Quaternions and particle dynamics in the Euler fluid equations

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In honour of Darryl Holm on his 60th birthday
Some papers with Darryl on this topic


Summary of this talk

Motivation: Do the 3D Euler equations possess some subtle geometric structure that guides the growth & direction of vorticity? (Peter Constantin, Geometric statistics in turbulence, SIAM Rev. 36, 73–98, 1994).

   Numerical studies: A history of investigations on the development of a finite time singularity in $\omega$ in 3D Euler. Work on the direction of vorticity.

2. Quaternions: what are they & why are they now considered to be important?

3. Lagrangian particle dynamics: Explicit equations are displayed for the Lagrangian derivatives of an ortho-normal co-ordinate system for a particle

4. The 3D-Euler equations: Ertel’s Theorem shows how these & other problems fit naturally into this framework (JDG, Holm et al 2006).

5. Modelling the pressure Hessian: Restricted Euler equations; tetrad model.
3D Euler equations – still the same after 250 years!

1. The 3D incompressible Euler equations in terms of the velocity field \( u(x, t) \):

\[
\left( \frac{\partial}{\partial t} + u \cdot \nabla \right) u = -\nabla p; \quad \text{div} \ u = 0
\]

\( \text{div} \ u = 0 \) constrains the pressure \( p \) to obey \( \{ S = \frac{1}{2}(u_{i,j} + u_{j,i}) \ \text{strain matrix} \} \)

\[-\Delta p = Tr S^2 - \frac{1}{2} \omega^2.\]

2. 3D incompressible Euler in terms of the vorticity field \( \omega = \text{curl} \ u \):

\[
\left( \frac{\partial}{\partial t} + u \cdot \nabla \right) \omega = \omega \cdot \nabla u = S \omega.
\]

3. Why the interest in singularities?

- **Physically** their formation may signify the onset of turbulence & may be a mechanism for energy transfer to small scales.
- **Numerically** they require very special methods – a great challenge to CFD.
- **Mathematically** their onset would rule out a global existence result.
The Beale-Kato-Majda-Theorem

Beale-Kato-Majda Theorem (1984): There exists a global solution of the 3D Euler equations $u \in C([0, \infty]; H^s) \cap C^1([0, \infty]; H^{s-1})$ for $s \geq 3$ if

$$\int_0^T \|\omega(\cdot, \tau)\|_{L^\infty(\Omega)} d\tau < \infty,$$

for every $T > 0$.

Remark: See also Kozono & Taniuchi (2000) for a version using the BMO norm.

Corollary to BKM Thm: If a singularity is observed in a numerical experiment

$$\|\omega(\cdot, t)\|_{L^\infty(\Omega)} \sim (T - t)^{-\beta}$$

then it is necessary to have $\beta \geq 1$ for the singularity to be genuine & not an artefact of the numerics.
Numerical search for singularities
(a revised & up-dated version of a list originally compiled by Rainer Grauer)


9. Kerr (1993, 2005): Used Chebyshev polynomials with anti-parallel initial conditions; resolution $512^2 \times 256$. Found amplification of vorticity by 18. Observed $\|\omega\|_{L^\infty(\Omega)} \sim (T - t)^{-1}$. **Singularity: yes.**


   - Cichowlas & Brachet: **Singularity: no.**
   - Pelz & Ohkitani: **Singularity: no.**
   - Gulak & Pelz: **Singularity: yes.**

16. Hou & Li (2006): Agrees with Kerr (1993) until the final stage and then growth slows. **Singularity: no.**
Direction of vorticity: the work of CFM & DHY

a) Constantin, Fefferman & Majda (1996) discussed the idea of vortex lines being “smoothly directed” in a region of greatest curvature. They argued that if the velocity is finite in a ball \((B_{4\rho})\) & \(\lim_{t \to T} \sup_{W} \int_{0}^{t} \|\nabla \hat{\omega}(\cdot, \tau)\|_{L_{\infty}(B_{4\rho})}^{2} d\tau < \infty\) then there can be no singularity at time \(T\).

b) Deng, Hou & Yu (2006) take the arc length \(L(t)\) of a vortex line \(L_{t}\) with \(\hat{n}\) the unit normal and \(\kappa\) the curvature. If \(M(t) \equiv \max \left(\|\nabla \cdot \hat{\omega}\|_{L_{\infty}(L_{t})}, \|\kappa\|_{L_{\infty}(L_{t})}\right)\) they argue that there will be no blow-up at time \(T\) if

1. \(U_{\hat{\omega}}(t) + U_{\hat{n}}(t) \lesssim (T - t)^{-A} \quad A + B = 1,\)
2. \(M(t)L(t) \leq \text{const} > 0\)
3. \(L(t) \gtrsim (T - t)^{B}.\)
Lord Kelvin (William Thompson) once said:

Quaternions came from Hamilton after his best work had been done, & though beautifully ingenious, they have been an unmixed evil to those who have touched them in any way.


http://www-groups.dcs.st-and.ac.uk/ history/Mathematicians/Hamilton.html

Kelvin was wrong because quaternions are now used in the avionics & robotics industries to track objects undergoing sequences of tumbling rotations.

They are also used in the computer animation business:


A quote from Hanson’s introduction:

Although the advantages of the quaternion forms for the basic equations of attitude control – clearly presented in Cayley (1845), Hamilton (1853, 1866) & especially Tait (1890) – had been noticed by the aeronautics & astronautics community, the technology did not penetrate the computer animation community until the land-mark Siggraph 1985 paper of Shoemake.

The importance of Shoemake’s paper is that it took the concept of the orientation frame for moving 3D objects & cameras ... exposed the deficiencies of the then-standard Euler-angle methods & introduced quaternions to animators as a solution.
What are quaternions? (Hamilton 1843)

Quaternions are constructed from a scalar $p$ & a 3-vector $q$ by forming the tetrad

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

based on the Pauli spin matrices that obey the relations $\sigma_i \sigma_j = -\delta_{ij} - \epsilon_{ijk} \sigma_k$

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

Thus quaternions obey the multiplication rule (associative but non-commutative)

$$ p_1 \otimes p_2 = [p_1 p_2 - q_1 \cdot q_2, \quad p_1 q_2 + p_2 q_1 + q_1 \times q_2]. $$

They have a close connection with the Cayley-Klein parameters & thus the Euler angles of a rotation (Whittaker 1944).
Quaternions, Cayley-Klein parameters & Rotations

Let $\hat{p} = [p, q]$ be a unit quaternion with inverse $\hat{p}^* = [p, -q]$ with $p^2 + q^2 = 1$. For a pure quaternion $r = [0, r]$ the transformation $r \rightarrow R = [0, R]$ gives the Euler-Rodrigues formula for the rotation $O(\theta, \hat{n})$ by an angle $\theta$ of $r$ about its normal $\hat{n}$. Cayley-Klein parameters ($SU(2)$) are the elements of $\hat{p} = \pm[\cos \frac{1}{2} \theta, \hat{n} \sin \frac{1}{2} \theta]$

If $\hat{p} = \hat{p}(t)$ then

$$\dot{R}(t) = (\dot{\hat{p}} \otimes \hat{p}^*) \otimes R - ((\dot{\hat{p}} \otimes \hat{p}^*) \otimes R)^*,$$

$$\dot{R} = \Omega_0(t) \times R$$

The angular velocity is $\Omega_0(t) = 2\text{Im}(\dot{\hat{p}} \otimes \hat{p}^*)$: the rigid body result: see Marsden-Ratiu 2003.
It don’t mean a thing if it ain’t got that swing! (Duke Ellington)

Consider the general Lagrangian evolution equation for a 3-vector \( \mathbf{w} \) such that
\[
\frac{D\mathbf{w}}{Dt} = \mathbf{a}(\mathbf{x}, t) \quad \frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla
\]
transported by a velocity field \( \mathbf{u} \). Define the scalar \( \alpha_a \) the 3-vector \( \chi_a \) as
\[
\alpha_a = |\mathbf{w}|^{-1}(\hat{\mathbf{w}} \cdot \mathbf{a}) , \quad \chi_a = |\mathbf{w}|^{-1}(\hat{\mathbf{w}} \times \mathbf{a}) ,
\]
for \( |\mathbf{w}| \neq 0 \). Using the parallel/perp decomposition
\[
\mathbf{a} = \alpha_a \mathbf{w} + \chi_a \times \mathbf{w} ,
\]
\[
\frac{D|\mathbf{w}|}{Dt} = \alpha_a |\mathbf{w}| , \quad \frac{D\hat{\mathbf{w}}}{Dt} = \chi_a \times \hat{\mathbf{w}} .
\]

- \( \alpha_a \) is the ‘growth rate’ (Constantin 1994)

- Note that \( \chi_a = 0 \) when \( \mathbf{w} \) and \( \mathbf{a} \) align.

- For Euler when \( \mathbf{w} = \omega \) aligns with \( S\omega \) (straight tube/sheet) \( \Rightarrow \chi = 0 \).
Define the quaternions

\[ q_a = [\alpha_a, \chi_a], \quad w = [0, w]. \]

The above decomposition allows us to write \( Dw/Dt = a \) as

\[ \frac{Dw}{Dt} = q_a \otimes w, \]

which is associated with an ortho-normal frame – the “quaternion frame”

\[ \{ \dot{w}, \hat{\chi}_a, (\dot{w} \times \hat{\chi}_a) \}. \]

- The Lagrangian evolution of this frame can be explicitly found – next slide.
- It provides us with an ortho-normal basis in which to expand other vectors – see later for a Theorem regarding the pressure.
- The frame collapses when \( a \) and \( w \) align; i.e., when \( \chi_a = 0 \).
Theorem: (JDG/Holm 06) If \( a \) is differentiable in the Lagrangian sense s.t.
\[
\frac{Da}{Dt} = b(x, t),
\]

(i) \( q_a \) and \( q_b \) satisfy the Riccati equation \(|w| \neq 0\),
\[
\frac{Dq_a}{Dt} + q_a \otimes q_a = q_b;
\]

(ii) The Lagrangian time derivative of the ortho-normal frame \((\hat{w}, \hat{\chi}_a, \hat{w} \times \hat{\chi}_a) \in SO(3)\) is expressed as
\[
\frac{D\hat{w}}{Dt} = D_{ab} \times \hat{w},
\]
\[
\frac{D(\hat{w} \times \hat{\chi}_a)}{Dt} = D_{ab} \times (\hat{w} \times \hat{\chi}_a),
\]
\[
\frac{D\hat{\chi}_a}{Dt} = D_{ab} \times \hat{\chi}_a,
\]

where the Darboux angular velocity vector \( D_{ab} \) is defined as
\[
D_{ab} = \chi_a + \frac{c_b}{\chi_a} \hat{w}, \quad c_b = \hat{w} \cdot (\hat{\chi}_a \times \chi_b).
The orientation frame of a particle

The dotted line represents a particle (●) trajectory moving from \((x_1, t_1)\) to \((x_2, t_2)\).

The orientation of the orthonormal unit vectors 
\[ \{ \hat{w}, \hat{\chi}_a, (\hat{w} \times \hat{\chi}_a) \} \]

is driven by the Darboux vector 
\[ D_{ab} = \chi_a + \frac{c_b}{\chi_a} \hat{w} \] where 
\[ c_b = \hat{w} \cdot (\hat{\chi}_a \times \chi_b). \]

Thus we need the ‘quartet’ of vectors to make this process work
\[ \{ u, w, a, b \}. \]

The frame orientation is a visual diagnostic in addition to the path.
Figure 1: \textbf{u-field is Arter-flow:} \( b(x(t)) = [\sin(k_1x(t)); \sin(k_2y(t)); \sin(k_3z(t))]; \) \( k = [1, 2, 0.5]. \) The initial \( a(x_0, t_0) = [0.5, 0.2, 0.6] \) and the initial \( w(x_0, t_0) = [0.1, 0.2, 0.3] \) with \( x_0 = [0.1, 0.2, 0.3] \) as the initial particle position. \textbf{Computation by Matthew Dixon.}
The 3D Euler equations and Ertel’s Theorem

\[ \frac{D\omega}{Dt} = \omega \cdot \nabla u = S\omega \quad \text{Euler in vorticity format} \]

**Theorem:** (Ertel 1942) If \( \omega \) satisfies the 3D incompressible Euler equations then any arbitrary differentiable \( \mu \) satisfies

\[ \frac{D}{Dt}(\omega \cdot \nabla \mu) = \omega \cdot \nabla \left( \frac{D\mu}{Dt} \right) \implies \left[ \frac{D}{Dt}, \omega \cdot \nabla \right] = 0. \]

**Proof:** Consider \( \omega \cdot \nabla \mu \equiv \omega_i \mu, i \)

\[
\frac{D}{Dt}(\omega_i \mu, i) = \frac{D\omega_i}{Dt} \mu, i + \omega_i \left\{ \frac{\partial}{\partial x_i} \left( \frac{D\mu}{Dt} \right) - u_{k,i} \mu, k \right\} \\
= \left\{ \omega_j u_{i,j} \mu, i - \omega_i u_{k,i} \mu, k \right\} + \omega_i \frac{\partial}{\partial x_i} \left( \frac{D\mu}{Dt} \right)
\]

In characteristic (Lie-derivative) form, \( \omega \cdot \nabla(t) = \omega \cdot \nabla(0) \) is a Lagrangian invariant (Cauchy 1859) and is “frozen in”.
Various references


The pressure Hessian

Define the Hessian matrix of the pressure

\[ P = \{p_{ij}\} = \left\{ \frac{\partial^2 p}{\partial x_i \partial x_j} \right\} \]

Ohkitani (1993) & Klainerman (1984) took \( \mu = u_i \).

**Result:** The vortex stretching vector \( \omega \cdot \nabla u = S\omega \) obeys

\[
\frac{D(\omega \cdot \nabla u)}{Dt} = \frac{D(S\omega)}{Dt} = \omega \cdot \nabla \left( \frac{D u}{Dt} \right) = -P \omega
\]

Thus for Euler, via Ertel’s Theorem, we have the identification:

\[
w \equiv \omega \quad a \equiv \omega \cdot \nabla u = S\omega \quad b \equiv -P\omega
\]

with a quartet

\[
(u, w, a, b) \equiv (u, \omega, S\omega, -P\omega).
\]
Euler: the variables $\alpha(x, t)$ and $\chi(x, t)$


$$S\hat{\omega} = \alpha \hat{\omega} + \chi \times \hat{\omega}$$

$$(\alpha_a) \quad \alpha = \hat{\omega} \cdot S\hat{\omega}$$

$$(\alpha_b) \quad \alpha_p = \hat{\omega} \cdot P\hat{\omega}$$

$$\chi = \hat{\omega} \times S\hat{\omega} \quad (\chi_a)$$

$$\chi_p = \hat{\omega} \times P\hat{\omega} \quad (\chi_b)$$

$$q = [\alpha, \chi]$$

$$q_b = -[\alpha_p, \chi_p]$$

$$\frac{Dq}{Dt} + q \otimes q + q_p = 0,$$

constrained by $\text{div } u = 0 \implies -TrP = \Delta p = u_{i,j}u_{j,i} = TrS^2 - \frac{1}{2}\omega^2$. 
Lagrangian frame dynamics of an Euler fluid particle

The dotted line represents the fluid packet (●) trajectory moving from \((\mathbf{x}_1, t_1)\) to \((\mathbf{x}_2, t_2)\). The orientation of the orthonormal unit vectors

\[
\{ \hat{\omega}, \hat{\chi}, (\hat{\omega} \times \hat{\chi}) \}
\]

is driven by the Darboux vector

\[
\mathcal{D} = \chi + \frac{c_p}{\chi} \hat{\omega}, \quad c_p = -\hat{\omega} \cdot (\hat{\chi} \times \chi_p).
\]

Thus the pressure Hessian within \(c_1\) drives the Darboux vector \(\mathcal{D}\).
**Remark:** the $\alpha$ and $\chi$ equations

In terms of $\alpha$ and $\chi$, the Riccati equation for $q$

$$\frac{Dq}{Dt} + q \otimes q + q_p = 0;$$

becomes

$$\frac{D\alpha}{Dt} = \chi^2 - \alpha^2 - \alpha_p,$$

$$\frac{D\chi}{Dt} = -2\alpha\chi - \chi_p.$$

Stationary values are

$$\alpha = \gamma_0, \quad \chi = 0, \quad \alpha_p = -\gamma_0^2$$

which correspond to **Burgers’-like vortices**.

When tubes & sheets bend & tangle then $\chi \neq 0$ and $q$ becomes a full tetrad driven by $q_p$ which is coupled back through the elliptic pressure condition.

**Note:** Off-diagonal elements of $P$ change rapidly near intense vortical regions across which $\chi_p$ and $\alpha_p$ change rapidly.
A summary of quartets \{u, w, a, b\} for other 3D problems

\[
\frac{D}{Dt} = \frac{\partial}{\partial t} + u \cdot \nabla
\]

<table>
<thead>
<tr>
<th>System</th>
<th>u</th>
<th>w</th>
<th>a</th>
<th>b</th>
<th>BKM</th>
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<tr>
<td>incom Euler</td>
<td>u</td>
<td>\omega</td>
<td>S\omega</td>
<td>-P\omega</td>
<td>\int_0^T |\omega|_\infty dt</td>
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<tr>
<td>baro-Euler</td>
<td>u</td>
<td>\omega/\rho</td>
<td>(\omega/\rho) \cdot \nabla u</td>
<td>-(\omega_j/\rho)\partial_j(\rho\partial_i p)</td>
<td>\int_0^T (|\omega|<em>\infty + |J|</em>\infty) dt</td>
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<tr>
<td>MHD</td>
<td>v^\pm</td>
<td>v^\mp</td>
<td>B \cdot \nabla v^\mp</td>
<td>-PB</td>
<td>\int_0^T |\delta \ell|_\infty dt</td>
</tr>
<tr>
<td>Mixing</td>
<td>u</td>
<td>\delta \ell</td>
<td>\delta \ell \cdot \nabla u</td>
<td>-P\delta \ell</td>
<td>\int_0^T |\delta \ell|_\infty dt</td>
</tr>
</tbody>
</table>

For MHD, \(v^\pm = u \pm B\), \(J = \text{curl } B\) and

\[
\frac{D^\pm}{Dt} = \frac{\partial}{\partial t} + v^\pm \cdot \nabla
\]

The \(\int_0^T (\|\omega\|_\infty + \|J\|_\infty) dt < \infty\) MHD result is due to Caflisch, Klapper & Steel 1998.
Restricted Euler equations: modelling the Hessian $P$

The gradient matrix $M_{ij} = \partial u_j / \partial x^i$ satisfies ($\text{tr } P = -\text{tr } (M^2)$)

$$\frac{DM}{Dt} + M^2 + P = 0, \quad \text{tr } M = 0.$$ 

Several attempts have been made to model the Lagrangian averaged pressure Hessian by introducing a constitutive closure. This idea goes back to Léorat (1975); Vieillefosse (1984); Cantwell (1992) who assumed that the Eulerian pressure Hessian $P$ is isotropic. This results in the restricted Euler equations with

$$P = -\frac{1}{3} I \text{tr } (M^2), \quad \text{tr } I = 3.$$ 

• Constantin’s distorted Euler equations (1986): Euler can be written as

$$\frac{\partial M}{\partial t} + M^2 + Q(t) Tr(M^2) = 0, \quad Q_{ij} = R_i R_j$$

with the Riesz transform $R_i = (-\Delta)^{-1/2} \partial_i$. ‘Distorted Euler equns’ appear with $Q(t)$ replaced by $Q(0) \Rightarrow$ rigorous blow up.
• **Tetrad model** of Chertkov, Pumir & Shraiman (1999), recently developed by Chevillard & Meneveau (2006). Underlying its mean flow features is the assumption that the Lagrangian pressure Hessian is isotropic.

For $P$ to transform as a Riemannian metric and satisfy $\text{tr} \ P = -\text{tr} \ (M^2)$

$$P = - \frac{G}{\text{tr} \ G} \text{tr} \ (M^2), \quad G(t) = I \quad \Rightarrow \quad \text{restricted Euler}.$$  

$\text{tr} \ P = -\text{tr} \ (M^2)$ is satisfied for *any* choice of $G = G^T$

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

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 flow laws for $G$ would also determine the evolution of the driving term $q_b$ in the Riccati equation.
Frame dynamics & the Frenet-Serret equations

With \( \hat{\mathbf{w}} \) as the unit tangent vector, \( \hat{\mathbf{\chi}} \) as the unit bi-normal and \( \hat{\mathbf{w}} \times \hat{\mathbf{\chi}} \) as the unit principal normal, the matrix \( \mathbf{N} \) can be formed

\[
\mathbf{N} = \left( \hat{\mathbf{w}}^T, (\hat{\mathbf{w}} \times \hat{\mathbf{\chi}})^T, \hat{\mathbf{\chi}}^T \right),
\]

with

\[
\frac{D\mathbf{N}}{Dt} = \mathbf{G} \mathbf{N}, \quad \mathbf{G} = \begin{pmatrix} 0 & -\chi & 0 \\ \chi & 0 & -c_1\chi^{-1} \\ 0 & c_1\chi^{-1} & 0 \end{pmatrix}.
\]

The Frenet-Serret equations for a space-curve are

\[
\frac{d\mathbf{N}}{ds} = \mathbf{F} \mathbf{N} \quad \text{where} \quad \mathbf{F} = \begin{pmatrix} 0 & \kappa & 0 \\ -\kappa & 0 & \tau \\ 0 & -\tau & 0 \end{pmatrix},
\]

where \( \kappa \) is the curvature and \( \tau \) is the torsion.
The arc-length derivative $d/ds$ is defined by

$$\frac{d}{ds} = \mathbf{w} \cdot \nabla.$$ 

The evolution of the curvature $\kappa$ and torsion $\tau$ may be obtained from Ertel's theorem expressed as the commutation of operators $\left[ \frac{D}{Dt}, \mathbf{w} \cdot \nabla \right] = 0$

$$\alpha_a \frac{d}{ds} + \left[ \frac{D}{Dt}, \frac{d}{ds} \right] = 0.$$ 

This commutation relation immediately gives

$$\alpha_a F + \frac{DF}{Dt} = \frac{dG}{ds} + [G, F].$$

Thus Ertel's Theorem gives explicit evolution equations for the curvature $\kappa$ and torsion $\tau$ that lie within the matrix $F$ and relates them to $c_1, \chi_a$ and $\alpha_a$. 