Lagrangian particle paths & ortho-normal quaternion frames

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Abstract

Experimentalists now measure intense rotations of Lagrangian particles in turbulent flows by tracking their trajectories and Lagrangian-average velocity gradients at high Reynolds numbers. This paper formulates the dynamics of an orthonormal frame attached to each Lagrangian fluid particle undergoing three-axis rotations, by using quaternions in combination with Ertel’s theorem for frozen-in vorticity. The method is applicable to a wide range of Lagrangian flows including the three-dimensional Euler equations and its variants such as ideal MHD. The applicability of the quaternionic frame description to Lagrangian averaged velocity gradient dynamics is also demonstrated.

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1 Introduction

1.1 General background

On 16th October, 1843, Hamilton wrote the expression for quaternion multiplication,

\[ I^2 = J^2 = K^2 = IJK = -Id, \]

as an algebraic rule for composing “turns” (directed arc lengths of great circles) in orienting his telescope. This feature – that multiplication of quaternions represents composition of rotations – has made them the technical foundation of modern inertial guidance systems in the aerospace industry where tracking the paths and the orientation of satellites and aircraft is of paramount importance [1]. The graphics community also uses them to control the orientation of tumbling objects in computer animations because they avoid the difficulties incurred at the north and south poles when Euler angles are used [2].

Given the utility of quaternions in explaining the dynamics of rotating objects in flight, one might ask whether they would also be useful in tracking the orientation and angular velocity of Lagrangian particles in fluid dynamical situations. Recent experiments in turbulent flows have developed to the stage where the trajectories of tracer particles can be detected at high Reynolds numbers [3, 4, 5, 6, 7, 8, 9, 10, 11, 12]; see Figure 1 in [3]. Numerical differentiation of these trajectories gives information about the Lagrangian velocity and acceleration of the particles. In particular the curvature of the particle paths can be used to extract statistical information about velocity gradients from a single trajectory [12].

The usual practice in graphics problems is to consider the Frenet-frame of a trajectory which consists of the unit tangent vector, a normal and a bi-normal [2, 12]. In navigational language, this represents the corkscrew-like pitch, yaw and roll of the motion. In turn, the tangent vector and normals are related to the curvature and torsion. While the Frenet-frame describes the path, it ignores the dynamics that generates the motion. Here we will discuss another ortho-normal frame associated with the motion of each Lagrangian fluid particle, designated the quaternion-frame. This may be envisioned as moving with the Lagrangian particles, but their evolution derives from the Eulerian equations of motion.

The first main contribution of this paper lies in the explicit calculation of the evolution equations of this quaternion frame. Secondly, this formulation is shown to apply to a wide range of Lagrangian problems, as the next sub-section shows. Thirdly, the evolution of the quaternion frame is related to an associated Frenet frame. Finally, it is shown how the pressure Hessian, which plays a key role in driving the quaternion frame for Euler fluid flow, can be modelled using constitutive relations.

1.2 An appropriate class of Lagrangian flows

Suppose \( \mathbf{w} \) is a contravariant vector quantity attached to a particle following a flow along characteristic paths \( \frac{d\mathbf{x}}{dt} = \mathbf{u}(\mathbf{x}, t) \) of a velocity \( \mathbf{u} \). Let us consider the abstract Lagrangian flow equation

\[
\frac{D\mathbf{w}}{Dt} = \mathbf{a}(\mathbf{x}, t), \quad \frac{D\mathbf{u}}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla. \tag{1.1}
\]

where the material derivative has its standard definition. Examples of systems that (1.1) might represent are:
1. The vector \( \mathbf{w} \) in (1.1) could be the velocity of a tracer particle in a fluid transported by a background velocity field \( \mathbf{u} \) with \( \mathbf{a} \) as the particle’s acceleration.

2. \( \mathbf{w} \) could be the vorticity \( \omega = \text{curl} \mathbf{u} \) of the incompressible Euler fluid equations, in which case \( \mathbf{a} = \omega \cdot \nabla \mathbf{u} \) and \( \text{div} \mathbf{u} = 0 \). The case of the Euler equations with rotation \( \Omega \) would make \( \mathbf{w} \equiv \tilde{\omega} = \rho^{-1}(\omega + 2\Omega) \).

3. For the barotropic compressible Euler fluid equations (where the pressure \( p = p(\rho) \) is only density dependent) then \( \mathbf{w} \equiv \omega_\rho = \rho^{-1}\omega \), in which case \( \mathbf{a} = \omega_\rho \cdot \nabla \mathbf{u} \) and \( \text{div} \mathbf{u} \neq 0 \).

4. The vector \( \mathbf{w} \) could represent a small vectorial line element \( \delta \ell \) transported by a background flow \( \mathbf{u} \), in which case \( \mathbf{a} = \delta \ell \cdot \nabla \mathbf{u} \). For example, using Moffatt’s analogy between the (magnetic) \( \mathbf{B} \)-field in ideal MHD and fluid vorticity [13], taking \( \delta \ell \equiv \mathbf{B} \) in the equations for incompressible ideal MHD, then \( \mathbf{a} = \mathbf{B} \cdot \nabla \mathbf{u} \) and \( \text{div} \mathbf{B} = 0 \). In a slightly generalized form it could also represent the Elsasser variables \( \mathbf{w}_\pm = \mathbf{u} \pm \mathbf{B} \) in which case \( \mathbf{a}_\pm = \mathbf{w}_\pm \cdot \nabla \mathbf{u} \) with two material derivatives [13]. In each of the cases (2-4) the vectors \( \mathbf{w} \) and \( \mathbf{u} \) satisfy the standard Eulerian form

\[
\frac{D\mathbf{w}}{Dt} = \mathbf{w} \cdot \nabla \mathbf{u}.
\]  

Consequently, it follows from Ertel’s Theorem [14] [15] [16] that

\[
\frac{D(\mathbf{w} \cdot \nabla \mu)}{Dt} = \mathbf{w} \cdot \nabla \left( \frac{D\mu}{Dt} \right),
\]  

for any differentiable function \( \mu(x, t) \). Choosing \( \mu = \mathbf{u}(x, t) \) as in [15] and identifying the flow acceleration as \( \frac{D\mathbf{u}}{Dt} = \mathbf{Q}(x, t) \) yields the second derivative relation

\[
\frac{D^2\mathbf{w}}{Dt^2} = \mathbf{w} \cdot \nabla \left( \frac{D\mathbf{u}}{Dt} \right) = : \mathbf{w} \cdot \nabla \mathbf{Q}.
\]

In each of the cases (2-4) above the acceleration vector \( \mathbf{Q} \) in (1.4) is readily identifiable. Thus, in these cases we have

\[
\frac{D\mathbf{w}}{Dt} = \mathbf{a}(x, t) \quad \text{and} \quad \frac{D\mathbf{a}}{Dt} = \mathbf{w} \cdot \nabla \mathbf{Q} =: \mathbf{b}(x, t) \quad \text{along} \quad \frac{D\mathbf{x}}{Dt} = \mathbf{u}(x, t).
\]

These are the kinematic rates of change of the vectors \( \frac{D\mathbf{w}}{Dt} = \mathbf{a} \) and \( \frac{D\mathbf{a}}{Dt} = \mathbf{b} \) following the characteristics of the velocity vector \( \mathbf{u} \) along the path \( x(t) \) determined from \( \frac{D\mathbf{x}}{Dt} = \mathbf{u}(x, t) \).

The plan of the paper is as follows: [3] shows that the quartet of 3-vectors \( \{\mathbf{u}, \mathbf{w}, \mathbf{a}, \mathbf{b}\} \) appearing in (1.5) determines the quaternion-frame and its Lagrangian dynamics: indeed, a knowledge of \( \mathbf{b} \) is essential to determining the dynamical process. Modulo a rotation around \( \mathbf{w} \), the quaternion-frame turns out to be the Frenet-frame attached to lines of constant \( \mathbf{w} \). In case (2) where \( \mathbf{w} = \omega \), lines of constant \( \mathbf{w} \) are vortex lines and the particles are fluid parcels. As described in [15] – see also [16] for a history – in this case Ertel’s Theorem for Euler’s fluid equations [14] ensures that \( \mathbf{b} = -\text{P} \omega \) where \( \text{P} \) is the Hessian matrix of spatial derivatives of the pressure. In some practical situations, however, the vector \( \mathbf{b} \) may not be known, or may not exist for every system for every triad \( \{\mathbf{u}, \mathbf{w}, \mathbf{a}\} \). For example no explicit relation for \( \mathbf{b} \) is known for the Euler equations in velocity form for which \( \{\mathbf{u}, \mathbf{w}, \mathbf{a}\} \equiv \{\mathbf{u}, \mathbf{u} - \nabla p\} \).

Section [4] elaborates three examples: the Euler equations with rotation; the barotropic compressible Euler equations; and ideal MHD in Elsasser variables. Section [5] demonstrates the applicability of the quaternionic frame description to turbulence models of Lagrangian averaged velocity gradient dynamics, in which approximate constitutive relations for the pressure Hessian and auxiliary equations for the constitutive parameters are introduced.
2 Quaternions and rigid body dynamics

Rotations in rigid body mechanics has given rise to a rich and long-standing literature in which Whittaker’s book is a classic example [17]. This gives explicit formulae relating the Euler angles and what are called the Cayley-Klein parameters of a rotation. In fact the use of quaternions in this area is not only much more efficient but avoids the immensely complicated inter-relations that are unavoidable when Euler angle formulae are involved [18, 19].

In terms of any scalar \( p \) and any 3-vector \( q \), the quaternion \( q = [p, q] \) is defined as (Gothic fonts denote quaternions)

\[
q = [p, q] = pI - \sum_{i=1}^{3} q_i \sigma_i ,
\]

where \( \{\sigma_1, \sigma_2, \sigma_3\} \) are the three Pauli spin-matrices defined by

\[
\sigma_1 = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix},
\]

and \( I \) is the \( 2 \times 2 \) unit matrix. The relations between the Pauli matrices \( \sigma_i \sigma_j = -\delta_{ij} I - \epsilon_{ijk} \sigma_k \)

then give a non-commutative multiplication rule

\[
q_1 \odot q_2 = [p_1 p_2 - q_1 \cdot q_2, p_1 q_2 + p_2 q_1 + q_1 \times q_2].
\]

It can easily be demonstrated that quaternions are associative.

Let \( \hat{p} = [p, q] \) be a unit quaternion with inverse \( \hat{p}^* = [p, -q] \); this requires \( \hat{p} \odot \hat{p}^* = [p^2 + q^2, 0] = [1, 0] \) for which we need \( p^2 + q^2 = 1 \). For a pure quaternion \( r = [0, r] \) there exists a transformation from \( r = [0, R] \rightarrow R = [0, \mathcal{R}] \)

\[
\mathcal{R} = \hat{p} \odot r \odot \hat{p}^*.
\]

This associative product can explicitly be written as

\[
\mathcal{R} = \hat{p} \odot r \odot \hat{p}^* = [0, (p^2 - q^2)r + 2p(q \times r) + 2q(r \cdot q)].
\]

Choosing \( p = \pm \cos \frac{\theta}{2} \) and \( q = \pm \hat{n} \sin \frac{\theta}{2} \), where \( \hat{n} \) is the unit normal to \( r \), we find that

\[
\mathcal{R} = \hat{p} \odot r \odot \hat{p}^* = [0, r \cos \theta + (\hat{n} \times r) \sin \theta] \equiv O(\theta, \hat{n})r ,
\]

where

\[
\hat{p} = \pm[\cos \frac{\theta}{2}, \hat{n} \sin \frac{\theta}{2}].
\]

Equation (2.6) is the famous Euler-Rodrigues formula for the rotation \( O(\theta, \hat{n}) \) by an angle \( \theta \) of the 3-vector \( r \) about its normal \( \hat{n} \); the quantities \( \theta, \hat{n} \) are called the Euler parameters. The elements of the unit quaternion \( \hat{p} \) are the Cayley-Klein parameters\(^1\) which are related to the Euler angles [17].

**Lemma 1** The unit quaternions form a representation of the Lie group \( SU(2) \).

\(^1\)The Cayley-Klein parameters of the quaternion \( q = [\alpha, \chi] \) of \( \mathbb{C}^3 \) are given by

\[
\hat{q} = \left[ \frac{\alpha}{\alpha^2 + \chi^2}, \frac{\chi}{\alpha^2 + \chi^2} \right].
\]
Proof: From (2.1), the matrix representation of a unit quaternion is

\[ J = p I - i q \cdot \sigma = \begin{pmatrix} p - i q_3 & -i q_1 - q_2 \\ -i q_1 + q_2 & p + i q_3 \end{pmatrix} \] (2.8)

where \( J \in SU(2) \); that is, \( J \) is a unitary \( 2 \times 2 \) matrix with unit determinant. Hence, we may rewrite the map (2.4) for quaternionic conjugation equivalently in terms of the Hermitian Pauli spin matrices as

\[ R \cdot \sigma = J r \cdot \sigma J^\dagger \] (2.9)

This is the standard representation of \( SO(3) \) rotations as a double covering (\( \pm J \)) by \( SU(2) \) matrices, which is now seen to be equivalent to quaternionic multiplication: for more discussion of this theorem see a modern treatise on mechanics such as [20]. The (\( \pm \)) in the Cayley-Klein parameters reflects the 2:1 covering of the map \( SU(2) \rightarrow SO(3) \).

To investigate the map (2.4) when \( \hat{p} \) is time-dependent, the Euler-Rodrigues formula in (2.6) can be written as

\[ \mathcal{R}(t) = \hat{p} \otimes r \otimes \hat{p}^* = \hat{p} \otimes \mathcal{R}(t) \otimes \hat{p}. \] (2.10)

Thus \( \mathcal{R} \) has a time derivative given by

\[
\begin{align*}
\dot{\mathcal{R}}(t) &= \dot{\hat{p}} \otimes (\hat{p}^* \otimes \mathcal{R} \otimes \hat{p}) \otimes \hat{p}^* + \hat{p} \otimes (\hat{p}^* \otimes \mathcal{R} \otimes \hat{p}) \otimes \dot{\hat{p}}^* \\
&= \dot{\hat{p}} \otimes \hat{p}^* \otimes \mathcal{R} + \mathcal{R} \otimes \dot{\hat{p}} \otimes \hat{p}^* \\
&= (\dot{\hat{p}} \otimes \hat{p}^*) \otimes \mathcal{R} + \mathcal{R} \otimes (\dot{\hat{p}} \otimes \hat{p}^*)^* \\
&= (\dot{\hat{p}} \otimes \hat{p}^*) \otimes \mathcal{R} - ((\dot{\hat{p}} \otimes \hat{p}^*) \otimes \mathcal{R})^*,
\end{align*}
\] (2.11)

having used the fact on the last line that because \( \mathcal{R} \) is a pure quaternion, \( \mathcal{R}^* = -\mathcal{R} \). Because \( \hat{p} = [p, q] \) is of unit length, and thus \( p\dot{p} + q\dot{q} = 0 \), this means that \( \hat{p} \otimes \hat{p}^* \) is also a pure quaternion

\[ \hat{p} \otimes \hat{p}^* = [0, \Omega_0(t)]. \] (2.12)

The 3-vector entry in (2.12) defines the angular frequency \( \Omega_0(t) \) as

\[ \dot{\mathcal{R}} = \Omega_0 \times \mathcal{R}. \] (2.13)

For a Lagrangian particle, the equivalent of \( \Omega_0 \) is the Darboux vector \( \mathcal{D}_a \) in Theorem 1 of \( \S 3 \).

3 Lagrangian evolution equations and the quaternion picture

3.1 An ortho-normal frame and particle trajectories

Having set the scene in \( \S 2 \) by describing some of the essential properties of quaternions, it is now time to apply them to the Lagrangian relation (1.1) between the two vectors \( w \) and \( a \) which we shall repeat here

\[ \frac{Dw}{Dt} = a. \] (3.1)

Through the multiplication rule in (2.3) quaternions appear in the decomposition of the 3-vector \( a \) into parts parallel and perpendicular to another vector, which we choose to be \( w \). This decomposition is expressed as

\[ a = \alpha_a w + \chi_a \times w = [\alpha_a, \chi_a] \otimes [0, w], \] (3.2)
where the scalar $\alpha_a$ and 3-vector $\chi_a$ are defined as
\[
\alpha_a = w^{-1}(\hat{w} \cdot a), \quad \chi_a = w^{-1}(\hat{w} \times a).
\] (3.3)

Equation (3.2) thus shows that the quaternionic product is summoned in a natural manner. It is now easily seen that $\alpha_a$ is the growth rate of the scalar magnitude ($\hat{w} = |\hat{w}|$) which obeys
\[
\frac{Dw}{Dt} = \alpha_a w,
\] (3.4)
while $\chi_a$, the swing rate of the unit tangent vector $\hat{w} = \hat{w} w^{-1}$, satisfies
\[
\frac{D\hat{w}}{Dt} = \chi_a \times \hat{w}.
\] (3.5)

Figure 1: The dotted line represents the tracer particle ($\bullet$) path moving from $(x_1, t_1)$ to $(x_2, t_2)$. The solid curves represent lines of constant $\hat{w}$ to which $\hat{w}$ is a unit tangent vector. The orientation of the quaternion-frame $(\hat{w}, \hat{\chi}_a, \hat{w} \times \hat{\chi}_a)$ is shown at the two space-time points; note that this is not the Frenet-frame corresponding to the particle path but to lines of constant $\hat{w}$.

Now define the two quaternions
\[
q_a = [\alpha_a, \chi_a], \quad w = [0, w],
\] (3.6)
where $w$ is a pure quaternion. Then (3.1) can automatically be re-written equivalently in the quaternion form
\[
\frac{Dw}{Dt} = q_a \circ w.
\] (3.7)

Moreover, if $a$ is differentiable in the Lagrangian sense (see (1.5))
\[
\frac{Da}{Dt} = b,
\] (3.8)
then, exactly as for $q_a$, a quaternion $q_b$ can be defined which is based on the variables
\[
\alpha_b = w^{-1}(\hat{w} \cdot b), \quad \chi_b = w^{-1}(\hat{w} \times b),
\] (3.9)
where
\[
q_b = [\alpha_b, \chi_b].
\] (3.10)

It is now clear that there exists a similar decomposition for $b$ as that for $a$ as in (3.2)
\[
\frac{D^2w}{Dt^2} = [0, b] = [0, \alpha_b w + \chi_b \times w] = q_b \circ w.
\] (3.11)
Using the associativity property, compatibility of (3.11) and (3.7) implies that $(w = |w| \neq 0)$

$$\left( \frac{Dq_a}{Dt} + q_a \otimes q_a - q_b \right) \otimes w = 0,$$

which establishes a Riccati relation between $q_a$ and $q_b$

$$\frac{Dq_a}{Dt} + q_a \otimes q_a = q_b,$$  \hspace{1cm} (3.13)

whose components yield

$$\frac{D}{Dt} \left[ \alpha_a, \chi_a \right] + \left[ \alpha^2_a - \chi^2_a, 2\alpha_a \chi_a \right] = \left[ \alpha_b, \chi_b \right],$$  \hspace{1cm} (3.14)

where $\chi_a = |\chi_a|$. From (3.13), or equivalently (3.14), there follows the first main result of the paper:

**Theorem 1** The ortho-normal quaternion-frame $(\hat{w}, \hat{\chi}_a, \hat{w} \times \hat{\chi}_a) \in SO(3)$ has Lagrangian time derivatives expressed as

$$\frac{D\hat{w}}{Dt} = \mathcal{D}_a \times \hat{w},$$  \hspace{1cm} (3.15)

$$\frac{D(\hat{w} \times \hat{\chi}_a)}{Dt} = \mathcal{D}_a \times (\hat{w} \times \hat{\chi}_a),$$  \hspace{1cm} (3.16)

$$\frac{D\hat{\chi}_a}{Dt} = \mathcal{D}_a \times \hat{\chi}_a,$$  \hspace{1cm} (3.17)

where the Darboux angular velocity vector $\mathcal{D}_a$ is defined as

$$\mathcal{D}_a = \chi_a + \frac{c_b}{\chi_a} \hat{w}, \quad c_b = \hat{w} \cdot (\hat{\chi}_a \times \chi_b).$$  \hspace{1cm} (3.18)

**Remark:** The Darboux vector $\mathcal{D}_a$ sits in a two-dimensional plane and is driven by the vector $b$ which sits in $c_b$ in (3.18). The analogy with rigid body rotation expressed in (2.13) is clear.

**Proof:** To find an expression for the Lagrangian time derivatives of the components of the frame $(\hat{w}, \hat{\chi}_a, \hat{w} \times \hat{\chi}_a)$ requires the derivative of $\hat{\chi}_a$. To find this it is necessary to use the fact that the 3-vector $b$ can be expressed in this ortho-normal frame as the linear combination

$$w^{-1}b = \alpha_b \hat{w} + c_b \hat{\chi}_a + d_b (\hat{w} \times \hat{\chi}_a).$$  \hspace{1cm} (3.19)

where $c_b$ is defined in (3.18) and $d_b = - (\hat{\chi}_a \cdot \chi_b)$. The 3-vector product $\chi_b = w^{-1}(\hat{w} \times b)$ yields

$$\chi_b = c_b (\hat{w} \times \hat{\chi}_a) - d_b \hat{\chi}_a.$$  \hspace{1cm} (3.20)

When split into components, equation (3.14) becomes

$$\frac{D\alpha_a}{Dt} = \chi_a^2 - \alpha_a^2 + \alpha_b$$  \hspace{1cm} (3.21)

and

$$\frac{D\chi_a}{Dt} = -2\alpha_a \chi_a + \chi_b.$$  \hspace{1cm} (3.22)

From the latter it is easily seen that

$$\frac{D\chi_a}{Dt} = -2\alpha_a \chi_a - d_b$$  \hspace{1cm} (3.23)
from which it follows
\[ \frac{D\tilde{\chi}}{Dt} = c_b\chi_a^{-1}(\tilde{\omega} \times \hat{\chi}_a), \quad \frac{D(\tilde{\omega} \times \hat{\chi}_a)}{Dt} = \chi_a \tilde{\omega} - c_b\chi_a^{-1}\hat{\chi}_a, \] (3.24)

which gives equations (3.15)-(3.18).

Theorem 1 is the main result of the paper and is the equivalent for a Lagrangian particle undergoing fluid motion of the well-known formula (2.13) for a rigid body undergoing rotation about its center of mass.

3.2 The evolution of the $b$-field in equation (3.8)

The Lagrangian rate of change of acceleration $D\alpha_a/Dt = b$ is important for tracking passive tracer particles. However, the vector $b$ cannot be calculated directly from Ertel’s Theorem in (1.5). As shown below, the Lagrangian evolution of $q_b$ appearing in the quaternionic Riccati relation (3.13) may be described without approximation in terms of three arbitrary scalars.

**Theorem 2** The Lagrangian time derivative of the quaternion $q_b$ in the Riccati relation (3.13) can be expressed as
\[ \frac{Dq_b}{Dt} = q_a \otimes q_b + \mathcal{Q}_{a,b}, \]
(3.25)
\[ \mathcal{Q}_{a,b} = \lambda_1 q_b + \lambda_2 q_a + \lambda_3 \text{Id}, \] (3.26)
where $\lambda_1(x, t)$, $\lambda_2(x, t)$, $\lambda_3(x, t)$ are arbitrary scalar functions and $\text{Id} = [1, 0]$ is the identity for the quaternions.

**Remark:** Without further constraints $\lambda_1(x, t)$, $\lambda_2(x, t)$ and $\lambda_3(x, t)$ would be arbitrary.

**Proof:** To establish (3.25), we differentiate the orthogonality relation $\chi_b \cdot \tilde{\omega} = 0$ and use the Lagrangian derivative of $\tilde{\omega}$
\[ \frac{D\chi_b}{Dt} = \chi_a \times \chi_b + s_0, \quad \text{where} \quad s_0 = \mu \chi_a + \lambda \chi_b. \] (3.27)
$s_0$ lies in the plane perpendicular to $\tilde{\omega}$ in which $\chi_a$ and $\chi_b$ also lie and $\mu = \mu(x, t)$ and $\lambda = \lambda(x, t)$ are arbitrary scalars. Explicitly differentiating $\chi_b = w^{-1}(\tilde{\omega} \times b)$ gives
\[ w^{-1}(\tilde{\omega} \cdot b) + s_0 = -\alpha_b \chi_b - \alpha_b \chi_a + w^{-1}(\tilde{\omega} \cdot b) + w^{-1} \left( \tilde{\omega} \times \frac{Db}{Dt} \right), \] (3.28)
which can easily be manipulated into
\[ \tilde{\omega} \times \left\{ \frac{Db}{Dt} - \alpha_b a - \alpha_a b \right\} = w s_0. \]
(3.29)
This means that
\[ \frac{Db}{Dt} = \alpha_b a + \alpha_a b + s_0 \times w + \varepsilon w, \]
(3.30)
where $\varepsilon = \varepsilon(x, t)$ is a third unknown scalar in addition to $\mu$ and $\lambda$ in (3.27). Thus the Lagrangian derivative of $\alpha_b = w^{-1}(\tilde{\omega} \cdot b)$ is
\[ \frac{D\alpha_b}{Dt} = \alpha_a \alpha_b + \chi_a \cdot \chi_b + \varepsilon. \]
(3.31)
Lagrangian differential relations have now been found for $\chi_b$ and $\alpha_b$, but at the price of introducing the triplet of unknown coefficients $\mu$, $\lambda$, and $\varepsilon$ which are re-defined as

$$\begin{align*}
\lambda &= \alpha_a + \lambda_1, \\
\mu &= \alpha_b + \lambda_2, \\
\varepsilon &= -2\chi_a \cdot \chi_b + \lambda_2\alpha_a + \lambda_1\alpha_b + \lambda_3.
\end{align*}$$

The new triplet has been subsumed into the tetrad defined in (3.26). Then (3.27) and (3.31) can again be written in the quaternion form (3.25).

In §5 we shall discuss an approach for determining $q_b$ by introducing an approximate constitutive relation for the pressure Hessian $P$ and auxiliary equations for the constitutive parameters.

### 3.3 Frame dynamics and the Frenet equations

![Figure 2](http://example.com/figure2.png)

**Figure 2:** The ortho-normal frame $(\hat{w}, \hat{w} \times \hat{\chi}_a, \hat{\chi}_a)$ as the Frenet-frame to lines of constant $\hat{w}$.

Modulo a rotation around the unit tangent vector $\hat{w}$, with $\hat{\chi}_a$ as the unit bi-normal $\hat{b}$ and $\hat{w} \times \hat{\chi}_a$ as the unit principal normal $\hat{n}$, the matrix $F$ can be formed

$$F = (\hat{w}^T, (\hat{w} \times \hat{\chi}_a)^T, \hat{\chi}_a^T),$$

and (3.15)–(3.17) can be re-written as

$$\frac{DF}{Dt} = AF,$$

where

$$A = \begin{pmatrix}
0 & -\chi_a & 0 \\
\chi & 0 & -c_b\chi_a^{-1} \\
0 & c_b\chi_a^{-1} & 0
\end{pmatrix}.$$

For a space curve parameterized by arc-length $s$, then the Frenet equations relating $dF/ds$ to the curvature $\kappa$ and the torsion $\tau$ of the line of constant $\hat{w}$ are

$$\frac{dF}{ds} = NF$$

where

$$N = \begin{pmatrix}
0 & \kappa & 0 \\
-\kappa & 0 & \tau \\
0 & -\tau & 0
\end{pmatrix}.$$

It is now possible to relate the $t$ and $s$ derivatives of $F$ given in (3.34) and (3.35). At any time $t$ the integral curves of the vorticity vector field define a space-curve through each point $\mathbf{x}$. The arc-length derivative $d/ds$ is defined by

$$\frac{d}{ds} = \hat{w} \cdot \nabla.$$
The evolution of the curvature $\kappa$ and torsion $\tau$ of a vortex line may be obtained from Ertel’s theorem in (1.3), expressed as the commutation of operators

\[
\left[ \frac{d}{ds}, \frac{D}{Dt} \right] = \alpha_a \frac{d}{ds}.
\]  

(3.37)

Applying this to $F$ and using the relations (3.34) and (3.35) establishes the following Theorem

**Theorem 3** The matrices $N$ and $A$ satisfy the Lax equation that relates the evolution of the curvature $\kappa$ and the torsion $\tau$ to $\alpha_a$, $\chi$ and $c_b$ defined in equations (3.2) and (3.18)

\[
\frac{DN}{Dt} - \alpha_a N = \frac{dA}{ds} + [A, N].
\]  

(3.38)

Thus, if $\chi = 0$ the curvature $\kappa$ is stationary.

### 4 Three further examples

The quaternionic formulation can be applied to other situations, such as the stretching of fluid line-elements, incompressible and compressible motion of Euler fluids and ideal MHD [21].

**(i) The Euler fluid equations for incompressible flow in a rotating frame:** The velocity form of Euler’s equations for an incompressible fluid flow in a frame rotating at frequency $\Omega$

\[
\frac{Du}{Dt} = (u \times 2\Omega) - \nabla p, \quad \text{with} \quad \text{div} \, u = 0.
\]  

(4.1)

Taking the curl yields ($\omega = \text{curl} \, u$)

\[
\frac{D\tilde{\omega}}{Dt} = \tilde{\omega} \cdot \nabla u, \quad \text{with} \quad \tilde{\omega} = \rho^{-1}(\omega + 2\Omega).
\]  

(4.2)

The triad of vectors $(u, w, a)$ in this case represents $(u, \tilde{\omega}, \tilde{\omega} \cdot \nabla u)$ with $\omega = \text{curl} \, u$ and $\text{div} \, u = 0$. Then Ertel’s theorem becomes

\[
\frac{D}{Dt}(\tilde{\omega} \cdot \nabla \mu) = \tilde{\omega} \cdot \nabla \left( \frac{D\mu}{Dt} \right).
\]  

(4.3)

Upon taking $\mu = u$ in Ertel’s theorem as in [15] and using the motion equation gives a relation in the moving frame

\[
\frac{D}{Dt}(\tilde{\omega} \cdot \nabla u) = \tilde{\omega} \cdot \nabla (u \times 2\Omega) - \nabla p
\]

\[
= -P\tilde{\omega} + \tilde{\omega} \cdot \nabla (u \times 2\Omega),
\]  

(4.4)

where $P$ is the Hessian matrix of the pressure defined by

\[
P = \frac{\partial^2 p}{\partial x_i \partial x_j}.
\]  

(4.5)

Thus (4.3) and (4.4) identify $a$ and $b$ as $a = \tilde{\omega} \cdot \nabla u$ and $b = -P\tilde{\omega} + \tilde{\omega} \cdot \nabla (u \times 2\Omega)$; the particles are now fluid packets and not passive tracer particles. The divergence-free constraint $\text{div} \, u = 0$ implies that

\[
-\Delta p = u_{i,j}u_{j,i} - \text{div} \, (u \times 2\Omega) = \text{tr} \, S^2 - \frac{i}{2}\omega^2 - \text{div} \, (u \times 2\Omega).
\]  

(4.6)
Equation (4.6) places an implicit condition upon the relation between the strain matrix $S$ and the pressure Hessian $P$ in addition to the Riccati equation (3.12). This situation has been discussed at greater length in [16] in the absence of rotation.

(ii) Euler’s equations for a barotropic compressible fluid: The pressure of a barotropic compressible fluid is a function of its mass density $\rho$, so it satisfies $\nabla \rho \times \nabla p = 0$. The velocity form of Euler’s equations for incompressible fluid motion in a frame rotating at frequency $\Omega$ is

$$
\frac{Du}{Dt} = -\frac{1}{\rho} \nabla p(\rho) =: -\nabla h(\rho),
$$

(4.7)

$$
\frac{D\rho}{Dt} + \rho \text{div } u = 0.
$$

(4.8)

Taking the curl yields

$$
\frac{D\omega_{\rho}}{Dt} = \omega_{\rho} \cdot \nabla u, \quad \text{with } \omega_{\rho} = \omega/\rho \quad \text{and } \omega = \text{curl } u.
$$

(4.9)

Then Ertel’s theorem takes the same form as above, and the second Lagrangian time derivative yields the Ohkitani relation for a barotropic compressible fluid,

$$
\frac{D^2 \omega_{\rho}}{Dt^2} = \frac{D}{Dt}(\omega_{\rho} \cdot \nabla u) = -\omega_{\rho} \cdot \nabla (\nabla h(\rho)) \equiv b,
$$

(4.10)

in terms of the Hessian of its specific enthalpy, $h(\rho)$. This has the same form as for incompressible fluids, except the acceleration term $b = -\omega_{\rho} \cdot \nabla (\nabla h(\rho))$ has its own dynamical equation. Thus, the methods in [16, 22] also apply for barotropic fluids. For isentropic compressible fluids, the situation is more complicated.

(iii) The equations of incompressible ideal MHD: These are

$$
\frac{Du}{Dt} = B \cdot \nabla B - \nabla p,
$$

(4.11)

$$
\frac{DB}{Dt} = B \cdot \nabla u,
$$

(4.12)

together with $\text{div } u = 0$ and $\text{div } B = 0$. The pressure $p$ in (4.11) is $p = p_f + \frac{1}{2} B^2$ where $p_f$ is the fluid pressure. Elsasser variables are defined by the combination

$$
v^\pm = u \pm B.
$$

(4.13)

The existence of two velocities $v^\pm$ means that there are two material derivatives

$$
\frac{D^\pm}{Dt} = \frac{\partial}{\partial t} + v^\pm \cdot \nabla.
$$

(4.14)

In terms of these, (4.11) and (4.12) can be rewritten as

$$
\frac{D^\pm v^\mp}{Dt} = -\nabla p,
$$

(4.15)

with the magnetic field $B$ satisfying (div $v^\pm = 0$)

$$
\frac{D^\pm B}{Dt} = B \cdot \nabla v^\pm.
$$

(4.16)
Thus we have a pair of triads \((v^\pm, B, a^\pm)\) with \(a^\pm = B \cdot \nabla v^\pm\), based on Moffatt’s identification of the \(B\)-field as the important stretching element \[13\]. From \[16, 22\] we also have

\[
\frac{D^\pm a^\pm}{Dt} = -PB,
\]

where \(b^\pm = -PB\). With two quartets \((v^\pm, B, a^\pm, b)\), the results of Section 2 follow, with two Lagrangian derivatives and two Riccati equations

\[
\frac{D^\pm q_i}{Dt} + q_i^\pm \otimes q_i^\mp = q_b.
\]

5 Approximate constitutive relations for the pressure Hessian

In this section, we discuss an approach for determining \(q_b\) by introducing an approximate constitutive relation for the pressure Hessian \(P\) in the Euler equations and auxiliary equations for these constitutive parameters. Recall Euler’s familiar equations for an incompressible fluid flow with velocity \(u\), written as

\[
\frac{Du}{Dt} = -\nabla p, \quad \text{with} \quad \text{div}\, u = 0.
\]

Taking the gradient yields the matrix Riccati equation

\[
\frac{DM}{Dt} + P + M^2 = 0,
\]

where the velocity gradient tensor \(M = \nabla u\) has Cartesian components \(M_{ij} = \partial u_j/\partial x^i = u_{j,i}\) and the (symmetric) pressure Hessian \(P = \nabla \nabla p\) has Cartesian components \(P_{ij} = \partial^2 p/\partial x^i \partial x^j\).

Because of the incompressibility condition \(\text{div}\, u = 0\), the trace of the velocity gradient tensor \(\text{tr}\, M\) vanishes, thereby requiring \(\text{tr}\, P = -\text{tr}\, (M^2)\), which is a Poisson equation for the pressure. For laminar flow in a bounded domain, the Poisson equation determines both the pressure in the exact Euler equations and its Hessian appearing in the velocity gradient equations \[5.2\].

However, in turbulent flows, modern diagnostics for both numerical simulations and fluid measurements make extensive use of average values of the velocity gradients moving in a coarse-grained volume element following the mean flow \[23\]. The process of averaging following a fluid parcel is called Lagrangian averaging. By its definition, Lagrangian averaging commutes
with the material derivative, but with not the spatial gradient. In contrast, Eulerian averaging does the opposite. With its two Eulerian spatial gradients, the Lagrangian averaged Hessian is a challenging object to compute. Several attempts have been made to model the Lagrangian averaged pressure Hessian in \([5.2]\) by introducing a constitutive closure for it. This idea goes back to Léorat \([24]\), Vieillefosse \([25]\) and Cantwell \([26]\) who assumed that the Eulerian pressure Hessian \(P\) is isotropic; see also \([27, 28]\). This assumption results in the restricted Euler equations \([5.1]\) and \([5.2]\) with
\[
P = -\frac{\text{Id}}{3} \text{tr} (M^2),
\]
where \(\text{Id}_{ab} = \delta_{ab}\) and \(\text{tr} (\text{Id}) = 3\) in three dimensions, so that taking the trace satisfies the relation required for incompressibility \([30]\). Conversely, one may assume that the Lagrangian pressure Hessian is isotropic. The latter assumption underlies the mean flow features of the tetrad model of Chertkov, Pumir and Shraiman \([31]\); see Chevillard and Meneveau \([32]\) for a recent review of this approach and results on its use in turbulence diagnostics.

A more general model that encompasses the mean flow features of both the restricted Euler equations and the tetrad model emerges from the transformation properties of the pressure Hessian under the Lagrangian flow map. The pressure Hessian transforms from Eulerian to Lagrangian coordinates by the flow map \(\phi_t : X \to x(t)\) in which \(x(t)\) denotes the present position of a certain fluid particle, at time \(t\), that started initially at position \(X = x(0)\) at time \(t = 0\). This flow map preserves volume. Consequently, it is invertible and its Jacobian, the deformation gradient tensor, \(D^i_A(X, t) = \partial x^i / \partial X^A\) has unit determinant \(\det(D) = 1\). If it were frozen into the flow, the pressure Hessian would transform under the flow map as
\[
\frac{\partial^2 p(t)}{\partial x^i \partial x^j} dx^i(t) \otimes dx^j(t) = \phi_t \circ \left( \frac{\partial^2 p(0)}{\partial X^A \partial X^B} dX^A \otimes dX^B \right).
\]
This is the way that a Riemannian metric \(G\) transforms under a time-dependent change of spatial coordinates. Namely, the transformation of a Riemannian metric gives the evolving quantity \(G(t)\) in terms of the reference metric \(G(0)\) and the change of basis governed by the evolution of Jacobian matrix \((D^{-1})_A^i(t) = \partial X^A / \partial x^i\) of the inverse flow map in tensor index notation as
\[
G_{ij}(t) = G_{AB}(0) (D^{-1})^A_i(t)(D^{-1})^B_j(t).
\]
In short, a Riemannian metric in the Lagrangian reference configuration transforms under the flow map \(\phi_t\) as
\[
G(t) = D^{-1}(t) G(0) D^{-1}(t),
\]
where the material time derivative of \(D^{-1}(t)dx(t) = dx(0)\) determines the evolution of \(D^{-1}(t)\).

For the pressure Hessian to transform as a Riemannian metric and also to satisfy the Poisson equation for its trace, it must take the following algebraic form
\[
P = -\frac{G}{\text{tr} G} \text{tr} (M^2).
\]
Setting \(G(t) = \text{Id}\) recovers the restricted Euler equations of \([25, 26]\), while setting \(G(0) = \text{Id}\) reformulates the mean flow part of the tetrad model \([31]\).

\(^{2}\)The metric \(G(t)\) is called the Finger tensor in nonlinear elasticity. For its history and a modern application of the Finger tensor, see \([33, 34, 29]\).
In fact, the Poisson equation for pressure is satisfied for any choice of the nonsingular symmetric matrix $G = G^T$ in equation (5.7) for the Hessian. Moreover, it may even be satisfied by choosing a linear combination of symmetric matrices in the form

$$P = - \left[ \sum_{\beta=1}^{N} c_\beta \frac{G_\beta}{\text{tr} G_\beta} \right] \text{tr} (M^2), \quad \text{with} \quad \sum_{\beta=1}^{N} c_\beta = 1,$$

(5.8)

so long as an evolutionary flow law is provided for each of the symmetric tensors $G_\beta = G_\beta^T$ with $\beta = 1, \ldots, N$. Any choice of these flow laws would also determine the evolution of the driving term $q_b$ in the Riccati equation (3.13).

6 Conclusions

The review of rigid body rotations in §2 shows that, if handled properly, quaternions have a computational advantage over Euler angle formulations. For example, the Euler-Rodrigues formula (2.6) arises from a simple multiplication of quaternions. When this approach is applied to Lagrangian evolution equations, as in §3, it demonstrates that quaternions are a natural and efficient way of calculating the orientation and angular velocity of Lagrangian particles in motion through the introduction of the concept of ortho-normal quaternion-frames travelling with each particle. For any problem in this class, knowledge of the quartet of 3-vectors $(u, w, a, b)$ is sufficient for the application of Theorem 1, which is the paper’s main result. The complexity of the various versions of the 3D Euler equations comes through the ortho-normal dynamics via the pressure field which is itself coupled back through $\Delta p = -u_{i,j}u_{j,i}$. This has been discussed more fully in [35, 36]. Adaptations of these ideas when more physics is added to the Euler equations has been discussed in section §4. For the 3D Euler equations the pressure affects the coefficient $c_b$ in the Darboux vector $D_{ab}$ of Theorem 1 through the pressure Hessian $P$. The pressure Hessian also figures prominently in Lagrangian averaged models of velocity gradient dynamics in turbulence. These models employ approximate constitutive relations for the pressure Hessian. The potential applicability of the present quaternionic frame description in these Lagrangian averaged turbulence models was demonstrated in §5.

It is also possible that the general formulation could be modified to include viscous effects, particularly if experimental data becomes available in a quaternionic format: the reader is referred to the review [37] and also to [38]. While the current formulation depends only on $\hat{\omega}$ and not $\nabla \hat{\omega}$, the latter dependence could not be avoided if viscosity were included. An equivalent formulation for the compressible Euler equations ([39, 40]) may give a clue to the nature of the incompressible limit.

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