Lagrangian particle paths & ortho-normal quaternion frames

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Abstract

New optical methods now allow experimentalists to track the trajectories of Lagrangian tracer particles in fluid flows at high Reynolds numbers. Independently, quaternions are used in the aerospace and computer graphics industries to track the paths of objects undergoing three-axis rotations. It is shown here that quaternions are a natural way of selecting an appropriate ortho-normal quaternion-frame (not the Frenet-frame) for a Lagrangian particle and of obtaining the equations for its dynamics. The method is applicable to a wide range of Lagrangian flows.

1 Introduction

Hamilton discovered the multiplication rule for quaternions on 16th October, 1843, as a composition rule for orienting his telescope, which had four cranks. This feature – that multiplication of quaternions represents compositions of rotations – has made them the technical foundation of modern inertial guidance systems in the aerospace industry where tracking the paths of moving rotating satellites and aircraft is of paramount importance (Kuipers 1999). 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 (Hanson 2006).

Given the utility of quaternions in tracking the paths of rotating objects one might ask whether they would also be useful in tracking Lagrangian particles in fluid dynamical situations. Recently by using optical methods developed for tracking particles created in cosmic ray bursts, experiments in turbulent flows have developed to the stage where the trajectories of tracer particles can be detected at high Reynolds numbers (Voth *et al.* 2002); see Figure 1 in [La Porta *et al.* (2001)]. 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 (Hanson 2006). In navigational language, this represents the corkscrew-like pitch, yaw and roll of the motion. 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 particle, designated the *quaternion-frame*. Quaternion-frames may be envisioned as moving with the Lagrangian particles, but their evolution derives from the Eulerian equations of motion.

Suppose $\boldsymbol{w}$ is a contravariant vector quantity attached to a tracer particle following the flow along characteristic paths $d\boldsymbol{x}/dt = \boldsymbol{u}(\boldsymbol{x}, t)$ of a velocity $\boldsymbol{u}$. Being contravariant, the components of $\boldsymbol{w}$ evolve under the coordinate transformation $\boldsymbol{x}(0) \to \boldsymbol{x}(t)$ along the characteristic path by the change of coordinates rule

$$\boldsymbol{w}(t) \cdot \frac{\partial}{\partial \boldsymbol{x}(t)} = \boldsymbol{w}(0) \cdot \frac{\partial}{\partial \boldsymbol{x}(0)} \,. \tag{1.1}$$

That is, the vector field $\boldsymbol{w} \cdot \boldsymbol{\nabla}$ keeps its value (is preserved) along the characteristics of the flow of the velocity vector $\boldsymbol{u}$ (which is also contravariant). Since it keeps its value, the Lagrangian rate of change of $\boldsymbol{w} \cdot \boldsymbol{\nabla}$ must vanish, so that

$$\frac{d}{dt}\left(\boldsymbol{w}(\boldsymbol{x}(t), t) \cdot \frac{\partial}{\partial \boldsymbol{x}(t)}\right) = 0\,, \quad \text{along} \quad \frac{d\boldsymbol{x}}{dt} = \boldsymbol{u}(\boldsymbol{x},\, t)\,. \tag{1.2}$$

Upon expansion of the derivative, this takes the Eulerian form,

$$\frac{D\boldsymbol{w}}{Dt} - \boldsymbol{w} \cdot \boldsymbol{\nabla}\boldsymbol{u} = 0 \quad \text{with} \quad \frac{D}{Dt} = \frac{\partial}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla}\,. \tag{1.3}$$

As a physical example of this process, consider the case when $\boldsymbol{w}$ is a stretching line-element $\boldsymbol{w} = \boldsymbol{\ell}$ transported passively in the flow of a prescribed velocity $\boldsymbol{u}(\boldsymbol{x},\, t)$, as discussed in [Batchelor (2000)]. As another physical example, $\boldsymbol{w} = \boldsymbol{B}$ may be the frozen-in magnetic field in the kinematic dynamo equation, which again takes the form in (1.3).

Given (1.2), it follows from Ertel's Theorem (Ertel 1942) that

$$\frac{D(\boldsymbol{w} \cdot \boldsymbol{\nabla}\boldsymbol{\theta})}{Dt} = \boldsymbol{w} \cdot \nabla \left(\frac{D\boldsymbol{\theta}}{Dt}\right)\,, \tag{1.4}$$

for any differentiable function $\boldsymbol{\theta}(\boldsymbol{x},\, t)$. In particular, we may choose $\boldsymbol{\theta} = \boldsymbol{u}$ and identify $D\boldsymbol{u}/Dt = \boldsymbol{Q}(\boldsymbol{x},\, t)$ as the prescribed acceleration. In this case, we find

$$\frac{D\boldsymbol{w}}{Dt} = \boldsymbol{w} \cdot \boldsymbol{\nabla}\boldsymbol{u}\,, \tag{1.5}$$

and

$$\frac{D^2\boldsymbol{w}}{Dt^2} = \frac{D(\boldsymbol{w} \cdot \nabla\boldsymbol{u})}{Dt} = \boldsymbol{w} \cdot \boldsymbol{\nabla}\left(\frac{D\boldsymbol{u}}{Dt}\right) =: \boldsymbol{w} \cdot \boldsymbol{\nabla}\boldsymbol{Q}\,, \tag{1.6}$$

with prescribed flow and acceleration $\boldsymbol{u}(\boldsymbol{x},\, t)$ and $\boldsymbol{Q}(\boldsymbol{x},\, t)$.

In what follows, we will develop a quaternionic picture of this process of Lagrangian flow and acceleration. Thus, we consider the abstract Lagrangian flow equation,

$$\frac{D\boldsymbol{w}}{Dt} = \boldsymbol{a}(\boldsymbol{x},\, t)\,, \tag{1.7}$$

whose Lagrangian acceleration equation is given by

$$\frac{D^2\boldsymbol{w}}{Dt^2} = \frac{D\boldsymbol{a}}{Dt} = \boldsymbol{b}(\boldsymbol{x},\, t)\,. \tag{1.8}$$

So far, these are just kinematic rates of change following the characteristics of the velocity generating the path $\boldsymbol{x}(t)$ determined from $d\boldsymbol{x}/dt = \boldsymbol{u}(\boldsymbol{x},\, t)$.

Section 2 will show that the quartet of vectors $(\boldsymbol{u},\, \boldsymbol{w},\, \boldsymbol{a},\, \boldsymbol{b})$ determines the quaternion-frame and its Lagrangian dynamics. Modulo a rotation around $\boldsymbol{w}$, the quaternion-frame turns out to be the Frenet-frame attached to lines of constant $\boldsymbol{w}$. If the particles are not passive tracers but are fluid parcels, the individual elements in the triad $(\boldsymbol{u},\, \boldsymbol{w},\, \boldsymbol{a})$ may not be independent; for instance, for the three-dimensional incompressible Euler equations in vorticity form, we have

$(\boldsymbol{u},\,\boldsymbol{w},\,\boldsymbol{a}) \equiv (\boldsymbol{u},\,\boldsymbol{\omega},\,\boldsymbol{\omega}\cdot\boldsymbol{\nabla u})$ with the vorticity $\boldsymbol{\omega} = \mathrm{curl}\,\boldsymbol{u}$ and $\mathrm{div}\,\boldsymbol{u} = 0$. As described in Ohkitani (1993) – see also Gibbon *et al.* (2006) for a history – in this case Ertel's Theorem for Euler's fluid equations ensures that $\boldsymbol{b}$ exists and takes the form $\boldsymbol{b} = -P\boldsymbol{\omega}$ where P is the Hessian matrix of spatial derivatives of the pressure. Because $\hat{\boldsymbol{w}} = \hat{\boldsymbol{\omega}}$ in this case, lines of constant $\boldsymbol{w}$ are vortex lines. Modulo a rotation around $\hat{\boldsymbol{\omega}}$, the quaternion-frame is then the Frenet-frame for these vortex lines. Examples such as Euler's equations for a rotating incompressible fluid, for a barotropic fluid and for ideal MHD are examples where the above conditions are fulfilled; these are outlined in Section 3. In some practical situations, however, the vector $\boldsymbol{b}$ may not exist for every system for every triad $(\boldsymbol{u},\,\boldsymbol{w},\,\boldsymbol{a})$. For example no $\boldsymbol{b}$ is known for the Euler equations in velocity form for which $(\boldsymbol{u},\,\boldsymbol{w},\,\boldsymbol{a}) \equiv (\boldsymbol{u},\,\boldsymbol{u},\,-\boldsymbol{\nabla}p)$.

The quaternion picture: Three-axis rotations lie at the heart of the definition of a quaternion. In terms of any scalar[1] p and any 3-vector $\boldsymbol{q}$, the quaternion $\mathfrak{q} = [p,\,\boldsymbol{q}]$ is defined as (Gothic fonts denote quaternions)

$$\mathfrak{q} = [p,\,\boldsymbol{q}] = pI - \sum_{i=1}^{3} q_i\sigma_i\,, \tag{1.9}$$

where $\{\sigma_1,\,\sigma_2,\,\sigma_3\}$ are the three Pauli spin-matrices and I is the 2×2 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

$$\mathfrak{q}_1 \circledast \mathfrak{q}_2 = [p_1p_2 - \boldsymbol{q}_1\cdot\boldsymbol{q}_2,\; p_1\boldsymbol{q}_2 + p_2\boldsymbol{q}_1 + \boldsymbol{q}_1\times\boldsymbol{q}_2]\,. \tag{1.10}$$

It can easily be demonstrated that quaternions are associative. As will be recalled in Section 4 the individual elements of a unit quaternion provide the Cayley-Klein parameters of a rotation. This representation is a standard alternative to using Euler angles in describing the orientation of rotating objects (Whittaker 1944).

2 Lagrangian evolution equations in quaternionic form

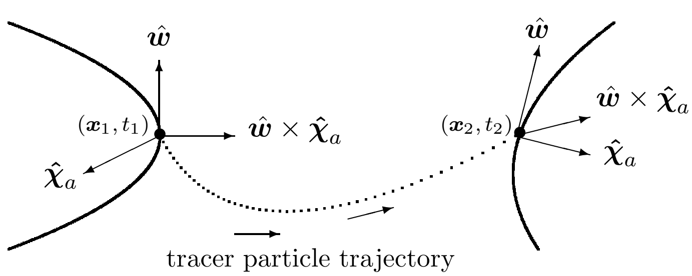

Figure 1: The dotted line represents the tracer particle ($\bullet$) path moving from $(\boldsymbol{x}_1, t_1)$ to $(\boldsymbol{x}_2, t_2)$. The solid curves represent lines of constant $\boldsymbol{w}$ to which $\hat{\boldsymbol{w}}$ is a unit tangent vector. The orientation of the quaternion-frame $(\hat{\boldsymbol{w}}, \hat{\boldsymbol{\chi}}_a,\; \hat{\boldsymbol{w}}\times\hat{\boldsymbol{\chi}}_a)$ 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 $\boldsymbol{w}$.

Given the Lagrangian equation (1.7), define the scalar α_a and the 3-vector $\boldsymbol{\chi}_a$ as

$$\alpha_a = w^{-1}(\hat{\boldsymbol{w}}\cdot\boldsymbol{a})\,, \qquad\qquad \boldsymbol{\chi}_a = w^{-1}(\hat{\boldsymbol{w}}\times\boldsymbol{a})\,. \tag{2.1}$$

The 3-vector $\boldsymbol{a}$ can be decomposed into parts that are parallel and perpendicular to $\boldsymbol{w}$

$$\boldsymbol{a} = \alpha_a\boldsymbol{w} + \boldsymbol{\chi}_a\times\boldsymbol{w} = [\alpha_a,\,\boldsymbol{\chi}_a] \circledast [0,\,\boldsymbol{w}]\,, \tag{2.2}$$

[1]The scalar entry p in the quaternion $\mathfrak{q}$ should not be confused with pressure.

and thus the quaternionic product is summoned in a natural manner. By definition, the growth rate α_a of the scalar magnitude $w = |\boldsymbol{w}|$ obeys

$$\frac{Dw}{Dt} = \alpha_a w\,, \tag{2.3}$$

while the unit tangent vector $\hat{\boldsymbol{w}} = \boldsymbol{w}w^{-1}$ satisfies

$$\frac{D\hat{\boldsymbol{w}}}{Dt} = \boldsymbol{\chi}_a \times \hat{\boldsymbol{w}}\,. \tag{2.4}$$

Now identify the quaternions

$$\mathfrak{q}_a = [\alpha_a,\, \boldsymbol{\chi}_a]\,, \qquad\qquad \mathfrak{q}_b = [\alpha_b,\, \boldsymbol{\chi}_b]\,, \tag{2.5}$$

where $\alpha_b,\ \boldsymbol{\chi}_b$ are defined as in (2.1) for $\alpha_a,\ \boldsymbol{\chi}_a$ with $\boldsymbol{a}$ replaced by $\boldsymbol{b}$. Let $\mathfrak{w} = [0,\, \boldsymbol{w}]$ be the pure quaternion satisfying the Lagrangian evolution equation (1.7) with $\mathfrak{q}_a$ defined in (2.5). Then (1.7) can automatically be re-written equivalently in the quaternion form

$$\frac{D\mathfrak{w}}{Dt} = [0,\, \boldsymbol{a}] = [0,\, \alpha_a\boldsymbol{w} + \boldsymbol{\chi}_a \times \boldsymbol{w}] = \mathfrak{q}_a \circledast \mathfrak{w}\,. \tag{2.6}$$

Moreover, if $\boldsymbol{a}$ is differentiable in the Lagrangian sense as in (1.8) then it is clear that a similar decomposition for $\boldsymbol{b}$ as that for $\boldsymbol{a}$ in (2.2) gives

$$\frac{D^2\mathfrak{w}}{Dt^2} = [0,\, \boldsymbol{b}] = [0,\, \alpha_b\boldsymbol{w} + \boldsymbol{\chi}_b \times \boldsymbol{w}] = \mathfrak{q}_b \circledast \mathfrak{w}\,. \tag{2.7}$$

Using the associativity property, compatibility of (2.7) and (2.6) implies that

$$\left(\frac{D\mathfrak{q}_a}{Dt} + \mathfrak{q}_a \circledast \mathfrak{q}_a - \mathfrak{q}_b\right) \circledast \mathfrak{w} = 0\,, \tag{2.8}$$

which establishes a *Riccati relation* between $\mathfrak{q}_a$ and $\mathfrak{q}_b$

$$\frac{D\mathfrak{q}_a}{Dt} + \mathfrak{q}_a \circledast \mathfrak{q}_a = \mathfrak{q}_b\,. \tag{2.9}$$

From (2.9) there follows the main result of the paper:

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

$$\frac{D\hat{\boldsymbol{w}}}{Dt} = \boldsymbol{\mathcal{D}}_a \times \hat{\boldsymbol{w}}\,, \tag{2.10}$$

$$\frac{D(\hat{\boldsymbol{w}} \times \hat{\boldsymbol{\chi}}_a)}{Dt} = \boldsymbol{\mathcal{D}}_a \times (\hat{\boldsymbol{w}} \times \hat{\boldsymbol{\chi}}_a)\,, \tag{2.11}$$

$$\frac{D\hat{\boldsymbol{\chi}}_a}{Dt} = \boldsymbol{\mathcal{D}}_a \times \hat{\boldsymbol{\chi}}_a\,, \tag{2.12}$$

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

$$\boldsymbol{\mathcal{D}}_a = \boldsymbol{\chi}_a + \frac{c_b}{\chi_a}\hat{\boldsymbol{w}}\,, \qquad\qquad c_b = \hat{\boldsymbol{w}} \cdot (\hat{\boldsymbol{\chi}}_a \times \boldsymbol{\chi}_b)\,. \tag{2.13}$$

Moreover, the Lagrangian time derivative of $\mathfrak{q}_b$ *can be expressed as*

$$\frac{D\mathfrak{q}_b}{Dt} = \mathfrak{q}_a \circledast \mathfrak{q}_b + \mathfrak{P}_{a,b}\,, \tag{2.14}$$

$$\mathfrak{P}_{a,b} = \mu_1\mathfrak{q}_a + \lambda_1\mathfrak{q}_b + \varepsilon_1\mathbb{I}\,, \tag{2.15}$$

where $\mu_1(\boldsymbol{x},\, t)$, $\lambda_1(\boldsymbol{x},\, t)$ *and* $\varepsilon_1(\boldsymbol{x},\, t)$ *are arbitrary scalars* ($\mathbb{I} = [1,\, 0]$).

Remark 1: The frame orientation is controlled by the Darboux vector $\boldsymbol{\mathcal{D}}_a$ which itself sits in a two-dimensional plane. In turn this is driven by $c_b = \hat{\boldsymbol{w}} \cdot (\hat{\boldsymbol{\chi}}_a \times \boldsymbol{\chi}_b)$ in (2.13).

Remark 2: The existence of the Lagrangian derivative of $\mathfrak{q}_b$ is unusual but comes at a price through the necessary introduction of the three arbitrary scalars $\mu_1\,, \lambda_1$ and ε_1.

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

$$w^{-1}\boldsymbol{b} = \alpha_b\,\hat{\boldsymbol{w}} + c_b\hat{\boldsymbol{\chi}}_a + d_b(\hat{\boldsymbol{w}} \times \hat{\boldsymbol{\chi}}_a)\,. \tag{2.16}$$

where c_b is defined in (2.13) and $d_b = -\,(\hat{\boldsymbol{\chi}}_a \cdot \boldsymbol{\chi}_b)$. The 3-vector product $\boldsymbol{\chi}_b = w^{-1}(\hat{\boldsymbol{w}} \times \boldsymbol{b})$ yields

$$\boldsymbol{\chi}_b = c_b(\hat{\boldsymbol{w}} \times \hat{\boldsymbol{\chi}}_a) - d_b\hat{\boldsymbol{\chi}}_a\,. \tag{2.17}$$

To find the Lagrangian time derivative of $\hat{\boldsymbol{\chi}}_a$, we use the 3-vector part of the equation for the quaternion $\mathfrak{q}_a = [\alpha_a,\, \boldsymbol{\chi}_a]$ in Theorem 1

$$\frac{D\boldsymbol{\chi}_a}{Dt} = -2\alpha_a\boldsymbol{\chi}_a + \boldsymbol{\chi}_b\,, \qquad \Rightarrow \qquad \frac{D\chi_a}{Dt} = -2\alpha_a\chi_a - d_b\,, \tag{2.18}$$

where $\chi_a = |\boldsymbol{\chi}_a|$. Using (2.17) and (2.18) there follows

$$\frac{D\hat{\boldsymbol{\chi}}_a}{Dt} = c_b\chi_a^{-1}(\hat{\boldsymbol{w}} \times \hat{\boldsymbol{\chi}}_a)\,, \qquad \frac{D(\hat{\boldsymbol{w}} \times \hat{\boldsymbol{\chi}}_a)}{Dt} = \chi_a\,\hat{\boldsymbol{w}} - c_b\chi_a^{-1}\hat{\boldsymbol{\chi}}_a\,, \tag{2.19}$$

which gives equations (2.10)-(2.13).

To establish (2.14), we differentiate the orthogonality relation $\boldsymbol{\chi}_b \cdot \hat{\boldsymbol{w}} = 0$ and use the Lagrangian derivative of $\hat{\boldsymbol{w}}$

$$\frac{D\boldsymbol{\chi}_b}{Dt} = \boldsymbol{\chi}_a \times \boldsymbol{\chi}_b + \boldsymbol{s}_0\,, \qquad \text{where} \qquad \boldsymbol{s}_0 = \mu\boldsymbol{\chi}_a + \lambda\,\boldsymbol{\chi}_b\,. \tag{2.20}$$

$\boldsymbol{s}_0$ lies in the plane perpendicular to $\hat{\boldsymbol{w}}$ in which $\boldsymbol{\chi}_a$ and $\boldsymbol{\chi}_b$ also lie and $\mu = \mu(\boldsymbol{x}, t)$ and $\lambda = \lambda(\boldsymbol{x}, t)$ are arbitrary scalars. Explicitly differentiating $\boldsymbol{\chi}_b = w^{-1}(\hat{\boldsymbol{w}} \times \boldsymbol{b})$ gives

$$w^{-1}\hat{\boldsymbol{w}}\,(\boldsymbol{\chi}_a \cdot \boldsymbol{b}) + \boldsymbol{s}_0 = -\alpha_a\boldsymbol{\chi}_b - \alpha_b\boldsymbol{\chi}_a + w^{-1}\hat{\boldsymbol{w}}\,(\boldsymbol{\chi}_a \cdot \boldsymbol{b}) + w^{-1}\left(\hat{\boldsymbol{w}} \times \frac{D\boldsymbol{b}}{Dt}\right)\,, \tag{2.21}$$

which can easily be manipulated into

$$\hat{\boldsymbol{w}} \times \left\{\frac{D\boldsymbol{b}}{Dt} - \alpha_b\,\boldsymbol{a} - \alpha_a\,\boldsymbol{b}\right\} = w\,\boldsymbol{s}_0\,. \tag{2.22}$$

This means that

$$\frac{D\boldsymbol{b}}{Dt} = \alpha_b\boldsymbol{a} + \alpha_a\boldsymbol{b} + \boldsymbol{s}_0 \times \boldsymbol{w} + \varepsilon\boldsymbol{w}\,, \tag{2.23}$$

where $\varepsilon = \varepsilon(\boldsymbol{x}, t)$ is a third unknown scalar in addition to μ and λ in (2.20). Thus the Lagrangian derivative of $\alpha_b = w^{-1}(\hat{\boldsymbol{w}} \cdot \boldsymbol{b})$ is

$$\frac{D\alpha_b}{Dt} = \alpha\alpha_b + \boldsymbol{\chi}_a \cdot \boldsymbol{\chi}_b + \varepsilon\,. \tag{2.24}$$

Lagrangian differential relations have now been found for $\boldsymbol{\chi}_b$ and α_b, but at the price of introducing the triplet of unknown coefficients μ, λ, and ε which are re-defined as

$$\lambda = \alpha_a + \lambda_1\,, \qquad \mu = \alpha_b + \mu_1\,, \qquad \varepsilon = -2\boldsymbol{\chi}_a \cdot \boldsymbol{\chi}_b + \mu_1\alpha_a + \lambda_1\alpha_b + \varepsilon_1\,. \tag{2.25}$$

The new triplet has been subsumed into the tetrad defined in (2.15). Then (2.20) and (2.24) can be written in the quaternion form (2.14). ∎

3 Three further examples

This 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 (Majda & Bertozzi 2001).

(i) The incompressible Euler equations in a rotating frame: The velocity form of Euler's equations for an incompressible fluid in a frame rotating at frequency $\boldsymbol{\Omega}$ is

$$\frac{D\boldsymbol{u}}{Dt} = \underbrace{(\boldsymbol{u}\times 2\boldsymbol{\Omega})}_{Coriolis} - \boldsymbol{\nabla}p\,, \quad \text{with} \quad \operatorname{div}\boldsymbol{u} = 0\,. \tag{3.1}$$

Taking the curl yields

$$\frac{D\boldsymbol{q}}{Dt} = \boldsymbol{q}\cdot\boldsymbol{\nabla}\boldsymbol{u}\,, \quad \text{with} \quad \boldsymbol{q} = \rho^{-1}(\boldsymbol{\omega} + 2\boldsymbol{\Omega}) \quad \text{and} \quad \boldsymbol{\omega} = \operatorname{curl}\boldsymbol{u} \tag{3.2}$$

Then Ertel's theorem becomes

$$\left[\frac{D}{Dt}, \boldsymbol{q}\cdot\boldsymbol{\nabla}\right]\boldsymbol{\theta} = 0\,, \quad \text{or} \quad \frac{D}{Dt}(\boldsymbol{q}\cdot\boldsymbol{\nabla}\boldsymbol{\theta}) = \boldsymbol{q}\cdot\boldsymbol{\nabla}\left(\frac{D\boldsymbol{\theta}}{Dt}\right)\,. \tag{3.3}$$

A second Lagrangian time derivative of (3.2) yields the Ohkitani relation in a rotating frame. Upon taking $\boldsymbol{\theta} = \boldsymbol{u}$ in Ertel's theorem and using the motion equation gives

$$\frac{D^2\boldsymbol{q}}{Dt^2} = \frac{D}{Dt}(\boldsymbol{q}\cdot\boldsymbol{\nabla}\boldsymbol{u}) = \boldsymbol{q}\cdot\boldsymbol{\nabla}\left(\frac{D\boldsymbol{u}}{Dt}\right) = \boldsymbol{q}\cdot\boldsymbol{\nabla}\big(\boldsymbol{u}\times 2\boldsymbol{\Omega} - \boldsymbol{\nabla}p\big)\,. \tag{3.4}$$

The triad of vectors $(\boldsymbol{u},\,\boldsymbol{w},\,\boldsymbol{a})$ in this case represents $(\boldsymbol{u},\,\boldsymbol{q},\,\boldsymbol{q}\cdot\boldsymbol{\nabla}\boldsymbol{u})$ with $\boldsymbol{\omega} = \operatorname{curl}\boldsymbol{u}$ and $\operatorname{div}\boldsymbol{u} = 0$. The particle is no longer a passive tracer but is a fluid parcel. Ertel's Theorem and the fluid motion equation in this case yields

$$\frac{D(\boldsymbol{q}\cdot\boldsymbol{\nabla}\boldsymbol{u})}{Dt} = -P\boldsymbol{q} + \boldsymbol{q}\cdot\boldsymbol{\nabla}\big(\boldsymbol{u}\times 2\boldsymbol{\Omega}\big)\,, \quad \text{with} \quad P = \frac{\partial^2 p}{\partial x_i \partial x_j}\,, \tag{3.5}$$

where P is the Hessian matrix of the pressure. Thus (3.5) identifies $\boldsymbol{a}$ and $\boldsymbol{b}$ as $\boldsymbol{a} = \boldsymbol{q}\cdot\boldsymbol{\nabla}\boldsymbol{u}$ and $\boldsymbol{b} = -P\boldsymbol{q} + \boldsymbol{q}\cdot\boldsymbol{\nabla}\big(\boldsymbol{u}\times 2\boldsymbol{\Omega}\big)$. The divergence-free constraint $\operatorname{div}\boldsymbol{u} = 0$ implies that

$$-\Delta p = u_{i,j}u_{j,i} - \operatorname{div}\big(\boldsymbol{u}\times 2\boldsymbol{\Omega}\big) = Tr\,S^2 - \tfrac{1}{2}\omega^2 - \operatorname{div}\big(\boldsymbol{u}\times 2\boldsymbol{\Omega}\big)\,. \tag{3.6}$$

Equation (3.6) places an implicit condition upon the relation between S and P in addition to the Riccati equation (2.8) and it will also place constraints upon the scalars λ_1, μ_1 and ϵ_1 in Theorem 1. This situation has been discussed at greater length in Gibbon *et al.* (2006) 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 ρ, so it satisfies $\boldsymbol{\nabla}\rho\times\boldsymbol{\nabla}p = 0$. The velocity form of Euler's equations for incompressible fluid motion in a frame rotating at frequency $\boldsymbol{\Omega}$ is

$$\frac{D\boldsymbol{u}}{Dt} = -\frac{1}{\rho}\boldsymbol{\nabla}p(\rho) =: -\boldsymbol{\nabla}h(\rho)\,, \quad \text{with} \quad \frac{D\rho}{Dt} + \rho\operatorname{div}\boldsymbol{u} = 0\,. \tag{3.7}$$

Taking the curl yields

$$\frac{D\boldsymbol{q}}{Dt} = \boldsymbol{q}\cdot\boldsymbol{\nabla}\boldsymbol{u}\,, \quad \text{with} \quad \boldsymbol{q} = \boldsymbol{\omega}/\rho \quad \text{and} \quad \boldsymbol{\omega} = \operatorname{curl}\boldsymbol{u}\,. \tag{3.8}$$

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,

$$\frac{D^2\boldsymbol{q}}{Dt^2} = \frac{D}{Dt}(\boldsymbol{q}\cdot\boldsymbol{\nabla}\boldsymbol{u}) = \boldsymbol{q}\cdot\boldsymbol{\nabla}\left(\frac{D\boldsymbol{u}}{Dt}\right) = -\,\boldsymbol{q}\cdot\boldsymbol{\nabla}\left(\boldsymbol{\nabla}h(\rho)\right)\,, \tag{3.9}$$

in terms of the Hessian of its specific enthaply, $h(\rho)$. This has the same form as for incompressible fluids, except the acceleration term $\boldsymbol{b} = -\,\boldsymbol{q}\cdot\boldsymbol{\nabla}\left(\boldsymbol{\nabla}h(\rho)\right)$ has its own dynamical equation. Thus, the methods of Gibbon *et al.* (2006) also apply for barotropic fluids. For isentropic compressible fluids, the situation is more complicated.

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

$$\frac{D\boldsymbol{u}}{Dt} = \boldsymbol{B}\cdot\boldsymbol{\nabla}\boldsymbol{B} - \boldsymbol{\nabla}p\,, \tag{3.10}$$

$$\frac{D\boldsymbol{B}}{Dt} = \boldsymbol{B}\cdot\boldsymbol{\nabla}\boldsymbol{u}\,, \tag{3.11}$$

together with $\operatorname{div}\boldsymbol{u} = 0$ and $\operatorname{div}\boldsymbol{B} = 0$. The pressure p in (3.10) is $p = p_f + \frac{1}{2}B^2$ where p_f is the fluid pressure. Elsasser variables are defined by the combination

$$\boldsymbol{v}^{\pm} = \boldsymbol{u} \pm \boldsymbol{B}\,. \tag{3.12}$$

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

$$\frac{D^{\pm}}{Dt} = \frac{\partial}{\partial t} + \boldsymbol{v}^{\pm}\cdot\boldsymbol{\nabla}\,. \tag{3.13}$$

In terms of these, (3.10) and (3.11) can be rewritten as

$$\frac{D^{\pm}\boldsymbol{v}^{\mp}}{Dt} = -\boldsymbol{\nabla}p\,, \tag{3.14}$$

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

$$\frac{D^{\pm}\boldsymbol{B}}{Dt} = \boldsymbol{B}\cdot\boldsymbol{\nabla}\boldsymbol{v}^{\pm}\,. \tag{3.15}$$

Thus we have a pair of triads ($\boldsymbol{v}^{\pm}$, $\boldsymbol{B}$, $\boldsymbol{a}^{\pm}$) with $\boldsymbol{a}^{\pm} = \boldsymbol{B}\cdot\boldsymbol{\nabla}\boldsymbol{v}^{\pm}$, based on Moffatt's (1985) identification of the $\boldsymbol{B}$-field as the important stretching element. From Gibbon (2002) and Gibbon *et al.* (2006) we also have

$$\frac{D^{\pm}\boldsymbol{a}^{\mp}}{Dt} = -P\boldsymbol{B}\,, \tag{3.16}$$

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

$$\frac{D^{\mp}\mathfrak{q}_a^{\pm}}{Dt} + \mathfrak{q}_a^{\pm}\circledast\mathfrak{q}_a^{\mp} = \mathfrak{q}_b\,. \tag{3.17}$$

In consequence, MHD-quaternion-frame dynamics needs to be interpreted in terms of two sets of ortho-normal frames $\left(\hat{\boldsymbol{B}},\,\hat{\boldsymbol{\chi}}^{\pm},\,\hat{\boldsymbol{B}}\times\hat{\boldsymbol{\chi}}^{\pm}\right)$ acted on by their opposite Lagrangian time derivatives.

$$\frac{D^{\mp}\hat{\boldsymbol{B}}}{Dt} = \boldsymbol{\mathcal{D}}^{\mp}\times\hat{\boldsymbol{B}}\,, \tag{3.18}$$

$$\frac{D^{\mp}}{Dt}(\hat{\boldsymbol{B}}\times\hat{\boldsymbol{\chi}}^{\pm}) = \boldsymbol{\mathcal{D}}^{\mp}\times(\hat{\boldsymbol{B}}\times\hat{\boldsymbol{\chi}}^{\pm})\,, \tag{3.19}$$

$$\frac{D^{\mp}\hat{\boldsymbol{\chi}}^{\pm}}{Dt} = \boldsymbol{\mathcal{D}}^{\mp}\times\hat{\boldsymbol{\chi}}^{\pm}\,, \tag{3.20}$$

where the pair of Elsasser Darboux vectors $\boldsymbol{\mathcal{D}}^{\mp}$ are defined as

$$\boldsymbol{\mathcal{D}}^{\mp} = \boldsymbol{\chi}^{\mp} - \frac{c_B^{\mp}}{\chi^{\mp}}\hat{\boldsymbol{B}}\,, \qquad\qquad c_B^{\mp} = \hat{\boldsymbol{B}}\cdot[\hat{\boldsymbol{\chi}}^{\pm}\times(\boldsymbol{\chi}_{pB}+\alpha^{\pm}\boldsymbol{\chi}^{\mp})]\,. \tag{3.21}$$

4 Quaternions and Rotations

The purpose of this paper has been to introduce the concept of ortho-normal quaternion-frames that travel with Lagrangian particles. The calculations are not complicated once the formulation has been made and show that quaternions are ideally suited to studying Lagrangian evolution equations of all types.

It is also possible that the general formulation of (1.7) and (1.8) could be modified to include viscous effects, particularly if experimental data becomes available: the reader is referred to the review by Falkovich *et al.* (2001). One advantage of the current formulation is that it is that is only dependent on $\hat{\boldsymbol{w}}$ and not $\boldsymbol{\nabla}\hat{\boldsymbol{w}}$, although this could not be avoided if viscosity were included.

It has been mentioned already in Section 1 that quaternions are used in the aerospace and computer graphics industries to avoid difficulties with Euler angles. Here we briefly sketch the relation between quaternions and one of the many ways that have been used to describe rotating bodies in the rich and long-standing literature of classical mechanics. Whittaker (1944) shows how quaternions and the *Cayley-Klein parameters* (Klein 2004) are intimately related and gives explicit formulae relating these parameters to the Euler angles.

Let $\hat{\mathfrak{q}} = [p,\,\boldsymbol{q}]$ be a unit quaternion with inverse $\hat{\mathfrak{p}}^* = [p,\,-\boldsymbol{q}]$: this requires $\hat{\mathfrak{q}}\circledast\hat{\mathfrak{q}}^* = [p^2+q^2,\,0] = [1,0]$ for which we need $p^2+q^2=1$. For a pure quaternion $\mathfrak{r} = [0,\,\boldsymbol{r}]$ there exists a transformation from $\mathfrak{r}\to\mathfrak{r}' = [0,\,\boldsymbol{r}']$

$$\mathfrak{r}' = \hat{\mathfrak{p}}\circledast\mathfrak{r}\circledast\hat{\mathfrak{p}}^*\,. \tag{4.1}$$

This associative product can explicitly be written as

$$\mathfrak{r}' = \hat{\mathfrak{q}}\circledast\mathfrak{r}\circledast\hat{\mathfrak{q}}^* = [0,\,(p^2-q^2)\boldsymbol{r} + 2p(\boldsymbol{q}\times\boldsymbol{r}) + 2\boldsymbol{q}(\boldsymbol{r}\cdot\boldsymbol{q})]\,. \tag{4.2}$$

Choosing $p = \pm\cos\frac{1}{2}\theta$ and $\boldsymbol{q} = \pm\,\hat{\boldsymbol{n}}\sin\frac{1}{2}\theta$, where $\hat{\boldsymbol{n}}$ is the unit normal to $\boldsymbol{r}$, we find that

$$\mathfrak{r}' = \hat{\mathfrak{q}}\circledast\mathfrak{r}\circledast\hat{\mathfrak{q}}^* = [0,\,\boldsymbol{r}\cos\theta + (\hat{\boldsymbol{n}}\times\boldsymbol{r})\sin\theta]\,, \tag{4.3}$$

where

$$\hat{\mathfrak{q}} = \pm[\cos\tfrac{1}{2}\theta,\,\hat{\boldsymbol{n}}\sin\tfrac{1}{2}\theta]\,. \tag{4.4}$$

Equation (4.3) represents a rotation by an angle θ of the 3-vector $\boldsymbol{r}$ about its normal $\hat{\boldsymbol{n}}$. The elements of the unit quaternion $\hat{\mathfrak{q}}$ are the Cayley-Klein parameters which are related to the Euler angles. All terms in the (4.2) are quadratic in p and $\boldsymbol{q}$, and thus possess the well-known $\pm$ equivalence.

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References

[Batchelor (2000)] BATCHELOR, G. K. 2000 *An Introduction to Fluid Dynamics*, Cambridge Mathematical Library, Cambridge University Press (Cambridge).

[Ertel (1942)] ERTEL, H. 1942 Ein Neuer Hydrodynamischer Wirbelsatz. *Met. Z.*, **59**, 271–281.

[Falkovich *et al.* (2001)] FALKOVICH, G., GAWEDZKI, K. AND VERGASSOLA, M. 2001 Particles and fields in fluid turbulence. *Rev. Mod. Phys.*, **73**, 913-975.

[Galanti *et al.* (1997)] GALANTI, B., GIBBON, J. D. & HERITAGE, M. 1997 Vorticity alignment results for the $3D$ Euler and Navier-Stokes equations. *Nonlinearity*, **10**, 1675–1695.

[Gibbon (2002)] GIBBON, J. D. 2002 A quaternionic structure in the three-dimensional Euler and ideal magneto-hydrodynamics equation. *Physica D*, **166**, 17–28.

[Gibbon *et al.* (2006)] GIBBON, J. D., HOLM, D. D., KERR, R. M. AND ROULSTONE, I. 2006 Quaternions and particle dynamics in Euler fluid flow. To appear in *Nonlinearity.* http://arxiv.org/abs/nlin.CD/0512034.

[Hanson (2006)] HANSON, ANDREW J. 2006 *Visualizing Quaternions*, Morgan Kaufmann Elsevier (London).

[Klein (2004)] KLEIN, F. 2004 *The Mathematical Theory of the Top: Lectures Delivered on the Occasion of the Sesquicentennial Celebration of Princeton University*, Dover Phoenix Edition No 2.

[Kuipers (1999)] KUIPERS, J. B. 1999 *Quaternions and rotation Sequences: a Primer with Applications to Orbits, Aerospace, and Virtual Reality*, Princeton University Press, (Princeton).

[La Porta *et al.* (2001)] LA PORTA, A., VOTH, G. A., CRAWFORD, A., ALEXANDER, J. AND BODENSCHATZ, E. 2001 Fluid particle accelerations in fully developed turbulence. *Nature*, **409**, 1017-1019.

[Majda & Bertozzi (2001)] MAJDA, A. J. & BERTOZZI, A. 2001 *Vorticity and incompressible flow.* Cambridge Texts in Applied Mathematics (No. 27), Cambridge University Press (Cambridge).

[Moffatt (1978)] MOFFATT, H. K. 1978 *Magnetic field generation by fluid motions*, Cambridge University Press (Cambridge).

[Ohkitani (1993)] OHKITANI, K. 1993 Eigenvalue problems in three-dimensional Euler flows. *Phys. Fluids A*, **5**, 2570–2572.

[Voth *et al.* (2002)] VOTH, G. A., LA PORTA, A., CRAWFORD, A., BODENSCHATZ, E. AND ALEXANDER, J. 2002 Measurement of particle accelerations in fully developed turbulence. *J. Fluid Mech.*, **469**, 121-160.

[Whittaker (1944)] WHITTAKER, E. T. 1944 *A treatise on the analytical dynamics of particles and rigid bodies*, Dover, New York.