Topological Aspects of Material Interface Reconstruction: Challenges and Perspectives

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Abstract. Multi-fluid simulations, especially volume of fluid datasets, confront visualization experts with the challenge of reconstructing appropriate material interfaces that accurately delimit fluid boundaries. In general this reconstruction problem does not have an unique solution, leading to possible spatial and temporal inconsistencies in the reconstructed interfaces. In this paper we present and discuss challenges and directions for topology based analysis of volume of fluid data and its interfaces. We investigate the suitability of established topological methods for solving these challenges, analyze their potential and drawbacks, and propose future research directions.

1 Introduction

Topological methods have long served the visualization community as fundamental tools to generate insightful methods for visual data analysis. These type of approaches have enabled the interpretation of ambiguous data in a robust fashion, and allowed the characterization of salient features in data through a notion of connectivity. Many applications have benefited in this respect, ranging from the reconstruction of molecular surfaces over the structural analysis of vector fields to the identification of biological structures.

Material Interface Reconstruction (MIR) – the reconstruction of boundary surfaces from volume averages or volume fractions – has so far received little attention from the research community with respect to a rigorous topological treatment. Corresponding simulation techniques that generate volume fraction data, have risen in popularity for some years. For example, the volume-of-fluid method (VOF) for multi-phase flows is often employed to model the flow of multiple fluids around moving boundaries. Through the implicit representation of fluid distribution in terms of volume fractions in the cells of a computational mesh, this method has proven strongly advantageous in comparison to other simulation techniques that involve re-meshing or explicit interface propagation through level sets, while achieving similar simulation accuracy [1]. Volume fraction data is not only limited to flow analysis, however, but is also found in modern medical applications, received through MRI or EM scans, and a variety of other domains. Thus, robust and reliable visualization and analysis methods are needed to accommodate this class of problems.
In general, as there is an infinite number of possible interfaces fitting given volume fraction, MIR is a vastly under-constrained problem. In order to arrive at practical approaches, previous approaches to MIR have mostly focused on adding constraints aimed at high-quality visualization, such as interface continuity and smoothness and accurate reproduction of volume fractions. While the resulting methods have proven sufficient for some application areas the topological configuration of the resulting interface has thus far not been studied in depth, nor incorporated as a primary factor in the reconstruction process.

In this paper, it is our intent to document the need for, and stimulate further research into the topological aspects of MIR. For this purpose, we briefly introduce the MIR problem and provide a short survey on state-of-the-art MIR algorithms. We focus on highlighting topological aspects of the discussed methods, and point out individual shortcomings. We conclude with a short discussion of possible avenues towards incorporating topological considerations into MIR techniques.

2 Topology and Material Interface Reconstruction

To understand the motivation behind integrating topological aspects into material interface reconstruction, we first briefly highlight the application of topological methods in a variety of research areas. This establishes a conceptual framework for the analysis of reconstruction methods as presented in the second half of this section.

2.1 Topology in Visualization

In scientific visualization the concept of topology allows for the analysis of an intuitive notion of connectivity of objects, providing an important tool to enrich classic analysis that is purely based on object geometry. Although the mathematical idea of topology came into focus of the visualization community around twenty years ago (cf. for example the work by Helman and Hesselink [2]), the variety of topological representations, methods, and analysis techniques has grown steadily. A complete survey is clearly beyond the scope of this paper; instead we highlight important work in computational topology that is closely related to the challenges presented in this paper.

A large body of work has been published about the notion of vector field topology in flow simulations. One goal of such topological approaches is to go beyond the geometrical representation of flows and find regions where streamlines behave similarly in their limit, i.e. share common sources and sinks. Two examples of work in this field are given by Reich et al. [3] and Scheuermann et al. [4]. Note that while a large portion of MIR data stems from flow simulations, volume fractions itself lack in general the information about flow direction and velocity hence methods from vector field topology are often not applicable.

Scalar field topology constitutes a second major area in the fields of topological analysis and visualization, where topology is used to identify critical features
like minima, maxima, and their corresponding plateaus and basins. Topology was integrated into visual analysis tools to provide abstract views onto the fields, especially benefitting large and high dimensional data sets [5,6]. Moreover, topological field abstraction and simplification can also be used to intuitively compare different scalar fields [7]. For two-material cases, the input data for material interface reconstruction techniques corresponds to a scalar field representing the local density of one of the two materials, i.e. volume fractions.

The capability of topological abstractions to facilitate high-level comparisons of features has spawned a third focus of topology analysis that is driven by the desire to track and compare identified (topological) features in vector or scalar fields over time. For example, Weber et al. [8], Edelsbrunner et al. [9], or Szymczak [10], make use of Reeb graphs and contour trees data representations to achieve tracking and efficient comparisons.

In all these publications it becomes clear that topological methods are a valuable extension to the classic geometrical visualization and analysis. As we demonstrate in the following, the challenges present in material interface reconstruction resemble classic problems studied in topological analysis, leading us to expect that strong potential improvements can be obtained from combining these two areas of research.

2.2 Material Interface Reconstruction

Although MIR and topological analysis have common application areas like flow simulation and medical visualization, they are relatively new approaches in visualization. Interaction between both research directions has so far been limited. Hence, the impact, influence, and challenges of topological methods in MIR have not yet been studied in a concise fashion. To encourage such studies, we first summarize the MIR problem definition and existing work in the field before discussing challenges and perspectives of topological analysis in MIR.

**Reconstruction Problem** MIR problems can be found in research fields like computational fluid dynamics or medicine, where multi-fluid simulations or medical scans are a typical source of data. The technical and computational limits of those simulation and measurement techniques lead to discretized and approximated data. Inaccurate scans, the need of fast algorithms and impracticality of continuous representations therefore force a discretization of the original domain \( D \), usually \( D \subseteq \mathbb{R}^2 \) or \( D \subseteq \mathbb{R}^3 \) into finite number of cells.

Instead of the providing pointwise material properties, the result of the scans and simulations is approximated over those cell. One example of such an approximation is the *volume-of-fluid* (VOF) method [11], in which for each cell only the volumes of the different fluids or materials as a fraction of the cell’s total volume are given. Although there are other methods that approximate the original data, e.g. through mass conserving density fields [12], we focus on VOF-type data throughout this work.

Formally, for a set of \( n \) materials, each cell in the domain corresponds to an \( n \)-dimensional vector over the interval \([0, 1]\) which indicates the fraction of each
material present in that cell. Note that in some representation only a \( (n - 1) \)-dimensional vector is used since the last fraction is given implicitly. For two materials this results in a scalar-field representation of the data.

As an example, consider a section of a flow simulation in a finite tank \( T \subset \mathbb{R}^3 \) with two materials as illustrated in Figure 1. The left images shows the original simulation and the segmentation of the domain into four cells, while the right image only shows the volume fractions for each of these cells.

![Fig. 1. Volume fractions in a two-material example.](image)

Each cell \( c \) is either pure, i.e. it is completely filled with one material, or contains multiple materials and hence a boundary (interface) between the two materials. Note however that the geometric information of the interfaces is not contained in this approximation.

Hence, a series of methods were introduced to reconstruct those boundaries with the ultimate goal of obtaining the material interfaces. However, Figure 2 illustrates that this is a strongly under-determined problem if only the volume fractions are given since all of the shown material surfaces produce the volume fractions as given by the data (Figure 1 (right)) exactly. Furthermore note the significant difference in interface properties such as smoothness and topology among these examples.

![Fig. 2. Several sketches of interfaces that accurately provide the same volume fraction as in Figure 1. This illustration demonstrates the ambiguity of the MIR problem.](image)

It is clear that interface reconstruction is an infeasible task without the availability of further prior knowledge of interface properties. However, since those
properties and of course the original data itself are usually unknown, this requirement is usually dropped. Instead reconstructions focus on reproducing volume fractions accurately while fulfilling other more abstract requirements such as continuity or smoothness. This additional, important family of requirements rises from the needs in visualization to obtain meaningful surface structures with appropriate normal approximations. While for fluids smooth surfaces with $C^1$ or higher continuity are preferred, in object scans reconstruction results that are able to model sharp edges and may therefore be $C^0$ often come closer to the original data. By adding and prioritizing different requirements including computational efficiency and scalability, stability over time, etc., a wide range of different reconstruction methods were developed. To give an adequate overview the next section provides a compact survey of MIR methods.

![Fig. 3. Four sketches of the same cell showing the results of different reconstruction methods. The partially seen cells are all pure while the center cell has an original volume fraction of (0.28, 0.72).](image)

**Reconstruction Methods** One of the first methods, by Noh and Woodward [13], simply moves sequentially for each material an axis-parallel plane through each cell until the volume fractions in the reconstruction match the prescribed volume fractions. This method, called *Simple Line Interface Calculation* (SLIC), obviously does not produce continuous interfaces. See, for example in Figure 3(a) the border between the center and the partial shown pure cell in the middle-left.

Even an extension, namely *Piecewise Linear Interface Calculation* (PLIC) by Youngs [14], which moves the plane along a gradient computed from the volume fraction in the neighbor cells does not produce continuity. Figure 3(b) shows a simple sketch of such a reconstruction with the arrow indicating the gradient of respective material volume fractions. Hence for realistic visualization of fluids new approaches were required which specially focus on smoothness.

The current approaches can be classified either as grid-based or as discrete methods. Grid-based methods move from cells to dual meshes like Bonnell et al. [15] or to grids like in Feng et al. [16] or Meredith [17] where information is stored at the cell corners. The latter method by Meredith for example averages
the fractions of the adjacent cells at each corner. Sequentially for each material an interpolation function over those average values places a plane in the cell. Since the different grids cells share common corners with their neighbors the resulting interfaces are generally continuous. Figure 3(c) shows the averages for the first material at each corner while the second values follow implicitly.

Note however that in all those grid-based methods the original fraction information in the cells is lost, which results in errors in the volume reconstruction for most cells. This is illustrated in Figure 3(c) in which the volume fraction is changed from (0.28, 0.72) to (0.5, 0.5). In summary, accuracy within single cells was traded off in favor of smoother interfaces over the whole domain.

Another class of approaches therefore focuses more on the accuracy requirement. First exemplified by the method of Anderson et al. [18] (termed DA in the following), these approaches first discretize each cell into smaller subcells or single particles, each randomly labeled with a material such that their labeling approximates the volume fraction of the cell. An energy function based on the subcells models desirable interface properties. Using simulated annealing by swapping random pairs of subcells, the subcells iteratively move to a minimal configuration, see Figure 3(d).

Extensions, like the method by Anderson et al. [19] (SA) use the subcells next to material borders in the final configuration as base for interpolating a continuous interface. Or, as in Garimella et al. [20], use the centroids of the different material particles for a power diagram [21] to built a determine interfaces. Especially for SA the question arises whether these extensions also change the topology of the interfaces with respect to the DA method. Furthermore, with regard to the discrete method, it is unclear whether the simulated annealing algorithm also leads to different topologies when applied twice on the same data.

Not only these internal changes of topology but also in general the varying topologies between different reconstructions and between those and the original data are known and pointed out in most of the mentioned publications. However, thus far this aspect of MIR has never been pursued in detail or analyzed thoroughly, and tools to analyze those ambiguities and therefore also the differences in the reconstruction methods have not been discussed in the literature. In the following we aim towards analyzing challenges, solutions, and perspectives of (automatic) topological analysis of the MIR task.

3 Challenges and Directions

In the following we present a set of scenarios or problem settings and discussion where topological methods could contribute to the design of new reconstruction method or lead to improved reconstruction analysis.

As a remark, we do not claim that the presented methods are optimal for these problems. They are only first ideas to show that topology can be a possible approach in the scenarios. We even assume that many of the readers associated with computational topology research come up with more and possible better
ideas. After all, this paper’s main purpose is to simply emphasis further research in this direction.

3.1 Scenario 1: Intra-Method Inconsistency

Some of the presented reconstruction methods from Section 2.2 rely on parameters. In the following, we will illustrate how parameter changes in PLIC can also change the topology of the reconstructed interfaces. Here, the parameter is the ordering of the materials.

In PLIC, material planes are aligned orthogonally to material gradient directions and translated within the cell until the volume fraction for the current material agrees with the original fraction. Figure 4 shows an example for a single cell with three materials and eight pure neighbor cells (partially shown). Arrows in the middle of the cell indicate the gradient vectors for the three materials and numbers represent the order in which the materials are reconstructed. Note that in Figure 4(b) the two dark gray areas are no longer connected while in 4(a) they still share a common edge. If we assume cases with thousands to millions of cells such a small detail is easily overlooked in a purely geometric visualization, but can cause major problems in automatic post-processing steps. However, a topology-oriented analysis based on connected components can immediately find and highlight those discrepancies and provide a simple visual support and analysis tool to evaluate the quality of a reconstruction.

Furthermore, in the PLIC method, changes in the parameters only change the topology implicitly. The next method, DA, shows an example where the topological changes are independent of any parameters, but depend in a more complex fashion on the outcome of a probabilistic part of the algorithm. Defining a parameter for DA that explicitly influences the topology of the result, e.g. through explicit topology-based terms in the energy function, remains a challenge for future work.

In order to go more into detail, the global energy function $E$ in DA sums up the energy of each subcell $x$ with corresponding material label $f_x$, namely

![Fig. 4. Two interfaces for a three-material example. The numbers indicate the order in which the materials are reconstructed.](image)
\[ \sum_{y \in N} \omega_{x,y} \delta(f_x \neq f_y) \] with \( \omega_{x,y} \) a suitable weighting function, \( N \) the local neighborhood of \( x \) even beyond the cell boundaries, and \( \delta = \{ \text{true} : 1, \text{false} : 0 \} \).

While DA optimally converges to a global minimum for this energy function \( E \), such a global minimum might not exist or DA may converge to a local minimum in case the simulated annealing stops the movement within the single cells too early.

With this in mind, consider the volume fraction for two materials in four cells as illustrated in Figure 5. The adjacent partially shown cells are pure, i.e. they are completely filled with one of the two materials. Next to this figure are two possible reconstructions for those volume fractions, Figure 5(b) and 5(c). With \( \omega_{x,y} = 1 \) for all subcells, both interfaces result in identical energy values, hence are both possible outcomes of DA though they are topologically distinct.

Figure 5. A volume fraction (a) and two interfaces (b,c) with exactly the same energy function w.r.t. DA. However note that (b) and (c) have two different topologies since different materials are connected or separated, respectively.

As mentioned above, a possible step to address this problem is to integrate additional topological constraints into the energy function. A topological analysis on the volume fractions can even provide good and case-specific parameters before the actual reconstruction. An analysis based for example on a contour tree \cite{22} for one of the materials is possible, using its volume fractions to build contours along the cell edges. Future applications could allow to choose a subtree to decide if groups of pure cells, peaks and troughs in the contour map, are within the same material boundaries in the final reconstruction. In this case the nodes in the contour tree would represent groups of connected cell whose volume fraction of the current material is above a given threshold.

Hence, due to their capability to measure the influence of the method parameter or to design new ones to control those influences, topological approaches provide striving perspectives for the inclusion of topological methods into the MIR method design process. This might provide new reconstruction methods that can fit to different applications like fluids (large connected components, with occasional drops), aerosols (high topological complexity) or objects that obviously have different topological constraints (like scans in material engineering) by changing a single parameter describing topological complexity. Additionally,
a visual representation of the topology of the volume fraction data could take a supporting role in choosing suitable method parameters prior to the actual reconstruction.

### 3.2 Scenario 2: Inter-Method Inconsistency

The previous scenario illustrated how the same method can result in topologically different interface reconstructions. Obviously, these differences can also be present when comparing different methods, leading to the next challenge, namely to find suitable topological representations to qualitatively analyze and compare MIR methods.

First, we refer to Anderson et al. [19] where it is nicely illustrated that the grid-based methods, here that by Meredith, lose small features like bubbles or thin layers. Hence, a scenario as it is presented in Figure 6 is possible. The left figure shows the original interface and the separation of the domain into cells. Figure 6(b) and Figure 6(c) show possible results as they might be produced by DA and by Meredith’s method, respectively. An obvious topological tool to compare those two reconstructions is the so-called Reeb graph [23, 24]. Figure 6(d) shows such graphs for the two results and the original data using height as the Morse-function. Especially for large data such an abstract view on the reconstructions allows easy comparison and evaluations of the different MIR methods. Next to the choice of the right topological representation there are however still many open challenges, like in case of higher dimensional or extremely diverse, complex, and large data. Higher dimensionality complicates the definition of a suitable Morse-function, while for large scale data one needs to find a good transition between local and global approaches. Local variations of genus computation or connected component analysis may enable effective detail comparisons of different reconstruction techniques. Global techniques, on the other hand, can provide an intuitive summary of the comparisons however generally suffer from computational complexity due to non-local operations.
3.3 Scenario 3: Inconsistency over Time

Another usage of the Reeb graph representation is to track topological features over time. Some approaches are already incorporated in existing work, namely in the work by Chen et al. [25] and Bremer et al. [26]. Both show the usage of the Reeb graph to intuitively follow splits and merges of a material in a fluid simulation, or, respectively, flame propagation over time. Chen et al. furthermore emphasized that topological changes between time step can occur due to inaccuracy in the interpolation methods. This leads to two questions: First, do topological changes within the interface reconstruction happen over time? And second, are these changes based on equivalent changes in the underlying interfaces or caused by inconsistent reconstruction?

As an example, consider an atomized fluid, e.g. from a hair sprayer that floats almost motionless in the air over time. Figure 7 shows a sketch of two time steps of this case, separated into five cells where each cell has roughly the same fluid density. Figure 7(b) and 7(c) show reconstruction of the fluid interfaces using SLIC and DA, respectively, for both time steps. Note that the interface in the second time step in Figure 7(c) is just a reflection of the first one. Therefore both have the same energy function and therefore are both equiprobable in the DA approach. While the topology for SLIC obviously stays the same, the last image,

![Fig. 7](image)

**Fig. 7.** An atomized fluid (a) and possible reconstructions from SLIC (b) and discrete Anderson (c), as well as the Reeb graph (d) for the latter reconstruction using time as the Morse-function.

Figure 7(d), shows a Reeb graph representing the movement of the singular subcells in 7(c) over time. As one option on how to follow such movements in mesh-based reconstructions we point out the work of Obermaier et al. [27].

Note how this graph differs from a graph based on the interfaces in Figure 7(a) or 7(b). Especially if we consider the atomized drops in 7(a) as one connected object or cloud, we observe the interesting result that from a topological point
of view SLIC fits better to the original interface than the DA method. However note that this is only an extremely special case and not suited for a qualitative analysis of the two methods.

We note that topological tracking over time can be used to build new requirements for MIR methods, for example topological stability. Two approaches of this type were described by Mueller-Fischer et al. [12] and by Garimella et al. [28]. Both assumed a constant topology with regard to connected components. However in the former work this resulted in all single offshoots of the same material being connected to each other by very thin strings. The latter, despite smoothing, still results in discontinuous interfaces similar to PLIC. Thus, topology as a non-constant design parameter for a smooth reconstruction remains a promising open challenge.

One step towards solving this challenge is first to efficiently recognize if and where inconsistencies in the topology appear, e.g. using pattern recognition techniques on the topological representation. Furthermore, one has to evaluate whether these inconsistencies, especially topological oscillation like those that probably appear when we add more time steps in Figures 7(c) and 7(d), actually indicate incorrect reconstructions. This leads to a set of challenges, for example about scalability, efficiency or representation methods for time-varying topological analysis, whose discussion however is beyond the scope of this paper.

3.4 Scenario 4: Multi-Material Reconstruction

Up to this point we mainly presented two-material examples to illustrate the effects on topology of MIR. The following figure shows a more challenging problem. Figure 8 presents two subfigures each showing the interfaces for three materials. This can be, for example, the results of a reconstruction method from two separate time steps, cells, or two possible reconstructions of a single cell. Regardless of the exact scenario, note that the topology of each single material stays the same in both figures. However, all the introduced topological representations so far are not suitable to emphasize that in 8(a) material M1 is split by material M2 while in 8(b) this is caused by material M3. For each of the above ideas on

![Fig. 8. Two three-material interfaces in which material M1 is split in half by one of the other two materials.](image)
using topology as either an analysis tool or as design parameter, one also has to consider multiple materials and their connectivities. Hence, for each analysis method one has to examine whether the methods can be used on each material separately or if inter-material factors exist and how to integrate those into the topological analysis. In case of Reeb graph representation one may combine the graphs for the single materials using a connectivity graph. This then leads to the task to visualize the changes in local, single material topology and global connectivity over time in a simple and intuitive way.

Hence, while MIR can greatly benefit from topological analysis, it at the same time creates new challenges with respect to topological methodology and visual representation.

4 Conclusions

In this paper, we provided an overview of topological considerations, or the lack thereof, in Material Interface Reconstruction research, with the aim of identifying interesting research challenges in this area. Through four scenarios we emphasized the potential utility of incorporating topological approaches

– in pre-reconstruction visualization, e.g. through material density based contour trees,
– as a design parameter allowing MIR methods to incorporate different topological constrains, and
– as an analysis tool to perform intra-, inter-methods comparisons and evaluate over time.

Especially for the scenarios which incorporate time as a relevant factor, Reeb graphs seems immediately useful where time can serve as a suitable Morse-function. For single time steps, however, other functions are needed to build such a graph, for example, fluid density or coordinate functions. However, next to finding a suitable function for Reeb graph construction, other approaches like Morse-smale complexes [29] or Alpha complexes [24] can become focus of interest in future work.

Another promising direction for future work is the use of topology either as new requirement or as interactive support for new reconstruction methods. For example by forcing the method to produce a stable topology over time or as additional parameter for the MIR method. For the latter one can consider the integration of topological constraints into the energy function in Anderson’s discrete method, as an example.

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