Parallel Vectors Criteria for Unsteady Flow Vortices

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Abstract—Feature-based flow visualization is naturally dependent on feature extraction. To extract flow features, often higher order properties of the flow data are used such as the Jacobian or curvature properties, implicitly describing the flow features in terms of their inherent flow characteristics (for example, collinear flow and vorticity vectors). In this paper, we present recent research that leads to the (not really surprising) conclusion that feature extraction algorithms need to be extended to a time-dependent analysis framework (in terms of time derivatives) when dealing with unsteady flow data. Accordingly, we present two extensions of the parallel-vectors-based vortex extraction criteria to the time-dependent domain and show the improvements of feature-based flow visualization in comparison to the steady versions of this extraction algorithm both in the context of a high-resolution data set, that is, a simulation specifically designed to evaluate our new approach and for a real-world data set from a concrete application.

Index Terms—Vortex feature detection, time-varying data visualization.

1 INTRODUCTION

In this paper, we present a solution to the challenge of feature extraction when dealing with time-dependent simulation data from computational fluid dynamics. We aim at feature-based flow visualization with focus on vortices and their central locations. In an extension of the state of the art, we present two new methods for the extraction of vortex core lines (also known as vortex axes) in unsteady flow that are truthful to the time-dependent nature of the extracted features.

A lot of work has been done in the field of feature extraction from steady/time-independent flow data, especially focusing on vortices. In the context of time-dependent flow, previous work focussed on extracting features from individual time steps by interpreting the flow data as a “stack” of steady flow fields (one per time step) and by applying extraction methods for steady flow data accordingly. The time-dependent nature of these features was taken into account by connecting them afterwards over time, for example, by tracking. In Section 2, we go into more detail with respect to related previous work.

1. In other fields, for example, in fluid mechanics, vortex cores are considered to be of regional type (and not of line type). In this paper, we use the term vortex core line for line-type curve features, which represent central locations in vortices.

It is favorable to inherently consider time already during feature extraction and not separately in a second step. Doing so, we find ourselves aligned with others (such as Hussain already in 1983 [10]), who demand the joint consideration of space and time when investigating features in time-dependent flow data. Accordingly, we propose to formulate the extraction criterion in a way that temporal derivatives are used for the local characterization of vortices and not only the Jacobian of the flow. This is synonymous to considering pathlines for feature extraction from unsteady flow instead of streamlines. Even though we experienced in exchange with colleagues, reviewers, and others that this extension is easily and quickly considered to be logical and straightforward, the results improved more than expected.

Very often, flow phenomena such as gas flow during combustion or air flow around a vehicle are time dependent in nature and steady representations are just an approximation. Data sets with time-independent flow are useful for domain experts as they provide information, about general or large-scale characteristics of the flow, at a relatively low cost in terms of data set size, simulation time, and analysis time. However, we still observe a clear trend toward more unsteady flow data in scientific and in commercial applications mostly because of better results, especially when doing a more careful or detailed flow analysis and also because of the availability of increased computing and storage resources.

Accordingly, we consider it important to explicitly demonstrate that feature extraction based on time is not only logical to do but also, indeed, yields better results. In certain cases, we can even observe that the traditional streamline-oriented approaches lead to displaced “features.” Furthermore, we can find an improved agreement of the new approach with physical extraction schemes such as the low-pressure assumption in the midst of vortices (no need for a correction step). In Sections 3 and 5, we exemplify our point by means of selected cases both in analytic and computed form. The need for a new approach is...

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demonstrated, as well as the gain through improved results. The contributions of this paper include two mathematical examples that model real-world problems. Based on the results of these examples, we derive simple modifications of existing vortex core line detection algorithms to extend them to the unsteady flow domain. Real-world applications where the original approaches fail are presented, and it is shown that the results improve using the modified approach. Finally, a numerical study evaluates the impact of time-derivative estimation on the feature extraction process. In the appendix, we give details on implementation details for unstructured grid data.

2 RELATED WORK

Feature-based flow visualization has been an active field of research for many years, and it is beyond the scope of this paper to provide a comprehensive discussion of all of this work—we refer to Post et al. [18], who published an extended overview recently. In this section, we focus on selected pieces of previous work, which are tightly related to our new approach.

The algorithms, which we take as a basis for developing our new approach, are the proven method for extracting vortex core lines from steady flow data by Sujudji and Haines [24], as well as the related higher order method by Roth and Peikert [21]. Both approaches were successfully applied in many cases, especially when dealing with time-independent data. As such, we consider them as a strong starting point for approaching the case of unsteady flow data. To do so, we adopt the principle of the parallel vectors approach [16] for extracting the vortex core lines in conjunction with modified extraction criteria that are based on temporal derivatives.

Reinders et al. [19] use a graph view to show the development of flow features over time and to indicate events such as birth, death, and annihilation of features. Bauer and Peikert [2] discuss the tracking of vortices in scale space, which improves the consideration of important features. Garth et al. [6] show the movement of singularities relative to an axis, which is of special importance compared to the others. Theisel and Seidel [25] introduce the concept of the feature flow field and use it to improve feature tracking: The paths of the critical points are tracked as the streamlines of a new vector field, that is, the feature flow field constructed from the original vector field.

The idea of considering pathlines when analyzing time-dependent flow data is not new as such. Theisel et al. [26] present a pathline-oriented approach to extracting the topology of 2D time-dependent vector fields—similar to a streamline-based approach, they distinguish features according to attracting, repelling, or saddlelike behavior. Haller [7] describes vortices through the stability of manifold structures that are related to fluid trajectories, that is, pathlines, and extracts vortex regions in unsteady flow data based on this information. Sadlo and Peikert [22] extract ridges from 3D finite-time Lyapunov exponents (FTLE) for the extraction of Lagrangian coherent structures (LCS). Moreover, Garth et al. [5] present a method for the direct visualization of 2D FTLE information, which results in expressive images of time-dependent flow.

In general, we observe a new motivation in the field to approach even very complex cases in 3D time-dependent flow visualization. Peikert and Sadlo [17] discuss feature-based visualization for the investigation of vortex rings and vortex breakdown bubbles in recirculating flow, and Tricoche et al. [27] describe a slice-based visualization for understanding intricate flow structures where the slices are placed orthogonal to trajectories of the flow.

Another interesting class of approaches are physical criteria (instead of geometric ones) for feature extraction. Banks and Singer [1] propose a method to find vortex core lines based on a predictor/corrector method that steps through the field in the direction of the vorticity vector. At each step, the normal plane is constructed, and the point is reset to the nearest local pressure minimum. Jankun-Kelly et al. [11] present an improvement of this approach using a function fitting procedure to locate the extreme values, stepping along the real eigenvector of the velocity gradient. Stegmaier et al. [23] present an algorithm that combines the \( \lambda_2 \) method by Jeong and Hussain [12] with the predictor/corrector method by Banks and Singer. For growing the skeleton, they step in the direction of the vorticity vector. In this context of physical approaches, other several methods have been presented, for example, the Q-criterion by Hunt et al. [9], also known as the elliptic version of the Okubo-Weiss criterion by Okubo [15] and Weiss [29], or the extension of considering acceleration terms by Hua et al. [8], which includes temporal derivatives and expresses the feature extraction process from the Lagrangian perspective.

In an upcoming paper, Weinkauf et al. [28] approach the question of vortex core line extraction in a similar fashion. For finding “swirling particle cores,” they analyze the real eigenvector of the velocity gradient and the acceleration vector. Even though they arrive at a similar extraction method, they reason differently (and use other related vectors for their approach). Our solution, as presented in this paper, is based on physical principles, resulting in a corresponding modification of existing algorithms. The swirling particle cores method is based on the space-time framework and builds primarily on a geometric approach. In future work, we plan to evaluate and compare the two approaches thoroughly. In this paper, we are also able to demonstrate our work in the context of an application, compare it to other simulated quantities related to vortices and show its good numerical behavior regarding time step width in the data set.

3 ANALYTIC CONSIDERATIONS

In the following, we discuss two analytic examples that can be considered as models for related phenomena in actual flow data. This way, we can concentrate on the demonstration of the need for a new approach. Looking at analytic cases, we can avoid issues such as aspects related to sampling and reconstruction. This approach is analogous to the work of others who use analytic examples for motivation and for demonstration [24], [21], [7].

3.1 A Tilting Vortex

To construct our first synthetic vortex example, we aimed at a, as simple as possible, flow model that still can demonstrate the difference between a streamline-and a
pathline-based approach. To avoid a simultaneous discussion of whether our approach is Galilean invariant, we decided to go for one simple vortex that tilts over time. Accordingly, we specify our flow model as

\[
\mathbf{u}(x, y, z, t) = \begin{pmatrix} -y + tz \\ -x - tz \\ \dot{z} \end{pmatrix}.
\]

The vortex in \( \mathbf{u} \) is linearly strained in the \( z \)-direction and contains a tilt which increases over time. Considering \( \mathbf{u} \) in just one time step \( t = t_a \) and analyzing its—in all locations equal—Jacobian

\[
J|_{t = t_a} = \begin{pmatrix} 0 & -1 & t_a \\ 1 & 0 & -t_a \\ 0 & 0 & 1 \end{pmatrix}.
\]

By considering the only one real eigenvector \((t_a, 0, 1)^T\) of this matrix, we observe a virtual rotation of the instantaneous flow field around an axis that is aligned with this vector and tilts into the positive \( x \)-direction. In Figs. 1a and 1b, this situation is illustrated for two time steps \( t_a = 0 \) (Fig. 1a) and \( t_a = 0.3 \) (Fig. 1b).

We abandon the restriction to only consider the flow in just one time step and see a different picture (Figs. 1c and 1d). In addition to the abovementioned \( x \)-tilt, there is another tilt toward the viewer. The corresponding vortex core line illustrated in yellow in Fig. 1d reflects this additional \( y \)-tilt.

The design of this flow model allows to analytically find explicit solutions for stream- and pathlines. If we first consider just one time step \( t = t_a \), we derive the streamline for seed location \((x_0, y_0, z_0)^T\) in parameterized form as

\[
\begin{align*}
x(\tau) &= (x_0 - t_a z_0) \cos(\tau) - y_0 \sin(\tau) + t_a z_0 e^{\tau}, \\
y(\tau) &= (x_0 - t_a z_0) \sin(\tau) + y_0 \cos(\tau), \\
z(\tau) &= z_0 e^{\tau}.
\end{align*}
\]

The \( t_a z_0 e^{\tau} \) term in the \( x \)-component of streamlines reflects the above discussed \( x \)-tilt. In the \( y \)-component of streamlines, we do not see any corresponding tilt term.

Considering pathlines next, we derive the following solution (now parameterized with time \( t \)):

\[
\begin{align*}
x(t) &= (x_0 + \frac{1}{2} z_0) \cos(t) - (y_0 + \frac{1}{2} z_0) \sin(t) + (t - \frac{1}{2}) z_0 e^{t}, \\
y(t) &= (x_0 + \frac{1}{2} z_0) \sin(t) + (y_0 + \frac{1}{2} z_0) \cos(t) - \frac{1}{2} z_0 e^{t}, \\
z(t) &= z_0 e^{t}.
\end{align*}
\]

Now, we see corresponding tilt terms in both the \( x \)- and the \( y \)-components of the pathlines, and the vortex axis is found to be along the vector \((t, -t, 1)\).

### 3.2 A Rotating Vortex Rope

As a second example, we construct a simple synthetic model of a rotating vortex rope that has characteristics that are related to an important flow phenomenon in the draft tube of large water turbines. To start, we consider the flow field:

\[
\mathbf{u} = \begin{pmatrix} -(y - y_1) \cdot s \\ (x - x_1) \cdot s \\ 1 \end{pmatrix}.
\]

For the degenerated case of \( x_1 = y_1 = 0 \), this simply is a rigid rotation about the \( z \)-axis. Assuming that the points \((x_1, y_1, z)\) lie on a helix with radius \( R \) and pitch \( \frac{2\pi}{s} \), which rotates around the \( z \)-axis with angular frequency \( \omega \) and phase 0, that is, with

\[
\begin{align*}
x_1 &= R \cdot \cos(kz + \omega t) \quad \text{and} \\
y_1 &= R \cdot \sin(kz + \omega t),
\end{align*}
\]

we get a rotating vortex, that is, a time-dependent flow field as desired—see Fig. 2 for selected streamlines and pathlines. Note that we assume that \(|k + \omega| < s\) to ensure that the structure of the helix dominates the rotation about it.

Based on this model, we can analytically derive several variants of vortex core lines (according to different extraction schemes). In all cases, we obtain a helix with the same pitch, frequency, and phase but with different radii. See Table 1 for an overview of the results.

The employed methods are three state of the art approaches for steady flow data: the method proposed by Levy et al. (curl parallel to velocity [13]), the one by Sujudi and Haines (parallel first and second derivatives of streamlines [24]), and the higher order method by Roth and Peikert (parallel first and third derivatives of streamline [21]). We apply them to the flow data of individual time steps as discussed above.

We contrast these results with those of our new approach, that is, the unsteady extension by Sujudi and Haines’ (as described in Section 4.1) and the unsteady
version of the higher order approach (as described in Section 4.2). We see that the traditional approaches miss the rotation of the vortex rope (missing \( + \omega \) terms in all cases), since it obviously cannot be detected from considering an individual time step only.

We also compute a correct vortex core line for this unsteady flow by using a symmetry argument. On each slice orthogonal to the \( z \)-axis \( (z = z_{\text{const}}) \), there is just one point \( (x, y, z_{\text{const}})^T \), with

\[
 x = \frac{R \cdot \cos(kz)}{1 - (k + \omega)/s} \quad \text{and} \quad y = \frac{R \cdot \sin(kz)}{1 - (k + \omega)/s},
\]

such that a particle that is released from this point at time 0 moves along a pathline of exact helical shape. Particles that are released from any other location yield pathlines of more complicated geometry (Fig. 2). In this case, we see that the material line (time line), which consists of all of these special particles, coincides with the correct vortex core line. This curve has the same radius as the helical pathlines but exhibits a different pitch of \( \omega/x \) versus \( \omega/s \). We note, however, that the fact that the vortex core line also is a material line is specific to this example and does not generally hold for arbitrary cases.

By comparing the different radii in Table 1 with the correct solution and by considering the geometric series \((1 - p)^{-1} = (1 + p + p^2 + \ldots)\) here, with \( p = (k + \omega)/s \), we can see a nice alignment of our new approach with the correct solution. The modified variant of the approach by Sujudi and Haimes is the first-order approximation of the correct solution, and the modified variant of the higher order approach is its second-order approximation.

The deviation of the Sujudi-Haimes lines from the correct vortex core lines is the phenomenon first observed in the “bent helix” example [20], and it is due to the combination of a weakly rotating vortex and a strongly curved vortex core line. The error becomes negligible if \(|k + \omega| \ll |s|\), that is, if the sum of the spatial and the temporal frequency is much smaller than \( s \) controlling the swirl around the vortex core line. The higher order method yields an additional term of the Taylor series in this example.

We have seen that the extension to unsteady flow for both methods results in improved results in comparison with the time frozen analysis of vortex flow features. To understand what is happening with unsteady vortices, it is necessary to extend the steady versions of the vortex extraction criteria.

## 4 Pathline Geometry-Based Feature Detectors

We can generalize existing feature extraction algorithms to unsteady flow data by replacing streamlines with pathlines in the underlying model. This way, they remain unchanged for steady flows.

### 4.1 Sujudi-Haimes

In this section, we modify the approach by Sujudi and Haimes [24] to include time derivatives.

#### 4.1.1 Original Definition

In the original definition, the first step is to compute the eigenvalues of \( \nabla \times \mathbf{u} \) per tetrahedral cell. Only cells where a pair of complex eigenvalues exists are further processed. The existence of two complex eigenvalues is determined by the discriminant of the characteristic polynomial [4].

The next step is to compute the single real eigenvector \( \mathbf{e}_r \) for the candidate cells to extract the local direction of the vortex core line. In the final step, the algorithm searches for locations where \( \mathbf{e}_r \) is parallel to \( \mathbf{u} \). Linear interpolation is used between the nodes of a grid cell when searching for parallel locations. A modification in order to get connected lines instead of disjoint straight line segments is to estimate velocity gradients per node and compute parallel positions on cell faces.

#### 4.1.2 Equivalent Definition

The eigenvector computation required by the original method is quite expensive. A more efficient method [16] is to compute the matrix-vector product \( \mathbf{a}_s = (\nabla \mathbf{u}) \mathbf{u} \) instead. Given that \( \mathbf{e}_r \) is the only real eigenvector of \( \nabla \mathbf{u} \), it is parallel to \( \mathbf{u} \) exactly if \( \mathbf{a}_s \) is. Hence, Sujudi-Haimes vortex core lines can be equivalently defined as the locus of points, 

| Different Extraction Schemes, All Result in Helical Vortex Core Lines but with Different Radii |
|---------------------------------|-----------------|------------------|
| **streamline-based**            | **pathline-based (new)** |
| Levy et al.                     | \((1 + \frac{k}{s^2})R\)  | \((1 + \frac{k + \omega}{s})R\)  |
| Sujudi & Haimes                 | \((1 + \frac{k}{s^2})R\)  | \((1 + \frac{k + \omega}{s})R\)  |
| higher-order                    | \((1 + \frac{k + \omega}{s})R\)  | \((1 + \frac{k + \omega}{s})R\)  |
| correct                        | \((1 + \frac{k + \omega}{s})R\)  | \((1 + \frac{k + \omega}{s})R\)  |

We compare the results for the algorithms by Levy et al. [13], Sujudi and Haimes [24], the higher order method by Roth and Peikert [21], and an analytically determined correct variant.
where $u$ and $a_u$ are parallel, restricted to points where the velocity gradient has a pair of complex eigenvalues. In this context, two vectors are said to be parallel also if one or both of them is zero.

### 4.1.3 Modification for Unsteady Flow

The original formulation of the Sujudi-Haines criterion is expressed in terms of the velocity field and its gradient tensor field. Using this formulation, we cannot include the time derivative information since these quantities are the same for steady and unsteady flow. In contrast, the parallel vectors formulation allows for a different extension to unsteady flow. The vector $a_u = (\nabla u)u$ can be viewed as the steady case of the acceleration vector

$$a_u = Du/Dt = (\nabla u)u + \partial u/\partial t$$

of a particle. An obvious modification is now to use the true acceleration vector instead of the vector $a_u$, that is, to look for points where $a_u$ and $u$ are parallel. Besides the justification as being the natural extension to unsteady flow, this modification is also backed up by the following observation.

Sujudi-Haines vortex core lines can be defined in a third equivalent way, namely, as the locus of zero streamline curvature, again constrained to points where the velocity gradient has a pair of complex eigenvalues. The equivalence is shown as follows: The curvature of a curve with (time) parameter is $\kappa = |x \times \dot{x}|/\|\dot{x}\|^3$, where the dots denote temporal derivatives. For a streamline, $\dot{x} = u$ and $\ddot{x} = a_u$; so, the streamline curvature is zero exactly where the Sujudi-Haines criterion is met. For a pathline, $\dddot{x}$ is $Du/Dt$, so, the pathline curvature is zero exactly where the modified Sujudi-Haines criterion is met.

In principle, the zero curvature points of streamlines or pathlines could be computed to yield vortex core lines according to the original or modified Sujudi-Haines criterion. However, numerical integration and curvature computation are too expensive operations to make this a practical alternative to the parallel vectors method.

It was a long standing open question from our application partners why the vortex core lines resulting from the original algorithm by Sujudi and Haines very often exhibit a small phase-shift in relation to regions of low pressure. Therefore, it is a common approach to do a correction step toward pressure minima when extracting vortex core lines [1], [11]. In Fig. 3, we can see that the yellow vortex core lines extracted using the classical approach by Sujudi and Haines [24] deviates from the center of pressure isosurface. The modification to time derivative aware extraction of the vortex core line improves the results visibly.

Fig. 3. For the vortex rope in the depicted data set, isovales of pressure give good insight on where the vortex core line is located. We can clearly see how the yellow core line (extracted using the classical approach by Sujudi and Haines [24]) deviates from the center of pressure isosurface. The modification to time derivative aware extraction of the vortex core line improves the results visibly.

In this section, we modify the higher order approach to work on pathlines.

#### 4.2.1 Original Definition

Roth and Peikert [21] present an extension of the vortex extraction approach by Sujudi and Haines to bent vortices. The eigenvector is based on a straight-line model for the vortex core line. In real-world data sets, we can find many types of bent vortices though. Common types are hairpin-, horseshoe-, and ring-shaped vortices. Roth and Peikert showed [20] that the eigenvector method introduces an error as soon as the vortex is bent.

To overcome these drawbacks, we can weaken the conditions on a vortex core line such that we can detect bent vortices as well, but the amount of false positives will increase significantly. It is not possible to model a curved vortex based on linear fields; therefore, one has to take into account higher order derivatives when searching for vortex core lines. The second derivative following a particle in a steady velocity field is $b_x = (\nabla a)u$.

Based on the torsion of a parametric curve in $\mathbb{R}^3$, we can relax the condition on vortex core lines such that torsion is zero and that zero torsion is preserved as much as possible when following the streamline. The extraction algorithm is based on the fact that for the bent vortex model, the torsion at the vortex core line is not only restricted to the $<\hat{u},a_u>$ plane but that the best choice is to require that $b_x$ is parallel to $u$. Thus, we can state the following definition for a vortex core line: The vortex core line is the location of all points, where $b_x$ is parallel to $u$.

#### 4.2.2 Modification for Unsteady Flow

The problems observed for curved vortices in steady flow data [21] obviously extend to curved vortices on unsteady flow data. In Section 3.2, we have seen that the modified version of the higher order model will reproduce the correct vortex core line of the bent time dependent model if we ignore the terms of higher order in the Taylor expansion. Therefore, we can use the parallel vectors operator to apply the higher order approach to unsteady flows.
therefore to replace the vector core line detection algorithm, the required modification is streamline-based geometries. For the higher order vortex will show the same inconsistencies as observed for restriction. However, for strongly bent vortices, the result for straight vortex core lines. The line that is classified as the vortex core lines, we can derive additional attributes such as an attribute measuring the distance from the core line for further analysis.

A criterion based on zero curvature in principle searches for straight vortex core lines. The line that is classified as the vortex core line by the parallel vectors approach of the previous section can deviate to some extend from this restriction. However, for strongly bent vortices, the result will show the same inconsistencies as observed for streamline-based geometries. For the higher order vortex core line detection algorithm, the required modification is therefore to replace the vector $b_t$ by the actual jerk vector (rate of change of acceleration) $b_t = \frac{D^2u}{Dt^2}$. See Fig. 7 for an example.

### 4.3 Interactive Vortex Core Line Extraction and Filtering

Both the eigenvector method and the higher order method produce many line segments that cannot be considered as vortex core lines. For this reason, we use the interactive visual analysis features of the SimVis framework to extract the meaningful vortex core lines. This way, we get confidence in the extracted vortex core lines and can improve their quality. Here, we rely on smooth expressions of vortex detectors to select the vortex core lines of interest [3]. In the other way round, we use the extracted core lines to derive other attributes in the data. Fig. 4 illustrates this approach.

To our knowledge, there is no fully satisfying approach to extract only the relevant vortex core lines automatically from the data. The interactive multifield approach of SimVis handles this problem using visual analysis. To be able to do this, we modify the parallel vectors algorithm slightly:

1. Generate additional field $a_t$ or $b_t$ (see Section 4.1.3, Section 4.2.2, and Appendix A).
2. Compute closed parallel vectors lines without additional criteria (see Appendix A.3).
3. Use interactive region of interest specification to extract correct subsections of the lines (see Fig. 4).

The delta discriminant used as an additional criterion both by the method of Sujudi and Haimes and the higher order method was introduced by Chong et al. [4]. This physics-based criterion does not take into account the time-dependent components of the flow. Nevertheless, physics-based criteria such as delta, $Q$, and $\lambda_2$ are often directly applicable to unsteady flow, when it is possible to derive them from instantaneous properties of the flow. The delta criterion is prone to finding false positives in large regions of the flow (for example, in the turbine data set, it is true almost everywhere). In our experience, it has shown to reduce the number of spurious solutions to use additional vortex core region detectors in combination with the delta criterion. Another type of additional criteria includes information derived from the vortex core line [16]. Examples are the angle between flow and vortex core line, number of core line segments, and vortex strength. These are difficult to tune optimally. By combining multiple vortex region criteria, as suggested in [3], we can avoid criteria involving the extracted vortex core line.

Building on the information that we got from the extracted vortex core lines, we get access to a whole new type of information that we can use in further analysis steps. To include information on the vortex core line, we derive for each cell an attribute that measures the distance from the final vortex core line in a simple breadth-first traversal, starting with cells that contain a vortex core line segment.

### 5 Application Study—Engine Data Sets

We have implemented the presented vortex core line (Fig. 5) detection algorithms in the SimVis framework [31] and applied it to two engine data sets to verify the approach on real-world data. For these data sets, we have found that using the Green-Gauss approach for computing gradients gives better results than a least squares approach (see Appendix A).

The first data set results from a simulation of the compression and combustion phase in the combustion chamber of a standard engine model. In Fig. 6, we can see the vortex core lines based on the original and the modified
versions of the parallel vectors criteria. Obviously, the results differ significantly, and one of the vortex core lines is not extracted at all using the original algorithm.

The second data set is a high-performance two-stroke engine data set (Fig. 7), which contains the complete simulation results from the injection and the combustion of fuel during one crank revolution. The engine geometry is shown in Fig. 8. Table 2 shows a comparison of the data sets discussed in the following sections.

5.1 Impact of Time Derivatives

The question remains whether and where the time derivative information has significant impact on the vortex core line extraction results. In the engine data sets, we have found the vortex core lines extracted by the modified and the unmodified methods to be similar but shifted for most time steps. However, in Fig. 6, we can observe that in a time step shortly after ignition, the vortex core line based on \( \mathbf{a}_t \) and the vortex core line based on \( \mathbf{a}_s \) can differ significantly. This is due to the strong impact of the time derivative in these time steps. To illustrate the close correlation between these two vectors in early time steps and the large impact of the time derivative after ignition, we show the magnitudes of the vectors normalized with mean and standard deviation in scatterplots (see Fig. 9). Very often, the time steps that include large changes over time are critical for the application. They have vital impact on mixing, material wear, and engine performance, and therefore, the analysis benefits from improving vortex core line extraction in these time steps.

<table>
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<th>T-junction</th>
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<td>46792</td>
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<tr>
<td>hexahedra</td>
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<td>125960</td>
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<td>214 – 428</td>
<td>6505</td>
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<tr>
<td>Timesteps</td>
<td>48</td>
<td>91</td>
<td>1570</td>
</tr>
</tbody>
</table>

Since the grids of the engine data sets vary over time the number of cells changes accordingly.
5.2 Equivalence Ratio (ER)

One key attribute that is related both to emission and engine performance is ER, which is the relation between fuel and air within a volume cell. It is crucial that ER lies in the optimal interval between 0.7 and 1.4 for most fluid cells at the moment of ignition. The mixing process happens at earlier time steps during compression when the influence of the time derivative is less than after ignition. Even though the difference between the core lines generated by the modified version is smaller, it is still not negligible. In Fig. 10a, we show isovalues of the \( \lambda_2 \) vortex detector and concentrate on the vortex core lines detected for this vortex. In the center of the combustion chamber of the two-stroke engine, we can see the large vortex region that plays a central role in the mixing process. The question in this example is, why the vortex core region is not of tubular shape. The second vortex core line (3) is not detected by the original approach. Combining (1) and (3), we can gain insight into the controlling skeleton of the main tumble vortex. In Fig. 10b, we can distinguish the regions of suboptimal and optimal to very high concentrations of fuel at an isovalue surface of 0.7. The bend part of vortex core line (3) closely follows the boundary of this region. In Fig. 10c, the surface describes the boundary of the region defined by slightly suboptimal to high-mixing and high-\( \lambda_2 \) values. The core line generated for this vortex with the original vortex core extraction method (1) and the modified approach (2) are similar, and both traverse the full region detected by the \( \lambda_2 \) vortex region detector. Another core line is not detected though. Obviously, we miss an important aspect without the second vortex core line since we can see in Fig. 10c that it influences the region of the vortex where nonoptimal mixing occurs.

6 Assessment of Numerical Behavior

In engineering applications, it is not common to store all the information computed in the course of the CFD simulation permanently. Especially that time derivative information is not generally stored in the data. Furthermore, the solver does not include all the time steps computed in the solution file. In general, we can expect the simulation design regarding cell types and cell sizes to be adequately chosen by the simulation designer. The simulation designer considers the necessary resolution for postprocessing such that reliable streamlines and pathlines can be constructed. From experience, we know these settings work well for computing vortex core lines in the steady case. Since time-derivative information is not stored and not all time steps are written out into the final data set, we need to evaluate the impact of larger step widths on the feature extraction process. Our application partners from Arsenal Research [30] have computed an unsteady solution to a pulsating flow in a tube t-junction (see Fig. 11). Time dependent boundary conditions are used to produce flow separation inside the tube. The total mesh size is about 170,000 cells.

During simulation, 1,570 time steps have been generated resulting in 26 Gbytes of compressed information. This is 10 times the temporal resolution our application partners would have stored usually for this simulation setting. To exclude possible interference from numerical problems introduced by the plane fitting technique, we use to estimate the material derivatives also the Jacobian computed during the simulation have been included in the data set. This way, we can analyze how strong the impact of larger time steps is when computing vortex core lines. We can use the time derivative computed for step width 1 as reference for the other step widths and measure the influence of larger step...
widths by computing the difference between the reference derivative and the respective derivative for the given step width. In Fig. 11, the magnitude of this difference is mapped to color. To analyze the impact on vortex extraction, we focus on a horseshoe vortex directly behind the top inlet. We see the difference between the acceleration vector from step width of 1 and step widths 10 and 20. The vortex core lines resulting from smaller step widths than 10 do not differ significantly from each other. This is exactly the default step width resulting from the standard simulation procedure. For larger step widths, the resulting vortex core line begins to deteriorate due to the noise introduced by the time derivative component of the acceleration vector. At step width of 20, we still get a similar but jagged result. At larger step widths, the extracted line no longer resembles the horse shoe vortex in the data set. At step width 100, the line breaks into three unconnected components that follow the vortex core line for some length and then trail off in random directions.

We conclude that for standard step widths in well-prepared simulations, the time-aware vortex core line extraction method produces reliable results. Both for the especially designed data set and the real-world examples (where the Jacobian had to be estimated), we did not find the estimation of the time derivatives to introduce significant additional noise.

7 CONCLUSION

This paper proposes a new method to find vortex core lines in unsteady flows. Localization of vortices has been shown to be dependent on the temporal developments of the flow. We have given examples where vortex core extraction on time-frozen fields fails and have shown how to solve this problem. This result is not only relevant to vortex core extraction algorithms but to unsteady flow feature extraction methods in general. Since we could demonstrate that vortex core extraction algorithms have to include the temporal developments of the flow, it can be expected that similar results can be achieved for other flow features as well. Therefore, we expect to see significant similar results in this direction in the future.

Based on the insight that it is necessary to include the time-derivative information into the feature extraction process, we proposed a natural extension of the feature extraction process to unsteady flow data. By changing the underlying geometry from a streamline to a pathline-based approach, we can generalize existing feature extraction algorithms to unsteady flow data in a way that does not change their behavior on steady flows. We presented an algorithm that follows this approach extending parallel vectors operator criteria. Due to the consistent extension of the approach, the algorithms change in a natural way, and (given an implementation of the parallel vectors operator) the extension can be implemented quickly. The additional computation cost amounts to computing finite differences to estimate the time derivatives, therefore, the difference to the original parallel vectors implementation is small.

We could confirm on real-world data that the extracted vortices can differ significantly in position from the method by Sujudi and Haimes, and in the large majority of the cases, the extracted core lines are the same or better than those we got with the standard methods.

We conclude that for unsteady data, the modified version of the algorithm by Sujudi and Haimes is the default choice. The higher order method generally performs very similar to the method by Sujudi and Haimes, but it intensifies numerical issues. Also, it requires additional computation. Therefore, only if after inspection of the data, the results of the unsteady version by Sujudi and Haimes do not perform as expected, we suggest to switch to the modified higher order method.

APPENDIX A

ALGORITHM DETAILS

The vortex core line extraction process consists of three stages:

1. estimate velocities at vertices and faces (Appendix A.1),
2. reconstruct gradients at vertices and faces using estimated velocities (Appendix A.2), and
3. for each cell, subdivide into tetrahedra and use reconstructed gradients to find vortex core positions (Appendix A.3).

Depending on the type of simulation data, storage can be either vertex or cell centered (see Fig. 12). In the third vortex core line extraction step, we need gradients at the nodes of the grid, and the gradient reconstruction step varies slightly for the two storage types.
A.1 Velocity Estimation

To reconstruct velocities, we use a standard inverse geometric weighted interpolation scheme.

For estimating face velocities from cell centers, we define the distance between the center of a cell and one of its faces as the distance between the cell center and the center of gravity of the face. The velocity at face $u_f$ is computed as

$$u_f := \alpha u_C + (1 - \alpha) u_N,$$

where $C$ and $N$ are the two cells adjacent to the face $f$. Here, the weighting geometric factor $\alpha$ can be computed as

$$\alpha := \frac{d(f, N)}{d(f, C) + d(f, N)}$$

where $d(., .)$ denotes the euclidean distance (see Fig. 13a). When working with vertex-centered volume representation, the velocity at a face can be computed by taking the average of the surrounding vertices.

The velocity at a node $v$ can be computed from the surrounding cell centers by using the cell values of the surrounding cells. The segments surround the median dual control volume, (a) The surrounding surface uses cell centers (green) and midpoints (gray). (b) In this detail illustration of the lighter gray section from (a), we see the full configuration for a single surrounding tetrahedron.

A.2 Gradient Reconstruction

In addition to the velocity values at the vertices to the cell, we also need the velocity gradients. To compute the gradients, we suggest to use the Green-Gauss reconstruction method that works with velocity values from the faces of the cell. The least squares linear reconstruction method can be used when no connectivity values are present. To compute the derivative at the center of the control volume, we assume that $\nabla \varphi$ is constant over the control volume, and the volume integral over $\nabla \varphi$ reduces to the volume of $\Omega$ times $\nabla u$:

$$\int_{\Omega} \nabla \varphi d\Omega = \int_{S} \varphi dS.$$

Finally, we can approximate the integral over the bounding surface using face values. That is

$$\nabla \varphi = \frac{1}{|\Omega|} \sum_{faces} \varphi \cdot area(face_i) \cdot n_f,$$

where $area(triangle)$ is the surface area of a triangle.

To compute the derivative at a vertex, we can use the control volume depicted in Fig. 14 and get

$$\Omega_C^{\nabla u} \approx \sum_{t=0}^{N_t(v)} \sum_{i=1}^{3} area(s_{t,i}) \cdot u_{t,i}^v.$$

Here, $N_t(v)$ is the number of tetrahedra at vertex $v$. Here, we are using an interpolated velocity vector at the midpoints $u_{t,i}^m := \frac{1}{2}(u_{t,i}^v + u_{t,i})$ and the velocity at the cell center to
construct the surface velocity $u^s_{ij} := \frac{1}{2}(u_{t,i}^m + u_{t,i+1}^m + u_c)$ (with $u_{t,1}^m := u_{t,1}^m$). See Fig. 14 for an illustration.

A.2.2 Least Squares Linear Reconstruction

Here, the gradient is estimated by fitting a hyperplane to the cell such that the difference between the extrapolated value for the surrounding cells and the present values of the surrounding cells are minimized.

For each edge of the resulting mesh incident to the vertex $v_0$, an edge projected gradient constraint equation is constructed using inverse distance weights for each edge:

$$
\frac{d}{C11k}(r_u)_{C0\times x,0} = \frac{d}{C11k}\left[ \frac{2}{C0}\right]_{0\times x_0}.
$$

The gradient construction is obtained by solving a least squares optimization problem to minimize the sum of the distances between the estimated values and the vertex values. This approach implicitly smoothes the data and can improve the results when working with noisy data.

Which weighting scheme works best is still an open question. Mavriplis [14] stresses that the minimization problem will be much better conditioned when using inverse distance weighting. On the other hand, when the mesh is irregularly sampled and, on one side of a cell, we have a large number of small triangles and, on the other side, just a few larger triangles, this can lead to a gross misrepresentation of small triangles. Therefore, we use unweighted direct neighbors for estimating the gradient at a cell by default and only change this procedure when necessary.

A.3 Pseudocode

Figs. 15 and 16.


[23] S. Stegmaier, U. Rist, and T. Ertl, “Opening the Can of Worms: Visualization, including interactive visual analysis, medical visualization, and the combination of scientific and information visualization. He is a member of the IEEE.

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