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Quaternions and particle dynamics in the Euler fluid equations

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Abstract

Vorticity dynamics of the three-dimensional incompressible Euler equations are cast into a quaternionic representation governed by the Lagrangian evolution of the tetrad consisting of the growth rate and rotation rate of the vorticity. In turn, the Lagrangian evolution of this tetrad is governed by another that depends on the pressure Hessian. Together these form the basis for a direction of vorticity theorem on Lagrangian trajectories. Moreover, in this representation, fluid particles carry ortho-normal frames whose Lagrangian evolution in time are shown to be directly related to the Frenet–Serret equations for a vortex line. The frame dynamics suggest an elegant Lagrangian relation regarding the pressure Hessian tetrad. The equations for ideal MHD are similarly considered.

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1. Introductory and historical remarks

Hamilton's determined concentration on the idea of quaternions is often depicted by mathematical historians as an obsession. Lord Kelvin wrote that (O'Connor and Robertson 1998)

> *Quaternions came from Hamilton after his really good work had been done, and though beautifully ingenious, (they) have been an unmixed evil to those who have touched them in any way.*

Having fallen in and out of fashion over the last century and a half (Tait 1890), quaternions currently play an important part in the theory of 4-manifolds, through which it has been shown that the essential physics of particles and fields is governed by geometric principles. Fluid turbulence is one of the great unsolved problems of modern science. While viscosity plays a dominant role in the late development of an incompressible turbulent flow through the Navier–Stokes equations, the inviscid Euler equations determine the early and intermediate dynamics. The Euler fluid equations are known to be essentially geometrical, so it would not be surprising if quaternions were helpful in understanding their solutions.

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A quaternion can be constructed from a scalar s and a 3-vector $\boldsymbol{r}$ by forming the tetrad[4] $\mathfrak{q} = [s, \boldsymbol{r}]$ that is defined by

$$\mathfrak{q} = [s, \boldsymbol{r}] = sI - \boldsymbol{r}\cdot\boldsymbol{\sigma}, \tag{1.1}$$

where $\boldsymbol{r}\cdot\boldsymbol{\sigma} = \sum_{i=1}^{3} r_i\sigma_i$ and I is the 2×2 unit matrix. $\{\sigma_1, \sigma_2, \sigma_3\}$ are the Pauli spin matrices

$$\sigma_1 = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \tag{1.2}$$

that obey the relations $\sigma_i\sigma_j = -\delta_{ij}I - \epsilon_{ijk}\sigma_k$. A multiplication rule between two tetrads $\mathfrak{q}_1 = [s_1, \boldsymbol{r}_1]$ and $\mathfrak{q}_2 = [s_2, \boldsymbol{r}_2]$ can easily be determined from these properties

$$\mathfrak{q}_1 \circledast \mathfrak{q}_2 = [s_1s_2 - \boldsymbol{r}_1\cdot\boldsymbol{r}_2, s_1\boldsymbol{r}_2 + s_2\boldsymbol{r}_1 + \boldsymbol{r}_1\times\boldsymbol{r}_2]. \tag{1.3}$$

This shows that quaternions are not commutative, although their associativity is easily demonstrated. They are found to be extremely useful in modern inertial navigation systems, robotics and graphics that are specifically designed to control or track rapidly moving objects undergoing three-axis rotations (Hanson 2006, Kuipers 1999). In fact, Hamilton discovered them in the context of an algorithm for rotating the telescope in his observatory. If Kelvin were alive today, he might be forced to revise his negative opinion of their importance.

Given the evidence, it is natural to reformulate Euler vorticity dynamics in terms of quaternions, particularly in tracking a fluid particle that carries its own ortho-normal co-ordinate system. Instead of setting Euler variables in standard function spaces, in which delicate geometric information might be lost, the principal aim of this paper is to investigate the Lagrangian evolution of these variables in appropriate quaternionic form in order to preserve their inherent geometric properties. The language of quaternions thus provides us with an alternative and unique look at the problem of Euler vortex dynamics. These manipulations are not specifically dependent upon the nature of the domain $\mathbb{D}\subset\mathbb{R}^3$ but for those parts of our work where the direction of vorticity is discussed, the local existence in time of classical solutions is necessary (Kato 1972). Thus, we restrict $\mathbb{D}$ to a three-dimensional periodic domain, although other more general forms of $\mathbb{D}\subset\mathbb{R}^3$ are also valid (see Majda and Bertozzi 2001). Otherwise our manipulations should be considered to be formal, particularly since Euler data gets rough very quickly.

Three-dimensional Euler vorticity growth is driven by the stretching vector $\boldsymbol{\omega}\cdot\nabla\boldsymbol{u}$. This term plays a fundamental role in determining whether or not a singularity forms in finite time. Major computational studies can be found in Brachet *et al* (1983, 1992); Pumir and Siggia (1990); Kerr (1993, 2005); Grauer *et al* (1998), Pelz (2001) and Hou and Li (2006). The Beale–Kato–Majda theorem (Beale *et al* 1984) has been the main cornerstone of Euler analysis: one version of this theorem is the precise statement that $\int_0^t \|\boldsymbol{\omega}\|_{L^\infty(\mathbb{D})}\mathrm{d}\tau$ must be finite to prevent singular behaviour on $\mathbb{D}$. A BMO-version of this theorem has been proved by Kozono and Taniuchi (2000). However, it has become clear that not only the magnitude but also the direction of vorticity is important. The papers by Constantin (1994), Constantin *et al* (1996), Cordoba and Fefferman (2001), Deng *et al* (2005, 2006) and Chae (2003a, 2005, 2006) are variations on this theme. References and a more global perspective on the Euler equations can be found in the book by Majda and Bertozzi (2001). Shnirelman (1997) has constructed very weak solutions which have some realistic features but whose kinetic energy monotonically decreases in time and which are everywhere discontinuous and unbounded. For work on Euler limits see Brenier (1999, 2000) and for its dynamics in the more exotic function spaces see the papers by Tadmor (2001) and Chae (2003b, 2004).

[4] We avoid the direct nomenclature '4-vector' because of the meaning assigned to this in gauge theories.

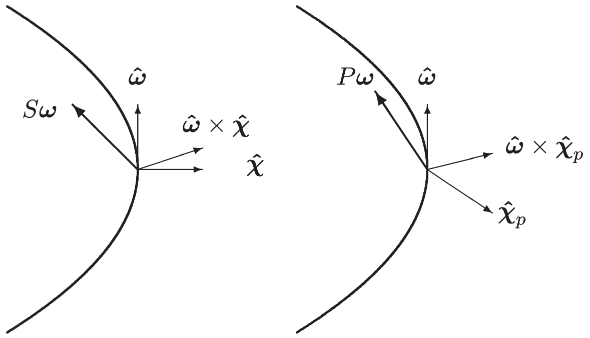

Figure 1. A vortex line with unit tangent vorticity vector $\hat{\omega}$. The normal vectors $\chi = \hat{\omega} \times S\hat{\omega}$ and $\chi_p = \hat{\omega} \times P\hat{\omega}$ are defined in (2.9) and (2.10). Thus, the three unit vectors $[\hat{\omega}, \hat{\chi}, \hat{\omega} \times \hat{\chi}]$ form an ortho-normal co-ordinate system. Moreover, $\hat{\omega}$, $S\omega$ and $\hat{\omega} \times \hat{\chi}$ are co-planar, as are $\hat{\omega}$, $P\omega$ and $\hat{\omega} \times \hat{\chi}_p$.

The new results in this paper displayed in sections 1–6 can be summarized as follows.

A well-known variable is the scalar growth rate $\alpha = \hat{\omega}\cdot S\hat{\omega}$ (Constantin 1994). Associated with this is the 3-vector rotation or swing rate $\chi = \hat{\omega} \times S\hat{\omega}$, where $\hat{\omega}$ is the unit vorticity and $S = \frac{1}{2}(u_{i,j} + u_{j,i})$ is the strain matrix. Together these form a natural tetrad[5] $\mathfrak{q} = [\alpha, \chi]$. Theorem 1 of section 2 shows that the Lagrangian advection equation for the vorticity tetrad $\mathfrak{w} = [0, \omega]$ can then be written as

$$\frac{\mathrm{D}\mathfrak{w}}{\mathrm{D}t} = \mathfrak{q} \circledast \mathfrak{w}. \tag{1.4}$$

All these quaternionic variables are Eulerian variables, i.e. point-wise functions of space and time, but undergoing Lagrangian evolution in time.

The tetrad $\mathfrak{q}$ satisfies its own Lagrangian advection equation driven by the effect of the pressure Hessian $P = \{p_{,ij}\}$ through the variables $\alpha_p = \hat{\omega}\cdot P\hat{\omega}$ and $\chi_p = \hat{\omega} \times P\hat{\omega}$. Together these also form a natural tetrad $\mathfrak{q}_p = [\alpha_p, \chi_p]$. Figure 1 shows how $S\omega$, $P\omega$ and the three orthonormal vectors $(\hat{\omega}, \hat{\chi}, \hat{\omega} \times \hat{\chi})$ are related. In addition to (1.4), theorem 1 also contains the results for the Lagrangian advection of $\mathfrak{q}$ and $\mathfrak{q}_p$. Simply stated this is

$$\frac{\mathrm{D}\mathfrak{q}}{\mathrm{D}t} + \mathfrak{q} \circledast \mathfrak{q} + \mathfrak{q}_p = 0. \tag{1.5}$$

The result in (1.5) enables us to prove a theorem in section 2 on the direction of vorticity based on Lagrangian trajectories: '*Provided $\|\chi_p\|_{L^\infty(\mathbb{D})}$ is integrable in time up to $t^* > 0$ on a periodic domain $\mathbb{D}$, no Euler singularity is possible at t^*, with the exception of the case where $\hat{\omega}$ becomes collinear with an eigenvector of P at t^**'. Although different in detail, this result is in the same style as the direction of vorticity theorems cited above and is a variant of the BKM theorem. Ohkitani and Kishiba (1995) have observed in computations that at maximum points of enstrophy, ω becomes collinear with the most negative eigenvector of P. Collinearity may therefore be an important process in vorticity growth. The pressure Hessian P and its interplay with the strain matrix S has appeared in the Euler and Navier–Stokes literature in various places; see the references in Galanti *et al* (1997), Majda and Bertozzi (2001) and Chae (2006).

At each point in space-time a fluid particle carries its own ortho-normal co-ordinate system $(\hat{\omega}, \hat{\chi}, \hat{\omega}\times\hat{\chi})$: see figure 1. Explicit equations for Lagrangian time derivatives of this frame are

[5] In Gibbon (2002) $\mathfrak{q} = [\alpha, \chi]$ was denoted as ζ. The change of notation to Gothic variables for tetrads has been introduced to avoid confusion between these and 3-vectors.

given in section 3. The corresponding Darboux vector is the particle rotation rate. The frame-equations are then shown to be directly related to the Frenet–Serret relations of differential geometry that govern the curvature and torsion of a vortex line through the arc-length derivative of its tangent, principal unit normal and bi-normal. Using Ertel's theorem, explicit differential equations for the curvature and torsion are then found.

It is shown in section 4 how to find Lagrangian differential equations for α_p and χ_p. The relation between $\mathfrak{q}_p$ and $\mathfrak{q}$ is given in theorem 3 where they are shown to satisfy

$$\frac{\mathrm{D}\mathfrak{q}_p}{\mathrm{D}t} = \mathfrak{q} \circledast \mathfrak{q}_p + \mathfrak{P}. \tag{1.6}$$

$\mathfrak{P}$ is a tetrad linear in $\mathfrak{q}$ and $\mathfrak{q}_p$ whose arbitrary scalar coefficients, in principle, are determined by the Poisson pressure relation.

The vorticity vector-field $\boldsymbol{\omega}\cdot\nabla$ is frozen into the Euler flow. Any system with a frozen-in vector-field will also have an associated form of Ertel's theorem and a corresponding tetrad $\mathfrak{q} = [\alpha, \chi]$. Thus, the Lagrangian-quaternionic format displayed in this paper is more generally applicable, as illustrated by the equations for ideal MHD in section 5. Two time-clocks and two tetrads $\mathfrak{q}^{\pm} = [\alpha^{\pm}, \chi^{\pm}]$ appear as a result because of the two Lagrangian derivatives that naturally arise through the use of Elsasser variables.

Previous attempts at formulating Euler vorticity dynamics using quaternions have met with only partial success. Past results have appeared in reverse order: the relations between α and χ to be displayed in theorem 1 were derived first by Galanti *et al* (1997) (see also Gibbon *et al* 2000), which were then shown to be expressible in a quaternionic form (Gibbon 2002). That story was incomplete, however, because the Lagrangian advection equation for $\mathfrak{w}$ was missing, as were the ideas on particle frame dynamics, the pressure relation (1.6) and results on the direction of vorticity. Roubtsov and Roulstone (1997, 2001) have also formulated semi-geostrophic theory in terms of quaternions.

2. Vorticity dynamics in quaternion form

In their vorticity form, the three-dimensional incompressible Euler equations are

$$\frac{\mathrm{D}\boldsymbol{\omega}}{\mathrm{D}t} = \boldsymbol{\omega}\cdot\nabla\boldsymbol{u} = S\boldsymbol{\omega}, \tag{2.1}$$

where the strain matrix is written as $S = \frac{1}{2}(u_{i,j} + u_{j,i})$ and $\boldsymbol{\omega} = \operatorname{curl}\boldsymbol{u}$ is the vorticity (Majda and Bertozzi 2001). Equation (2.1) arises from taking the curl of the Euler equations in their velocity formulation

$$\frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t} = -\nabla p, \qquad \operatorname{div}\boldsymbol{u} = 0, \tag{2.2}$$

in which the Lagrangian (material) derivative is defined as

$$\frac{\mathrm{D}}{\mathrm{D}t} = \frac{\partial}{\partial t} + \boldsymbol{u}\cdot\nabla. \tag{2.3}$$

The vorticity can be expressed as a tetrad by taking the quaternionic curl of $\mathfrak{U} = [0, \boldsymbol{u}]$

$$\boldsymbol{\nabla} \circledast \mathfrak{U} = [-\operatorname{div}\boldsymbol{u},\ \operatorname{curl}\boldsymbol{u}]. \tag{2.4}$$

Thus, there exists a natural vorticity tetrad $\mathfrak{w}$ which has the divergence-free constraint built into it

$$\mathfrak{w} = [0,\ \boldsymbol{\omega}]. \tag{2.5}$$

The results in this paper employ Ertel's theorem (Ertel 1942), which is widely used in geophysical fluid dynamics in the study of potential vorticity: see Hide (1983, 2004) and Hoskins, *et al* (1985). More generally it applies to any fluid system whose flow preserves a vector field, as the Euler equations preserve $\boldsymbol{\omega}\cdot\nabla$. For the extensive history behind this result, which seems to have originated with Cauchy, see Truesdell and Toupin (1960), Kuznetsov and Zakharov (1997) and Viudez (1999). The most general form of Ertel's theorem says that if $\boldsymbol{\omega}$ satisfies (2.1) then for an arbitrary differentiable vector $\boldsymbol{\theta}$

$$\frac{\mathrm{D}}{\mathrm{D}t}(\boldsymbol{\omega}\cdot\nabla\boldsymbol{\theta}) = \boldsymbol{\omega}\cdot\nabla\left(\frac{\mathrm{D}\boldsymbol{\theta}}{\mathrm{D}t}\right). \tag{2.6}$$

The choice of $\boldsymbol{\theta}$ as the Euler velocity field $\boldsymbol{u}$ (Ohkitani 1993) implies that the vortex stretching vector $\boldsymbol{\omega}\cdot\nabla\boldsymbol{u} = S\boldsymbol{\omega}$ is governed by

$$\frac{\mathrm{D}(S\boldsymbol{\omega})}{\mathrm{D}t} = -P\boldsymbol{\omega}, \tag{2.7}$$

where $P = \{p_{,ij}\} = \{\partial^2 p/\partial x_i\partial x_j\}$ is the Hessian matrix of the pressure. Thus, the combination of (2.1) and (2.7) gives Ohkitani's relation (Ohkitani 1993):

$$\frac{\mathrm{D}^2\boldsymbol{\omega}}{\mathrm{D}t^2} + P\boldsymbol{\omega} = 0. \tag{2.8}$$

To understand how the *direction* in which the vorticity vector stretches (compresses) in relation to its growth rate requires an understanding of its relationship with the matrices S and P. The scalar and vector variables α and $\boldsymbol{\chi}$ are defined by

$$\alpha = \hat{\boldsymbol{\omega}}\cdot S\hat{\boldsymbol{\omega}}, \qquad \boldsymbol{\chi} = \hat{\boldsymbol{\omega}}\times S\hat{\boldsymbol{\omega}}, \tag{2.9}$$

$$\alpha_p = \hat{\boldsymbol{\omega}}\cdot P\hat{\boldsymbol{\omega}}, \qquad \boldsymbol{\chi}_p = \hat{\boldsymbol{\omega}}\times P\hat{\boldsymbol{\omega}}. \tag{2.10}$$

The left part of figure 1, based upon $S\hat{\boldsymbol{\omega}}$, shows the ortho-normal co-ordinate system $\hat{\boldsymbol{\omega}}$, $\hat{\boldsymbol{\chi}}$ and $\hat{\boldsymbol{\omega}}\times\hat{\boldsymbol{\chi}}$; the right-hand part of the figure shows the same figure with S replaced by P. Thus, $S\hat{\boldsymbol{\omega}}$ can be decomposed into its components along the two orthogonal vectors $\hat{\boldsymbol{\omega}}$ and $\boldsymbol{\chi}\times\hat{\boldsymbol{\omega}}$

$$S\hat{\boldsymbol{\omega}} = \alpha\hat{\boldsymbol{\omega}} + \boldsymbol{\chi}\times\hat{\boldsymbol{\omega}}. \tag{2.11}$$

From (2.1) and (2.11), the Lagrangian derivatives of $|\boldsymbol{\omega}|$ and $\hat{\boldsymbol{\omega}}$ are given by

$$\frac{\mathrm{D}|\boldsymbol{\omega}|}{\mathrm{D}t} = \alpha|\boldsymbol{\omega}|, \qquad \frac{\mathrm{D}\hat{\boldsymbol{\omega}}}{\mathrm{D}t} = \boldsymbol{\chi}\times\hat{\boldsymbol{\omega}}. \tag{2.12}$$

The quantities $(\alpha, \boldsymbol{\chi})$ are, respectively, the rates of change in vorticity magnitude and direction; that is, one may, respectively, call α and $\boldsymbol{\chi}$ the stretching rate[6] and the rotation or swing rate. These variables form natural tetrads associated with $\mathfrak{w} = [0,\ \boldsymbol{\omega}]$

$$\mathfrak{q} = [\alpha, \boldsymbol{\chi}], \qquad \mathfrak{q}_p = [\alpha_p, \boldsymbol{\chi}_p]. \tag{2.13}$$

The following theorem shows how Euler vorticity dynamics can be formulated using quaternions.

Theorem 1 (Euler vorticity dynamics in terms of quaternions). *The vorticity tetrad* $\mathfrak{w}(\boldsymbol{x}, t)$ *satisfies the relation*

$$\frac{\mathrm{D}\mathfrak{w}}{\mathrm{D}t} = \mathfrak{q}\circledast\mathfrak{w}, \tag{2.14}$$

while Ohkitani's relation (2.8) becomes

$$\frac{\mathrm{D}^2\mathfrak{w}}{\mathrm{D}t^2} + \mathfrak{q}_p\circledast\mathfrak{w} = 0. \tag{2.15}$$

The tetrads $\mathfrak{q}(\boldsymbol{x}, t)$ *and* $\mathfrak{q}_p(\boldsymbol{x}, t)$ *defined in (2.13) satisfy the compatibility relation (Riccati equation)*

$$\frac{\mathrm{D}\mathfrak{q}}{\mathrm{D}t} + \mathfrak{q}\circledast\mathfrak{q} + \mathfrak{q}_p = 0. \tag{2.16}$$

[6] α and α_p are Rayleigh quotient estimates for eigenvalues of S and P, respectively, although they are only exact eigenvalues when $\boldsymbol{\omega}$ aligns with one of their eigenvectors. Constantin (1994) has a Biot–Savart formula for α.