Multi Scale Color Coding of Derived Curvature and Torsion Fields on a Multi-Block Curvilinear Grid

Nathan Brener
Department of Computer Science
Louisiana State University
USA 70808, Baton Rouge, LA
brener@csc.lsu.edu

Farid Harhad, Bijaya Karki
Department of Computer Science
Louisiana State University
USA 70808, Baton Rouge, LA
fharha1@tigers.lsu.edu, karki@csc.lsu.edu

Werner Benger
Center for Computation & Technology
Louisiana State University
USA 70808, Baton Rouge, LA
werner@cct.lsu.edu

Sumanta Acharya
Department of Mechanical Engineering
Louisiana State University
USA 70808, Baton Rouge, LA
acharya@me.lsu.edu

Marcel Ritter
Institute for Astro- and Particle Physics
University of Innsbruck
Austria A-6020, Technikerstrasse 25/8, Innsbruck
marcel.ritter@uibk.ac.at

S. Sitharama Iyengar
School of Computing & Info. Sciences
Florida International University
USA 33199, Miami, FL
iyengar@cis.fiu.edu

ABSTRACT

We present a method to compute and visualize the curvature and torsion scalar fields derived from a vector field defined on a multi-block curvilinear grid. In order to compute the curvature and torsion fields, we define a uniform Cartesian grid of points in the volume occupied by the curvilinear grid and interpolate from the curvilinear grid to the Cartesian grid to get the vector field at the Cartesian grid points. We can then use finite difference formulas to numerically compute the derivatives needed in the curvature and torsion formulas. Once the curvature and torsion have been computed at the Cartesian grid points, we employ a multi scale color coding technique to visualize these scalar fields in orthoslices of the Cartesian grid. This multi scale technique allows one to observe the entire range of values of the scalar field, including small, medium and large values. In contrast, if uniform color coding is used to visualize curvature and torsion fields, it sometimes shows most of the values in a single predominant color, which makes it impossible to distinguish between the small, medium and large values. As an example of this multi-scale technique, we displayed the curvature and torsion fields in a computational fluid dynamics (CFD) simulation of an industrial stirred tank and used these images to identify regions of low, medium and high fluid mixing in the tank.

Keywords

Curvature, Torsion, Vector Field Visualization, Nonlinear Color Map, Transfer Function Generation, Computational Fluid Dynamics.

1 INTRODUCTION

In computational fluid dynamics (CFD), visualization of scalar fields derived from vector fields is an important tool in identifying and understanding flow patterns and complex fluid flow motions. There are a number of visualization methods (cf. (Post et al., 2002) for a survey of flow visualization techniques) that are suitable for various circumstances. In this work, we propose to use multi-scale color coding to visualize the curvature and torsion scalar fields derived from a vector field defined on a multi-block curvilinear grid in order to investigate fluid mixing in CFD simulations of an industrial stirred tank. Implementing this type of visualization on a multi-block curvilinear grid presents considerable challenges compared to a uniform grid.

1.1 Related Work

Computing the curvature of an entire vector field was introduced by (Theisel, 1995) for 2D vector fields, then later was generalized for 3D vector fields by (Weinkauf and Theisel, 2002) and included torsion, Gaussian curvature, and mean curvature, as well. They showed that at the critical points, the curvature tends to infinity. We extend their work to time-dependent vector fields defined on multi-block curvilinear grids as opposed to static vector fields defined on uniform grids.

(de Leeuw and van Wijk, 1993) introduced an interactive probe to visualize a vector and other derived quantities from the velocity gradient tensor such as acceleration, curvature, torsion, and shear. They visualized the curvature as a bended arrow, and the torsion as twisted stripes around the bended arrow. While this approach is explicit and very informative, this probe is impractical for an entire curvature field because the visualization would quickly become cluttered. Instead, we opted for a scalar visualization method. We examined the curvature and torsion fields using orthoslices. For this approach, it becomes crucial to choose the right color mapping technique.

Research on generating color maps focuses on making the scalar values more prominent and easy to visualize. (Kindlmann and Durkin, 1998) introduced a semi-automatic method of generating transfer functions to find material boundaries in a volume. They created a histogram volume which measured the relationship between the scalar values and their first and second derivatives, and used this information to construct opacity functions. Later they further extended this approach to include curvature information in their multi-dimensional transfer functions. Other approaches of generating transfer functions include topological-controlled methods as done by (Zhou and Takatsuka, 2009). Alternatively, (Tzeng et al., 2003) introduced a user interface that allows the user to paint directly on slices of a volume, then automatically define high-dimensional classification functions using artificial neural networks. There also exists other work in this area involving automatic (Hafen et al., 2013) and manual (Pfister et al., 2001) generation of functions to construct color maps.

These color mapping approaches focus on isolating a specific region in space. In contrast, our multi scale color coding technique allows us to show all of the major ranges of a scalar field by simultaneously displaying all of the variations in the curvature and torsion across any given orthoslice.

We previously used multi scale color coding to display the curvature and torsion along integration lines (pathlines) in a vector field (Khurana et al., 2012). In this paper we extend our previous work from integration lines to scalar fields of the entire vector field. Thus here we generate the curvature and torsion everywhere in the stirred tank instead of just along pathlines.

2 METHOD

In this method, the two major parts are 1) computation of the curvature and torsion scalar fields, and 2) rendering the scalar fields as orthoslices using multi scale color mapping. In the first part, we read a data file, of size 350 GB in binary HDF5 format, that contains the vector field (fluid velocity) at the grid points of the multi-block curvilinear grid used in the CFD stirred tank simulations. This curvilinear grid is subdivided into 2088 blocks and contains 3.1 million grid points. The CFD simulation was run over 5700 time steps representing 25 rotations of the stirred tank impeller (Roy et al., 2010). We then do the following steps:

1. Define a 3D Cartesian grid of points in the stirred tank that will be used to calculate the curvature and torsion fields.
2. Since these Cartesian grid points are different from the curvilinear grid points where the vector field is given, we have to get the vector field at the Cartesian points by interpolation. We do this using the Direct Interpolation method which is described in (Bohara et al., 2010).
3. Compute the first, second, and mixed derivatives of the vector field with respect to x, y, and z at the Cartesian grid points using finite difference formulas.
4. Use these derivatives to calculate the curvature and torsion at the Cartesian grid points. This gives us the curvature and torsion fields for the entire stirred tank.

In part two, we render the resulting scalar fields as follows:

1. Construct a histogram of the scalar values, then design a multi scale color map. We show that the use of conventional uniform color coding for the whole range of these scalar values often gives a single predominant color, making it impossible to visualize variations in the scalar values. In contrast, multi scale color coding gives different colors for the small, medium, and large scalar values, thereby enabling one to visualize the entire range of these values.
2. Extract a plane (orthoslice) from the Cartesian grid on which the scalar fields are computed, and apply the multi scale color map to the orthoslice. This technique enables one to visualize the variations in the scalar values throughout the orthoslice.

In the following subsections, we describe parts one and two in more detail.

2.1 Curvature and Torsion Computation

The CFD simulation models an ideal continuous stirred tank reactor in which the fluid velocity $\mathbf{V}$ (vector field) is continuous everywhere inside the tank. Since the discrete vector field in the simulation represents an actual continuous vector field, we can assume that the equality of mixed partial derivatives is true for our discrete representation. Also we neglect any possible critical points in the vector field and assume that its derivatives are defined everywhere in the discrete grid.

Let $\mathbf{V}$ be the fluid velocity (vector field) in the CFD stirred tank simulation:

$$\mathbf{V} = (u, v, w) \tag{1}$$

where u, v and w are the x, y and z components of the fluid velocity. The first derivatives of $\mathbf{V}$ with respect to x, y and z are:

$$\mathbf{V}_x = (u_x, v_x, w_x) \tag{2}$$
$$\mathbf{V}_y = (u_y, v_y, w_y) \tag{3}$$
$$\mathbf{V}_z = (u_z, v_z, w_z) \tag{4}$$

where u_x, v_x, and w_x are the first derivatives of u, v, and w with respect to x, etc.

The second derivatives and mixed derivatives of $\mathbf{V}$ are:

$$\mathbf{V}_{xx} = (u_{xx}, v_{xx}, w_{xx}) \tag{5}$$
$$\mathbf{V}_{yy} = (u_{yy}, v_{yy}, w_{yy}) \tag{6}$$
$$\mathbf{V}_{zz} = (u_{zz}, v_{zz}, w_{zz}) \tag{7}$$
$$\mathbf{V}_{xy} = (u_{xy}, v_{xy}, w_{xy}) \tag{8}$$
$$\mathbf{V}_{xz} = (u_{xz}, v_{xz}, w_{xz}) \tag{9}$$
$$\mathbf{V}_{yz} = (u_{yz}, v_{yz}, w_{yz}) \tag{10}$$

where u_{xx}, v_{xx}, w_{xx} are the second derivatives of u, v, w with respect to x, etc., and u_{xy}, v_{xy}, w_{xy} are the mixed derivatives of u, v, w with respect to x and y, and so on.

Let L be the position field of the fluid whose velocity field (vector field) is $\mathbf{V}$. Then the first, second and third derivatives of L with respect to time are given by:

$$\dot{L} = \mathbf{V} \tag{11}$$

$$\ddot{L} = u\mathbf{V}_x + v\mathbf{V}_y + w\mathbf{V}_z \tag{12}$$

$$\begin{aligned}\dddot{L} = &(uu_x + vu_y + wu_z)\mathbf{V}_x + \\ &(uv_x + vv_y + wv_z)\mathbf{V}_y + \\ &(uw_x + vw_y + ww_z)\mathbf{V}_z + \\ &u^2\mathbf{V}_{xx} + v^2\mathbf{V}_{yy} + w^2\mathbf{V}_{zz} + \\ &2uv\mathbf{V}_{xy} + 2uw\mathbf{V}_{xz} + 2vw\mathbf{V}_{yz}\end{aligned} \tag{13}$$

The curvature κ and torsion τ are then given as:

$$\kappa = \frac{|\ddot{L} \times \dot{L}|}{|\dot{L}|^3} \tag{14}$$

$$\tau = \frac{det[\dot{L}, \ddot{L}, \dddot{L}]}{|\ddot{L} \times \dot{L}|^2} \tag{15}$$

These formulas can be used to calculate the curvature and torsion at any point in the stirred tank Cartesian grid for any time step in the CFD simulations.

2.2 Multi Scale Color Coding

In designing a multi scale for color coding, one has to specify the number of divisions in the scale, the range of the scalar values in each division, and the color range for each division. Generally one needs to visualize the entire range of the scalar field values including small, medium and large values, but if the range of values is large, as in the case of curvature and torsion, uniform color coding often gives a single predominant color for most of the values which makes it difficult to distinguish between these values. We need to see the small and medium values of the curvature and torsion in addition to the large values in order to determine the degree of fluid mixing in different parts of the stirred tank. Thus we have to choose a set of parameters for the multi scale (the number of divisions and the range of scalar values and colors for each division) that will enable us to visualize the entire range of curvature and torsion values.

Various techniques can be used to construct the multi scale. In the method presented here, the number of divisions in the multi scale and the range of scalar values in each division are determined manually so as to facilitate the visualization of the scalar field variations of interest. A cumulative histogram of the scalar values is used to determine the boundaries of the divisions so that each division contains the desired percentage of scalar values. The user can choose any number of divisions and specify any range of scalar values and any range of colors for each division in order to enhance the visualization of the scalar values of interest.

An example of multi scale color coding is given in figure 1, which compares the uniform and multi scale color coded curvature field in an orthoslice in the xy plane at time step 1 in the CFD stirred tank simulations. A histogram of the curvature values, which range from 0 to more than 55, shows that about 41% of them are less than 1, 72% are less than 2, 86% are less than 3, 92% are less than 4, 96% are less than 6, etc. The curvature values were capped at 55 so that values greater than 55 were treated as outliers and set to 55. If uniform color coding is used to display the curvature values from 0 to 55 on a color scale that goes from red to violet, most of the values are shown as shades of red and cannot be distinguished from each other, making it impossible to visualize the small, medium and large values, as shown in figure 1(a).

In order to see the small, medium and large values of the curvature, we manually designed the following multi scale color mapping, which has 9 divisions and is piecewise linear in each division:

Division	Curvature Range	Percent Range
1	0 - 0.5	0 - 17.90
2	0.5 - 1	17.90 - 40.96
3	1 - 1.5	40.96 - 59.86
4	1.5 - 2	59.86 - 72.38
5	2 - 2.5	72.38 - 80.83
6	2.5 - 3	80.83 - 85.91
7	3 - 4	85.91 - 91.64
8	4 - 6	91.64 - 96.44
9	6 - 55	96.44 - 100

The curvature ranges and corresponding percent ranges used in this multi scale mapping were obtained manually from a cumulative histogram of the curvature values. The color scale that we are using goes from red to violet as its color index goes from 0 to 1. The color range for each division is specified by converting the percent range to decimal percents and using these as the starting and ending color indexes for that division (e.g., the starting and ending color indexes for division 2 are .1790 and .4096). Within each division, the color index varies linearly with the curvature value:

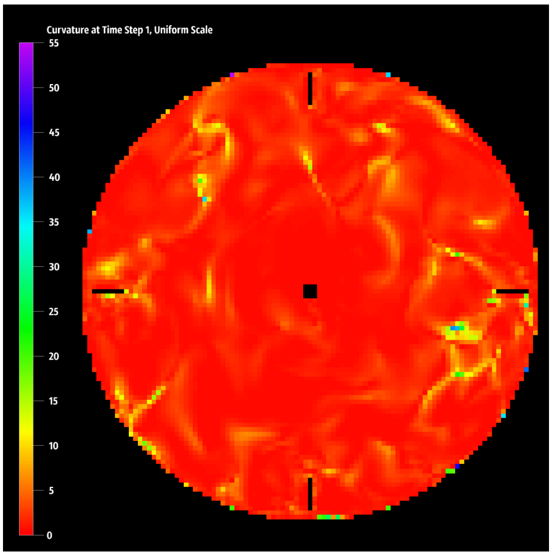
$$c = c_1 + \frac{(v - v_1).(c_2 - c_1)}{v_2 - v_1} \quad (16)$$

where v is the curvature value, c is the corresponding color index, v_1 and v_2 are the starting and ending curvature values of the division, and c_1 and c_2 are the starting and ending color indexes. Thus this multi scale color coding is piecewise linear.

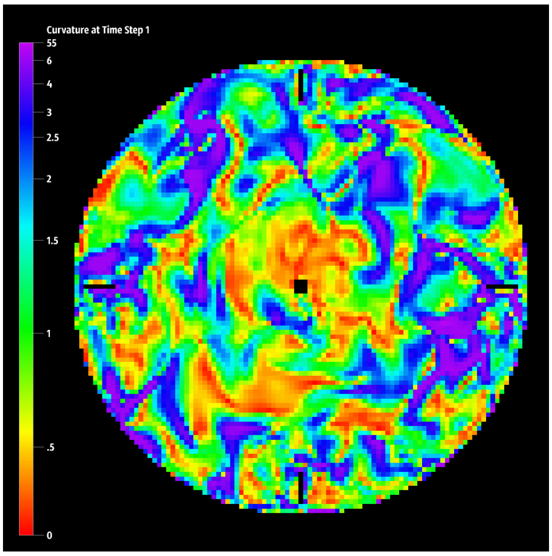
When this multi scale scheme is used to display the curvature in the orthoslice, one can now easily distinguish between the small, medium and large curvature values, as shown in figure 1(b). The red and orange areas, yellow and green areas, and blue and violet areas correspond to small, medium, and large curvature, respectively. Thus the red and orange areas indicate a small degree of fluid mixing while the blue and violet areas indicate a large degree of mixing.

3 RESULTS

We used the multi scale color coding technique described above to color code the curvature and torsion fields in a specified orthoslice of the stirred tank's uniform Cartesian grid. The orthoslice we used is parallel to the xy plane and is located around the middle of



(a) Uniform scale color coding for curvature



(b) Multi scale color coding for curvature

Figure 1: Comparison of uniform and multi scale color coding of an orthoslice of the curvature field.

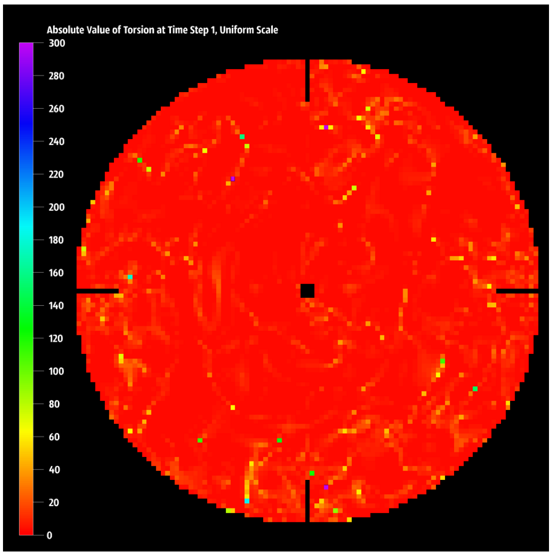
the stirred tank. The main idea is to visualize the variations of the curvature to see the regions of high and low straining of the fluid elements, and to visualize the variations of the torsion to see where fluid elements get twisted the most. These are shown in separate sections which compare the uniform and multi scale color coding methods for each quantity. The dimensions of the orthoslices are 100 × 100 × 1 in the x, y, and z directions respectively. We rendered both uniform scale and multi scale color coded orthoslices of the curvature and torsion fields at time step 1 in order to compare the uniform and multi scale color coding methods (figures 2 and 3). We then rendered 12 multi scale color coded orthoslices, including 6 for the curvature field and 6 for the torsion field at time steps 1, 1000, 2000, 3000, 4000, and 5000, in order to observe the scalar fields at different time steps (figure 3).

3.1 Curvature Field

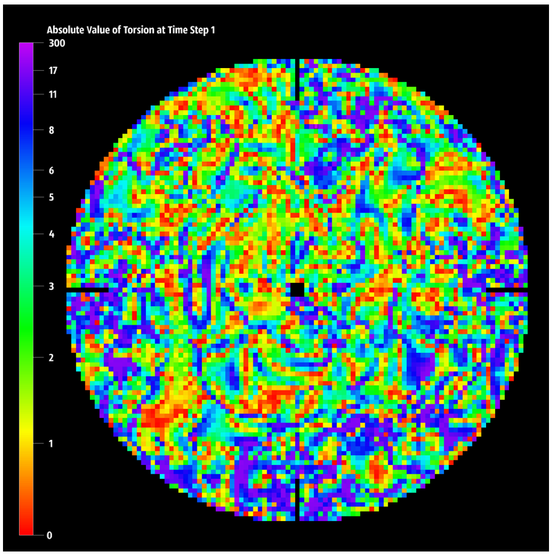
In figure 1(a), uniform color coding is used to display the curvature field in an orthoslice in the *xy* plane at time step 1. As mentioned previously, a cumulative histogram of the curvature values shows that about 92% of them are less than 4, but in the uniform color scale shown in the figure, curvature values less than 4 are in the bottom 7% of the color scale which contains only shades of red. Thus when uniform color coding is employed, 92% of the curvature values are displayed using only 7% of the color scale and hence these curvature values all appear as shades of red and cannot be distinguished from one another. This means that in general, uniform color coding cannot distinguish between the small, medium and large curvature values. It can only distinguish the very large ones from the others.

In order to visualize the small, medium and large curvature values, we used the multi scale color map described above to display the curvature field in the orthoslice, which is shown in figure 1(b). In this multi scale method, the lowest 92% of the curvature values are displayed using 92% of the color scale instead of only 7%, the lowest 96% of the curvature values are displayed using 96% of the color scale, etc. This causes the small, medium, and large values to be shown in distinctively different colors (red and orange, yellow and green, and blue and violet, respectively) so that one can easily distinguish between them. In the figure we can clearly see that in general the outer regions near the baffles of the stirred tank produce significant curvature and flow distortion. This reaffirms the expectation that the baffles disturb the rotation of the fluid causing distortion and stretching of the fluid elements, which promotes mixing. In general the lowest curvature values appear to be near the inner rotating shaft, as expected.

Figures 4(a)-4(f) show the multi scale color coded curvature images in the orthoslice at time steps 1, 1000, 2000, 3000, 4000 and 5000. The multi scale used in these 6 images is similar to the one described in Section 2.2 except that the upper end point of the curvature range in the last division is 200 instead of 55 (i.e., the curvature values are capped at 200 instead of 55) and the percent ranges for the 9 divisions are slightly different at each of the 6 time steps. Thus figure 4(a) is the same as figure 1(b) except that the curvature values in figure 4(a) are capped at 200 instead of 55 in order to be consistent with figures 4(b)-4(f). In all of these images, the multi scale color coding enables one to clearly visualize the small, medium and large curvature values as the red and orange, yellow and green, and blue and violet areas, respectively. It can be observed in these time series images that in general the regions of high and low curvature do not change spatial locations significantly with time. This type of visualization and analysis is not possible with uniform color coding.



(a) Uniform scale color coding for torsion



(b) Multi scale color coding for torsion

Figure 2: Comparison of uniform and multi scale color coding of an orthoslice of the torsion field.

3.2 Torsion Field

Figure 2(a) shows the uniform color coded torsion field in the orthoslice at time step 1. As mentioned in Section 1.2, the torsion values can be positive or negative, but we are visualizing only the absolute value of the torsion, neglecting whether the twist is clockwise or counterclockwise since the degree of fluid mixing depends primarily on the magnitude of the torsion rather than its direction. A cumulative histogram of the absolute value

 ISBN 978-80-86943-71-8

of the torsion values shows that about 94% of them are less than 17, but in the uniform color scale shown in the figure, torsion values less than 17 are in the bottom 6% of the color scale which contains only shades of red. Thus uniform color coding uses only 6% of the color scale to display 94% of the torsion values and hence these torsion values all appear as shades of red and cannot be distinguished from each other. This means that in general, as in the case of curvature, uniform color coding cannot distinguish between the small, medium and large torsion values. It can only distinguish the very large ones from the others.

In order to visualize the small, medium and large torsion values, we manually constructed the following multi scale color mapping, which has 10 divisions and is piecewise linear in each division:

Division	Absolute Value of Torsion Range	Percent Range
1	0 - 1	0 - 18.61
2	1 - 2	18.61 - 36.07
3	2 - 3	36.07 - 50.59
4	3 - 4	50.59 - 61.18
5	4 - 5	61.18 - 68.69
6	5 - 6	68.69 - 74.13
7	6 - 8	74.13 - 82.30
8	8 - 11	82.30 - 89.55
9	11 - 17	89.55 - 94.40
10	17 - 300	94.40 - 100

The absolute value of torsion ranges and corresponding percent ranges used in this multi scale mapping were obtained manually from a cumulative histogram of the torsion values, which were capped at 300. The above multi scale color map was used to display the torsion field in the orthoslice, which is shown in figure 2(b). In this multi scale method, the lowest 94% of the torsion values are displayed using 94% of the color scale instead of only 6%. This enables one to easily visualize the small, medium, and large torsion values, which are shown in red and orange, yellow and green, and blue and violet, respectively.

Figures 4(g)-4(l) show the multi scale color coded torsion images in the orthoslice at time steps 1, 1000, 2000, 3000, 4000 and 5000. The multi scale used in these 6 images is similar to the one used in figure 2(b) except that the upper end point of the torsion range in the last division is 600 instead of 300 and the percent ranges for the 10 divisions are slightly different at each of the 6 time steps. Thus figure 4(g) is the same as figure 2(b) except that the torsion values in figure 4(g) are capped at 600 instead of 300 in order to be consistent with figures 4(h)-4(l). In all of these images, the multi scale color coding enables one to clearly distinguish between the small, medium and large torsion values, which is not possible with uniform color coding.

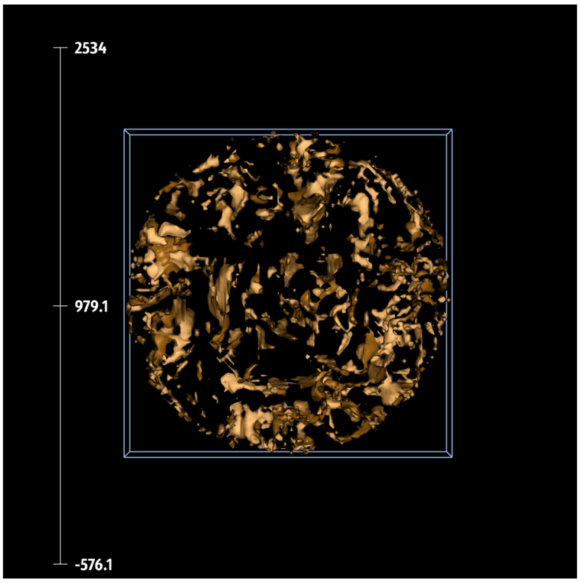


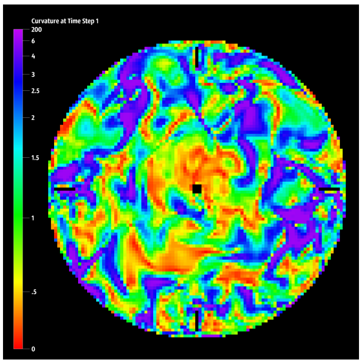
Figure 3: Torsion isosurface of a sub grid of the stirred tank.

The regions of high torsion are associated with fluid elements that are significantly distorted in the angular plane and hence likely to be well mixed. As in the case of curvature, in general the outer regions of the stirred tank near the baffles produce areas of high torsion and hence high mixing, while low and medium torsion areas, which indicate low and medium mixing, are primarily located in the interior of the tank.

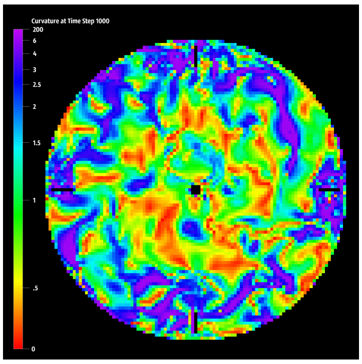
Figure 3 shows a sample non color coded torsion isosurface for the iso value 979.1. In future work we plan to generate multi scale color coded isosurfaces for both curvature and torsion to complement the multi scale color coded orthoslices.

4 DOMAIN EXPERT REVIEW

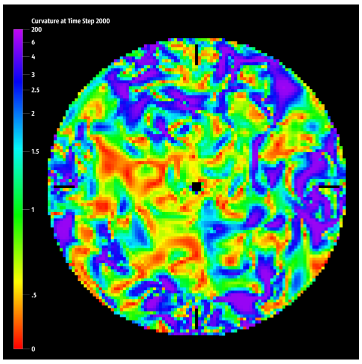
Images for the orthoslices considered here are generated using both the multi scale and the uniform color coding techniques. The multi scale images can be observed for analysis of mixing performance as they are capable of displaying both the well and poorly mixed zones in the stirred tank. The greater the values of curvature and torsion, the greater the mixing of the fluids in that region. In figure 4, there are many regions (blue and violet) of high curvature and torsion indicating high mixing. These regions are typically located in the near-baffle regions close to the stirred tank wall. Similarly, there are areas (red and orange) of low curvature and torsion which indicate low mixing and are typically located in the interior of the tank. These types of observations are not possible in the uniformly color coded images as they are visually incapable of providing a definitive analysis of the scalar fields.



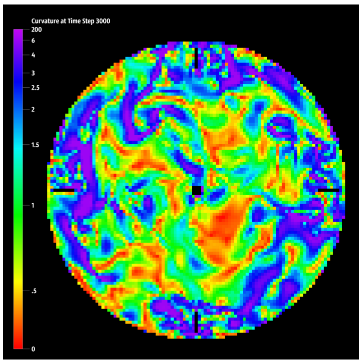
(a) Curvature at time step 1



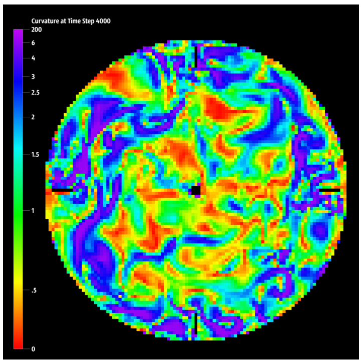
(b) Curvature at time step 1000



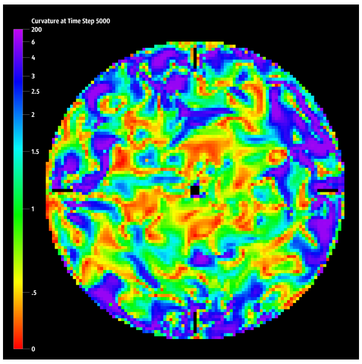
(c) Curvature at time step 2000



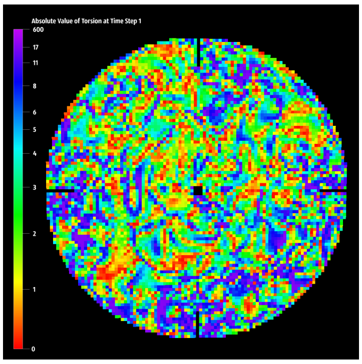
(d) Curvature at time step 3000



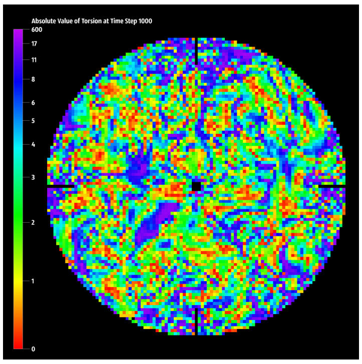
(e) Curvature at time step 4000



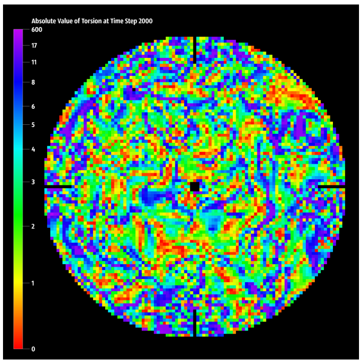
(f) Curvature at time step 5000



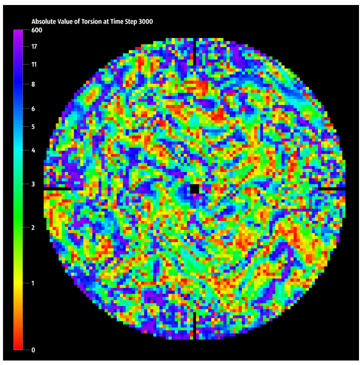
(g) Torsion at time step 1



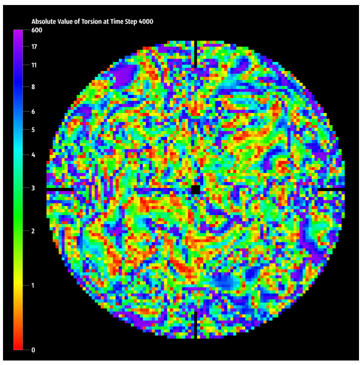
(h) Torsion at time step 1000



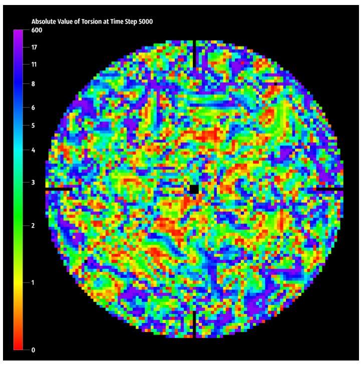
(i) Torsion at time step 2000



(j) Torsion at time step 3000



(k) Torsion at time step 4000



(l) Torsion at time step 5000

Figure 4: Curvature and torsion fields at various time steps, displayed using multi scale color coding.

 ISBN 978-80-86943-71-8

5 CONCLUSION

In this paper, we demonstrated the computation and visualization of curvature and torsion scalar fields that are derived from a vector field (the fluid velocity) defined on a multi-block curvilinear grid used to model a stirred tank reactor. We showed that if uniform color coding is used to display the scalar quantities, then most of them are shown in the same color (red), making it impossible to distinguish between the small, medium and large values. Instead, we used a multi scale color coding technique that displays the small, medium, and large values in distinctively different colors (red and orange, yellow and green, and blue and violet, respectively) so that one can easily distinguish between them. This enables one to estimate the degree of fluid mixing in different parts of the stirred tank since curvature and torsion are indicators of fluid mixing (the greater the curvature and torsion, the greater the mixing). Thus if the values of a scalar field are not uniformly distributed between the lowest and highest values, which is usually the case, then multi scale color coding is needed to effectively display these values. In future work we plan to generate multi scale color coded isosurfaces of the curvature and torsion fields, which will complement the multi scale color coded orthoslices shown in this paper.

6 ACKNOWLEDGMENTS

This multi scale visualization method was implemented in the VISH visualization system (Benger et al., 2007). This research employed resources of the Center for Computation & Technology at Louisiana State University. This work was supported by an oil spill grant from BP through LSU, and by a grant from the Louisiana Board of Regents Post Katrina Support Fund Initiative. It was also supported by the Austrian Science Foundation FWF DK+ project Computational Interdisciplinary Modeling (W1227) and grant P19300. Werner Benger is affiliated with the Institute for Astro- and Particle Physics, University of Innsbruck, Technikerstrasse 25/8, A-6020 Innsbruck, Austria. In addition both Werner Benger and Marcel Ritter are affiliated with the AirborneHydroMapping GmbH, Technikerstrasse 21a, A-6020 Innsbruck, Austria.

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