Fiber Orientation Fields in Turbulence

by

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Dedication

This thesis is dedicated to my parents, Mary and Bruce, who have supported me endlessly, especially in my love for math and science.
Abstract

We study the orientation field of fibers in homogeneous isotropic turbulence. As small rod-like particles (referred to as fibers) are advected through a turbulent flow, they rotate and follow Jeffery’s equation, which may be used to calculate their orientations at any time in the flow. However, this method depends on the initial orientation chosen for each particle. Instead, we examine the preferential alignment of the particles, which is given by the largest stretching direction of the surrounding fluid. We calculate this using the left Cauchy-Green strain tensor, which measures the strain deformation undergone by the fluid over a finite time interval. The most extensional eigenvector of the left Cauchy-Green strain tensor gives the stretching direction and thus the preferential fiber orientation. This does not depend on the initial orientation of the particle. We show that the independence of initial conditions extends further: as we calculate this field using longer integration times (by considering earlier initial sampling times), the field converges to an invariant state. We visualize the spatial structures of the orientation field and observe, for the first time in 3D turbulence, surfaces across which the orientation rapidly rotates by \( \pi \). These surfaces become thinner as we increase integration time, and create regions of very sharp change in the otherwise smooth orientation field. We measure these spatial structures statistically through the orientation structure function and demonstrate the fractal structure of the field caused by these alignment-inversion surfaces.
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Chapter 1

Introduction

1.1 Fiber Orientation Fields

Spatial structures within fluid flows present a rich topic for many different scientific domains. Material mixing, and the tracking of passive scalars, present one such problem with extensive study. An intuitive model examines the behavior of passive particles, which do not affect the flow, suspended within the flow of interest. Such a situation occurs in many natural and industrial flows, such as the water transport of material sediment suspensions. The motion of particles in such systems is important in determining environmental effects such as deposition, motivating their study. Some of these flows, such as ocean flows of plankton, consist of anisotropic particles. Unlike isotropic (spherical) particles, anisotropic particles have a shape that varies in the different directions, and thus their behavior in flow depends on their orientations. This adds an extra dimension to the problem. The simple example of a thin rod-like particle, referred to as a fiber, comes with an inherent axial orientation. The field of these fiber orientations plays a significant role in many applications. A suspension will scatter electromagnetic radiation in a way that depends on the relative alignment between fibers [2]. In the case of a cloud, ice crystals of many different shapes are advected in atmospheric turbulence. Among them are rod-like crystals, and their ensuing solar scattering depends on the crystals’ orientations [3]. Understanding more about the fiber orientation field in turbulence will provide critical insights into important anisotropic particle suspension problems. Previous study of advected director orientation fields
has led to substantial advances in the theory of dynamical systems and, particularly, in the study of chaotic and turbulent flows. Extending that work into turbulent and multiphase flows will provide powerful information to the large community investigating turbulence.

Orientation fields in turbulent flows have been studied in a variety of contexts, including the evolution of magnetic field lines in magnetohydrodynamics, as well as the motion of thin rods or material line segments [4]. Because magnetic field lines do not affect the flow, they are considered passive vectors. Thin rods, material line segments, and fibers are similar, but they have symmetry and are thus considered passive directors. The passive vector problem provides key insights that connect to the problem of passive directors. We account for the appropriate considerations of symmetry and magnitude where they arise, but otherwise express the fiber’s director as a vector during calculation. Consider an infinitesimal ellipsoidal particle (a fiber) beginning at position $\mathbf{x}(t_i)$; its major axis aligns with the vector $\mathbf{p}(t_i)$. Jeffery’s equation describes the motion of the passive vector $\mathbf{p}(t)$ aligning with the particle at position $\mathbf{x}(t)$ at any time in the flow [3]. When we integrate his equation along a particle’s trajectory to find $\mathbf{p}(t)$ we must start from a known initial orientation, $\mathbf{p}(t_i)$ [5].

To gain insight into the orientation field problem, Pumir and Wilkinson tracked ellipsoidal particles in a numerical simulation of turbulence using Jeffery’s equation [5]. They found a strong correlation between director orientation and the vorticity vector [5]. The vorticity measures the rotation of the fluid around any one point in the flow, and is a property of the velocity field which is instantaneous. Thus, the vorticity depends only on the time at which it is measured and not some initial condition from earlier in the flow. Such comparisons, between rod orientations and other fields that are independent of initial orientation, have shown strong connections between particle orientations and other dynamics of the turbulent flow.

As another initial orientation-independent field, the Lagrangian stretching direction determines the single preferential orientation for a particle at a given time and position in the flow. The preferential orientation is an average of orientations that are calculated by integrating Jeffery’s equation. For a single fiber with a single trajectory, a large distribution of initial orientations is used to calculate corresponding final orientations. When examining the statistics of the resulting set of final orientations, the mean orientation is the preferential fiber alignment. Parsa et. al [6] found that thin rods align strongly with the Lagrangian stretching direction in 2D chaotic flow, and Ni et. al [4] found the same for 3D turbulent flow. These findings were also used to explain
the correlation between rod orientation and the vorticity vector [4]. Such findings motivate our study of the field of preferential fiber orientations using the Lagrangian stretching direction. It offers a strong simplification that removes the initial orientation dependence from the orientation field.

1.2 Lagrangian Stretching

1.2.1 Velocity Gradient

Before considering Lagrangian stretching, which represents fluid stretching over some time interval, we must consider the deformation rate that the fluid incurs at any one moment in the flow. This instantaneous rate of deformation is contained in the velocity gradient. The velocity gradient at any point measures the relative velocity of the fluid close to that point in each direction. In a velocity field \( u(x) \), this is measured by the second rank tensor

\[
A = \frac{\partial u_i}{\partial x_j}
\]

where entry \( ij \) is the derivative of the \( i^{th} \) component of the velocity field with respect to the \( j^{th} \) spatial direction. Take 2D simple shear flow for example. The velocity field is defined by:

\[
u(x) = (kx_2,0)
\]

for some constant k. The field is shown in figure 1.1.

We can find the velocity gradient tensor \( A \) using the partial derivatives:

\[
A = \begin{bmatrix}
\frac{\partial u_1}{\partial x_1} & \frac{\partial u_1}{\partial x_2} \\
\frac{\partial u_2}{\partial x_1} & \frac{\partial u_2}{\partial x_2}
\end{bmatrix}
\]

Since the \( x_2 \) velocity is constant 0, and the \( x_1 \) velocity scales linearly with \( x_2 \), the simple shear flow has the following velocity gradient:

\[
A = \begin{bmatrix}
0 & k \\
0 & 0
\end{bmatrix}
\]
or stretched and compressed by the flow, which deforms the fluid. Each of these actions is the result of the relative velocity of the surrounding fluid with respect to the point of interest, so they are measured by the velocity gradient. When we decompose the velocity gradient tensor, we see these two motions in the vorticity tensor $\Omega$ (the antisymmetric rotation portion) and the strain rate tensor $S$ (the symmetric stretching portion):

$$A = \Omega + S$$  \hspace{1cm} (1.5)

$$\Omega = \frac{1}{2} (A - A^T)$$  \hspace{1cm} (1.6)

$$S = \frac{1}{2} (A + A^T)$$  \hspace{1cm} (1.7)

Since the strain rate tensor deforms the fluid (while the vorticity only rotates it), the deformation rate is given by the symmetric strain rate tensor $S$. In the following section, we calculate deformation gradient from the velocity gradient tensor. The total deformation gradient comes from this symmetric portion of the velocity gradient.
1.2.2 Deformation

To find the Lagrangian stretching direction, consider a fluid element at position $X$ at initial time $t_i$. The small fluid element, in our 2D example, begins as a circle. As time passes, this fluid gets deformed according to the velocity gradient at its position at each moment. As this is happening, the fluid is being advected in the flow, so we take into account the trajectory of the fluid element when assessing the velocity gradient at each time. Finally, after some finite time $\Delta t$, the fluid is at position $x(X,t)$. For a very small fluid element, the circle deforms into an ellipse, as shown in figure 1.2. We measure the shape of this ellipse, with respect to the initial circle, using the deformation gradient:

$$F = \frac{\partial x_i}{\partial X_j}$$

which quantifies the deformation that the fluid has experienced during the time interval. Since the velocity gradient is the time derivative of the deformation gradient, we calculate the total deformation by integrating the velocity gradient tensor according to the differential equation:

$$\frac{dF}{dt} = AF$$

with the initial condition that $F = I$, the identity tensor, because the circle begins with no deformation. The deformation gradient tensor now tells us how the fluid has been stretched and rotated by the flow along its trajectory from initial time $t_i$ to the current time $t$. 

Figure 1.2: A circular fluid element in the velocity field deforms into an ellipse after some small time, and as $\Delta t$ approaches $\infty$, the ellipse aligns with $e_1$. 
For our case of simple shear, the fluid element experiences the same velocity field throughout the entire trajectory, so we do not need to numerically integrate the various velocity gradients that it experiences (as we do in the turbulent case). Instead, we can determine the deformation gradient by the original definition $F = \partial x_i / \partial X_j$. For our velocity field, any point experiences only a constant velocity in the $x_1$ direction, which is linear with the point’s $x_2$ position (which remains constant). So, the final position $x$ after time $\Delta t$ of any initial point $X$ is given by:

\[ x_1 = X_1 + k\Delta t X_2 \quad (1.10) \]
\[ x_2 = X_2 \quad (1.11) \]

from which we can calculate the deformation:

\[ F = \begin{bmatrix} \partial x_1 / \partial X_1 & \partial x_1 / \partial X_2 \\ \partial x_2 / \partial X_1 & \partial x_2 / \partial X_2 \end{bmatrix} = \begin{bmatrix} 1 & k\Delta t \\ 0 & 1 \end{bmatrix} \quad (1.12) \]

### 1.2.3 Cauchy-Green Strain Tensors

We then use the left Cauchy-Green strain tensor, $C^L$, to find the stretching directions of the fluid element:

\[ C^L = FF^T \quad (1.13) \]

The eigenvectors of $C^L$ correspond to the principal axes of the ellipse at final time $t$. The most extensional eigenvector, $\hat{e}_{L1}$, indicates the direction in which the fluid element has been stretched the most (the Lagrangian stretching direction), as shown in figure 1.2.

In our case of simple shear flow, we will calculate $\hat{e}_{L1}$ from the deformation in the previous subsection:

\[ C^L = FF^T = \begin{bmatrix} 1 & k\Delta t \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ k\Delta t & 1 \end{bmatrix} = \begin{bmatrix} 1 + (k\Delta t)^2 & k\Delta t \\ k\Delta t & 1 \end{bmatrix} \quad (1.14) \]

We now solve for the eigenvalues and eigenvectors of $C^L$. The eigenvalues, $\lambda_i$, are the solutions of:

\[ |C^L - \lambda I| = 0 \quad (1.15) \]

\[ \begin{vmatrix} 1 + (k\Delta t)^2 & k\Delta t \\ k\Delta t & 1 \end{vmatrix} - \begin{bmatrix} \lambda & 0 \\ 0 & \lambda \end{bmatrix} = 0 \quad (1.16) \]
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\[
\begin{bmatrix}
1 + (k\Delta t)^2 - \lambda & k\Delta t \\
\lambda & 1 - \lambda
\end{bmatrix} = 0
\quad (1.17)
\]

from which the eigenvalues are
\[
\lambda = \frac{2 + (k\Delta t)^2 \pm \sqrt{(2 + (k\Delta t)^2)^2 - 4}}{2}
\]
We use the largest eigenvalue, \(\lambda = \frac{2 + (k\Delta t)^2 + \sqrt{(2 + (k\Delta t)^2)^2 - 4}}{2}\), to find the most extensional eigenvector \(\hat{e}_{L1}\):

\[
[C^L - \lambda I] \hat{e}_{L1} = 0
\quad (1.18)
\]

\[\hat{e}_{L1}\] and \(e_1\) as \(\Delta t\) increases. In the limit of small \(\Delta t\) (\(\Delta t \to 0\)), the angle is \(\pi/4\). As \(\Delta t\) increases (\(\Delta t \to \infty\)), the angle approaches 0, indicating that \(\hat{e}_{L1}\) aligns with the horizontal axis for this case of simple shear flow.

\[\hat{e}_{L1}\] numerically for increasing \(\Delta t\) and shows that:

\[
\lim_{\Delta t \to \infty} \hat{e}_{L1} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}
\quad (1.19)
\]

We see this result in figure 1.2 as the ellipse’s major axis approaches horizontal after long \(\Delta t\).

For the case of turbulence, the fluid elements that we examine experience a different velocity.
gradient at each moment during the flow. Instead of finding the deformation as we did for simple shear, we must carry out the numerical integration of \( \frac{dF}{dt} = \mathbb{A}F \). This allows us to calculate \( C^L \) in turbulence, and likewise find the stretching direction \( \mathbf{e}_{L1} \).

If we consider a fiber (a thin rod-like particle) that is at the center of our ellipse at the end of this trajectory \( (x(X,t)) \), it would have begun at the center of the circle \( (X) \) at \( t_i \) and followed our fluid element over the whole time interval. The alignment of that fiber at \( t \) is most likely to be \( \mathbf{e}_{L1} \). Note that this is the preferential alignment of such a fiber. The orientation of any individual fiber depends on what its orientation is at \( t_i \), which Jeffery’s equation takes into account. Averaging over many possible initial orientations results in a preferential final alignment of \( \mathbf{e}_{L1} \), which becomes very strong for longer \( \Delta t \).

Note that \( \mathbf{e}_{L1} \) depends on time \( t \), position \( x \), and integration time \( \Delta t \) for which it is calculated. Also, \( \mathbf{e}_{L1} \) is a director because stretching direction, fiber orientation, and eigenvectors are all identical to their inverses. For example, in the field of Cauchy-Green eigenvectors, \( \mathbf{e}_{L1} \) and \( -\mathbf{e}_{L1} \) are equivalent.

The alignment of fibers with \( \mathbf{e}_{L1} \), independent of initial orientation, greatly simplifies the passive director problem. While the left Cauchy-Green eigenvector field measures fiber alignment almost perfectly [4], it remains a characteristic inherent to the flow and not to specific fibers. Calculating fiber orientations from only velocities and velocity gradients - well-defined and easily tracked quantities - proves to be a powerful tool for studying turbulent flows.

### 1.3 Lagrangian Stretching Applications and Studies

The field of fiber orientations presents many avenues for exploration: what patterns and structures do we see in the directors? How do these structures form? What effects do these structures have on other properties of the field?

Studies of the spatial structures within this field have shown interesting statistical properties with significant implications. Mehlig et al. [1] used stochastic models (in both 2D and 3D) and turbulent channel flow, and observed the scaling of fiber alignment with respect to the distance between fibers. In a smooth field, the relative orientation difference between fibers increases with the distance between fibers (since nearby fibers should have similar orientations). This
orientation difference should, in a smooth field, show a power law function whose exponent scales with the moment of distribution that is observed. Mehlig et al. discovered anomalous power law scaling exponents, which measure the degree of fractal structure in this field. This intermittency signifies a very interesting underlying structure whose pattern has exceptional effects on particle alignment: nearby fibers do not align as much as they would in a smooth field. The effects of unalignment on chemical, structural, and refractive properties warrant the need to further understand this field.

Hejazi et al. [7] studied a 2D time-periodic chaotic flow and demonstrated a possible cause for misalignment: scar lines. The actual pattern of the underlying structure has been observed to consist of a smooth field in most places, but to contain lines across which orientations display a large, sharp change. The flow history quantified by the Lagrangian stretching field demonstrates how these scars form. Fluid that is stretched in one direction initially, and later stretched in the orthogonal direction, experiences a cancellation of stretching and becomes a scar line across which fibers are unaligned. Such structures, which we identify in 3D flows, could explain the field’s anomalous scaling.

Studies of nematic liquid crystals in magnetic and electric fields have shown similar structures. Domain walls in electric and magnetic fields consist of vectors whose orientations change rapidly by $\pi$ over a small distance. These separate two domains, which have opposite orientations, on each side of the wall. Helfrich et. al [8] and Stieb et. al [9] studied nematic liquid crystals and found such surfaces in the director field in the presence of magnetic and electric fields. Such a director field corresponds more directly to the director field of fiber orientations. In these alignment-inversion walls (also referred to as kink walls [10]) the director orientation rotates rapidly by $\pi$, and the directors on each side of the wall demonstrate equivalent orientations. Alignment-inversion surfaces in liquid crystals demonstrate different types of such structures. In a twist wall, the orientation rotates by $\pi$ within the plane of the wall [9], similar to a Néel wall in a magnetic field [8]. A bend wall consists of directors which rotate in the plane perpendicular to the wall [9], and mimic a Bloch wall in a magnetic field [8]. We observe the same behavior in our alignment-inversion surfaces in the fiber orientation field.

The mathematicians studying flow in phase space in dynamical systems have also explored the idea of director alignment. The mathematics of dynamical systems correspond directly to the problem of mixing in a 2D flow. Giona et. al [11] show that a material line segment in 2D time
periodic flow approaches a unique, well-defined orientation. A small line in the field experiences the same flow pattern many times in periodic flow. When measuring a material line’s orientation, they then consider its orientation after each subsequent period. They find that this converges to a unique direction. This property is known as asymptotic directionality, and is a general feature of the dynamics in phase space of 2D periodic systems. The asymptotic convergence of such structures has also been referred to as the formation of a persistent pattern site [12,13], as well as a strange eigenmode [14].

Since such periodic systems show consistent repetition of certain dynamics, we may expect that some structures approach a steady state. In isotropic turbulence, however, such fields in the flow must be different at every time. We want to understand the direction in which a fiber will align in isotropic turbulence. Does this depend on the history of the flow, which varies in turbulence? If it does depend on flow history from a long time prior to the time of interest, then there may not be a unique alignment orientation. While the case of isotropic turbulence must present a different orientation field at each time in the flow, we observe the analogous asymptotic directionality.

The calculation of one field of preferential fiber alignments, calculated by the stretching direction \( \mathbf{e}_{L1} \), depends on \( \Delta t \). However, we find that in the limit of increasing \( \Delta t \) and observing stretching from a longer history, the field converges to a stable state. We study the structure of the field as well: scar lines from the 2D case are instead sheet-like in 3D, and they still cause anomalous scaling exponents that characterize a fractal field. By examining the field for different \( \Delta t \) we can determine the time at which stretching occurred to create a scar surface. The time dependence of this field proves to have some intricate properties, as longer integration times develop finer alignment-inversion surfaces (and create the fractal), but they take up exponentially less space in the field. The effect of the alignment-inversion surfaces converges to zero, so the field overall reaches a stationary state. We discuss these phenomena in depth in chapter 3.
Chapter 2

Methods

2.1 Direct Numerical Simulation

We study the field of preferential fiber orientations in a direct numerical simulation (DNS) obtained from the Johns Hopkins Turbulence Database [15–17]. The simulation is a triply periodic box with $1024^3$ resolution of forced homogeneous isotropic turbulence with Taylor-Reynolds number $R_\lambda = 418$. The simulation is stored at a time-step of $0.047\tau_\eta$, where $\tau_\eta$ is the Kolmogorov time scale. Details on the accuracy and resolution of the simulation are available at http://turbulence.pha.jhu.edu/.

To calculate a field of preferential orientations (i.e. a field of Cauchy-Green eigenvectors $\hat{e}_{L1}$) we select the final time $t$ to observe. We generate planar grids of $512^2$ points in the flow domain and calculate the stretching direction $\hat{e}_{L1}$ at time $t$. The stretching direction is determined by the history of the velocity gradients that the fluid point has experienced, so we track a particle from each point backward from time $t$ to an earlier time $t_i = t - \Delta t$, with $\Delta t = 59\tau_\eta$. Note that the trajectories are the history of the paths taken by the particles, leading up to their final positions in the grid at $t$. At each time step of the DNS along the trajectory, we store particle positions and the associated velocity gradients. The Johns Hopkins database provides a set of built-in functions that allow the calculation of particle trajectories and velocity gradients. We chose the option that uses sixth-order Lagrangian spatial interpolation for positions, and fourth-
order Lagrangian spatial interpolation for velocity gradients. We can then integrate the velocity
gradients along the trajectory of each particle leading up to $t$ and compute the preferential
orientation from the stretching direction $\hat{e}_{L1}$. We do this according to the process described in
chapter 1, except in this case we use tensors for three dimensional flow.

In the calculation of Lagrangian stretching direction we can sample data points at a higher
spatial resolution than that of the simulation. While the sampled particles end up in final
positions that are in between simulation nodes, the stretching for each is measured over a long
trajectory, during which the particles spend most of the time quite far apart, and their total
stretching is resolved by the simulation’s spatial resolution. Consider two adjacent data points in
our sample grid at final time $t$, such as the circle and square particles in figure 2.1. The JHTDB
interpolation scheme is sufficient to track the trajectories (shown in grey) of particles between
sample nodes in the simulation, so if we follow these two particles (backwards in time), we see
that they come from positions that are much farther apart. In fact, most of their trajectories
are easily resolved by the DNS resolution. Since the final orientation is defined by stretching
along the entire trajectory, which is almost completely resolved without interpolation, the two
particles that end up between DNS nodes will have orientations that are resolved as well.
Figure 2.1: (color). A simplified 2D concept depiction of sampled particles in the grid at final time $t_f$, and their prior trajectories from $t_i$, compared to DNS spatial resolution. Though the orientation field at $t$ refers to points between DNS nodes, the data for those points are calculated from their associated trajectories (which are not between DNS nodes) and are hence well resolved.
Chapter 3

Results

3.1 Scar Surfaces in 3D Passive Director Orientation Fields

Figure 3.1 shows alignment-inversion surfaces in the orientation field in isotropic turbulence. To capture the 3D spatial structure of the field, we sample several two dimensional planar cuts surrounding and crossing through a $17\eta$ cubic region (figure 3.1(a)), where $\eta$ is the Kolmogorov length scale. Note the thin spiraling lines that pass through this cube. An otherwise smooth region of the orientation field is split by a thin region across which the orientation changes rapidly. Drawing connections between similar features of the inner slices and nearby outer walls, we see that these structures (which appear as lines in a two dimensional cross-section) are two dimensional sheets. Two close fibers on opposite sides of the surface have the same orientation. The fibers between those, within the surface, demonstrate an abrupt rotation between the outer, aligned fibers. The sheets in figure 3.1(a) spiral around a vortex to form a tube. Figure 3.1(b) shows how the far right wall of figure 3.1(a) fits within a larger subsection at the scale of $140\eta$, displaying typical turbulent structures such as vortices and mushrooms. Note that figures 3.1 and 3.2 show the field for a relatively short integration time (because these are well resolved). At shorter times such as this, the surfaces are quite wide, so it may seem that orientations on one side of the surface do not quite match orientations on the other side. We calculate the field using longer time intervals in figure 3.4, where it is more apparent that the thin surfaces sharply divide regions with the same orientation on either side.
Figure 3.1: (color). The orientation field of fibers in a subsection of the flow, measured by the $x_1$ component of $\mathbf{e}_{L1}$ for $\Delta t = 9.4\tau_\eta$. The field is measured on: (a) three walls and three inner cross-sections of a $17\eta$ cube; (b) one $140\eta$ square cross-section and one $17\eta$ sub-square cross-section. The $17\eta$ (lower) square in (a) corresponds to the right outer wall square in (b).

Having established the geometric structures of these surfaces, we now explore more closely the phenomenology of the directors that they comprise. The director nature of the orientations is taken into account as we map the magnitude of the $x_1$ component of $\mathbf{e}_{L1}$. This will always have a value between zero and one and the resulting equivalence between $-\mathbf{e}_{L1}$ and $\mathbf{e}_{L1}$ in the visualization treats this properly as a director field. There is also slight information loss in observing one director component when there are two degrees of angular freedom. Since the surfaces contain fibers of many different orientations, it is very unlikely that these orientations are all perpendicular to the observed component. This is the only case in which such a structure would not appear in the visualization and we cross-check this in figure 3.2. Observing the $x_2$ and $x_3$ coordinates of the same orientation field, we see most alignment-inversion surfaces do appear in all three visualizations.
We further verify that these regions are not phenomena of individual components by measuring the gradient of the orientation field at each point. This second rank tensor measures the spatial rate of change of the orientation around one position in the field:

\[ \frac{\partial(\hat{e}_{L1})_i}{\partial x_j} \]  \hspace{1cm} (3.1)

We measure the total rate of orientation change with a scalar, given by the trace of the inner product of the gradient. A larger gradient at some position indicates that the orientations nearby change very rapidly, and that position has a sharp alignment rotation. Figure 3.3 shows that regions which appear to have strong component variation, indicating alignment-inversion surfaces, do have a large three dimensional gradient, and the strong orientation changes are therefore not component-specific. At this high resolution, we near the limit of our numerical calculation of the gradient, as we see some thin artifacts that seem to exhibit more surfaces than we observe in figure 3.2. The very thin black lines (at (16\eta, 6\eta) for example) are probably the result of noise as they are not resolved, and do not always separate actual distinct surfaces. For this reason, we observe the surfaces in the previous (component-based) visualizations, and use the gradient to confirm that these do correspond to overall orientation changes. The larger, more isolated surfaces (at (4\eta, 2\eta) for example) are well resolved and match the surfaces that we see in figure 3.2. What we visualize are in fact surfaces across which the fiber orientation sharply changes. Our later statistical analyses do not rely on specific components, so this does...
not affect those results, but reassures that our qualitative observations of the fiber behaviors are correct.

\[\text{Figure 3.3:} \quad \text{Magnitude (logarithmic color scale) of the tensor gradient of the orientation vector field. This measures the spatial rate of change in the orientation field. Lighter areas denote structures where orientation varies dramatically.}\]

Upon examining our visualizations, we see that these structures are a fascinating result of stretching [7], and are not simply regions of chaotic orientations. They actually demonstrate a specific rotation pattern within the surface. The area surrounding the surface is a relatively smooth field: the fibers on either side of the surface will have the same orientation. Although not always the case for the fields calculated with shorter time (as we have seen so far), which still have wider surfaces, as we increase the integration time and the surfaces shrink, the orientations surrounding them come to match. We observe this in figure 3.4. For sake of connecting with our visualization, consider the fibers just outside of one surface to align with the \(x_1\) axis: they will have a \(x_1\) component of 1, and form a smooth white region in our image. Moving through the surface we see that the \(x_1\) component changes continuously from 1 to 0, as the color shifts from white to black, so the fibers obtain every orientation from parallel to perpendicular to \(\hat{x}_1\). Then, the \(x_1\) component likewise shifts back from 0 to 1. The fibers display a full rotation by \(\pi\), turning over after they become perpendicular to the outer fibers, forming a surface in which their alignment inverts. Because a director is equivalent to itself under \(\pi\) rotation, the orientation originates from and returns to alignment with fibers surrounding the surface.
3.2 Preferential Orientation Invariance

This orientation field serves as an accurate model for particle-laden flows, and we wish to decipher just how simple of a picture it is. It somewhat simplifies the problem in its independence of fibers’ initial orientations. What other parameters does this field depend on, and of what parameters is it independent? Since the flow is turbulent, the orientation field must depend on the time and position at which it is measured. Does it depend on the amount of the flow history which is considered in its calculation? We find that it does not have to. We vary $\Delta t$ by selecting different $t_i$ along the trajectory, and integrating from $t_i$ to one final time $t$. This allows us to observe the orientation field for the same particles in the same positions at $t$, but for a longer integration time (larger $\Delta t$ and earlier $t_i$). Larger integration time allows for a more precise picture of the stretching field itself as it takes into account additional stretching that happened earlier in the flow history. To observe the effect we examine the field of $\hat{e}_{L1}$ as it develops with increasing $\Delta t$.

Figure 3.4 shows this development at the scale of both $140\eta$ and $17\eta$ for $\Delta t$ in the range from $7.1\tau_\eta$ to $42\tau_\eta$. For $\Delta t > 21\tau_\eta$, the larger scale structures of the orientation field do not change. This is the first qualitative indication of the field’s invariance. Examining the $17\eta$ cross-sections, we see that the only changes for larger $\Delta t$ are the developments of new, but increasingly thin, alignment-inversion surfaces, as described in the previous section. While this phenomena continues to change the field as $\Delta t$ increases, it only affects a set of points whose measure approaches 0. This is because the thickness of the new surface structures also approaches 0. In figure 3.1, the inversion surfaces that form between $7.1\tau_\eta$ and $14\tau_\eta$ have a small but evident thickness. However, the surfaces that form between $28\tau_\eta$ and $35\tau_\eta$ are much thinner, and new formations at $42\tau_\eta$ are unresolved entirely. The diminishing thickness of subsequent new surfaces creates negligible changes at large $\Delta t$, resulting in convergence towards a field that is overall stationary.

The convergence of the field with respect to integration time allows us to think of it as a simple, distinct field that is independent of distant past history. If stretching from much earlier in the flow history had a significant effect on the orientation field, the calculation of the field would always be missing information from stretching before $t_i$. In that case the calculated preferential orientations would depend strongly on the amount of integration time that is used to calculate the field. The stretching model would be horrendously variable with time and poorly
Figure 3.4: (color). The evolution of the fiber orientation field as integration time increases. Fibers are observed at the same time $t$ on the same $140\eta$ square and $17\eta$ sub-square cross-sections are observed for $\Delta t = (a)7.1\tau_\eta$, (b) $14\tau_\eta$, (c) $21\tau_\eta$, (d) $28\tau_\eta$, (e) $35\tau_\eta$, and (f) $42\tau_\eta$. With longer integration times, more alignment-inversion surfaces form as a result of stretching from earlier in the flow history. While these form continually, their effect on the orientation field becomes negligible, as the surface thickness falls off rapidly. This is apparent in the minimal change between (e) and (f).

defined. Fortunately, the effect of earlier stretching becomes negligible as it is only apparent in surfaces whose thickness decreases rapidly enough to not significantly change the field. Only the recent stretching history is relevant to fiber orientation, and we can find that simply using the preferential alignment field. The unique limit of the field under increasing $\Delta t$ is invariant. Every time $t$ of the flow has one such unique field, independent of $\Delta t$, which characterizes the preferential fiber orientations at that time. While a single calculation of the stretching field must be defined over a chosen finite time interval $\Delta t$, the convergence with increasing $\Delta t$ means that we can achieve results that are very close to the time-independent limit that represents the full orientation field. If we want to be within a specific small error of the invariant field, there exists a finite $\Delta t$ that can be used to calculate the stretching field within the desired error. As we see in the statistical results to come, this $\Delta t$ is quite reasonable to resolve the orientation field of very small scales in turbulence. More importantly, the existence of the invariant limit field allows the field to be a well-defined and powerful new tool for studying turbulent flows.

The convergence of the orientation field for growing $\Delta t$ is verified quantitatively when we find that the finite derivative of the field, with respect to integration time $\Delta t$, asymptotically approaches 0. We calculate this finite difference for a specific $\Delta t$ by computing the difference...
Chapter 3 - Results

Figure 3.5: (color). (a) The second moment of the finite orientation difference (with respect to $\Delta t$) converges to zero as integration time $\Delta t$ increases. The orientation field itself, then, converges to a unique field that is independent of integration time. The orientation change at each data point is measured as $|\hat{e}_{L1}(\Delta t) - \hat{e}_{L1}(\Delta t + \delta t)|^2$, where $\delta t = 0.5\tau_n$. (b) Log/linear PDF of finite orientation difference for individual points (whose mean is given in (a)) for $\Delta t$ values: $0.5\tau_n$, $12\tau_n$, $24\tau_n$, $36\tau_n$, $48\tau_n$. For larger $\Delta t$, although there are still points experiencing orientation change (in the tails of the PDF), the number of such points approaches zero so the field overall stabilizes.

between the orientation director for $\Delta t$ and the director at the same point for $\Delta t + \delta t$; $\delta t$ is small, in this case $\delta t = 0.5\tau_n$. We measure the change as the magnitude squared of the resulting vector difference $\delta \hat{e}_{L1} = \hat{e}_{L1}(\Delta t) - \hat{e}_{L1}(\Delta t + \delta t)$ at each point. To see the change in the field overall, figure 3.5(a) confirms that the finite difference of the whole field with respect to $\Delta t$, measured as the second moment over all points, converges to 0 as well.

Surprisingly, though the number of points that form inversion surfaces becomes negligible to the overall field, these structures do continue to form as $\Delta t$ increases, and create the interesting fractal structure of the field. The PDF in figure 3.5(a) demonstrates that with longer integration time, while almost all points exhibit no orientation change, there is always still a number (albeit converging towards 0) of points that experience an orientation change due to an alignment-inversion surface caused by earlier stretching. These are evident in the tails of the PDF, which always extend to the maximum value $\delta \hat{n}$ which is 2. We see that over time the number of points in these tails decreases, and converges towards 0, allowing the mean derivative of the field to converge to zero. Although their presence is not significant enough to create
integration time dependence in the invariant field limit, it is enough to create an unexpected fractal structure.

### 3.3 Orientation Field Intermittency

One characteristic of interest is the intermittency of the fiber orientation field. Since the inversion surfaces contain fibers at every orientation angle between 0 and $\pi$ (where 0 is the orientation of fibers immediately outside the sheet), they create points which are strongly unaligned with those nearby. As the surface thickness approaches zero, the fibers within the surface become essentially strongly unaligned from those surrounding the surface. We find that not only do these surfaces exist, but they are present at all small scales (below the Kolmogorov length) in the flow and create a fractal field. They appear in the tails of the PDF in figure 3.5(b), where some fibers change orientation under the formation of a new surface when integration time increases. Here we see the careful interplay of this field: for longer integration times there are always points where the preferential orientation changes (producing inversion surfaces and tails in figure 3.5(b)), but the number of such points approaches zero quickly enough that the overall field converges to a unique state, independent of integration time. We further demonstrate this feature in figure 3.6, where we plot the difference between the orientations of two fibers (a measure of their unalignment) as a function of the distance between them. For a smooth field, fibers will align with their nearby neighbors. As the distance $r$ increases between fibers, their second moment orientation difference will change with $r^2$ and have a scaling exponent of $\xi_2 = 2$. We see a similar effect for small integration time ($\cdot 0.5\tau_\eta$). This is because the orientation director is nearly the instantaneous strain rate direction, which is a smooth field. However, as integration time increases and the field converges, the structure function develops a scaling exponent of 0.29. This characterizes a highly intermittent field with structures of abrupt orientation change at these small scales.

### 3.4 Correspondence with Other Turbulent Flows

The orientation field of preferential fiber alignments is a powerful tool for examining homogeneous isotropic turbulence. It presents a unique, well-defined director field for each instant in
The structure function of the orientation field converges as integration time increases. Orientation director differences are calculated as $<|\delta e_{L1}|^2> = <|\hat{e}_{L1}(\vec{x}) - \hat{e}_{L1}(\vec{x} + \vec{r})|^2>$, and $r = |\vec{r}|$. Data are shown for $\Delta t = \{v_0, 5\tau \eta, 12\tau \eta, 23\tau \eta, 34\tau \eta, 46\tau \eta, 57\tau \eta\}$. The shortest integration time is close to the power law scaling of a smooth field, shown by the red dot-dashed line. As integration time increases, the function converges towards that of a fractal field, shown by the blue dashed line, with a scaling exponent of $0.29$.

The flow because it converges to a fixed field that does not depend on integration time. Our examination has so far uncovered a rich geometry of alignment-inversion surfaces that build a fractal pattern. The topology of these attributes - and their relation to well-known features of turbulence, such as vortices - presents a deep problem that warrants further investigation. These findings are particularly significant in their apparent universality across different forms of turbulence. Figure 3.6 demonstrates the fractal structure of the field as it affects the scaling exponents of various moments of the structure function. The scaling exponent $\xi_p$ is defined by $\langle|\delta e_{L1}|^p\rangle \propto r^{\xi_p}$, and corresponds to the slope of the log/log $p^{th}$ moment structure function, as shown in figure 3.6 for the second moment ($p = 2$) where $\xi_2 = 0.29$. All scaling exponents of the orientation field fall far below $\xi_p = p$, and saturate at larger $p$, signalling intermittency at these small scales. The homogeneous isotropic turbulence data has scaling exponents that are very similar to the turbulent channel flow. This provides evidence that the inversion surfaces and the resulting fractal pattern characterize turbulence more generally.
Figure 3.7: (color). Scaling exponents of the orientation structure function for □ homogeneous isotropic turbulence compared to + turbulent channel flow. Both scaling exponents fall far below the line $\xi_p = p$ (dashed line), which characterizes a smooth field. The fractal structure of the fiber orientation field appears to be a universal property of turbulence [1].
Conclusions

4.1 Alignment-Inversion Surfaces

Upon visualizing the fiber orientation field, we find that the dominant structures are thin surfaces across which the orientation changes rapidly by $\pi$. Most of the flow’s volume has a relatively smooth orientation field. But, there exist thin surfaces that show a sharp orientation change compared to the surrounding fibers. In our visualizations we see that the fiber orientations rotate rapidly by $\pi$ moving across each surface. The exact manner of rotation remains an interesting question for further study. Since orientations are directors, which are equivalent to their inverses, the orientation field is the same on each side of such surfaces. These outer fibers are parallel to the surface, and the fibers within the surface rotate through the orientation perpendicular to the stretching direction [7]. We see that these surfaces create a fractal structure in the orientation field.

4.2 Fractal Scaling

We find that the alignment-inversion surfaces create large alignment differences between fibers that are very close to each other. These sharp orientation changes cause the anomalous power law scaling that we find in the orientation structure functions when analyzing the field statistically.
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The orientation difference does not scale with distance between fibers as it would in a smooth field. Nearby fibers with larger differences cause the structure function to scale with $\xi_p < p$ for all moments $p$ of the function. Our anomalous scaling exponents agree with those from other numerical simulations of a different turbulent flow [1], suggesting that this fractal is a characteristic of turbulence in general. The field’s intermittency could play a large role in the understanding of multi-scale turbulence. The effects of intermittent structure on particle-laden fields, such as icy clouds [2], warrant further study into these fascinating structures. Ice crystals in clouds collide at rates determined by the relative orientations of nearby particles [1]. Such collisions affect droplet formation as well as other phenomena in clouds, and understanding the field of ice crystal orientations in turbulence will reveal further workings of such clouds.

4.3 Asymptotic Directionality

An important feature of the preferential fiber alignment field, given by Cauchy-Green eigenvectors $\hat{e}_{L1}$, is its independence of initial conditions. Unlike more explicit calculations of fiber orientations, for example tracking a fiber’s motion using Jeffery’s equation, the Cauchy-Green eigenvector field depends only on stretching and not on a specific initial fiber orientation, as it gives the most likely alignment averaged over all possible initial orientations. Calculation of any one $\hat{e}_{L1}$ does still depend on the initial time from which we start calculating the field, because it is defined over the finite time interval $\Delta t$ leading up to the time for which we calculate the field. We show that the orientation field becomes independent of this initial time at long times. Since rods align with the preferential alignments, $\hat{e}_{L1}$, for longer $\Delta t$, we focus on the $\hat{e}_{L1}$ field in the limit of increasing $\Delta t$. In this limit, we find that the field converges to a stable state. We have shown that the fiber orientation field presents the asymptotic directionality that has been found in periodic chaotic systems [11].

The asymptotic directionality of the fiber orientation field shows the intricate balance in the field’s time dependence. The field, calculated at any one time interval, does depend on the initial integration time. As we increase integration time, the field does change as new alignment-inversion surfaces form. However, they only change the orientation of a set of points whose size is exponentially decreasing. Recall that increasing $\Delta t$ allows us to calculate the orientation field at the same time $t$, but also takes into account deformation that occurred early in the flow history.
as we begin integrating from an earlier $t_i$. We see more alignment-inversion surfaces develop as we increase the integration time $\Delta t$. This indicates that more surfaces form as a result of deformation from further back in the flow history. But, observing stretching from further and further back in the flow history creates surfaces that become negligibly thin. As a result, the orientation field overall converges towards a steady state which is independent of the initial time from which it is calculated. This demonstrates the property of asymptotic directionality. This finding confirms that the orientation field - calculated by stretching direction $\hat{e}_{L1}$ - is a unique and well-defined characteristic of turbulent flow at any moment in time.
Appendix

5.1 MATLAB Scripting

The Johns Hopkins Turbulence Database provided raw data through their digital numerical simulation (DNS) of homogeneous isotropic turbulence. The JHTDB provides access through functions in C, Fortran, and Matlab using Web services. The key numerical integration of the velocity gradient tensor requires matrix operations, of which MATLAB has an extensive library. This reason, and the availability of database access, made MATLAB the strongest choice of programming language to analyze this field. The grid of orientations also fits well in a matrix, making it readily presentable through MATLAB’s strong plotting tools. In order to collect, analyze, and display the relevant data, I learned to write MATLAB scripts. As a prominent language in the scientific research community, MATLAB provided excellent experience in combining mathematical and computational aspects of physics.

Each function provided by JHTDB allows the user to query a different measurement of the flow, including velocity, velocity gradient, pressure, and many more. The user inputs one time instant and a matrix of spatial positions using coordinates of the three-dimensional simulation. The function then returns a matrix containing the chosen data measurement at each respective spatial point in the flow domain.

The goal is to find the orientation field: that is, calculate the preferential orientation at each
point in a grid within the flow domain at one time instant. We began by finding the orientation field on a full three-dimensional grid, of $64^3 = 262,144$ points. The time and data costs of this size prompted us to maintain that number of points for each data collection. However, the 64-point resolution did not sufficiently show the fine structure of the field. To increase resolution, we shifted to instead sample two-dimensional (planar) grids of data. The resulting square grids still contain 262,144 data points, but provide a sufficient resolution of 512 points per side. To visualize all three dimensions, we sample a few perpendicular grids, for example, a grid in the $x_1x_2$ plane, one in the $x_2x_3$ plane, and one in the $x_1x_3$ plane. In addition to aiding resolution, the 2D sampling grids provide a cleaner visualization: displaying a 3D orientation field on 2D paper mixes together the depths of different positions.

The codes used to collect, analyze, and visualize data are found on the Voth Group NAS2 server:

VothGroupNAS2\amasiphelps\paper codes
- \sheetsplit75.m
- \sheetcollect75.m

The script selects a time $t$ during the flow, and establishes a grid of positions within the flow domain. The data collection script considers a particle at each point in the grid and tracks its history: the trajectory that the particle followed leading up to this time, and the fluid stretching around the particle along the trajectory. For each step of the data collection, the script finds the position of each particle at one DNS time step earlier in the flow using the function GetPosition, which implements a Lagrangian velocity integration provided by Johns Hopkins. The code also calls the database function GetVelocityGradient to store the velocity gradient at each particle’s position at that earlier time. This process repeats for each time step during a large portion (1250 time steps = $59\tau_\eta$) of the simulation’s available flow time. Our final raw data then contains the positions of 262,144 particles scattered among the flow’s spatial domain at $t_i = t - 59\tau_\eta$. The data follow the trajectory of each particle forward in time over $59\tau_\eta$, at which point (at simulation time $t$) all of the particles lie in the grid that we created for sampling. We have also recorded the velocity gradient at each position along the trajectory of each particle, so we can calculate the stretching undergone by the fluid surrounding each particle.

- \DeformationIntegrator.m
This script performs the calculation described in section 1.2 for each particle in the grid created by the collection algorithm. The calculation iterates many times to compute the field using different integration times. It first calculates the field using the smallest integration time available, \( \Delta t = 0.5\tau_\eta \), using the data from \( t_i = t - 0.5\tau_\eta \) to \( t \) to find the orientations at \( t \). It then increases \( \Delta t \) by \( 0.5\tau_\eta \) and calculates the field using trajectories from \( t_i = t - \Delta t \) to \( t \). The code repeats this process for 125 different values of \( \Delta t \), ranging from \( 0.5\tau_\eta \) to \( 59\tau_\eta \). Our later analysis, describing the convergence of the field, examines the orientation field using these different integration times.

- \NumericalGradient.m

This calculates the numerical gradient of the orientation field.

- \integrationDifferencesPDF.m

To demonstrate the convergence of the orientation field, this script analyzes how the fields calculated above change as \( \Delta t \) increases. For each integration time \( \Delta t \) the script calculates the finite difference between the orientations in the field with \( \Delta t \) integration and those in the field with \( \Delta t + \delta t \) integration. This gives a numerical approximation for the derivative of the orientation field at \( \Delta t \) (with respect to increasing \( \Delta t \)). Calculating this difference for increasing \( \Delta t \) demonstrates the degree to which the field changes when it accounts for stretching that happened further back in the flow history. As we discuss in section 3.2, this finite difference approaches 0, demonstrating that the field converges toward a steady state.

- \eVexSFmultiPowers.m

This code calculates the orientation field structure function: a measure that has been used by Mehlig et al. [1] to demonstrate the fractal nature of this field. This function plots some moment \( p \) of the difference between two fiber orientations as a function of \( r \) the distance between the fibers. To calculate this, the code selects two data points from the orientation field. They represent fibers at final locations \( \mathbf{x}_1(\mathbf{X}_1, t) \) and \( \mathbf{x}_2(\mathbf{X}_2, t) \). The orientation calculation code has given their respective orientations, \( \mathbf{\hat{e}}_{L11}(\mathbf{X}_1, t) \) and \( \mathbf{\hat{e}}_{L12}(\mathbf{X}_2, t) \). It calculates \( r \) as the magnitude of the distance between the fibers: \( |r| = \sqrt{(\mathbf{x}_1(\mathbf{X}_1, t))^2 + (\mathbf{x}_2(\mathbf{X}_2, t))^2} \). When considering the difference between the fibers’ orientations, we take into account the symmetry of directors where \( \mathbf{\hat{e}}_{L1} \) is equivalent to \( -\mathbf{\hat{e}}_{L1} \). To do this we consider \( \mathbf{\hat{e}}_{L11}(\mathbf{X}_1, t) \) and consider the second orientation to be the vector \( \mathbf{\hat{e}}_{L12}(\mathbf{X}_2, t) \) or \( -\mathbf{\hat{e}}_{L12}(\mathbf{X}_2, t) \) which aligns more closely with \( \mathbf{\hat{e}}_{L11}(\mathbf{X}_1, t) \). For that
selected vector, the dot product with $\hat{e}_{L11}(X_1, t)$ will be positive, and we use this fact in our calculation.

If we place together the tails of these two unit vectors, the distance between their tips is given by $\sqrt{2 - 2(\hat{e}_{L11}(X_1, t) \ast \hat{e}_{L12}(X_2, t))}$. As described above, we want to find the smallest difference between these vectors, which occurs when their dot product is positive, so in the calculation of the difference we simply consider the absolute value of the dot product:

$$|\delta \hat{e}_{L1}| = \sqrt{2 - 2\hat{e}_{L11}(X_1, t) \ast \hat{e}_{L12}(X_2, t)}$$ (5.1)

The code evaluates this for many different pairs of fibers within the field, as well as distance $r$ between the fibers in each pair. We then sort the data with a MATLAB function to bin the values of $|\delta \hat{e}_{L1}|$ by their associated distances $r$. Within each $r$ bin, we calculate the $p^{th}$ moment of $|\delta_r \hat{e}_{L1}|$, which is $\langle |\delta_r \hat{e}_{L1}|^p \rangle$. To create the $p^{th}$ moment structure function, we plot $\langle |\delta_r \hat{e}_{L1}|^p \rangle$ as a function of $r^p$.

- \texttt{aggregateSFdisplay.m}
- \texttt{structureFunctionFit.m}
- \texttt{xiplot.m}

These codes, respectively, fit the structure functions to calculate $\xi_p$ and plot $\xi_p$ as a function of $p$ with corresponding data from Zhao et al. [1].
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