Tracking flame base movement and interaction with ignition kernels using topological methods

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Abstract. We segment the stabilization region in a simulation of a lifted jet flame based on its topology induced by the $Y_{OH}$ field. Our segmentation method yields regions that correspond to the flame base and to potential auto-ignition kernels. We apply a region overlap based tracking method to follow the flame-base and the kernels over time, to study the evolution of kernels, and to detect when the kernels merge with the flame. The combination of our segmentation and tracking methods allow us observe flame stabilization via merging between the flame base and kernels; we also obtain $Y_{CH_2O}$ histories inside the kernels and detect a distinct decrease in radical concentration during transition to a developed flame.

1. Introduction
In this section, we will motivate our work, and briefly discuss prior work.

1.1. Motivation
Non-premixed turbulent jet flames are useful configurations to study phenomena relevant to practical energy conversion devices. Laboratory scale jet flames have been studied experimentally [1] and proven useful for developing combustion models. Computational studies of canonical configurations, albeit at much smaller scales, produce exceptionally detailed flow information. Presently, we investigate a ‘direct numerical simulation’ of an ethylene slot jet surrounded by a co-flow of hot oxidizer. The flame may be stabilized by a variety of mechanisms: here, the temperature is elevated, so that the mixture may auto-ignite. The stabilization is influenced by chemical reactions occurring between the jet exit and the flame base. If the reactants are cold, or the velocities are large, the flame base may be stabilized by a propagating edge flame [2]. Unlike the edge flame, an auto-igniting front does not propagate in the traditional sense, but instead moves relative to the advected fluid by ‘sequential auto-ignition’ [3]. This flame base has been observed to periodically exhibit displacement speeds indicative of an auto-ignition front [4].

To further understand the stabilization mode, we wish to connect upstream reaction with the behaviour of the flame base. For this chemistry, the location of the quasi-steady non-premixed flame is described by the Hydroxyl ($Y_{OH}$) mass fraction, and the auto-ignition process is reflected in the evolution of radical species, such as Formaldehyde ($Y_{CH_2O}$). Our interests are threefold. First, is the stabilization of the flame due to auto-ignition alone, or is there some interplay with a local propagation. Second, can we relate the effective displacement speed and position of the
flame base to the nature of ‘ignition kernels’ formed upstream. Finally, can we relate the large scale flow structures to the propensity for formation of ignition kernels.

The first objective is relevant to describing the canonical configuration under consideration and framing the applicability of any conclusions drawn, the second and third together are steps in developing an effective combustion model to describe the stabilization mechanism. Accomplishing the second objective mandates a quantitative and unambiguous definition of the ‘ignition kernels’, and is the foremost motivation for applying topological methods to this problem. Further, this effort also begins to use a topological definition of the ignition kernels to explore the first objective.

1.2. Feature detection.
Topological based segmentation and feature detection methods have become increasingly popular. One of the most widely used topological structure is the contour tree [5, 6]. It encodes the topology of all level sets (also called isosurfaces) of a function. See [7, 8, 9] for applications. As described in Section 2, we base our segmentation method on [10]. This method employs the merge tree, a sub-structure of the contour tree, to represent the merging behaviour of level sets.

A closely related family of methods uses the Morse-Smale complex to represent features. The Morse-Smale complex was first introduced for triangulations by Edelsbrunner et al. [11]; extensions to 3D can be found in [12, 13].

1.3. Feature tracking.
It is often of important to track features in time-dependent data sets. Samtaney et al. [14] apply methods from object tracking in image processing to feature tracking in scientific datasets. In follow-up work, Silver and Wang [15] use volume overlap of features to identify correspondences. As discussed in Section 2 we use the vertex overlap induced by a triangulation of space-time to connect features in time. Laney et al. [16] use similar ideas to track bubble structures in turbulent mixing. Reinders et al. [17] use motion prediction to improve matching accuracy. Ji et al. [18] connect isosurfaces using the 4D space-time isosurface that contains them.

2. Segmentation and tracking
In this section, we briefly describe our feature segmentation and tracking methods. Our feature segmentation is based on [10].

2.1. Segmentation
Given a smooth function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ the level set of $f$ at isovalue $s$ is defined as all points in $\mathbb{R}^n$ with function value $s$. A connected component of a level set is called a contour. The merge tree of $f$ records the merging behavior of the contours of $f$ as the isovalue is swept top-to-bottom through the function range; see Figure 1. When the isovalue passes a maximum a new contour is born and a new leaf appears in the merge tree. When two contours meet at a saddle they merge into a single component represented in the merge tree as a joining of two branches.

Each branch of the merge tree can be used to represent the subset of $\mathbb{R}^n$ defined by the union of all its contours, indicated by the colored regions in Figure 1. For a data point $p$, the value $S(p)$ is the id of its corresponding merge tree branch. We are interested in regions around high $\nu_{\text{OH}}$ values and we define these regions starting from the leaf branches of the merge tree.
We want two neighboring regions with similar $Y_{OH}$ values to count as a single region. Following [10], we merge low persistence regions together and refine the merge tree arcs and the corresponding regions to create segments; see Figures 2(a) and 2(b). The relevance measure for a branch $b$ with maximum $u$ and saddle $v$, is defined as $\text{rel}(b) = (f(u) - f(v)) / (f(u) - f_{\text{min}})$ where $f_{\text{min}}$ is the global minimum of $f$. We are interested in regions around local maxima of $Y_{OH}$. Given a user defined threshold $r$, we can select regions around local maxima of $Y_{OH}$ whose set of arcs $B$ in the merge tree have relevance $\text{rel}(b) < r$ for all $b \in B$. Notice, that this final parameter choice represents a simple selection of a root branch $b$ and its sub-tree all of whose branches have a lower relevance value. Denote this root $b$ as the leader of the region, and say $b$ represents its region. In Figure 3, the segment labeled $S_t$ in the tree at time $t$ is the leader of the region corresponding to the segments in the subtree rooted at $S_t$. Note that, unlike conventional tree diagrams, the layout of the merge tree has the leaves on top; the subtree rooted at $S_t$ is obtained by walking up from $S_t$ towards the maxima nodes.

Selecting flame components Because we are interested in selecting and tracking the flame and kernels, and because the flame is defined as the $Y_{OH}$ level set of $s = 0.0005$, we have to modify our selection criterion to include these regions. This is easily accomplished: for every candidate leader arc $b$, we compare the local maximum in its subtree $f_{\text{max}}(b)$ with $s$. If $f_{\text{max}}(b) < s$, the region represented by $b$ does not include a component of the flame, and we select $b$. If $f_{\text{max}}(b) > s$, we select the arc $a$ in the subtree of $b$ that contains the value $s$.

2.2. Segment tracking

In this section, we describe how we track segments over time. Our method is simple; we connect successive time-steps in a triangulation, employ a weighted overlap measure to detect segment correspondence, and encode this correspondence in a tracking graph. This graph can be used to extract tracking information for an arbitrary choice of the relevance parameter at each time-step. The arc weights can be used to select an edge based on a user selected overlap threshold.

The tracking graph. The data at each time-step is sampled on a regular grid. We decompose the unit 4-cube defined by diagonally opposite points $p$ and $q$ into 4-simplices along the diagonal. The algorithm for computing the tracking graph $G_t$ between successive time-steps $t$ and $t + 1$, takes as input the segmented data for these time-steps and outputs a weighted graph encoding the correspondence between segments. We process every data point $p$ at time $t$, and decompose the 4-cube containing $p$ and its diagonally opposite point at time $t + 1$. We then process each edge connecting $p$ to data point $q$ in $t + 1$ and update the tracking graph: if arc $a = (S(p), S(q))$ belongs to $G_t$, then increment its weight $w(a)$ by unity, else insert $a$ with unit weight. The tracking graph $G_t$ contains segment correspondence for any arbitrary choice of relevance for
times $t$ and $t + 1$. Next we show how we extract the segment correspondence for a particular choice of relevance parameters.

Tracking with relevance selection. We describe the algorithm for computing the graph $H_t$ which encodes the tracking information for the choice of relevance parameters $R_t$ and $R_{t+1}$. Consider a region with leader segment $S_t$. Recall that the region is defined by all points whose segment id belongs to the subtree rooted at $S_t$. This collection of segments is connected to segments in $t + 1$ some of which might be selected for relevance $R_{t+1}$. Denote the leader of such a segment by $S_{t+1}$. Initialize $H_t$ to empty. For every segment $s$ with leader $S_t$ and arc $a = (s, s') \in G_t$ such that $s'$ is selected, update arc $b = (S_t, S_{t+1})$ in $H_t$. The update inserts arc $b$ if it does not exist in $H_t$ or increases its weight by $w(a)$ if it does exist.

We illustrate this algorithm in Figure 3. The figure shows a merge-tree at times $t$ and $t + 1$ with arcs colored if the corresponding segments are selected. Segment $S_t$ has two segments in its subtree that are connected to segments in the subtree of $S_{t+1}$; we accumulate their arc weights to obtain the arc between $S_t$ and $S_{t+1}$ with weight 145 shown at the right of the figure. Note that $S_t$ splits into two segments at $t + 1$ because a lower relevance value was chosen at $t + 1$.

3. Results
In this section, we present the results of segmenting and tracking the flame base and kernels using the $Y_{\text{OH}}$ field. The data consists of $2025 \times 1600 \times 400$ samples per time, and TTT time steps. For our experiments we focus on 30 timesteps of a $600 \times 200 \times 400$ block that includes part of one of the flame bases. Each timestep has a $2\mu\text{s}$ duration.

Segmentation and tracking. We segment the data for each timestep at a relevance of $R = 0.15$ and include all flame components by selecting segments that include the $Y_{\text{OH}} = 0.0005$ surface. The kernels are sufficiently large and slow moving that our overlap based tracking can successfully follow them over time. Figure 4(a) shows a zoomed in view of the tracking graph annotated with snapshots of the kernels and flame at various timesteps. As seen in the figure, components can merge and split before merging with the flame base and thereby stabilizing it. It appears that the upstream motion of the flame base is largely due to merging with kernels.

Tracking radical species. One of the goals of our analysis is to follow radical species concentrations in kernels as they develop so as to gain insight into the auto-ignition process.
The segmentation and tracking method described here enables this study. In our experiment, we follow the mass fraction of the Formaldehyde (\(Y_{\text{CH}_2\text{O}}\)) mass fraction at the local maximum in each kernel that is tracked. In Figure 4(b), we align the plots so that the times at which the kernels cross the flame threshold coincide. We observe that for almost all kernels the value of \(Y_{\text{OH}}\) mass fraction has a minimum at this time.

4. Conclusions
We have demonstrated that ignition kernels extracted using topological methods are instrumental in the stabilization of this flame. We observe that merging of the flame base with well developed kernels is responsible for the apparent upstream propagation of the flame base. We successfully track the kernels prior to merging with the flame base, allowing us to extract the evolution of radical species mass fractions. We have detected an interesting pattern of \(Y_{\text{CH}_2\text{O}}\) decrease near the time when the kernels transition to a developed flame. Further study of this phenomenon and other radical species behavior inside the tracked kernels will be in the future work.

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Figure 4: (a) Tracking graph showing kernels and flame base. Annotations show various topological changes experienced by the kernels and flame. (b) The mass fraction of $Y_{\text{CH}_2\text{O}}$ inside tracked kernels. We align each individual kernels plot so that the time at which they transition to burning is on the same vertical line (show by arrows). We notice that the $Y_{\text{CH}_2\text{O}}$ mass fraction drops at the transition time.