } t \in [t_{k}^{\Psi,-}, t_{k}^{\Psi,+}], \\ \ell(E_{k,m}; t) & \text{if } t \notin [t_{k}^{\Psi,-}, t_{k}^{\Psi,+}], \end{cases} \begin{cases} A_{k_{\text{primary}}} & \text{if } t > t_{k}^{\Psi,+} \\ 0 & \text{if } t \leq t_{k}^{\Psi,+} \end{cases} \quad (17)$$

with the immersed edge length $\ell(E; t) := |H_{k}^{-}(t) \cap H_{k}^{+}(s^*) \cap E|$ and the parameters

$$t_k^+ := \min_m \{ \phi_{G_2}(x_{k,m}) : \phi_{G_1}(x_{k,m}) \geq 0 \} \quad \text{and} \quad t_k^{-} := \min \{ \phi_{G_2}(x) : x \in \Gamma_1 \cap F_k \}, \quad (18)$$

where $t_k^{\Psi,+}$ and $t_k^{\Psi,-}$ are defined analogously with the respective maxima. See figure [10] for an illustration.

Remark 3.1 (Geometric interpretation). By $t_k^+$ ($t_k^{\Psi,+}$), we denote the smallest (largest) value of the signed distance $t$ for which the face $F_k$ is intersected by the PLIC plane $\Gamma_2$. For any $t \in [t_k^{-}, t_k^{\Psi,+}]$, the intersection $x_{0,k}(t)$ of the triple line $\Psi$ with the plane containing $F_k$ is contained in the convex hull of $F_k$. The case selection in eqs. (14) and (17) circumvents the numerical pitfall discussed in note 3.4.
Figure 10: Illustration of the delimiting parameters in eq. (18) for the computation of the immersed area $A_k$ of a truncated face $F_k$ with different intersection configurations. In the left panel, the intersection of $\Psi$ with the plane containing $F_k$ (●) is not located in its convex hull, implying that the original edges $E_{k,m}$ (bold) can be employed for the area computation (second case in eq. (17)). In the right panel, with $x_{0,k} \in \text{conv}(F_k)$, the truncated edges $E_{k,m}^\text{cut}$ (bold) are employed (first case in eq. (17)).

Equation (17) can be interpreted as follows: if $t \in [t_\Psi^-, t_\Psi^+]$, i.e. if $\Psi$ intersects the convex hull of $F_k$, the area is computed from the truncated edges $E_{k,m}^\text{cut}$ associated to $F_k$; cf. the right panel in figure 9. For $t < t_\Psi^-$, the negative halfspaces of $\Gamma_1$ and $\Gamma_2$ do not overlap in $F_k$, implying that the immersed area $A_k$ can be computed from the original (i.e., non-truncated) edges $E_{k,m}$. If the secondary PLIC plane $\Gamma_2$ does not intersect $F_k^\text{cut}$, one trivially obtains

$$A_k = \begin{cases} 0 & \text{if } t \leq t_k^-, \\ |F_k| - A_k^\text{primary} & \text{if } t \geq t_k^+. \end{cases}$$

(19)

**Note 3.5 (Topological classification).** Equation (19) induces a status of the faces, which allows to hierarchically infer the topological classification of the polyhedron described in figure 7. For a given signed distance $t$, the status is non-wetted if $t \leq \min_k t_k^-$, fully wetted if $t \geq \max_k t_k^+$ and triple otherwise.

The immersed edge length $\ell$ of a non-degenerately intersected ($\mathcal{S}_1 = 0$, cf. table 1) edge $E$ with vertices $\{\nu_1, \nu_2\}$ is computed as

$$\ell(E; t) = \|\nu_1 - \nu_2\| \begin{cases} \gamma_0^f + t\gamma_1^f & \text{if } \mathcal{S}_2(\nu_1) = -1, \\ 1 - \gamma_0^f - t\gamma_1^f & \text{if } \mathcal{S}_2(\nu_1) = 1, \end{cases}$$

(20)

with the generic coefficients

$$\gamma_0^f = \frac{\langle x\Gamma_0, \nu_1, n\Gamma_2 \rangle}{\langle \nu_2 - \nu_1, n\Gamma_2 \rangle} \quad \text{and} \quad \gamma_1^f = \frac{1}{\langle \nu_2 - \nu_1, n\Gamma_2 \rangle}.$$
For non-intersected edges ($S_1 \neq 0$, cf. table 1), one obtains

$$\ell(E) = \begin{cases} 0 & \text{if } S_1(E) \in \{1, 2\}, \\ ||\nu_1 - \nu_2|| & \text{if } S_1(E) \in \{-1, -2, 3\}. \end{cases}$$

(22)

**Remark 3.2** (Regularity). The status-based assignment in eq. (22) corresponds to assigning the left-sided limit to the derivatives of the immersed area $A_k$ with respect to $t$ for $t \in \{\langle x_{k,m}^2 \rangle - x_{T,0}^2, n_{T_2} \rangle\}$, i.e. when the plane $\Gamma_2$ passes through one of the faces vertices; cf. subsection 2.2 (Topological properties of geometric entities) in Kromer and Bothe [8].

For an original edge $E_{0,k,m}$ with $\nu_1 := x_{k,m}^2$ and $\nu_2 := x_{k,m+1}^2$, eq. (21) becomes

$$\gamma_{0,k,m}^{\ell} = \frac{x_{k,m+1}^2 - x_{k,m}^2}{x_{k,m+1}^2 - x_{k,m}^1, n_{T_2}} \quad \text{and} \quad \gamma_{1,k,m}^{\ell} = \frac{1}{x_{k,m+1}^2 - x_{k,m}^2, n_{T_2}}.$$  

(23)

The specific form of eq. (21) for a truncated edge $E_{k,m}^{cut}$ (cf. note 3.2 for the respective assignment of $\nu_1$ and $\nu_2$), depends on the logical status $S_1$ (see table 1) of its vertices with respect to the primary plane $\Gamma_1$, i.e.

$$\left\{ \gamma_0^{\ell}, \gamma_1^{\ell} \right\}_{k,m} = \begin{cases} \left[ \frac{\langle x_{\Gamma,0} - x_{k,m+1}^2, n_{T_2} \rangle}{\langle x_{k,m+1}^2 - x_{k,m}^2, n_{T_2} \rangle} \right] & \text{if } S_1(x_{k,m}^2) = -1, \\ \left[ \frac{\langle x_{\Gamma,0} - x_{k,m}^2, n_{T_2} \rangle}{\langle x_{k,m+1}^2 - x_{k,m}^2, n_{T_2} \rangle} \right] & \text{if } S_1(x_{k,m}^2) = 1, \end{cases}$$

(24)

**Remark 3.3** (Computational efficiency). Note that the coefficients in eq. (23) and eq. (24) are static in the sense that they are computed only once (after the primary plane $\Gamma_1$ is positioned).

The formulation of eq. (17) as a product allows to conveniently evaluate the derivatives of $A_k$ with respect to $t$, which are required for the root-finding part of the positioning procedure; cf. appendix A. So far, we have successfully extended the highly efficient divergence-based volume computation to twice truncated polyhedra.

### 4 Numerical experiments

With the volume computation of a sequentially truncated polyhedron, cf. eq. (12), at hand, figure 11 provides a flowchart of the adapted positioning algorithm.

As stated above, the present paper introduces an extension of the work of Kromer and Bothe [8] in terms of the volume computation for a twice truncated polyhedron. However, as can be seen in figure 11 the root-finding part, which was probed with an extensive set of normals and volume fractions for different convex and non-convex polyhedra, remains unchanged. In terms of the number of polyhedron truncations, constituting the relevant measure for computational effort, the root-finding algorithm of Kromer and Bothe [8] exhibits high efficiency: on average, the positioning requires 1–2 polyhedron truncations, thus outperforming existing methods; cf. appendix A. Hence, the authors consider it sufficient to conduct only a small set of numerical experiments. As pointed out by Marić [10], a meaningful assessment requires to consider the limiting cases of almost empty ($\alpha^* \approx 0$) or full ($\alpha^* \approx 1$) cells, where, for two planes to be positioned, all combinatorial configurations need
to be examined. Furthermore, while the volume fraction is invariant under linear transformations, the normal $n_\Gamma$ becomes distorted in general. In numerical experiments, this effect must be compensated by a sufficiently resolved sample set for $n_\Gamma$; cf. [8, note 1.2]. Subsection 4.1 covers the details of artificially generated instances. In order to assess the performance of our algorithm in comparison to existing methods, we restrict ourselves to cubes for the numerical tests. The reason for this is twofold:

1. The root-finding method employed was shown to be highly efficient for several classes of polyhedra [8]. Thus, only the augmented volume computation remains to be assessed. Due to the face-based formulation, the computational demand of the volume computation increases linearly with the number of faces, but is otherwise independent of the polyhedron topology. Hence, it is sufficient to consider a fairly simple polyhedron.

2. The flow solver, within which the present algorithm was originally implemented, resorts to a Cartesian mesh of cuboidal cells. The existing scheme, which will serve as a performance reference, combines a polyhedron decomposition for the volume computation with an accelerated bisection for the root-finding; cf. section 4.2 and appendix C for a detailed description.

### 4.1 Design of the numerical experiments

In the three-material case, the design of a meaningful numerical experiment, i.e. the sample sets for the normals and volume fractions, requires some preliminary considerations. While one can choose the normals $n_\Gamma_1$ and $n_\Gamma_2$ independently, the volume fractions must be chosen carefully, based on two user-defined tolerances $0 < \epsilon_1, \epsilon_2 \ll 1$ with $\epsilon_1 > \epsilon_2$. With $\epsilon_1$ being the most restrictive tolerance, note 3.1 induces the constraints

$$\epsilon_1 \leq \alpha_1^* \leq 1 - \epsilon_1, \quad \epsilon_1 \leq \alpha_2^* \leq 1 - \epsilon_1 \quad \text{and} \quad \epsilon_1 \leq \alpha_1^* + \alpha_2^* \leq 1 - \epsilon_1.$$  \hspace{1cm} (25)

For the two-phase case, corresponding to a single plane to be positioned, Kromer and Bothe [8] investigate volume fractions $\alpha^*$ from a sample set $S_{\alpha^*} \subset [\epsilon_1, 1 - \epsilon_1]$, which admits logarithmic spacing for volume fractions in the vicinity of zero and one, i.e. for $\alpha^* \in [\epsilon_1, \epsilon_2] \cap [1 - \epsilon_2, 1 - \epsilon_1]$, and linear spacing otherwise, i.e. in $[\epsilon_2, 1 - \epsilon_2]$, respectively indicated by $\circ$ and $\bullet$ in figure 12.
Figure 12: Illustration of sampling strategy for volume fractions \((\alpha_1^*, \alpha_2^*) \in [0,1]^2\) for tolerances \(\epsilon_1, \epsilon_2\) with admissible (log: \(\circ\), lin: \(\bullet\)) and non-admissible (log: \(\circ\), lin: \(\bullet\)) configurations. Note that both volume fractions refer to the volume of the original polyhedron \(P\).

In other words, \(\epsilon_1\) numerically replaces zero and \(\epsilon_2\) indicates the transition from logarithmic to linear spacing. As in [2], for the remainder of this manuscript, we employ \(\epsilon_1 = 10^{-9}\) and \(\epsilon_2 = 10^{-5}\). A naive extension for \((\alpha_1^*, \alpha_2^*)\), however, comprises configurations violating the condition \(\alpha_1^* + \alpha_2^* \leq 1 - \epsilon_1\). Besides the admissibility, figure 12 illustrates another distinct feature of the sequential positioning: due to the numerical zero-detection discussed in note 3.1, the accuracy of the reconstruction loses its symmetry. This numerical artifact is best illustrated by considering the case \(\alpha_1^* = 1 - \epsilon_1\). Compressing the second and third expression in eq. (25) then produces the conflicting condition \(\epsilon_1 \leq \alpha_2^* \leq 0\), implying that, in a numerical sense, the secondary phase will be neglected because the cell is fully occupied by the primary phase. In order to enforce a tolerance of \(\epsilon_1\) for the secondary phase, the upper bound for the primary volume fraction effectively reduces to \(1 - 2\epsilon_1\), where an analogous statement holds vice versa. Thus, eq. (25) becomes

\[
\epsilon_1 \leq \alpha_1^* \leq 1 - 2\epsilon_1, \quad \epsilon_1 \leq \alpha_2^* \leq 1 - 2\epsilon_1 \quad \text{and} \quad \epsilon_1 \leq \alpha_1^* + \alpha_2^* \leq 1 - \epsilon_1, \tag{25}
\]

corresponding to the shaded green region in figure 12. With the sample sets for the normal and volume fractions

\[
S_{n^*}(M_{n^*}) := \left\{ \cos \varphi \sin \theta, \sin \varphi \sin \theta, \cos \theta \right\}, \quad \left( \varphi, \theta \right) \in \left[ \frac{\pi}{2 M_{n^*}}, 1, 2, \ldots, 2 M_{n^*} \right] \times \left[ 0, 1, \ldots, M_{n^*} \right],
\]

\[
S_{\alpha^*}(M_{\alpha^*}) := \left\{ 10^{-4} + \frac{m - 1}{M_{\alpha^*} - 1} \left( 1 - 2 \cdot 10^{-4} \right) : 1 \leq m \leq M_{\alpha^*} \right\} \cup \left\{ 10^{-9}, 10^{-8}, 10^{-7}, 10^{-6}, 10^{-5} \right\} \cup \left\{ 1 - 10^{-5}, 1 - 10^{-6}, 1 - 10^{-7}, 1 - 10^{-8}, 1 - 2 \cdot 10^{-9} \right\},
\]

one obtains the following sets for the tupels of normals and volume fractions:

\[
S_{\alpha^*}^2 := \left\{ \left( x, y \right) \in S_{\alpha^*} \times S_{\alpha^*} : x + y \leq 1 - \epsilon_1 \right\} \quad \text{and} \quad S_{n^*}^2 := S_{n^*} \times S_{n^*}. \tag{26}
\]

Note that the size of their dyadic product, corresponding to the total number of instances, grows very quickly: choosing the moderate resolutions \(M_{n^*} = 10\) and \(M_{\alpha^*} = 20\), one already obtains \(|S_{\alpha^*}^2 \times S_{n^*}^2| \approx 1.45 \times 10^7\).

\(^4\)At the poles, i.e. for \(\theta \in \{0, \pi\}\), the azimuthal angle \(\varphi\) carries no information. Hence, the size of \(S_{n^*}(M_{n^*})\) effectively reduces from \(2M_{n^*} (M_{n^*} + 1)\) to \(2 + 2M_{n^*} (M_{n^*} - 1)\).
4.2 Baseline for the performance comparison: A decomposition-based accelerated bisection approach

The present method was compared to an existing method in FS3D based on polyhedron decomposition for the volume computation and an accelerated bisection for the root finding. The algorithm is presented in further detail in appendix C as the description is only available in a Master’s Thesis in German [13]. Summarising, this decomposition-based and also sequential PLIC positioning approach works as follows:

1. Rotate coordinate system that \( \langle \mathbf{n}_\Gamma, \mathbf{e}_1 \rangle \geq \langle \mathbf{n}_\Gamma, \mathbf{e}_2 \rangle \geq \langle \mathbf{n}_\Gamma, \mathbf{e}_3 \rangle \).

2. Exploit congruency, i.e. \( \{\alpha^*, \mathbf{n}_\Gamma\} \mapsto \{1 - \alpha^*, -\mathbf{n}_\Gamma\} \) for \( \alpha^* < \frac{1}{2} \).

3. For a cube, the volume function can be explicitly inverted using the formulae from appendix B, implying that the tentative positioning (blue boxes in figure 17) is carried out directly.

4. The primary position \( s^* \) is found with the explicit method from appendix B.

5. The secondary position \( t^* \) is found iteratively inside the remaining polyhedron with an accelerated bisection which makes use of the two-phase positioning of an extended volume fraction inside the original polyhedron \( \mathcal{P} \) and an error calculation of the position \( t \) inside the remaining polyhedron \( \mathcal{P}^{\text{cut}} \), cf. appendix C. The error is a lower limit for the change required for the iteration limits, thus is utilized to accelerate the bisection root-finding.

6. The computation of the truncated volume \( \alpha_2(t; \mathcal{P}^{\text{cut}}) \) relies on geometric decomposition, namely a sum of tetrahedrons, which relies on the polyhedrons being convex.

Both the volume computation and the intersection of a polyhedron with a plane require the computation of the connectivity, which requires multiple computationally expensive comparing and sorting operations. This may still be feasible for the cuboid meshes the algorithm was designed for, but already for cuboids the new method has huge advantages resulting both from the efficient, more elaborate root-finding and the more efficient volume computation shown in section 3. For other, possibly non-convex meshes a decomposition-based approach becomes infeasible and a fast convergence of the root-finding even more advantageous.

4.3 Numerical results

In what follows, we conduct numerical experiments based on the data sampling strategy outlined in subsection 4.1. First, recall from figure 11 that the sequential character of the algorithm implies that the primary positioning is carried out independently. Hence, the number of secondary polyhedron truncations, i.e. the number of truncations applied to \( \mathcal{P}^{\text{cut}} \), constitutes the relevant performance measure. We aggregate the number of secondary truncations \( N \) for each pair of volume fractions \( (\alpha_1^*, \alpha_2^*) \) by defining the average over the normals, i.e.

\[
N_{av}(\alpha_1^*, \alpha_2^*) := \frac{1}{|\mathcal{S}_{\mathcal{P}}|^2} \sum_{i=1}^{M_{\mathcal{P}}} \sum_{j=1}^{M_{\mathcal{P}}} N(\alpha_1^*, \alpha_2^*, \mathbf{n}_{\Gamma,i}, \mathbf{n}_{\Gamma,j}). \tag{27}
\]

For the interpretation of the results, it is instructive to disaggregate the averaged number of truncations based on the topological classification given in figure 7, which can be one of the following: triple, fully wetted or non-wetted. Recall from figure 11 that the degenerated configurations (\(|\langle \mathbf{n}_{\Gamma_1}, \mathbf{n}_{\Gamma_2} \rangle| = 1\)) are excluded a priori.
Note 4.1 (Performance impact of input data in practical applications). It is worth noting that the relative incidence of the intersection topologies strongly depends on the input data, i.e., on the volume fractions and normals; cf. figure 13. The physical properties of the involved fluid phases induce individual and highly dynamic spectra of configurations: e.g., consider a droplet (secondary) impinging on a structured super-hydrophilic wall (primary) in ambient gas: right before the impingement, there are only non-wetted (cyan) configurations. Once the contact line starts to form, the majority of the three-phase cells contains a triple line (green). With the wetted area (fully wetted/orange) being of codimension one and the advancing contact line being of codimension two, the ratio quickly shifts towards fully wetted cells.

In view of an application within a parallelized solver, where the phase boundaries and triple line may comprise several processes, load balancing becomes relevant. Thus, it is of paramount importance to ensure a robust performance with respect to the intersection topology.

Figure 13: Relative incidence of intersection topology (in %; cf. figure 7) as function of primary and secondary volume fraction. E.g., most of the non-wetted configurations (rightmost) are obtained if both the primary and secondary volume fraction are very small, i.e. $10^{-9} \leq \alpha_1^*, \alpha_2^* \leq 10^{-4}$.

Figure 13 depicts the relative incidence of topological classifications encountered, as a function of the volume fractions $(\alpha_1^*, \alpha_2^*)$, where “×” denotes zero incidence, i.e. for each combination of $(\alpha_1^*, \alpha_2^*)$, the values in the panels add up to 100 (%). Also, recall from eq. (25) that the choice of volume fractions is restricted, reproducing the lower triangular structure of figure 12. By further averaging over all combinations of volume fractions, one obtains the accumulated ratio of incidences (% in parentheses), i.e. the fraction of the respective classification with respect to the total number of instances $|S_{n_1^*}^2 \times S_{n_2^*}^2|$. As can be seen from the rightmost panel, roughly two thirds (65.97%) of all instances under consideration feature a triple line. For instances with $\alpha_2^* \lesssim 10^{-4}$, no fully wetted configurations were encountered (center panel in figure 13). Analogously, non-wetted configurations do not occur for $\alpha_2^* \gtrsim 1 - 10^{-4}$ (right panel in figure 13). It is crucial to note that the depicted relative incidence strongly depends on the underlying sample set of the normals $S_{n_1^*}^2$, given in subsection 4.1. Also, figure 13 exemplifies the performance considerations of note 11, while triple configurations can be found for nearly all combination of $\alpha_1^*$ and $\alpha_2^*$, a wetted configuration requires the secondary volume fraction to exceed a certain threshold. Figure 14 compares the average number of secondary truncations $N_{nv}$ (see eq. 27) of the proposed
algorithm to the existing decomposition-based accelerated bisection scheme of Potyka \cite{13}, cf. appendix \cite{3}

![Diagram](image)

(a) proposed algorithm

![Diagram](image)

(b) decomposition-based accelerated bisection approach (cf. appendix \cite{3} and \cite{13})

Figure 14: Number of polyhedron truncations $N_{av}$ (see eq. \ref{eq:27}) required for positioning the secondary plane $\Gamma_2$ as function of primary and secondary volume fraction for present divergence-based (top row) and decomposition-based positioning (bottom row), disaggregated by intersection topology; cf. figure \cite{7}. Note the non-coinciding ranges, respectively indicated to the left and right of the colorbars.

The main implications can be cast as follows:

1. By comparing the maximum number of truncations, indicated to the left and right of the respective color bar, the proposed method maintains the high efficiency of the single positioning of \cite{8}. This is to be expected, since we have only changed the method of volume computation. For all possible intersection classifications from figure \cite{4}, our approach requires, on average, between 1.41 and 2 truncations for the positioning of the secondary plane. Note that, with 1.41 truncations on average, our algorithm performs best in the presence of a triple-line, accounting for roughly two thirds of the instances.

2. For wetted intersection topologies, the average number of truncations slightly increases as the secondary volume fraction $\alpha_2^*$ approaches the value below which the intersection topology changes ($\times$ in figure \cite{14}). An analogous phenomenon occurs for non-wetted intersections when the sum of volume fraction approaches $1 - \epsilon_1$, i.e. for almost full cells, as well as for two distinct combinations ($\{1 - 10^{-4}, 10^{-9}\}$ and $\{1 - 10^{-4}, 10^{-8}\}$). The fact that no evident pattern, besides the aforementioned, can be found highlights the robustness with respect to the values of $\alpha_1^*$ and $\alpha_2^*$.

3. As can be seen from figure \cite{14} (bottom row, left), for configurations of triple-type, the number of truncations required by the accelerated decomposition-based bisection approach\cite{14} strongly depends on the volume fraction combination, which can be explained as follows:

\footnote{For a full description, see appendix \cite{3}}

19
(a) An orders of magnitude difference between the present volume fraction inside the whole cell \( \alpha_2(t; \mathcal{P}) \) which is utilized in the iteration and the calculated error \( \Delta \alpha_2(t; \mathcal{P}^{\text{cut}}) \), which is utilized for the acceleration, but has diminishing effect in the case of a large difference. This is leading to an algorithm close to pure bisection for \( \alpha_2 \) smaller than \( \alpha_1 \), as the update with the error has close to no effect on the change of the iterated volume fraction inside the whole cell. If this happens for the initial bracketing values, the whole iteration is close to pure bisection.

(b) If \( \alpha_1^* \) is large compared to \( \alpha_2^* \), the initial bracketing interval for the iteration is quite large, while the interval is small at small \( \alpha_1^* \), cf. figure 19.

(c) The convergence is slow when the value looked for is relatively close to an initial bracketing value, thus the opposite bound requires multiple updates in the beginning.

(d) For some cases, multiple negative effects on the convergence behaviour occur together.

**Note 4.2 (Topological classification).** The figure below shows the number of intersection topology mismatches between the present and decomposition-based approach (in %, relative to the number of possible normal combinations \( |S_{\mathcal{P}^2}| \), where \( x \) indicates zero mismatches; cf. eq. (27)) as function of primary and secondary volume fraction (\( \alpha_1^*, \alpha_2^* \)) (overall quota: 0.47%. Note that the absolute accuracy of the positioning is not degraded by a mismatch).

While the topological classification of the present algorithm is based on the tolerance for the signed distance \( t \) (\( \epsilon_{\text{zero}} = 10^{-14} \)), cf. note 3.3, the decomposition-based approach employs the tolerance used for the volume fraction (\( \epsilon = 10^{-12} \)); if the error \( \Delta \alpha_2 \) in the volume fraction for an assumed non-wetted \( (t') \) or wetted \( (t'') \) configuration falls below \( \epsilon = 10^{-12} \), the respective classification is assigned. In all other cases, i.e. if both \( |\Delta \alpha_2(t')| \) and \( |\Delta \alpha_2(t'')| \) exceed \( \epsilon \), the triple classification is at hand; cf. figure 17 and appendix C. This conceptual difference may produce dissenting classifications in the vicinity of a transition between two classifications. Note that, in general, no fixed choice of length and volume tolerances capable of resolving this artifact exists. From the right panel in the above figure, the rationale emerges from a simple geometric consideration: for some given signed distance, say \( t \), a small variation \( \delta t \) translates to a change of the volume fraction \( \delta \alpha = \alpha(t + \delta t) - \alpha(t) \approx \delta t \frac{\partial \alpha_2}{\partial t} \). In other words, for a consistent choice, the length and volume tolerances would have to be adjusted to the dynamic amplification \( \delta \alpha / \delta t \).

5 Summary

We have proposed an efficient method for the computation of the volume of a twice truncated arbitrary polyhedron. Employing the GAUSSIAN divergence theorem, the volume computation reduces to a summation of quantities associated to the faces of the original polyhedron, thus eliminating the necessity to establish...
intersection-dependent connectivity at runtime. From the numerical experiments in section 4 we draw the following conclusions:

1. For all instances under consideration, the algorithm maintains the high efficiency of Kromer and Bothe [8]: on average, the secondary plane can be positioned with 1–2 truncations. Furthermore, no connectivity needs to be extracted after the first positioning.

2. The performance is almost invariant with respect to the topological configuration (triple/non-wetted/fully wetted), indicating the suitability of the present algorithm for parallel application; cf. note 4.1.

3. In comparison to the decomposition-based bisection approach, the number of truncations required for the positioning was substantially reduced. Also, the present approach does not share the limitation to cuboids. In fact, the range of applicability covers arbitrary polyhedra with planar faces.

Once more, these findings highlight the superiority of divergence-based volume computation, which, besides versatility, allows to easily obtain and exploit the derivatives of the parametrized volume.

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The figures and flowcharts in this manuscript were produced using the versatile and powerful library pstricks. For further details and a collection of examples, the reader is referred to the book of Voß [20] and https://tug.org/PSTricks/main.cgi respectively.

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A Implicit bracketing

This section heavily draws from a previous work of the first and last author; [8, sections 2.3 and 2.4].

Within a bracket $B_i := [s_i, s_{i+1}]$, the volume fraction $\alpha(s)$ is an increasing cubic polynomial, denoted by $S_i(s)$. For any given $s^* \in B_i$, the polynomial reads

$$S_i(z; s^n) = \frac{\alpha'''(s^n)}{6} (z - s^n)^3 + \frac{\alpha''(s^n)}{2} (z - s^n)^2 + \alpha'(s^n) (z - s^n) + \alpha(s^n).$$

(28)

Hence, the truncation of the polyhedron $P$ at any $s^n$ (implicitly) provides the full information of $\alpha(s)$ within the containing bracket $B_i$. Exploiting that $\alpha_i = S_i(s_i; s^n)$ and $\alpha_{i+1} = S_i(s_{i+1}; s^n)$ suggests the following strategy:

1. if the current iteration $s^n$ is not located in the target bracket $B^*$ ($\alpha^* < \alpha_i$ or $\alpha_{i+1} < \alpha^*$), the next iteration is obtained from locally quadratic approximation (figure 15 left).

2. if the current iteration $s^n$ is located in the target bracket $B^*$ ($\alpha_i \leq \alpha^* \leq \alpha_{i+1}$), the sought $s^*$ corresponds to the root of $S_i - \alpha^*$, requiring no further truncation (figure 15 center).

![Figure 15: Implicit bracketing and locally quadratic approximation of volume fraction $\alpha(s)$](image)

The initial guess is obtained from a global cubic spline interpolation via

$$s^0(\alpha^*) := s_- + (s_+ - s_-) \left( \frac{1}{2} - \cos \left( \frac{\arccos(2\alpha^* - 1) - 2\pi}{3} \right) \right)$$

(29)

with $s_- = \min(\hat{S})$ and $s_+ = \max(\hat{S})$; cf. eq. [4]. Figure 15 illustrates the components of the strategy outlined above: with $s^0 \notin B_i$ (left), a quadratic approximation yields $s^1$, which lies within the target bracket $B^* = B_i$ (center). The rightmost configuration already starts with $s^0 \in B^*$, such that the spline interpolation directly yields the sought position $s^*$, implying that only a single truncation is required.

B An explicit inverse of the cuboid volume function

Note that any cuboid with edge lengths $\{\Delta x_i\}_{i=1}^3$ can be transformed to the reference cube with $\Delta x_i \equiv 1$. Furthermore, one can always find a rotation such that the components of the normal $n_\Gamma$ are positive and arranged in descending order. Let $n_i := (n_\Gamma, e_i)$ for ease of notation. Assuming that the second and third component of $n_\Gamma$ are zero ($n_2 = n_3 = 0$), the positioning problem becomes degenerate and one trivially obtains $s^* = \alpha^* \Delta x$. For two non-zero components ($n_3 = 0$), the normal can be parametrized by the polar angle $\varphi$ with
\[ \tan \varphi = \frac{n_2}{n_1}, \text{ and one obtains} \]

\[
s^* = \Delta x \begin{cases} 
\sqrt{\alpha^* \sin 2\varphi} & \text{for } \alpha^* \leq \frac{\tan \varphi}{2}, \\
\sin \varphi + \cos \varphi \left( \alpha^* - \frac{\tan \varphi}{2} \right) & \text{for } \frac{\tan \varphi}{2} < \alpha^* < 1 - \frac{\tan \varphi}{2}, \\
\cos \varphi + \sin \varphi - \sqrt{(1 - \alpha^*) \sin 2\varphi} & \text{for } \alpha^* \geq 1 - \frac{\tan \varphi}{2},
\end{cases}
\]  

(30)

where, due to the symmetry, the second case degenerates for \( \varphi = \pi/4 \). If all components of \( n_F \) are non-zero, the position reads

\[ s^* = S_k(\alpha^*) \text{ for } \alpha^* \in (\hat{\alpha}_k, \hat{\alpha}_{k+1}] \]  

(31)

with

\[
\hat{\alpha} = \begin{cases} 
\left[ 0, \frac{n_2}{6n_1n_2} - \frac{(n_2 - n_3)^2}{6n_1n_2n_3}, \frac{n_2 + n_3}{2n_1}, \frac{1}{2} \right] & \text{for } n_1 \geq n_2 + n_3, \\
\left[ 0, \frac{n_2}{6n_1n_2} - \frac{(n_2 - n_3)^2}{6n_1n_2n_3}, \frac{n_2^2 - (n_2 - n_3)^2}{6n_1n_2n_3}, \frac{1}{2} \right] & \text{for } n_1 < n_2 + n_3,
\end{cases}
\]  

(32)

and

\[
S_1(\alpha^*) = \sqrt[6]{6} \alpha^* n_1 n_2 n_3, \\
S_2(\alpha^*) = \frac{n_3}{2} + \sqrt{2\alpha^* n_1 n_2 - \frac{n_3^2}{12}}, \\
S_3(\alpha^*) = n_2 + n_3 - \sqrt{8n_2 n_3} \cos \left( \frac{1}{3} \arccos \left( \frac{3}{8} \sqrt{\frac{2}{n_2 n_3}} (n_2 + n_3 - 2n_1 \alpha^*) \right) + \frac{\pi}{3} \right), \\
S_4(\alpha^*) = \begin{cases} 
\frac{2\alpha^* n_1 + n_2 + n_3}{2} + 2\sqrt{p} \cos \left( \frac{1}{4} \arccos \left( \frac{3q}{2p} \sqrt{\frac{n_2 n_3}{p}} \right) - \frac{2\pi}{4} \right) & \text{for } n_1 \geq n_2 + n_3, \\
\frac{n_1 + n_3}{2} + 2\sqrt{p} \cos \left( \frac{1}{4} \arccos \left( \frac{3q}{2p} \sqrt{\frac{n_2 n_3}{p}} \right) - \frac{2\pi}{4} \right) & \text{for } n_1 < n_2 + n_3,
\end{cases}
\]  

(35)

(36)

with

\[
p = \frac{3}{4} \left( 2n_2^2 - (n_1 + n_2 + n_3)^2 + 2n_2^2 + 2n_3^2 \right) \text{ and } q = \frac{3n_1 n_2 n_3}{2}(2\alpha^* - 1).
\]  

(37)

Note that the point-symmetry of the cube volume fraction \( \alpha^* \) can be exploited to extend eq. (31) to \( \alpha^* > \frac{1}{2} \); cf. figure 16 for an illustration. A similar set of formulae was derived in Scardovelli and Zaleski and Lehmann and Gekle.

C A decomposition-based accelerated bisection approach for cuboids

The idea of this decomposition-based sequential positioning in three-phase cells is, that the positioning for two-phase cells is reused. This is feasible, if the positioning in two-phase cells is fast. In the case of a Cartesian grid the two-phase position is retrieved from an explicit formula, cf. appendix B. Therefore the requirement of a fast algorithm for two-phases is fulfilled. The first PLIC plane is positioned with the two-phase algorithm shown in appendix B which is a function of the volume fraction \( \alpha_1 \), the normal \( n_F \), and the grid cell’s dimensions \( \Delta x \).

An iterative algorithm, which reuses the two-phase positioning, is utilized to position the second PLIC plane. The initial minimum and maximum value for \( t \) are defined by the two extrema of the interface’s orientations.
Figure 16: Intersection topology for cube with normal $n_\Gamma = [4.2,1]^{T}_{/21}$ ($n_1 > n_2 + n_3$, blue) and $n_\Gamma = [4.3,2]^{T}_{/29}$ ($n_1 < n_2 + n_3$, red) at $\alpha_k$ (vertical lines) from eq. (32) with the respectively intersected vertices ($\bullet$).

where no contact line occurs:

1. The two interfaces do not interact inside the cell, they are independent, thus $t' = S(\alpha_2^*)$ and $\alpha_2^- = \alpha_2(t'; P)$

2. The second interface, the one of the fluid, fully wets the first interface of the solid, thus $t'' = S(\alpha_1^* + \alpha_2^*)$ and $\alpha_2^+ = \alpha_2(t''; P)$.

The initial bracketing values for $\alpha_2(t; P)$ and their corresponding positions $t$ are depicted in figure 19. Both limits can be retrieved from the two-phase PLIC positioning, cf. appendix B. For each tentative position $t^n$ from the volume fraction $\alpha_2(t^n; P)$ enclosed inside the whole cell $P$ the volume fraction $\alpha_2(t^n; P^{\text{cut}})$ inside the remnant polyhedron $P^{\text{cut}}$ is computed. The error in the enclosed volume

$$\Delta\alpha_2(t^n, P^{\text{cut}}) = \alpha_2^* - \alpha_2(t^n, P^{\text{cut}})$$  \hspace{1cm} (38)

of the present secondary position is compared to the true volume fraction $\alpha_2^*$. If either the secondary position at the minimum $\alpha_2^-$ or maximum $\alpha_2^+$ volume fraction inside the whole cell $P$ already yield an error below a given tolerance, a further iteration of the second PLIC plane’s position is not necessary, i.e. the liquid does not wet or fully wet the solid as no intersection volume is computed. If a contact line exists, the required tolerance is not reached with those two extreme positions. The calculated error is reused to refine the initial values enclosed by the PLIC plane inside the whole cell, as the eq. (38) is also a lower limit for the required adjustment in the volume enclosed below the secondary plane inside the whole cell $\alpha_2(t^n; P)$ for the next iteration, cf. figure 18. Depending on the sign of $\Delta\alpha_2(t^n; P^{\text{cut}})$, either the upper bound $\alpha_2^+$ or the lower bound $\alpha_2^-$ is adjusted with $\Delta\alpha_2(t^n; P^{\text{cut}})$. Both volume fractions are corresponding to the extended PLIC planes, the enclosed volume fraction in $P$. Therefore for this updated volume fraction appendix B is applicable to calculate the next update of $t^n$. A faster convergence is reached by combining a bisection based update with the calculated error. In each iteration, the volume fraction’s error eq. (38) is evaluated and $\alpha_2^+$ or $\alpha_2^-$ updated depending on the sign of $\Delta\alpha_2(t^n; P)$ like described above until the given tolerance is fulfilled in addition to employing a minimisation with bisection. The calculation of the error $\Delta\alpha_2(t^n; P^{\text{cut}})$ is depicted in figure 18. The flowchart in figure 17.
Figure 17: Flowchart of the accelerated decomposition-based bisection approach of Potyka [13] with \( \Delta \alpha_2(t) = \Delta \alpha_2(t, P_{\text{cut}}) := \alpha_2^+ - \alpha_2(t; P_{\text{cut}}) \) and \( \epsilon = 10^{-12} \); cf. figure 18 for an illustration. \( \alpha_2^+ \) and \( \alpha_2^- \) refer to the whole cell \( P \), thus the tentative positioning is performed with the two-phase algorithm, cf. appendix B.

Figure 18: Update strategy for decomposition-based approach of Potyka [13]: effectively, the updated position \( t^{n+1} \) is obtained by re-distributing the deviation \( \Delta \alpha_2(t^n; P_{\text{cut}}) \). Note that the domain overlap and the deviation of the next iteration (crosshatch) are coextensive, i.e. they admit the same volume. In other words, as the iterative position \( t^n \) approaches the true position \( t^* \), the associated deviation vanishes, i.e. \( \Delta \alpha_2(t^n; P_{\text{cut}}) \to 0 \) as \( t^n \to t^* \). The error \( \Delta \alpha_2(t^n; P_{\text{cut}}) \) at the same time is a lower bound for the required change of the volume fraction enclosed inside the whole cell \( \alpha_2(t^n; P) \).
illustrates the described procedure to determine the planes’ positions.

For robust convergence a few special cases are considered:

- A tolerance is needed to ensure that \( \alpha_2(t_n; P) + \Delta \alpha_2(t_n; P_{\text{cut}}) \) does not overshoot or undershoot the minimum and maximum boundaries, if the new volume fraction corresponds to \( t^* \) except for rounding errors during the computation.

- If the polyhedron’s dimensions become as small that there is up to a tolerance no difference between the minimum or maximum vertex point of the cell and an intersection point, \( \alpha_2(t_n; P) = 0 \) is set at the minimum or \( \alpha_2(t_n; P) = 1 \) at the maximum for the initial bracketing values.

The volume error computation consists of an intersection of the remnant polyhedron \( P_{\text{cut}} \) with \( t_n \) and the volume computation itself. For the computation of the intersection, all vertices are marked, if they are above, below or on the plane. All points which are below the plane and on the plane belong to the new polyhedron, but also new points have to be computed which are intersection points of the plane with the segments where one point is above and one below the plane. The connectivity of the original and intersected polyhedron are computed for the computation of a new point. This requires the information of common faces, thus multiple comparison operations are necessary. The volume computation of the polyhedron exploits, that the polyhedrons resulting from sequential cuts of a cuboid with one or two planes is convex. From an origin inside the polyhedron the volumes of tetrahedra are summed up. For each tetrahedron the connectivity has to be computed again by multiple comparisons, if the corner points have common faces. This requires significant computational effort already for cuboids with two intersections resulting in convex polyhedrons.