Multi Scale Color Coding of Fluid Flow Mixing Indicators along Integration Lines

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ABSTRACT

This paper presents a multi scale color coding technique which enhances the visualization of scalar fields along integration lines in vector fields. In particular, this multi scale technique enables one to see detailed variations in selected small ranges of the scalar field while at the same time allowing one to observe the entire range of values of the scalar field. This type of visualization, observing small variations as well as the entire range of values, is usually not possible with uniform color coding. This multi scale approach, which is linear within each division of the scale (piecewise linear), is a general visualization technique that can be applied to many different scalar fields of interest. As an example, in this paper we apply it to the visualization of fluid flow mixing indicators along pathlines in computational fluid dynamics (CFD) simulations. Pathlines are the trajectories of fluid particles over time in the CFD simulations, and applying multi scale color coding on the pathlines brings out quantities of interest in the flow such as curvature, torsion and specific measure of length generation, which are indicators of the degree of mixing in the fluid system. In contrast to uniform color coding, this multi scale scheme can display small variations in the mixing indicators and still show the entire range of values of these indicators. In this paper, the mixing indicators are computed and displayed only along line structures (pathlines) in the flow field rather than at all points in the flow field.

Keywords: transfer function generation, pathlines, nonlinear color map, computational fluid dynamics, vector field visualization, mixing indicators

1 INTRODUCTION

1.1 Motivation

This paper proposes a multi scale color coding scheme which can display nonuniform distributions of quantities that have small variations in some ranges and larger variations in other ranges. The paper shows the advantages of this multi scale technique compared to uniform color coding which usually cannot display both small and large variations in the same image. In this multi scale approach, the overall scale is divided up into intervals specified by the user, with a different linear scale inside each interval (i.e., it is piecewise linear). This technique enables one to see small variations in selected ranges of the quantity of interest and also observe the entire range of values of this quantity. This multi scale scheme is a general technique that can be used to visualize any scalar quantity of interest. As an example of this method, we use it to visualize fluid mixing indicators along integration lines (pathlines) in computational fluid dynamics simulations of fluid flow. In this paper the mixing indicators are computed and displayed only along the pathlines rather than at all points in the flow field.

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Computational fluid dynamics (CFD) uses numerical methods and analysis techniques to study fluid flow. The computational results from numerical models can yield data which is on the order of hundreds of gigabytes and consists of multiple blocks containing millions of cells. Computation on such a grid can take a substantial amount of time to trace the paths of fluid particles over time (pathlines). But once these pathlines have been calculated, fluid mixing indicators, such as curvature and torsion, can then be quickly computed and visualized at every point on the pathlines. Curvature and torsion computations along pathlines in a stirred tank CFD simulation were done earlier [3] and uniformly color coded, but the distribution of these values is not uniform. In this paper the multi scale color coding technique is used to display the nonuniform distributions of these quantities. The paper also adds another mixing indicator, the specific measure of length generation, to complement the curvature and torsion so as to better understand the mixing. In addition it uses higher order difference formulas to improve the accuracy of the curvature and torsion calculations. As mentioned above, the multi scale color coding scheme is a general method that can be used to visualize any scalar field of interest, such as pressure, which is also shown in the paper.

1.2 Fluid Mixing Indicators

In order to develop an understanding of the mechanical macro mixing process, we investigate the motion of the fluid particles in the flow domain. The flow domain considered is a mechanically agitated turbulent stirred tank with down-pumping pitched blade impellers. Water is considered as the working fluid in which a blob of a tracer is injected at a particular location. We look into the pathlines of a number of points associated with the injected tracer. These pathlines show exactly how tracer particles move inside the stirred tank volume. From the pathline visualizations, we try to qualitatively understand the stretching and distortions on the fluid elements by calculating the curvature and torsion at different points along the pathlines. A higher value of the curvature indicates more straining of the fluid element associated with it and also higher residence time of the fluid particle in that particular region resulting in prolonged inter-diffusion of the fluids, which promotes mixing [12]. The torsion is a measure of twisting strains on the fluid elements which also promotes the break up of the clumps and enhances mixing. Torsion can be positive or negative, but the degree of mixing in the stirred tank depends primarily on the magnitude of the torsion rather than its sign. Therefore, for visualizing torsion, we will show its absolute value (magnitude), neglecting whether the twist is clockwise or counterclockwise.

The curvature κ and torsion τ are given by

$$\kappa = \frac{|\ddot{q} \times \dot{q}|}{|\dot{q}|^3} \quad . \tag{1}$$

$$\tau = \frac{\dddot{q} \cdot (\ddot{q} \times \dot{q})}{|\ddot{q} \times \dot{q}|^2} \quad . \tag{2}$$

where $\dot{q}$ is the velocity of the fluid (vector field) and $\ddot{q}$ and $\dddot{q}$ are the first and second derivatives of the vector field with respect to time. In our approach we compute pathlines from the vector field first, based on user-specified initially defined seeding points, and then calculate curvature and torsion along the pathlines as a post-processing step.

Another measure of fluid mixing is the specific measure of length generation [13] defined as

$$\frac{d\ln(\lambda)}{dt} \tag{3}$$

where $\lambda = \frac{\delta}{L}$, δ being the increase in path length (which is proportional to the magnitude of the velocity) and L being the total path length (before the δ increment) at a particular time t. The proportional change of the path length will be larger at the start of the pathlines and smaller at their ends, thus this mixing indicator will be dominated by variations of the velocity as the pathlines get longer. The greater the specific measure of length generation, the greater the mixing. This quantity is also calculated as a post-processing step on the pathlines. It should be noted that in addition to the mixing indicators described above, there are also other principles that can be used to investigate the mixing of fluids.

1.3 Related Work

Automated generation of color maps has been the subject of research in scientific visualization for decades. Yet, still many visualization tools rely on manual specification of colors as the problem is highly application and problem specific. Taking over full control of color map generation from the user is usually not even desirable, leaving semi-automated assistance of color specification as the best compromise. A well known approach is the method of finding material boundaries by G. Kindlmann [8]. In this approach a Histogram Volume Structure is created which measures the relationship between the data values and their derivatives. In this volume, the three axes are f, f' and f'' , each axis is divided into some number of bins which contains the number of voxels falling in the same combination of ranges of these variables. This information facilitates a high-level interface to opacity function creation. In the winning entry of the IEEE Visualization 2004 Contest [6], the visualization system VisSym was highlighted, where the subset of data items were manually selected using techniques for information visualization such as scatter plots and histograms. These values were related to the dataset, e.g., for detecting the eye of the hurricane area, cells which exhibit low velocity and pressure regions were brushed out.

Our main objective is the depiction of scalar-valued fluid flow mixing indicators along pathlines. Fluid flow quantities such as curvature and torsion are common subjects of study. Weinkauf [15] demonstrated computation of curvature and torsion as a field over the entire data domain, allowing one to identify regions of interest within the full spatial domain. Due to the sheer amount of dynamic data in our application, which comprises about 300GB of binary data, this approach is not feasible and we need to restrict ourselves to displaying such field quantities on precomputed pathlines. One method for doing this is to use a geometric object [5] to visualize the fluid fields along the pathlines, however, if the number of pathlines is large, this approach is not visually appealing because the image is more cluttered and does not give global information about the flow. In the approach proposed here, we employ a simple but efficient way to display data values with a wide numerical range by specifying color mapping via histogram percentage rather than absolute data values. Rendering of these pathlines using the illuminated streamlines method [17] gives a 3D view of the lines using Phong Shading. The depth perception can be further enhanced by using the halos described in [7, 11] and we plan to implement this halo feature in future work on color coding line structures.

2 OUR APPROACH

The vector field in the stirred tank simulations produced scalar fields, such as curvature and torsion, which have a wide range of values in some parts of the stirred tank. The use of uniform color coding for the whole range of these scalar values often gives a single predominant color along most of the length of the pathlines, making it impossible to visualize small variations in these values. This paper describes the use of a multi scale color coding scheme which not only shows small variations in the scalar field but also enables one to see the entire range of values of the scalar field by just looking at the color coded pathlines. In this paper, the curvature and torsion, and also a new mixing indicator, the specific measure of length generation, are calculated for 300 time steps using more accurate higher order difference formulas and are then visualized using the multi scale color coding technique. Also another scalar quantity of interest, the pressure, is visualized using this approach. This multi scale color coding scheme enables one to easily draw conclusions about the behavior of the scalar fields without any uncertainty about the variations in the small values.

2.1 Higher Order Differentiation Schemes

The formulas for the curvature, eqn. (1), and torsion, eqn. (2), contain the first and second derivatives of the velocity with respect to time, and the specific measure of length generation is defined as the first derivative of $\ln(\lambda)$ with respect to time, eqn. (3). In this work we computed these derivatives with more accurate higher order difference formulas compared to previous work [3,4]. We used the following central difference formulas with fourth order accuracy for the first and second derivatives:

$$f'(x_0) \approx \left(\frac{1}{12} f(x_{-2}) - \frac{2}{3} f(x_{-1}) + \frac{2}{3} f(x_1) - \frac{1}{12} f(x_2) \right) \Big/ h_x \tag{4}$$

$$f''(x_0) \approx \left(-\frac{1}{12} f(x_{-2}) + \frac{2}{3} f(x_{-1}) - \frac{5}{2} f(x_0) + \frac{4}{3} f(x_1) - \frac{1}{12} f(x_2) \right) \Big/ h_x^2 \tag{5}$$

2.2 Multi Scale Color Coding

Designing a multi scale for color coding depends on several parameters like the number of divisions in the scale, the range of the scalar values in each division and the selection of the color range for each division. Generally one needs to visualize the entire range of 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 pathline which makes it difficult to distinguish between these values. For the mixing indicators described in this paper, we need to see the small and medium values in addition to the large values in order to determine where the mixing speed in the stirred tank is slow, intermediate and fast. Once the ranges of scalar values that need to be visualized in detail have been determined, one can then specify the number of divisions in the multi scale and the range of values and the color range for each division. There are a few considerations for the colors [9,16] that need to be addressed, including the fact that the human eye perceives more variation in the green than in the other colors. As an example of this, Figs. 6 and 7 contain a lot of green which enables one to readily see the variations in the scalar values. Other than these considerations, the colors can generally be chosen as the user desires.

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 one contains the desired percentage of scalar values. In this paper, all of the multi scales have three divisions and the same range of colors, but these are just examples to illustrate the multi scale method. In general 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. Currently this process is not automated but rather is done manually by the user. There also exists other work in this area which describes ways to come up with ranges of values from the scalar field. These involve automatic [10], semi-automatic [8] and manual generation of the functions to do this task [14].

Here, since we need to visualize small, medium and large values of the scalar field, three divisions were selected for the multi scale color coding. An example of these three divisions is given in Fig. 1, where the first, second and third divisions go from 0% to 10%, 10% to 30%, and 30% to 90% of the scalar values, and the third division is capped at 90%, with values above 90% being set to the 90% value. Capping the third division at 90% enables one to see the variation of the values between 30% and 90% in greater detail, which is more relevant to the mixing process than the variation of the large values between 90% and 100%. Each division has linear color gradients of R, G and B going from the left end point to the right end point of the division, but the overall color variation over all three divisions is not uniform but rather is multi scale in order to better show the variations in the small and medium scalar values. In the example shown in Figure 1, in the first division R varies linearly from 0 to 255, G=0, and B varies linearly from 255 to 0, in the second division R=255, G varies linearly from 0 to 255, and B=0, and in the third division R varies linearly from 255 to 0, G=255, and B=0. These color ranges for the three divisions were used to color code all four of the scalar fields shown in the paper, while the percents used for the boundaries between the divisions were different for each scalar field.

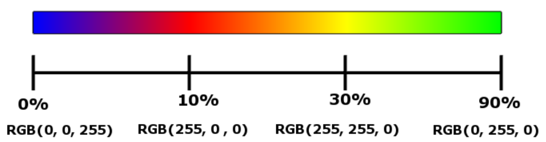


Figure 1: An example of Multi Scale Color Coding with different ranges of scalar values to distinguish regions of low values and medium values.

2.3 Rendering

For the final rendering step, we employ the method of illuminated streamlines [17], which provides improved depth perception as compared to homogeneously colored lines. While in its original form only monochrome illumination could be supported by OpenGL 1.0 hardware, modern OpenGL implementations support multi-texturing and thus allow an additional one-dimensional lighting model as proposed in [17]. Illumination of lines is done by using the Phong Reflection model which defines the intensity (I) at any point as

$$\begin{aligned} I &= I_{ambient} + I_{diffuse} + I_{specular} \\ &= k_a + k_d L \cdot N + k_s (V \cdot R)^n \end{aligned} \tag{6}$$

where L denotes the light direction, V the viewing direction and R the unit reflection vector (the vector in the L-N-plane with the same angle to the surface normal as the incident light). k_a, k_d and k_s are the ambient, diffuse and specular reflection constants respectively. For lines the normals and reflection vectors are undefined. So, intensity can be made dependent on the tangential vector T instead as

$$L \cdot N = |L_N| = \sqrt{1-(L \cdot T)^2} \tag{7}$$

and

$$\begin{aligned} V \cdot R = &(L \cdot T)(V \cdot T) - \\ &\sqrt{1-(L \cdot T)^2}\sqrt{1-(V \cdot T)^2} \quad . \end{aligned} \tag{8}$$

In order to enhance the color resolution, we use procedural color maps that are merely parametrized through linear functions between each key value. Generally, this linear mapping will be sufficient for each range of scalar values, but if a particular range needs to be subdivided, then that particular range can have more than one linear scale and additional colors. In the approach we have discussed, some idea of the scalar values can be derived from the histogram where, if more points are biased to a single value in that range, then nonlinear functions can be applied to map values to color for the single range. Only at the rendering step is the color map discretized into a texture, for instance one with 256 entries if sufficient, but a higher color resolution can be used if required.

3 RESULTS

We used the the multi scale color coding technique described above to color code the pathlines in the stirred tank. The main idea is to visualize the pathlines and color code them with different scalar quantities that indicate the mixing of the fluids. The quantities that were color coded are curvature, torsion, specific measure of length generation, and pressure. These are shown in separate sections which compare the uniform and multi scale color coding methods for each quantity. The pathlines are generated by introducing 36 seeding points or 516 seeding points on two spheres placed symmetrically about the z-axis in the stirred tank and traced for 300 timesteps totaling about 1.8 secs.

3.1 Curvature

The curvature and torsion values cover a large range and thus uniform color coding cannot represent the whole range efficiently and can be biased to a particular range of values. Even if the values are capped at a certain value, small variations are not visible. Figs. 2 and 3 compare the uniform and multi scale color coding methods for curvature images, and a lot of visible differences can be found.

From Fig. 2 it is clear that the uniform and multi scale color coding methods generate different images even when the range of scalar values is the same. One can see that, in general, multi scale color coding (Fig. 2(b)) gives more noticeable changes in color for the different ranges of scalar values as compared to uniform color coding. This is because variations within specified ranges of scalar values are highlighted in the multi scale technique but remain visibly indifferent in the case of uniform color coding.

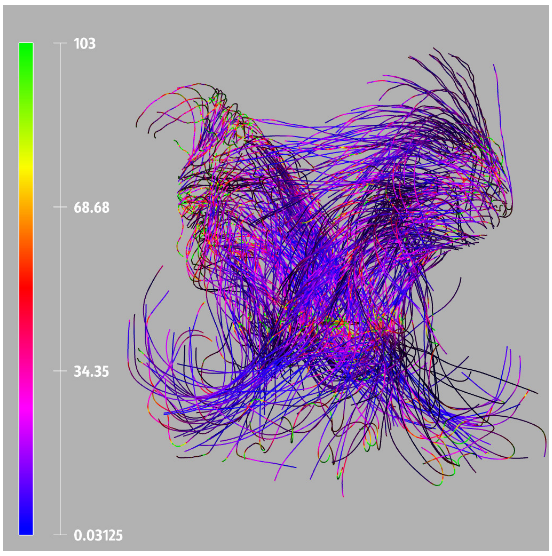
3.2 Torsion

Fig. 4 shows the uniform and multi scale color coded values of the magnitude of the torsion along pathlines in the stirred tank, and a wide range of colors can be seen in the multi scale image, indicating large variations in the torsion values even for pathline points that are close together. In contrast, the uniform color coded image is dominated by a small range of color along most of the length of the pathlines and hence one cannot see the large variations in the torsion.

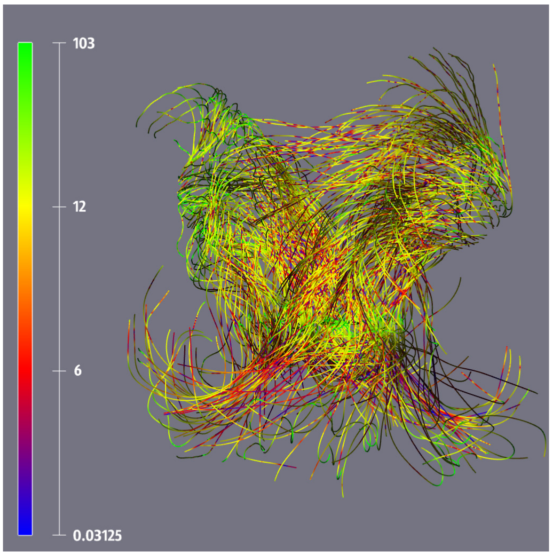
Alternatively, we may also employ Frenet Ribbons to geometrically encode the curvature and torsion [2] of a line in addition to its colorization. Here, the ribbons are rendered instead of the lines, which provide one more degree of freedom to the geometry, i.e., surface. Torsion can easily be visualized using ribbons, employing a geometry shader to generate the actual rendering primitives on the GPU with minimal performance impact as compared to rendering lines. In Fig. 5 we have used multi scale color coding to represent torsion. Areas with a lot of twist correlate to high torsion whereas the areas which seem consistently straight might have different colors due to changes in their torsion values.

3.3 Specific Measure of Length Generation

Fig. 6 shows the specific measure of length generation color coded using the uniform and multi scale methods.



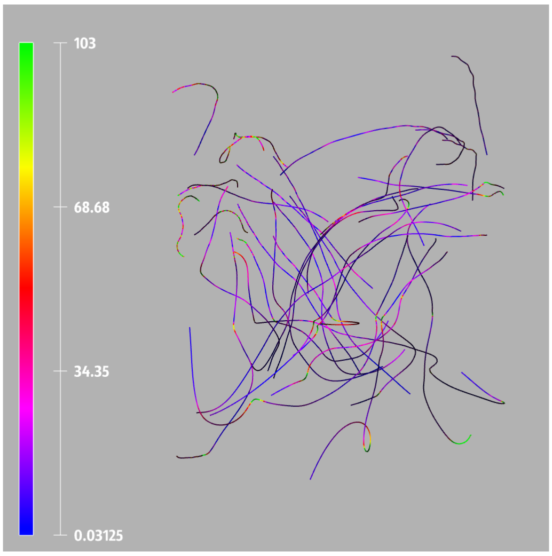
(a) Uniform color coding for curvature



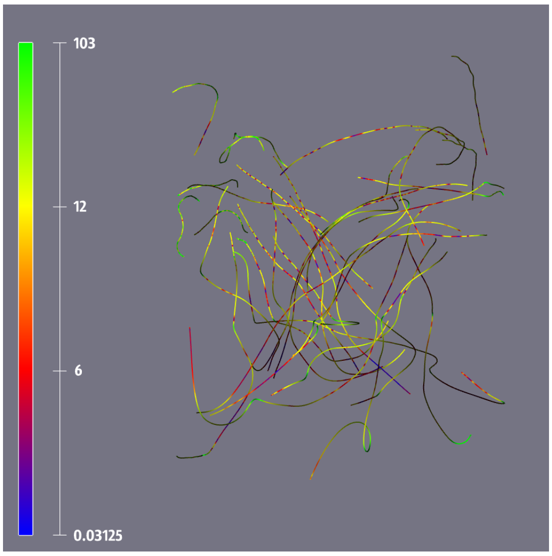
(b) Multi scale color coding for curvature

Figure 2: Comparison of uniform and multi scale color coding of curvature values on 516 pathlines for 300 time slices of stirred tank data. The curvature values were capped at the 95% value in both of the images. For the multi scale technique, the scale has three partitions: 0% to 11%, 11% to 32%, and 32% to 95%, which have the color ranges blue to red, red to yellow and yellow to green respectively.

In the uniform color coded image, almost the entire image is a single color so that one cannot see any variation in the specific measure of length generation values, while the multi scale image has more colors and shows variations in the values of this quantity.

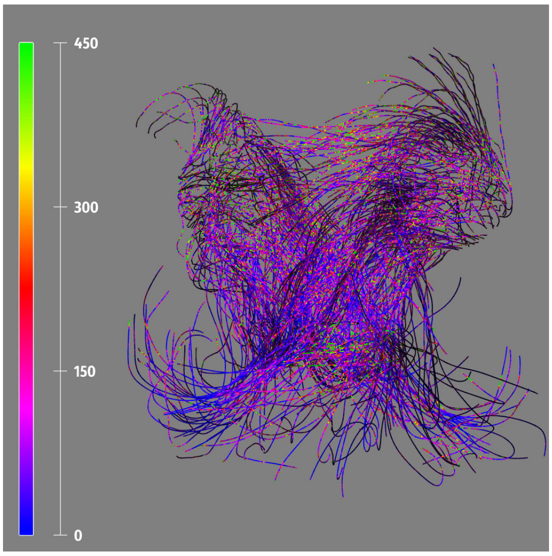


(a) Uniform color coding for curvature

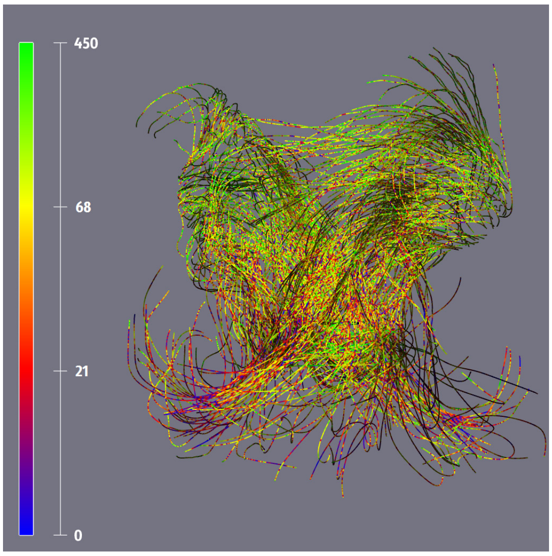


(b) Multi scale color coding for curvature

Figure 3: Comparison of uniform and multi scale color coding of curvature values on 36 pathlines for 300 time slices of stirred tank data. The curvature values were capped at the 95% value in both of the images. For the multi scale technique, the scale has three partitions: 0% to 11%, 11% to 32%, and 32% to 95%, which have the color ranges blue to red, red to yellow and yellow to green respectively.



(a) Uniform color coding for torsion



(b) Multi scale color coding for torsion

Figure 4: Comparison of uniform and multi scale color coding of torsion values on 516 pathlines for 300 time slices of stirred tank data. The values were capped at the 90% value in both the images. For the multi scale technique, the scale has three divisions: 0% to 15%, 15% to 40% and 40% to 90%, which have the color ranges blue to red, red to yellow and yellow to green.

3.4 Pressure

The pressure field is a scalar quantity of interest which is given at all of the grid points in the stirred tank simulation data set. Fig. 7 displays the values of the pressure using the uniform and multi scale color coding methods. As in Fig. 6, the uniform image is mostly a single color and thus shows very little variation in the pressure, while the multi scale image has more colors and shows significant variations in the pressure.

4 DOMAIN EXPERT REVIEW

Images for all of the fluid mixing indicators 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

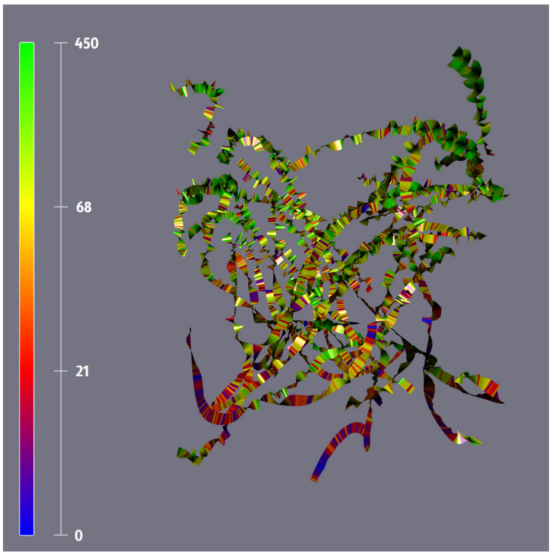
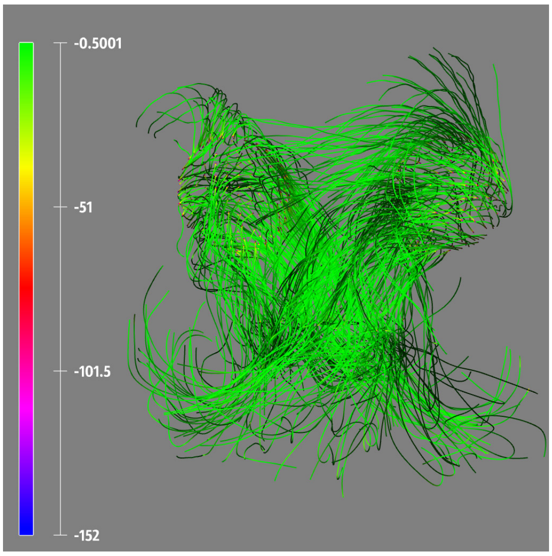


Figure 5: Multi scale color coding of torsion values on the pathlines visualized as ribbons. Values used to color code are the same as in Fig. 4(b)

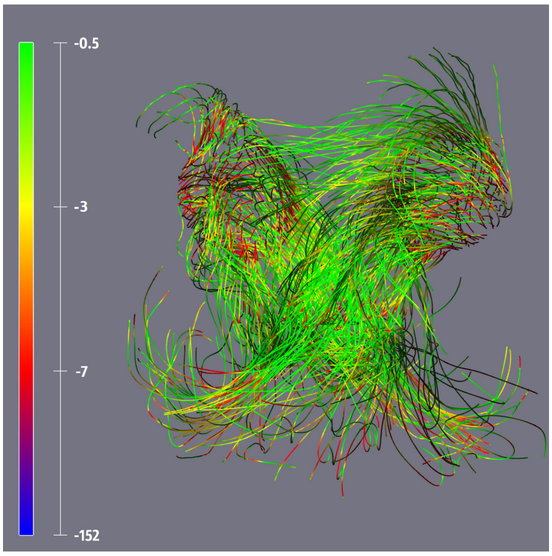
and poorly mixed zones. The larger values of the torsion, curvature or specific measure of length generation of the pathlines indicate the areas where the mixing is greater. There are some lines which can be observed to have the same green color in all of the multi scale images, indicating high mixing along that particular locus of the tracer particle. Similarly, certain lines can be found which have low values for all three mixing factors, indicating lower mixing in those regions of the stirred tank. These types of observations are not possible in the corresponding uniformly color coded images as they are visually incapable of providing a definitive analysis of the scalar fields.

5 CONCLUSION

The benefits of using a multi scale color coding scheme for the study of fluid flow, such as flows in large scale computational fluid dynamics simulations of a stirred tank, have been described in this paper. This technique allows one to identify areas of local variations in quantities of interest while also obtaining a global view of these quantities. Color coding of various mixing indicators along the fluid flow lines has been demonstrated. We provided a comparative study between the uniform and multi scale color coding methods for these pathline images, demonstrating that the mixing in the stirred tank can be visualized more clearly and effectively using the multi scale technique. This method has been implemented in the VISH visualization system [1] and yields an interactive way to study the fluid system in 3D.



(a) Uniform color coding for specific measure of length generation



(b) Multi scale color coding for specific measure of length generation

Figure 6: Comparison of uniform and multi scale color coding of specific measure of length generation on 516 pathlines for 300 time slices of stirred tank data. The values were capped at the 70% value in both of the images. For the multi scale technique, the scale has three partitions: 0% to 10%, 10% to 30%, and 30% to 70%, which have the color ranges blue to red, red to yellow and yellow to green respectively.

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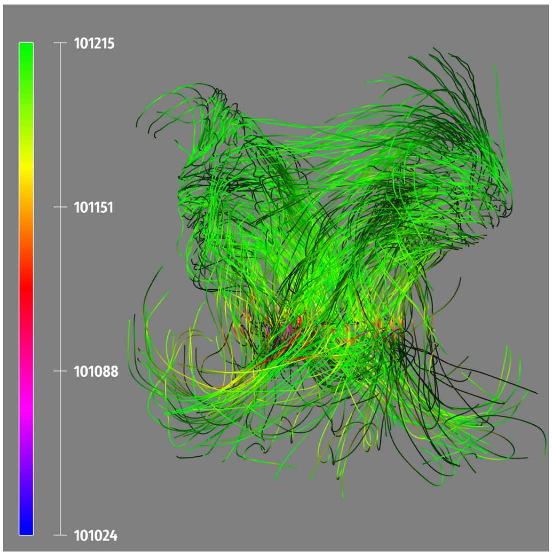
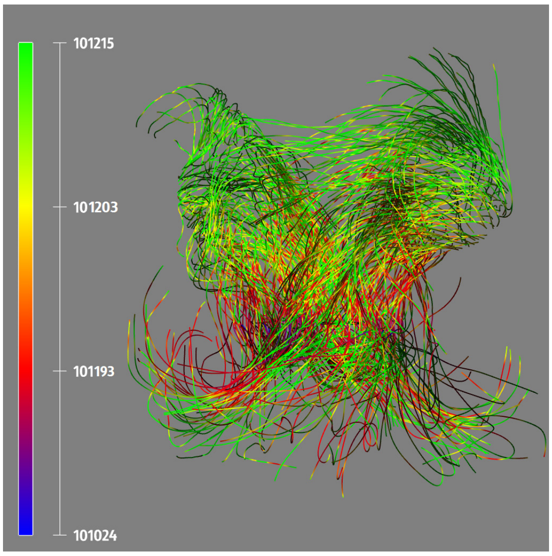


(a) Uniform color coding for pressure



(b) Multi scale color coding for pressure

Figure 7: Comparison of uniform and multi scale color coding of pressure on 516 pathlines for 300 time slices of stirred tank data. The values were capped at the 71% value in both of the images. For the multi scale technique, the scale has three partitions: 0% to 11%, 11% to 30%, and 30% to 71%, which have the color ranges blue to red, red to yellow and yellow to green respectively.

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