CURVATURE MEASURES OF 3D VECTOR FIELDS AND THEIR APPLICATIONS

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ABSTRACT

Tangent curves are a powerful tool for analyzing and visualizing vector fields. In this paper two of their most important properties are examined: their curvature and torsion. Furthermore, the concept of normal surfaces is introduced to the theory of 3D vector fields, and their Gaussian and mean curvature are analyzed. It is shown that those four curvature measures tend to infinity near critical points of a 3D vector field. Applications utilizing this behaviour for the (topological) treatment of critical points are discussed.

Keywords: flow visualization, vector fields, tangent curves, curvature, topology

1 INTRODUCTION AND RELATED WORK

The treatment and visualization of vector fields is of great importance to a wide area of sciences. Especially 3D vector fields appear in real world environments like fluid mechanics. But the visualization of 3D vector fields is still subject of ongoing research. Due to the high complexity of 3D vector fields and common problems of visualizing in three-dimensional space the majority of methods treats only parts or special properties of those fields ([Stolk92], [Leeuw93], [Zöck196]).

In this paper we will propose curvature measures for the treatment and visualization of 3D vector fields. Their properties give assistance in visualizing critical points and, therefore, the topology of vector fields. A classification of simple critical points can be found in [Batra98] or [Weink00]¹. Throughout this paper we want to consider vector fields with simple critical points only.

Leeuw et al introduced in [Leeuw93] a probe

for local flow field visualization which encodes (among other measures) the curvature of a tangent curve at a selected point of the vector field. The first use of curvature measures throughout the whole domain of the vector field is described by Theisel in [Theis95], but only for 2D vector fields. Weinkauf expanded this theory in [Weink00] for 3D vector fields and the results are published here.

Sections 2 and 3 present the theory of curvature measures, whereas section 4 examines their behaviour around critical points of 3D vector fields. Applications will be discussed in section 5 followed by a conclusion in section 6.

2 THEORETICAL BACKGROUND

A 3D vector field V shall be defined as a map $V : \mathbb{E}^3 \to \mathbb{R}^3$, where \mathbb{E}^3 denotes the euclidian 3D space equipped with a cartesian coordinate system (x, y, z) and \mathbb{R}^3 is a 3D vector space. Following the common notation, the components of V are called u, v and w. Partial derivatives of V will be denoted with $V_x = (u_x, v_x, w_x)^T$, where $u_x(x, y, z) = \frac{d}{dx} u(x, y, z)$. Same for V_y and V_z .

¹Some terms in this paper like "a critical point of class 4" refer to the terminology of [Batra98] resp. [Weink00] and will not be explained here.

2.1 Derivatives of Tangent Curves

In general, tangent curves can not be described explicitly, but implicitly as a solution of the following system of differential equations:

$$\frac{dx}{dt} = u(x, y, z)$$

$$\frac{dy}{dt} = v(x, y, z)$$

$$\frac{dz}{dt} = w(x, y, z)$$
(1)

This circumstance makes analyzing the properties of a vector field more difficult. But in order to compute measures like curvature or torsion of tangent curves it is necessary to know the derivatives of these curves. The definition of tangent curves states, that the first derivative vector \dot{L} of a tangent curve L at a point P equals the vector of the vector field V at the same point: $\dot{L}(P) = V(P)$. Although we do not know an explicit expression of tangent curves in general, we can compute their higher derivatives using the following $(\stackrel{1}{L} \doteq \dot{L}, \stackrel{2}{L} \doteq \ddot{L}, \ldots)$:

Lemma 1. Let $V = (u, v, w)^T$ be a 3D vector field, let L(t) be an arbitrary tangent curve of V and let $P \in L$ be an arbitrary point on L. Furthermore, let L(t) be parameterized in such a way, that $P = L(t_0)$ and $\dot{L}(t_0) = V(L(t_0))$. Then we obtain for the n-th derivative vector of L (n > 1):

$$\overset{n}{L}(t_0) = (u \cdot \overset{n-1}{L_x} + v \cdot \overset{n-1}{L_y} + w \cdot \overset{n-1}{L_z})(P) \quad (2)$$

Proof. We have:

$$\overset{n}{L} = \frac{d \overset{n-1}{L}}{dt}$$

To differentiate the function $\overset{n-1}{L}$ we have to apply the generalized chain rule. Doing this and paying attention to (1) we obtain:

$$\stackrel{n}{L} = \frac{d}{dt} \stackrel{n-1}{L} = \frac{L}{dx} \cdot \frac{dx}{dt} + \frac{L}{dy} \cdot \frac{dy}{dt} + \frac{L}{dz} \cdot \frac{dz}{dt}
 = \frac{L}{L_x} \cdot \frac{dx}{dt} + \frac{L}{L_y} \cdot \frac{dy}{dt} + \frac{L}{L_z} \cdot \frac{dz}{dt}
 = u \cdot \frac{L}{L_x} + v \cdot \frac{L}{L_y} + w \cdot \frac{L}{L_z}$$

Lemma 1 gives us the opportunity to compute the derivatives of tangent curves to any degree just by knowing the vector field and its partial derivatives. Using this, we are able to compute curvature and torsion of tangent curves.

2.2 Normal Surfaces

In this paper we want to introduce the concept of normal surfaces to the theory of 3D vector fields.

Definition. A surface $S \subseteq \mathbb{E}^3$ is called NORMAL SURFACE of a 3D vector field V, iff the following is satisfied for all points $P \in S$: The normal vector of S at P has the same direction as V(P).

Normal surfaces² are not defined at critical points. Neither they intersect nor touch each other, because of the unique direction of the vector field at every non-critical point. Therefore, there is one and only one normal surface through every non-critical point of a vector field. That is what they have in common with tangent curves. It is easy to see, that every point of a normal surface gets perpendicularly intersected by one tangent curve.

Just as tangent curves, normal surfaces can generally not be represented explicitly. To investigate the properties of normal surfaces we need to know their basic measures $\mathcal{E}, \mathcal{F}, \mathcal{G}, \mathcal{D}, \mathcal{D}'$ and \mathcal{D}'' of GAUSS'S THEORY OF SURFACES. For this we need 2 linear independent vectors \mathbf{a}_0 and \mathbf{b}_0 at every point $P_0 \in S$, which span the tangential plane in P_0 . Both have to be perpendicular to the normal vector in P_0 (which is given by the vector field itself) and can be computed by:

$$\mathbf{a_0} = \begin{pmatrix} \frac{-v}{\sqrt{u^2 + v^2}} \\ \frac{-w}{\sqrt{u^2 + v^2}} \\ 0 \end{pmatrix} \quad \mathbf{b_0} = \begin{pmatrix} 0 \\ \frac{-w}{\sqrt{v^2 + w^2}} \\ \frac{-w}{\sqrt{v^2 + w^2}} \end{pmatrix} \quad (3)$$

Knowing this, the basic measures of GAUSS'S IN-NER GEOMETRY OF SURFACES can be computed ([Spiva79]):

$$\mathcal{E} = \mathbf{a}_{0} \cdot \mathbf{a}_{0} = 1$$

$$\mathcal{F} = \mathbf{a}_{0} \cdot \mathbf{b}_{0} = -\frac{u \cdot w}{\sqrt{u^{2} + v^{2}} \cdot \sqrt{v^{2} + w^{2}}} \qquad (4)$$

$$\mathcal{G} = \mathbf{b}_{0} \cdot \mathbf{b}_{0} = 1$$

A first order taylor expansion of the vector field at P_0 gives us the possibility to compute the first derivatives of $\mathbf{a_0}$ and $\mathbf{b_0}$. Using this together with the normal vector of S at P_0 we get the basic measures \mathcal{D} , \mathcal{D}' and \mathcal{D}'' of GAUSS'S SECOND BASIC FORM OF SURFACE THEORY ([Spiva79]):

$$\mathcal{D} = -\frac{-u \cdot v \cdot v_x + u^2 \cdot v_y + v^2 \cdot u_x - v \cdot u \cdot u_y}{(u^2 + v^2) \cdot \|V(P_0)\|}$$
$$\mathcal{D}' = -\frac{v \cdot w \cdot (u_y + v_x) - 2 \cdot u \cdot w \cdot v_y - v^2 \cdot (u_z + w_x) + u \cdot v \cdot (v_z + w_y)}{2 \cdot \sqrt{u^2 + v^2} \cdot \sqrt{v^2 + w^2} \cdot \|V(P_0)\|}$$
$$\mathcal{D}'' = -\frac{-v \cdot w \cdot w_y + v^2 \cdot w_z + w^2 \cdot v_y - w \cdot v \cdot v_z}{(v^2 + w^2) \cdot \|V(P_0)\|}$$
(5)

²Following the terminology of tangent curves the name for these surfaces has been derived from the defining property: the normal vector.

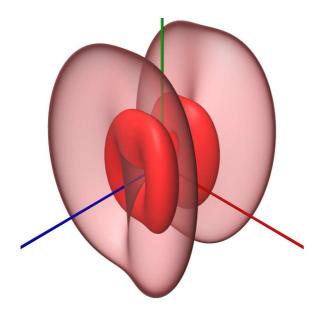
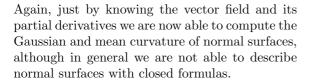


Figure 1: Isosurfaces of curvature field $\kappa(V_1^{\ell})$.



3 CURVATURE MEASURES

In this section we want to introduce 4 scalar fields defined by the already mentioned curvature measures and discuss their basic properties. To give an impression how the isosurfaces of those fields look like, we will visualize the curvature measures of the linear vector field $V_1^{\ell} = (-2x, -y, 2z)^T$, which has only one critical point at (0, 0, 0) with the class 1 topology (AN, S, S).³ Especially, very high positive (colored⁴ in red) or negative (colored in blue) isovalues will be used for this purpose. A detailed description of how the visualization is done and how it can be interpreted will be given in later sections.

3.1 Curvature and Torsion of Tangent Curves

The curvature of a curve is a measure for the curve's deviation from its own tangent. Therefore, a straight line has no curvature, whereas

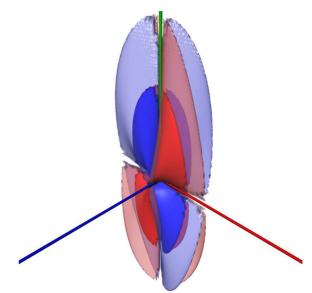


Figure 2: Isosurfaces of torsion field $\tau(V_1^{\ell})$.

the curvature on a circle is constant and different from zero. Furthermore, curves in 3D have always non-negative curvature. Using Lemma 1 we can compute the curvature of every point $P = L(t_0)$ of a tangent curve L ([Farin92]):

$$\kappa(t_0) = \frac{\|\dot{L}(t_0) \times \ddot{L}(t_0)\|}{\|\dot{L}(t_0)\|^3} \tag{6}$$

As we know that there is one and only one tangent curve through every non-critical point of the vector field V, we can define the CURVATURE FIELD $\kappa(V)$: A scalar field describing at every point the curvature of the tangent curve through that point. $\kappa(V)$ is not defined at critical points. Figure 1 gives an impression of how such a curvature field looks like.

The torsion is another important measure of curves. It describes how much the curve squirms out of its osculating plane. Therefore planar curves have no torsion. We can compute the torsion for a parameterized curve L(t) as follows ([Farin92]):

$$\tau(t_0) = \frac{\det\left[\dot{L}(t_0), \ddot{L}(t_0), \ddot{L}(t_0)\right]}{\left\|\dot{L}(t_0) \times \ddot{L}(t_0)\right\|^2}$$
(7)

Using this and Lemma 1 we can compute the torsion of any point of a tangent curve and therefore also for every non-critical point of a vector field. This defines the TORSION FIELD $\tau(V)$ at all noncritical points of a vector field and in conjunction with (6) it is easy to see, that also the torsion is not defined at points with curvature $\kappa = 0$ (as the denominator of (7) is zero at those points). Figure 2 shows an isosurface visualization of $\tau(V_1^{\ell})$.

³This abbreviation means that the flow in one eigenplane of the Jacobian matrix at the critical point has an attracting node topology, whereas the other two eigenplanes contain a saddle topology. See [Weink00] or [Batra98].

⁴If the images in this version of the paper are (printed) in greyscale, red colors might appear brighter than blue ones. Color versions of all images can be found at http://www.zib.de/weinkauf/.

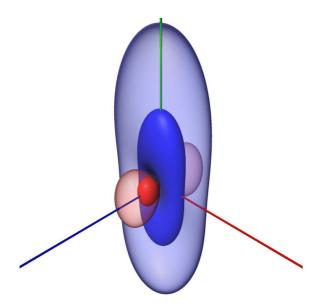


Figure 3: Isosurfaces of Gaussian curvature field $\mathcal{K}(V_1^{\ell})$.

3.2 Gaussian and Mean Curvature of Normal Surfaces

For every point on an arbitrary surface there are two main curvature values λ_1 and λ_2 , which represent the lowest and highest normal curvature of all curves on that surface that go through this point. The product of those two main curvatures is called Gaussian curvature $\mathcal{K} = \lambda_1 \cdot \lambda_2$ and can also be written in terms of differential geometry ([Spiva79]):

$$\mathcal{K} = \frac{\mathcal{D} \cdot \mathcal{D}'' - (\mathcal{D}')^2}{\mathcal{E} \cdot \mathcal{G} - \mathcal{F}^2}$$
(8)

Together with (4) and (5) we are now able to compute the Gaussian curvature of any point on a normal surface and as we know that there is one and only one normal surface through every non-critical point of a 3D vector field, we are able to define a scalar field $\mathcal{K}(V)$ on the same domain, which represents at every non-critical point the Gaussian curvature of the normal surface through that point. This scalar field shall be called GAUS-SIAN CURVATURE FIELD $\mathcal{K}(V)$ (Figure 3).

Gauss showed in his *Theorema egregium*, that the Gaussian curvature is invariant against isometrical mappings of the surface. As in general this might be a powerful property, it leads to the fact, that there is no difference between the Gaussian curvature fields of a vector field V and its inverse vector field $\check{V} = -V$, because only the direction of the normal surfaces differs between V and \check{V} .

In contrast, the mean curvature $\mathcal{H} = \frac{\lambda_1 + \lambda_2}{2}$ of a surface is *not* invariant against isometrical map-

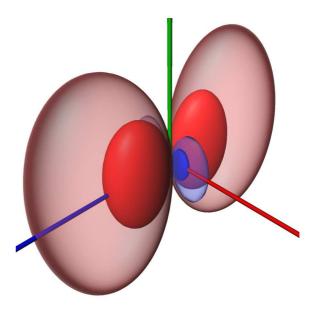


Figure 4: Isosurfaces of mean curvature field $\mathcal{H}(V_1^{\ell})$.

pings. It can also be defined in terms of differential geometry ([Spiva79]):

$$\mathcal{H} = \frac{\mathcal{E} \cdot \mathcal{D}'' - 2 \cdot \mathcal{F} \cdot \mathcal{D}' + \mathcal{G} \cdot \mathcal{D}}{2 \cdot (\mathcal{E} \cdot \mathcal{G} - \mathcal{F}^2)}$$
(9)

Following the definition of the Gaussian curvature field, we define the MEAN CURVATURE FIELD $\mathcal{H}(V)$ of a vector field V (Figure 4). In the next section we will show, that especially this scalar field has useful properties for analyzing vector fields.

4 BEHAVIOUR AROUND CRITICAL POINTS

In this section we want to study the behaviour of the 4 scalar fields introduced in section 3 around a critical point of a vector field. We will show, that the scalar values (depending on the examined scalar field itself and the topology of the critical point) mostly tend to infinity (diverge) near critical points - and only there. This property will be important for using curvature measures in visualization of vector fields. As the proof of divergence is quite similar for all 4 curvature measures, we will concentrate on the curvature of tangent curves. Detailed proofs for all 4 measures can be found in [Weink00].

As we consider critical points with simple topologies only, we can describe the vector field Varound a critical point with a first order approximation at this point⁵

$$V(x, y, z) = V_x \cdot x + V_y \cdot y + V_z \cdot z, \qquad (10)$$

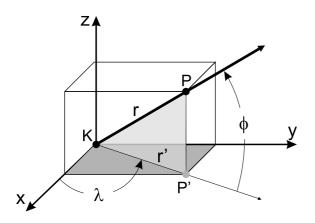


Figure 5: Transformation of coordinates using spherical coordinates.

where V_x , V_y and V_z are certain vector constants, which build up the Jacobian at the critical point (0, 0, 0). The Jacobian can be used to determine the topology of the critical point (see [Batra98]).

To prove the divergence, we consider the scalar values along an arbitrary ray starting at the critical point and we express (10) using spherical coordinates (see Figure 5):

$$V(r, \phi, \lambda) = r \cdot (V_x \cdot \cos \phi \cdot \cos \lambda + V_y \cdot \cos \phi \cdot \sin \lambda + V_z \cdot \sin \phi)$$
(11)

For a specific ray (decribed by ϕ and λ) the distance r from P to the critical point K is the only variable parameter in (11). Expressing the curvature field $\kappa(V)$ (known from (6)) with (11) and separating variable from constant parameters leads to (constant parts of the formula are denoted with an index 'c', e.g. $(\dot{L} \times \ddot{L})_u = r^2 (\dot{L}_c \times \ddot{L}_c)_u$):

$$\kappa(V) = \frac{r^2 \cdot \sqrt{(\dot{L}_c \times \ddot{L}_c)_u^2 + (\dot{L}_c \times \ddot{L}_c)_v^2 + (\dot{L}_c \times \ddot{L}_c)_w^2}}{r^3 \cdot \left(\sqrt{(\dot{L}_c)_u^2 + (\dot{L}_c)_v^2 + (\dot{L}_c)_w^2}\right)^3} \quad (12)$$

Now it is easy to show the divergence:

$$\lim_{r \to 0+0} \kappa(V) = \lim_{r \to 0+0} \frac{1}{r} \to \infty$$
(13)

This estimation can only be done, if the nominator of (12) is not constant zero for all possible rays. So we have to analyze in which cases $\kappa(V)$ is constant zero around a critical point:

$$\left(\dot{L}_c \times \ddot{L}_c\right)_u = \left(\dot{L}_c \times \ddot{L}_c\right)_v = \left(\dot{L}_c \times \ddot{L}_c\right)_w = 0$$
(14)

This leads to a linear system of equations with one non-degenerate solution

$$\left\{ \begin{aligned} u_x &= v_y = w_z \neq 0\\ u_y &= u_z = v_x = v_z = w_x = w_y = 0 \end{aligned} \right\}, \quad (15)$$

field	constant zero	divergence
$\kappa(V)$	class 4	$\lim_{r \to 0+0} \frac{1}{r} \to \infty$
$\tau(V)$	class 2 & 5	$\lim_{r \to 0+0} \frac{1}{r} \to \pm \infty$
$\mathcal{K}(V)$	center of class 7	$\lim_{r \to 0+0} \frac{1}{r^2} \to \pm \infty$
$\mathcal{H}(V)$	_	$\lim_{r \to 0+0} \frac{1}{r} \to \pm \infty$

Table 1: Behaviour of curvature measures around critical points.

which describes exactly a critical point with a star-topology of class 4: All tangent curves are straight lines starting or ending at the critical point. As straight lines have no curvature, $\kappa(V)$ has to be constant zero around such a star-topology, but for all other topologies (13) shows the divergence of the curvature field near the critical point.

Obviously, this condition is also sufficient: Considering equation (6) and keeping in mind that the vector field is piecewise analytic, we obtain that $\kappa(V)$ can tend to infinity only if the denominator of (6) converges to 0, i.e. we have a critical point.

Table 1 summarizes the behaviour of all 4 curvature measures around critical points. Regardless of the topology the mean curvature field $\mathcal{H}(V)$ tends to infinity in the area of a critical point, which is very important for analyzing vector fields with unknown topology. Furthermore, in [Weink00] was shown that $\mathcal{H}(V)$ describes an important subset of linear direction fields uniquely, which means that just by knowing the mean curvature field a reconstruction of the original vector field is possible (except for the magnitude of the vectors).

The results of this section show that curvature measures are very useful for finding critical points. In the next section we are going to propose some applications of them.

5 VISUALIZATION AND APPLICA-TIONS

The curvature measures introduced above have an unbounded co-domain, but many visualization techniques (e.g. colorization) need input parameters with bounded co-domains. Therefore, we normalize the scalar values s to the interval $\langle -1, 1 \rangle$ resp. $[0, 1 \rangle$ using the equation

$$s_{norm} = \operatorname{sgn}(s) \cdot (1 - e^{-\|s\| \cdot con}), \qquad (16)$$

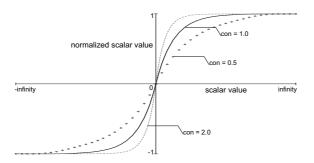


Figure 6: Plot of equation (16) with different contrast parameters.

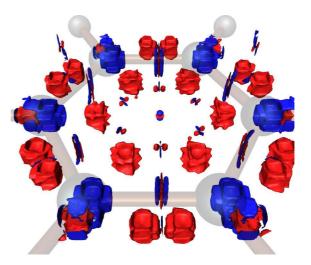
where *con* can be interpreted as a contrast parameter: Decreasing *con* emphasizes the critical points. Figure 6 illustrates this.

5.1 Isosurfaces

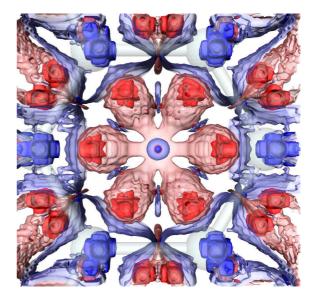
A lot of visualization techniques for scalar fields have been developed⁶, e.g. volume rendering and isosurface extraction. We found isosurface extraction especially suitable for visualizing the 4 introduced scalar fields. For this purpose very high or very low isovalues should be defined, because this ensures that the resulting isosurfaces are tightly bounded around the critical points of the vector field. Therefore, the positions of the critical points can easily be seen without a prior numerical analysis of the vector field, which would be necessary to visualize these positions otherwise.

The necessity of normalizing the curvature measures becomes very obvious for the definition of very high isovalues: It is very uncertain what a high value means in case of an unbounded codomain, but if the scalar values are bounded to $\langle -1, 1 \rangle$ resp. $[0, 1 \rangle$ this question is easy to answer. In the Figures 1, 2, 3 and 4 we used isovalues of 0.95 (colored in red) and -0.95 (colored in blue) for extracting the isosurfaces closest to the critical point. Somewhat smaller isovalues around ± 0.7 have been used for the transparent isosurfaces. It comes out that the isosurfaces defined by isovalues with the same sign are identical to each other except for scaling. This is ensured by the divergence behaviour of the curvature measures (see Table 1), but only true if an influence from other critical points can be excluded.

In Figure 7 we applied the isosurface visualization of the mean curvature field to a more complicated vector field: The electrostatic field around a benzene molecule, called *benzene data set*. It was calculated on a 101^3 regular grid using the



(a) Isosurfaces defined by very high and very low isovalues (±0.99). The positions of the critical points are obvious. Viewed from below.



(b) Isosurfaces defined by isovalues ± 0.99 (opaque) and ± 0.8 (transparent). Frontal view.

Figure 7: Benzene data set: Isosurfaces of mean curvature field. Positive mean curvature is colored red, negative is colored blue.

fractional charges method. For this paper we restrict the visualizations based on this data set to the inner ring of the molecule. The positions of the critical points can easily be seen in figure 7a, whereas figure 7b additionally gives an overview of the structure of the mean curvature field.

Isosurface visualization of curvature measures eases the determination of the positions of critical points, but does not include any directional information about the vector field.

 $^{^{6}\}mathrm{A}$ survey about visualization techniques for scalar fields can be found in [Schum00].

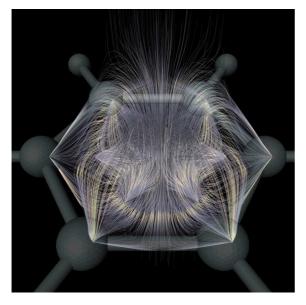


Figure 8: Benzene data set: Visualization of the vector field using illuminated streamlines.

5.2 Color Coding and Distribution of Streamlines

Another approach of applying the curvature measures to vector field visualization is to couple these measures with methods that include directional information of the vector field. A well-known method for this purpose is the visualization of streamlines. Zöckler et al proposed in [Zöckl96] the technique of *Illuminated Streamlines*, which incorporates a special lighting mechanism into the visualization of streamlines for a better visual recognition of their threedimensionality. In Figure 8 this technique was applied to the benzene data set, but the positions of the critical points and the flow around them are hard to see in this picture.

Therefore, we propose the use of curvature measures for colorization and distribution of illuminated streamlines. Colorizing the streamlines at positions of very high or very low curvature enables the viewer to detect critical points, and this eases the understanding of the flow to a very high degree. Furthermore, as the flow of a vector field around a critical point defines its topology, the resulting images support a visually performed topological analysis by a trained viewer. Figure 9 shows illuminated streamlines colorized by mean curvature.

Up to here, the seed points of the streamlines have been distributed homogeneous over the whole domain. Zöckler et al describe in [Zöckl96] a mechanism of distributing the seed points corresponding to regions of interest qualified by a certain scalar

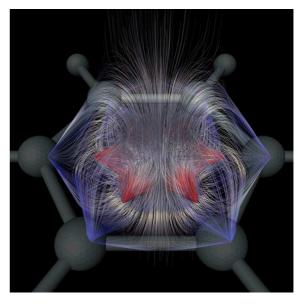


Figure 9: Benzene data set: Illuminated streamlines only influenced in color by the mean curvature field. Positive mean curvature is colored red, negative is colored blue.

quantity s, i.e. more seed points are placed in regions with high values of s. Choosing curvature measures as input of this mechanism increases the density of streamlines around critical points and decreases it in other regions⁷: The resulting visualization concentrates even more on the topology of the vector field. Furthermore, this effect can be intensified by applying a higher transparency to the streamlines at regions with lower (absolute) curvature. Figure 10 shows illuminated streamlines of the benzene data set influenced in color, distribution and transparency by the mean curvature field.

5.3 Other Applications

As the curvature measures tend to infinity around critical points of a vector field, a lot of other applications corresponding to the examination of critical points can be imagined. Only two examples shall be given here. At first, it might be helpful to use curvature measures instead of vector magnitude for finding critical points numerically. Especially in regions with an overall small magnitude the detection of critical points based on the criterion of a zero magnitude may be numerically unstable, whereas the curvature measures react rather sensitively to the appearance of critical points.

At second, curvature measures could be used as a criteria for subdividing vector fields, e.g. using an

⁷Absolute values have to be taken for this purpose.

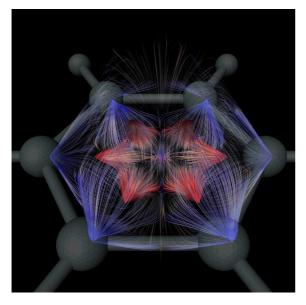


Figure 10: Benzene data set: Illuminated streamlines influenced in color, distribution and transparency by the mean curvature field. Positive mean curvature is colored red, negative is colored blue.

octree algorithm, if regions around critical points have to be subdivided into smaller pieces than other regions.

6 CONCLUSION AND ACKNOWL-EDGEMENTS

In this paper we presented the theory of curvature measures of 3D vector fields. We proofed their divergence around critical points according to table 1. This divergence is useful for many visualizations and applications with focus on critical points and the topology of a vector field. An isosurface visualization of the introduced scalar fields can be used to show the positions of critical points in vector fields, but this does not include any directional information about the vector field. Color coding and distributing streamlines by usage of curvature measures eliminates this drawback and leads to visualizations with a high topological expressiveness.

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