Understanding the Structure of the Turbulent Mixing Layer in Hydrodynamic Instabilities

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ABSTRACT

When a heavy fluid is placed above a light fluid, tiny vertical perturbations in the interface create a characteristic structure of rising bubbles and falling spikes known as Rayleigh-Taylor instability. Rayleigh-Taylor instabilities have received much attention over the past half-century because of their importance in understanding many natural and man-made phenomena, ranging from the rate of formation of heavy elements in supernovae to the design of capsules for Inertial Confinement Fusion.

We present a new approach to analyze Rayleigh-Taylor instabilities in which we extract a hierarchical segmentation of the mixing envelope surface to identify bubbles and analyze analogous segmentations of fields on the original interface plane. We compute meaningful statistical information that reveals the evolution of topological features and corroborates the observations made by scientists.

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1 INTRODUCTION

Understanding the turbulent mixing of fluids is one of the fundamental research problems in the area of fluid dynamics. Turbulent mixing occurs in a broad spectrum of phenomena ranging from boiling water to astrophysics and nuclear fusion. In the present work we apply topological techniques to the analysis of Rayleigh-Taylor instabilities.

Rayleigh-Taylor instability (RTI) occurs when two fluids of different density are accelerated opposite the mean density gradient. That is, a heavier fluid is accelerated against a lighter fluid. In this paper, the RTI occurs under the force of gravity, when a heavy fluid is placed above a light fluid and the planar interface between them (hereafter called the midplane) is seeded with perturbations. The heavy fluid accelerates downward, forming "spikes," while the light fluid moves upwards forming "bubbles." The bubbles and spikes are thought to be one way to characterize the large-scale behavior of the mixing process. At the same time, all bubbles and spikes are the result of fluid passing through the midplane, so understanding the properties of fields on the midplane is also an important goal.

Scientists analyzing these simulations are particularly interested in the number of bubbles (and spikes which behave nearly symmetrically) and their respective evolution. Large-scale models have been proposed based on bubble dynamics in which bubble growth, movement, and interaction (birth, merge, and death events). It is important to understand whether bubbles grow by merging with their neighbors or whether certain bubbles survive and continue to grow while others die-off. A key problem is to create a precise definition of a bubble given the multiscale nature of the fluid flow. Cook et al. [6] observe four phases in the mixing process resulting from the interaction of entrainment (the movement of one fluid by another) and diffusion:

1. Independent growth (I): The initial perturbations grow independently and no coupling occurs between them.
2. Weak turbulence (II): Coupling between modes occurs as instabilities develop, causing the fluid to begin taking on distinctive mushroom-cap (early bubble) shapes.
3. Mixing transition (III): The mixing rate dominates the entrainment rate, slowing the growth of the mixing layer.
4. Strong turbulence (IV): Mixing and entrainment become balanced, resulting in faster growth of the mixing layer.

These mixing phases affect the shape and number of bubbles. At sufficiently late times the width of the mixing layer has been assumed to be proportional to the square of the time since the start of the mixing [7, 5]. Thus, we expect that a study of bubble dynamics and bubble counts will show the effect of the different observed phases in the mixing process.

Analysis of the simulation data poses challenges at several levels:

1. Theoretical definitions: There exist no prevalent technical definitions of the "features," e.g. bubbles. How can we develop a theoretically sound definition of bubbles that enables design of efficient algorithms and their robust implementation?
2. Complexity: The late stage mixing creates extremely complex and chaotic structures which can cause numerical problems and highly degenerate configurations. How do we avoid numerical problems and not get bogged down by exhaustive case-by-case analysis of degeneracies?
3. Scale: The features of interest can change size drastically over time and must be analyzed independent of scale. How can our definitions and algorithms handle scale?
4. Data size: The simulations use high resolution regular grids (1152^3 and 3072^3 in our case) over a large number of time steps (here 755 and 224 respectively). Such large-sized data can render in-core implementations infeasible. How do we design our algorithms with this issue in mind?

This paper makes contributions to address each of these challenges. Our analysis is performed on two kinds of surfaces: envelope surfaces describing the boundary between undisturbed and "mixed" fluids, and height functions defined on the midplane.

For both types of surfaces, our definitions and algorithms are based on the mathematical foundations of Morse theory [18] which is discussed in Section 4. For envelope surfaces, we define bubbles using the constructs of the hierarchical Morse-Smale(MS) complex, implement a robust combinatorial algorithm to construct this complex, and use topological persistence to automatically clean-up noise and identify bubbles at any user-defined scale. Section 5
describes the algorithms used to extract bubbles and the different types of topological information gathered. We emphasize that all our algorithms are combinatorial in nature and are therefore robust in the presence of noise and degeneracies. The hierarchical nature of our constructions enable us to analyze the data at several scales in both space and time.

For analyzing midplanes, we also take advantage of the hierarchical Morse-Smale complex in order to provide persistence-based metrics. We note that Cook et al. [15] such that a full resolution envelope surface could be simplified through the original data and avoid storing intermediate results. In both space and time.

The second aspect of the research presented here is the tracking of features in iso-surfaces over time. Samtaney et al. [20] describe a general feature tracking algorithm based on extracting features at each time step, computing describing attributes, e.g. center of gravity, size, orientation, etc., and solving a best matching problem to create time correspondences. The results are presented as a graph encoding the birth, death, merging, and splitting of features. In some follow-up work they also use the volume overlap of features to decide correspondences [23]. Reinders et al. [19] use very similar ideas combined with motion prediction to improve matching accuracy.

Edelsbrunner et al. [10] develop theory and algorithms to compute time-varying Reeb graphs by connecting them using Jacobi sets [9] which are the paths traced by critical points. Ji et al. [16, 17] track the evolution of iso-surfaces in a time-dependent volume by extracting (two-dimensional) iso-surfaces within each time slice and define two such surfaces as linked if they are part of the same three dimensional space-time iso-surface. Sohn and Bajaj [1] compute correspondences between contour trees at successive time-steps by using volume matching as in [22] rather than the topological analysis used in [10]. They use this correspondence to encode the evolution of the iso-surface of a fixed iso-value over time in the Topology Change Graph.

Tracking of critical points and/or features is also common in flow field analysis typically based on integrating streamlines/surfaces through space-time. Work on two-dimensional flow fields can be found in [25] and three dimensional extensions in [12].

4 Background: Morse theory

This section reviews the formal definition of the Morse-Smale complex [18, 2] and strategies to compute and simplify it.

4.1 Morse-Smale complex

Let \( M \) be a continuous 2-manifold embedded in \( \mathbb{R}^3 \). Given a smooth function \( f : M \rightarrow \mathbb{R} \), a point \( c \in M \) is called critical if \( \nabla f(c) = 0 \) and its Hessian matrix of second derivatives is non-singular, and is classified as either a maximum, minimum, or saddle point. The unstable manifold of a critical point \( c \) is defined as the set of points for which the integral lines of \( \nabla f \) start/stop at \( c \). Assuming that no integral line starts and ends at a saddle, one can mutually refine the stable and unstable manifolds of \( M \) to create the Morse-Smale complex of \( f \) on \( M \) [2], see Figure 1(a)–(d).

A Morse-Smale complex defines a decomposition of \( M \) whose nodes are critical points of \( f \), whose arcs are integral lines connecting saddles with extrema and whose regions are the non-empty intersections of stable and unstable 2-manifolds. By definition, all integral lines within a region start at the same minimum and end at the same maximum and \( f \) is monotone. Therefore, the MS complex of \( f \) completely describes the topology of \( f \). Complete details on the definition of the Morse-Smale complex on 2-manifold triangle meshes and algorithms to compute it are given by Bremer et al. [2].
Integral lines (shown in black) ending at the canceled maximum are of a simplified complex; (f) Approximation of Figure 1: Morse-Smale complex construction, simplification and topologically valid approximation: (a) Small portion of the mixing layer of a Rayleigh-Taylor instability at an early time step; (b) Stable manifolds; (c) Unstable manifolds; (d) Morse-Smale complex; (e) Stable manifolds of a simplified complex; (f) Approximation of \( f \) corresponding to the topology of (e). Maxima are drawn red, minima blue, and saddles green.

Simplification. It is often useful to simplify an MS complex in order to remove noise as well as to analyze functions on multiple scales. Following [2] we use cancellations of connected critical point pairs to simplify an MS complex. The two possible cases are a maximum-saddle and a minimum-saddle cancellation, examples of the former are shown in Figure 2.

Figure 2: Two maximum-saddle cancellations merging adjacent stable manifolds. Saddles (shown in green) are canceled with their lowest neighboring maximum (shown in red). The corresponding persistences are indicated as \( p_1 \) and \( p_2 \). After the cancellation all integral lines (shown in black) ending at the canceled maximum are re-routed to end at the corresponding higher neighboring maximum.

Cancellations are ranked by their persistence—the absolute difference in function value between the two critical points they remove. Not all pairs can be canceled: A saddle \( v \) which is connected to the same extremum \( u \) twice cannot be canceled with \( u \) as this would change the genus of \( M \). It can be shown that greedily canceling the the pair with smallest persistence simplifies the topology of \( f \) in an \( L_\infty \)-optimal manner. Figures 1(e) and (f) shows an example of a topological simplification and a corresponding approximation.

Computation. In practice, one usually deals with piece-wise linear (PL)-functions given at the vertices of a triangulation. A detailed discussion on how the smooth theory discussed above is transferred to PL-functions can be found in [2]. In particular, we use a slightly modified version of the algorithms by Bremer and Pascucci [3] to efficiently compute and simplify MS complexes. Starting from saddles the arcs of the MS complex are computed as steepest monotone lines that do not cross each other. However, we avoid all mesh refinement by directly dealing with merging lines as well as multi-saddles. As a result we can use efficient static data structures to store the triangulation allowing us to compute Morse-Smale complexes of large data sets common in simulation.

5 Analysis

The focus of our research is to provide a set of dependable tools that scientists can use to analyze the mixing behavior. We cannot assume that there exist a particular objective other than to “better understand” the physics involved. Traditionally, application scientists provide some definition of interesting features (a tumor, a vortex core, etc.) and visualization aims to extract and highlight the particular object of interest. In the case of Rayleigh-Taylor simulations however, few concrete objectives exist besides the intuitive notion that the behavior of bubbles and spikes is important. Therefore, our goal is no longer primarily to provide a visualization of the data but to support the data analysis process in general.

An important consequence of analyzing little known phenomena is that results are difficult to validate. Therefore, techniques which cannot be independently proved to work as expected are of little use as they cannot necessarily be trusted. This section describes the various techniques we use to analyze different aspects of the data.

Data We analyze data from one large scale simulation. The data is defined on a regular grid that is periodic in the \( X \) and \( Y \) dimensions and closed in the \( Z \) dimension. The data set, which we denote the Borg data set, contains data defined on an \( 1152^3 \) grid at 759 distinct times. It utilizes a sub-grid scale model for diffusivity and viscosity. For each grid point the data contains 4-byte floating point values for density, pressure, and the three velocity components.

Segmentation of Bubbles One of the challenges in analyzing the mixing behavior is that there exists no prevalent mathematical definition for what constitutes a bubble/spike. In general, a bubble should be understood as a three dimensional feature composed of mainly lighter-density fluid moving upwards into a primarily heavier density fluid. Scalable 3-D Morse-Smale analysis is not yet available, so in consultation with physicists we have determined that segmenting bubbles based on the mixing envelope surface is a reasonable first step. We use the topological concepts introduced in Section 4 to define bubbles, spikes and other features of interest. Consider the images of the segmented mixing envelope surface at different times shown to the left, bottom, and right of the plot in Figure 3. During early time steps (3 upper left and middle left) it is natural to consider the mixing envelope as a time-varying functional surface defined over the \( xy \)-plane and associate local maxima with bubbles. This analogy fails at later time steps because the surface becomes non-functional. However, we can generalize this approach by treating the envelope surface as the domain of a function whose value at a point \( p \) is the \( z \)-coordinate of \( p \). It is natural to connect the maxima of this function to bubbles and compute the stable manifold of each maximum as a segmentation of the surface into bubbles. As can be seen in Figure 3, this segmentation corresponds very well to the human notion of a bubble. Symmetrically, we use the unstable manifolds of minima to define spikes. Potentially, other functions could be defined on the envelope surface that would result in a robust segmentation as well. For example, the \( Z \) velocity at all of the points on the envelope surface could be incorporated to capture the fact that bubbles should be moving upwards into the heavy fluid. Given the complexity of the problem, it has been determined to use the simplest, most intuitive segmentation if at all possible.

In general, topological based segmentations are often linked to important features: Maximal and minimal \( \chi \)-velocities on the mid-planes correspond to cores of rising and falling sections of fluids; Density extrema correspond to pockets of unmixed fluids. This makes topological methods flexible and allows us to analyze a variety of phenomena using the same methodology. Furthermore, the MS complex can be computed combinatorially [11, 2] which trans-
lates into provably correct and stable algorithms which are crucial when dealing with large and complex data.

**Multi-Scale Analysis** The MS complex, just as any other segmentation, usually contains some amount of noise. A simplification scheme can be used to remove noise and construct a series of approximations at decreasing resolution. Unlike many other techniques, topological segmentations allow a simplification scheme that is optimal wrt. the $L_\infty$-norm. One can formulate the problem of coarsening a segmentation in the following manner: Given a function $f$ and a segmentation $\mathcal{S}$ of the domain of $f$, what is the minimal change on $f$ such that $\mathcal{S}$ is coarsened? If the segmentation one considers is the MS complex of $f$ (or subsets of it) then it can be shown [2] that canceling a critical point pair with persistence $p$ in $f$ requires an approximation $\hat{f}$ with $|f - \hat{f}| \geq p/2$. Therefore, canceling critical points in order of increasing persistence corresponds to an $L_\infty$-optimal simplification.

For each MS complex we compute a sequence of cancellations which optimally simplifies the complex down to its minimal configuration. We can then create statistics showing the number of bubbles over time using a range of persistence thresholds. As shown in Section 6 the mixing behavior can differ significantly across scales and using the simplification sequences we capture the behavior on all scales without re-computing the MS complex.

**Interaction** We can visualize the bubble structure of an envelope surface at a given persistence by coloring each triangle according to index of its stable manifold. In order to interact with the MS-complex of an envelope surface at full resolution we store the parent-child information described in the previous paragraph in a separate file for each time step. This file contains one 16-bit integer for each triangle indicating the stable-manifold of lowest persistence to which it belongs, and a list of records, one for each stable manifold in the Morse complex. Each stable manifold record contains the position of its maximum, the persistence at which it is simplified, and the index of its parent in the hierarchy. For a given persistence threshold, the index of the stable manifold of each triangle is obtained by starting at its initial maximum and traversing that maximum’s chain of parents until the threshold is reached. We modified the streaming mesh viewer of Isenburg et al. [15] to read the parent-child information and simplify it along with an input mesh. The simplifier is grid-based, so that each cell in the grid ends up with a single vertex and only a subset of triangles survive in the simplified mesh. We simply keep the parent-child information of these simplified triangles so that each triangle can be colored appropriately at an interactively set persistence threshold.

### 6 Results

We present results for the Borg (1152³, 5.8Gb per time step) data set. Because of the extreme data sizes and limited available disc space we use every second time step on the simulation. The analysis was performed on 68 dual-processor nodes of a Linux based visualization cluster. In most cases jobs were parallelized over time across the nodes of the cluster.

| Borg          | T = 0         | T = 756       |
|---------------|---------------|---------------|
| Isosurface Ext.| 146 / 7.9Mb   | 276 / 15.4MB  |
| Isosurface Seg.| 2s / 62Kb    | 25s / 144Kb   |

Table 1: Performance data for different stages of our computing pipeline. Execution times as well as resulting file sizes are shown for both the first and last time step of both data sets.

Table 1 shows the running times and resulting file sizes for the selected operations using a single node of the cluster. Each operation is shown on the first and last time step of the corresponding data set which is roughly equivalent to the fastest and slowest execution across the temporal range. The size of the iso-surface refers to a standard obj file all others are uncompressed binary formats.

Figure 3 illustrates the bubble segmentation process. The images on the right side of the plot are all taken at the same time step for different persistences, showing that choosing the persistence threshold is important for getting an intuitively correct bubble segmentation. The images to the left and below are from the same curve, showing the increase in size of the bubbles, as indicated by the surface area of the set of Morse-Smale cells of all child maxima grouped with the parent maxima of each bubble.

The 2.59% persistence-threshold curve in Figure 3 shows three linear (power-law) regimes. The rate of decrease in the number of bubbles (which is correlated with increasing mixing width) is slow, then fast, then slow in Figure 3. There is an intriguing tail-off on all three curves in Figure 3, although it is not clear that running the simulation to later time was practical given the grid resolution and the subgrid-scale numerical models used.

### 7 Conclusion

In this paper we have demonstrated how topological segmentations based on Morse theory can be used to analyze the properties of mixing flow. This included a novel definition of bubbles in the mixing layer as stable manifolds of maxima of the height function. Furthermore, we have developed a suite of efficient algorithms algorithms forming a complete pipeline to perform multi-scale analysis of large and complex datasets. All algorithms are combinatorial making them stable even under extreme circumstances. It should be noted that the techniques described in this paper are in no-way limited to fluid dynamics research. On the contrary, the tools described here can be applied to any domain in which features can be indicated by the critical points of a function defined on a manifold.

We have extracted counts of critical points that correlate with growth of the mixing layer and the associated growth in the size (and therefore reduction in number) of features in the flow. We observe expected changes in the previously observed phases of the mixing process which suggest that a topological approach is valid. There are intriguing differences in the power-law behavior of the bubble counts derived from the envelope surfaces and the density minima counts on the midplanes. It is not clear at this time what accounts for these differences.

The results presented here highlight the need to develop more sophisticated metrics which do not require a qualitative approach to selecting a persistence threshold. It is clear that the flow features of interest are multi-scale, but it is not clear how to combine the different scales into a fully quantitative metric.

Finally, there exist some real limitations to attempting to track 3-D structures like bubbles using 2-D envelope surfaces due to the complexity of the internal structure of bubbles at late time is complex. It appears that a robust and scalable implementation of 3-D Morse-Smale complexes is required to capture all relevant information in the mixing process.

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Three regions of power-law behavior are shown by the curve fits in gray to the persistence curve at various times. Each maximum in the MS complex along with the Morse cells of its child-maxima are colored the same.

Figure 3: The plot depicts bubble counts as obtained by the Morse-Smale based segmentation of the envelope surface as shown in the rendered images. Three regions of power-law behavior are shown by the curve fits in gray to the 2.39% persistence curve. To the right of the figure images of the MS segmentation at three persistence values are shown for time 700. To the left and below the graph we show the bubble segmentation along the 2.39% persistence curve at various times. Each maximum in the MS complex, along with the Morse cells of its child-maxima are colored the same.

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