A frame-invariant definition of the Q-criterion

By **A. J. Banko** AND **J. K. Eaton**

1. Motivation and objectives

The identification of coherent structures is fundamental to understanding the real space dynamics of turbulent flows. One of the most widely used methods for classifying three-dimensional flow structures is the Q-criterion proposed by Hunt *et al.* (1988). It is defined in terms of the instantaneous velocity gradient tensor as (Chong *et al.* 1990)

$$Q = \frac{1}{2}\left((\nabla \cdot \mathbf{u})^2 - \nabla \mathbf{u} : \nabla \mathbf{u}^{\mathbf{T}}\right) = \frac{1}{2}\left((\nabla \cdot \mathbf{u})^2 + \|\mathbf{\Omega}\|_2^2 - \|\mathbf{S}\|_2^2\right). \quad (1.1)$$

Here, $\mathbf{u}$ is the velocity vector, $\mathbf{S}$ is the strain rate tensor, and $\mathbf{\Omega}$ is the rotation rate tensor. Thresholding Q to positive values identifies rotation-dominated regions of the flow, or vortices. Similarly, negative values of Q are associated with straining regions of the flow. These kinematic statements are made precise by considering a critical point analysis of the velocity gradient tensor (Chong *et al.* 1990). Note that other classification methods exist which also use scalar quantities derived from the velocity gradient tensor (Chong *et al.* 1990; Jeong & Hussain 1995; Horiuti & Fujisawa 2005).

The Q-criterion and related methods have been used to visualize important vortical structures in a variety of turbulent flows, including hairpins and attached eddies in turbulent boundary layers (Del Álamo *et al.* 2006; Adrian 2007; Wu & Moin 2009; Elsinga *et al.* 2010), vortex tubes surrounded by dissipation structures in isotropic turbulence (Bermejo-Moreno *et al.* 2009), the reorientation of vortices in shock-turbulence interactions (Larsson *et al.* 2013), horseshoe vortices producing significant scalar flux events in homogeneous shear flow (Vanderwel & Tavoularis 2011, 2016), and coherent structures in separated flows (Dubief & Delcayre 2000). Negative and positive values of Q are correlated with the clusters and voids formed by preferentially concentrated, inertial particles (Maxey 1987; Squires & Eaton 1991; Yoshimoto & Goto 2007; Toschi & Bodenschatz 2009). Q also has a dynamical role in incompressible flow as the source term in the pressure Poisson equation (Pope 2000; Bermejo-Moreno *et al.* 2009).

Despite its usefulness in practice, a fundamental problem of the Q-criterion is that it is not objective, specifically when considering rotating reference frames (Haller *et al.* 2005; Haller 2016). An objective quantity is invariant under coordinate transformations of the form

$$\mathbf{x}' = \mathbf{\Lambda}(t)\mathbf{x} + \mathbf{b}(t), \quad (1.2)$$

where $\mathbf{x}$ is a Cartesian coordinate system, $\mathbf{x}'$ is the transformed coordinate system, $\mathbf{\Lambda}(t)$ is a time-dependent proper orthogonal matrix, and $\mathbf{b}(t)$ is a time-dependent translation vector (Haller *et al.* 2005). Examination of Eq. (1.1) shows that Galilean transformations and linear accelerations of the origin preserve the value of Q, but that it is not invariant under the rotations corresponding to $\mathbf{\Lambda}(t)$. Therefore, observers undergoing rotational motion will calculate different values for Q, even leading to contradictory claims about the local flow structure. For example, a volume of fluid undergoing solid-body rotation will appear as a vortex to an inertial observer ($Q > 0$), but an observer rotating precisely with the flow will find no motion whatsoever ($Q = 0$). Moreover, an infinite number of possible rotating reference frames exist in between these, each yielding a different value for Q. A particular reference frame is singled out as physically relevant in special situations, such as that of the wall in turbulent pipe flow, but there is no preferred frame of reference in general (Carroll 2004; Haller *et al.* 2005). Therefore, it is problematic to ascribe dynamical significance to coherent structures identified from a quantity which depends on the coordinate system chosen.

In this work, we propose an extended formulation of the Q-criterion which is independent of any coordinate system by drawing on concepts from differential geometry and general relativity. In Sections 2.1 and 2.2, we first consider a fully relativistic definition in terms of a general spacetime manifold, the four-velocity of a fluid element, and the corresponding velocity gradient tensor computed using the covariant derivative. The expression is then simplified to the non-relativistic limit in Section 2.3, and example calculations are given for several linear flows in Section 3. The non-relativistic limit is also used to show that the results of this work are applicable to other scalar quantities used for vortex identification which are derived from the velocity gradient tensor (c.f. Jeong & Hussain (1995) and Horiuti & Fujisawa (2005)). We discuss the physical significance of the frame-invariant definition in Section 4. Conclusions are given in Section 5.

2. Frame-invariant definition

The extension follows directly from two requirements: First, tensorial expressions must be used to guarantee invariance, and second, the result should be consistent with Eq. (1.1) in the non-relativistic limit for an inertial observer. These requirements substantially restrict the possible definitions of Q so that the result, Eq. (2.8), immediately follows from the form of Eq. (1.1). Therefore, Section 2.1 is intended to provide an abridged background on the theory motivating Eq. (2.8). Some familiarity with the differential geometry underlying general relativity is assumed, and the reader is referred to Carroll (2004) for a detailed treatment of the subject. Table 1 summarizes the original formulation of Q, the frame-invariant formulation, and its simplification for non-relativistic flows.

2.1. *Background*

Events take place in spacetime, which is a 3+1-dimensional, differentiable manifold and exists independently of any coordinate system, as illustrated in Figure 1(a). The intrinsic geometry of the manifold is described by the metric tensor, a second-order symmetric tensor with components $g_{\mu\nu}$ and a Minkowski signature (Carroll 2004). The components are indexed by Greek symbols which run from zero to three, with zero denoting the time-like dimension (e.g., $(x^0, x^1, x^2, x^3) = (t, x, y, z)$ in Cartesian coordinates). Subscripts and superscripts denote covariant and contravariant indices, respectively.

Fluid elements moving through spacetime sweep out worldlines, as shown in Figure 1(b). These paths are also coordinate independent, and the objective notion of velocity is the tangent vector to the path, which necessarily has the same dimension as the manifold. In 3+1-dimensional spacetime, this is the four-velocity (Carroll 2004),

$$v^\mu = \frac{dx^\mu}{d\tau}. \tag{2.1}$$

The proper time τ is calculated from the metric tensor and an arbitrary parameterization

	Original	Relativistic	Non-relativistic
Dimensions	3 (space)	3+1 (spacetime)	3+1 (spacetime)
Velocity	$u^i = dx^i/dt$	$v^\mu = dx^\mu/d\tau$	$v^0 = 1\ ,\ v^i = u^i$
Derivative	∂_i	∇_μ	∇_μ
2Q	$\left(\partial_i u^i\right)^2 - \partial_i u^j \partial_j u^i\ {}^\dagger$	$\left(\widehat{\nabla}_\mu v^\mu\right)^2 - \widehat{\nabla}_\mu v^\nu \widehat{\nabla}_\nu v^\mu$	$\left(\widehat{\nabla}_\mu v^\mu\right)^2 - \widehat{\nabla}_\mu v^\nu \widehat{\nabla}_\nu v^\mu$
Transformations	$x^{i'} = f^{i'}(x^j) + b^i(t)$	$x^{\mu'} = f^{\mu'}(x^\nu)$	$x^{0'} = x^0 = t$ $x^{i'} = f^{i'}(x^j, t)$

Table 1. Summary of the original formulation of Q (Hunt *et al.* 1988; Chong *et al.* 1990), the extended formulation which is relativistic, and a simplification of the extended version to non-relativistic flows. The rows list important aspects of each formulation, including the number of space and/or time dimensions defining the tangent space of the manifold, the notion of velocity, the type of derivative used, the equation for Q, and the set of transformations under which Q is invariant. The Roman indices run over the spatial dimensions (e.g. $i \in \{1,2,3\}$), and the Greek indices run over the space and time dimensions (e.g., $\mu \in \{0,1,2,3\}$, with zero denoting the timelike dimension). The various functions f and b are arbitrary C^∞, bijective functions. †Note that the derivatives should be transformed appropriately (i.e., covariant derivatives should be used in the three spatial coordinates) if the coordinate system is non-Cartesian.

of the worldline of a fluid element as

$$\tau = \int_{s_1}^{s_2} \sqrt{-g_{\mu\nu}\frac{dx^\mu}{ds}\frac{dx^\nu}{ds}}\,ds. \tag{2.2}$$

It is the spacetime distance between two points, s_1 and s_2, on the worldline.

Accelerated motion is unambiguously defined using the intrinsic geometry of the manifold as paths which deviate from those taken by inertial observers, or geodesics. Observers on geodesics are in free-fall with respect to the background spacetime, and particles taking accelerated trajectories must be subject to net forces. For example, suppose that the spacetime in Figure 1 is flat, so that geodesics are straight lines. Then, without reference to any coordinate system, the worldlines of the two fluid elements shown are determined to be accelerating because they are curved. There must be a net viscous and pressure force exerted on the fluid elements to produce the accelerated motion.

In order to quantitatively measure the motion of fluid elements, observers must construct coordinates on the manifold. Figures 1(c) and 1(e) are examples of inertial and rotating Cartesian coordinate systems, respectively. Figures 1(d) and 1(f) display the projection of the fluid particle motion onto the spatial slices for each system. In the inertial coordinates, the particles move as in rigid-body motion and a rotational aspect of the flow is apparent. In the rotating system, the particles appear to remain at a fixed spatial location. These illustrations make the reason for the lack of objectivity of Q explicit. Although the spatial projection of the coordinates are Cartesian in both coordinate systems, the rotating coordinates in spacetime are curved, while the inertial coordinates are not curved. This aspect of the rotating system is not accounted for in the original formulation of the Q-criterion and hides the accelerated motion of the particles.

To avoid the lack of objectivity introduced by the coordinate system, tensorial expressions must be used to formulate the Q-criterion. The tensor transformation property guarantees that if all tensor components are zero in one frame of reference then they are zero in every frame of reference. Examples of tensors are the four-velocity, a first order

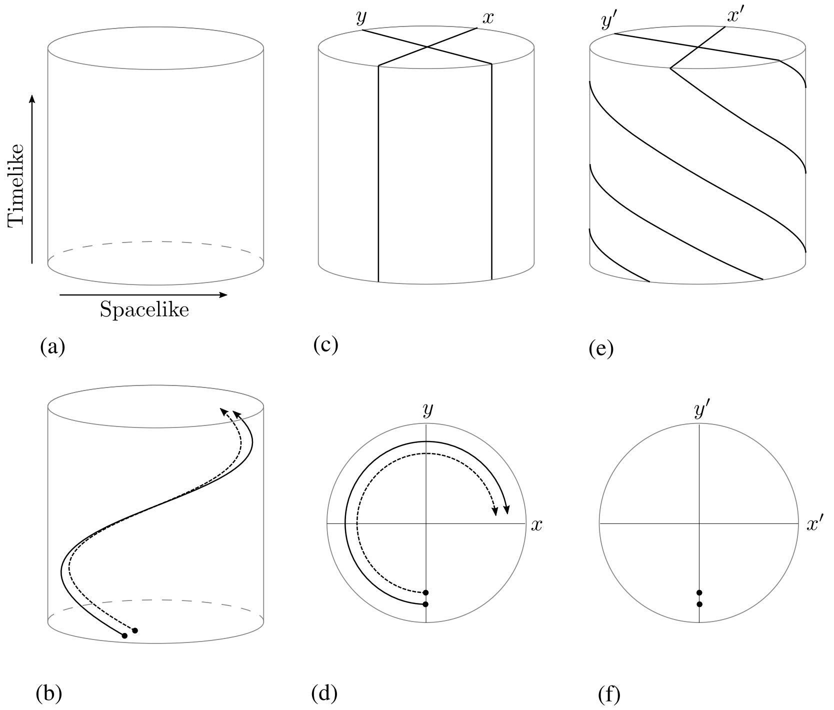

FIGURE 1. Depiction of fluid particle motion on a spacetime manifold with different coordinate systems constructed to measure the particle positions. (a) Spacetime manifold with the timelike and spacelike directions indicated. (b) Trajectory of nearby, accelerated fluid particles through spacetime, without reference to any coordinate system. (c) Coordinate system where the spatial coordinates are stationary in time. (d) Particle motion projected onto the x-y plane of the stationary coordinate system. (e) Coordinate system where the spatial coordinates rotate as time increases. (f) Particle motion projected onto the x'-y' plane of the rotating coordinate system.

tensor, and the metric tensor, a second-order tensor. A tensor with k covariant indices and l contravariant indices transforms according to (Carroll 2004)

$$T_{\mu'_1..\mu'_k}{}^{\nu'_1..\nu'_l} = \partial_{\mu'_1} x^{\alpha_1} .. \, \partial_{\mu'_k} x^{\alpha_k} \partial_{\beta_1} x^{\nu'_1} .. \, \partial_{\beta_l} x^{\nu'_l} T_{\alpha_1..\alpha_k}{}^{\beta_1..\beta_l}. \tag{2.3}$$

The Einstein summation convention is used for repeated Greek indices. The primed and unprimed systems are related through the C^{∞}, bijective coordinate transformation $x^{\mu'} = f^{\mu'}(x^{\nu})$. The three-velocity does not transform according to Eq. (2.3); therefore, the components may be nonzero in one frame but zero in another frame, as was illustrated above.

A version of the derivative which preserves the tensor transformation property is the covariant derivative. It accounts for the change in the tensor components due to changes in the coordinate basis vectors from one point on the manifold to another. The covariant derivative of a scalar field, ϕ, is simply the partial derivative: $\nabla_\mu \phi = \partial_\mu \phi$. Another familiar example of the covariant derivative arises in the transformation of the expression for the divergence of a vector field from Cartesian coordinates to spherical coordinates. In this work the covariant derivative is used in space and time, allowing non-trivial fluid motion to be identified in coordinate systems which are curved in time (Figure 1). Both the ordinary partial derivative in three-space and the covariant derivative in spacetime will identify a velocity gradient in Figure 1(d), while only the covariant derivative will correctly identify a non-zero velocity gradient in Figure 1(f). The following sections use the covariant derivative of the four-velocity given by

$$\nabla_\mu v^\nu = \partial_\mu v^\nu + \Gamma^\nu_{\mu\zeta} v^\zeta. \tag{2.4}$$

$\Gamma^\nu_{\mu\zeta}$ is the Christoffel symbol, which is computed in terms of the metric tensor as (Carroll 2004)

$$\Gamma^\nu_{\mu\zeta} = \frac{1}{2} g^{\nu\sigma} \left(\partial_\mu g_{\zeta\sigma} + \partial_\zeta g_{\sigma\mu} - \partial_\sigma g_{\zeta\mu} \right). \tag{2.5}$$

Here, $g^{\mu\nu}$ is the inverse metric tensor, so that $g^{\mu\alpha} g_{\alpha\nu} = \delta^\mu_\nu$, where δ^μ_ν is the Kronecker delta symbol.

Finally, we summarize some facts which are useful for calculations in the following sections. The metric tensor can be used to raise and lower indices; for example, $v_\mu = g_{\mu\alpha} v^\alpha$. For simplicity of notation, the timelike coordinate has been normalized using the speed of light so that the components of the metric tensor and the velocities are dimensionless, and the three-velocity is in the range of zero to unity. In this case, the four-velocity satisfies the normalization condition $v_\mu v^\mu = -1$. As a result of the normalization condition and the fact that the covariant derivative of the metric tensor is zero (Carroll 2004), one finds that $v_\nu \nabla_\mu v^\nu = 0$. Without gravity the spacetime is flat, and an inertial coordinate system can be chosen such that the metric tensor is equal to the Minkowski metric everywhere on the manifold (Carroll 2004). The Minkowski metric is $\eta_{\mu\nu} = \mathrm{diag}(-1, 1, 1, 1)$, where $\mathrm{diag}(\cdot)$ denotes the diagonal matrix. Specifically, this is achieved for an inertial frame of reference with Cartesian spatial coordinates. In an inertial frame but with curvilinear coordinates, such as a spherical coordinate system, the components of the metric will have a more complicated form.

2.2. *General formulation*

The natural extension of the Q-criterion is to replace the three-velocity in Eq. (1.1) by the four-velocity, and the partial derivatives by covariant derivatives as in Eq. (2.4). In addition, the velocity gradient tensor is projected onto the subspace orthogonal to the four-velocity vector. We show below that this projection results in the same value of Q as if the unprojected tensor were used, but that it is more readily interpreted in the relativistic setting. The projection tensor is

$$P_{\mu\nu} = g_{\mu\nu} + v_\mu v_\nu. \tag{2.6}$$

The properties of this tensor are summarized by Carroll (2004). The projected velocity gradient tensor is

$$\widehat{\nabla}_\mu v^\nu = P^\alpha{}_\mu P^\nu{}_\beta \nabla_\alpha v^\beta, \tag{2.7}$$

where the projection tensor with one contravariant and one covariant index is $P^\mu{}_\nu = g^{\mu\lambda} P_{\lambda\nu} = \delta^\mu_\nu + v^\mu v_\nu$.

Combining each of the aspects discussed above, the proposed extension of the Q-criterion is

$$Q = \frac{1}{2} \left(\left(\widehat{\nabla}_\mu v^\mu \right)^2 - \widehat{\nabla}_\mu v^\nu \widehat{\nabla}_\nu v^\mu \right). \tag{2.8}$$

It is straightforward to check that Q is invariant under any coordinate transformations of the form $x^{\mu'} = f^{\mu'}(x^\nu)$ because $\widehat{\nabla}_\mu v^\nu$ transforms as a second order tensor with one covariant index and one contravariant index.

According to the properties of the projection tensor, Q as defined in Eq. (2.8) is equal to the value calculated without projecting the velocity gradient tensor onto the subspace orthogonal to v^μ, as verified by the following calculation

$$\begin{aligned}
Q &= \frac{1}{2}\left(\left(\widehat{\nabla}_\mu v^\mu\right)^2 - \widehat{\nabla}_\mu v^\nu \widehat{\nabla}_\nu v^\mu\right)\\
&= \frac{1}{2}\left(\left(P^\alpha{}_\mu P^\mu{}_\beta \nabla_\alpha v^\beta\right)^2 - P^\alpha{}_\mu P^\nu{}_\beta P^\zeta{}_\nu P^\mu{}_\sigma \nabla_\alpha v^\beta \nabla_\zeta v^\sigma\right)\\
&= \frac{1}{2}\left(P^\alpha{}_\beta \nabla_\alpha v^\beta - P^\alpha{}_\sigma P^\zeta{}_\beta \nabla_\alpha v^\beta \nabla_\zeta v^\sigma\right)\\
&= \frac{1}{2}\left(\left(\left(\delta^\alpha_\beta + v^\alpha v_\beta\right)\nabla_\alpha v^\beta\right)^2 - \left(\delta^\alpha_\sigma + v^\alpha v_\sigma\right)\left(\delta^\zeta_\beta + v^\zeta v_\beta\right)\nabla_\alpha v^\beta \nabla_\zeta v^\sigma\right)\\
&= \frac{1}{2}\left(\left(\nabla_\mu v^\nu\right)^2 - \nabla_\mu v^\nu \nabla_\nu v^\mu\right). \qquad (2.9)
\end{aligned}$$

The third line has used the fact that $P^\mu{}_\alpha P^\alpha{}_\nu = P^\mu{}_\nu$, and the last line has used the identity $v_\nu \nabla_\mu v^\nu = 0$.

Although Q can be calculated directly from the four-velocity gradient tensor, its definition in terms of the projected velocity gradient tensor allows for an intuitive interpretation, even in relativistic flows. At any point on a spacetime manifold, one can construct locally inertial coordinates in which the metric tensor reduces to the Minkowski metric and the covariant derivative reduces to the partial derivative. The coordinates can be chosen such that the origin moves at the local fluid velocity, because the Minkowski metric is invariant under Lorentz transformations. Then, at this point $v^{\mu'} = \begin{bmatrix}1 & 0 & 0 & 0\end{bmatrix}$, and the projection tensor is $P^{\mu'}{}_{\nu'} = \delta^{\mu'}_{\nu'} - \delta^{\mu'}_{0'}\delta'^{0}_{\nu'} = \mathrm{diag}(0,1,1,1)$. In other words, this tensor projects onto the spatial coordinate directions. Explicit calculation of the velocity gradient tensor shows that

$$\widehat{\nabla}_{\mu'} v^{\nu'} = \begin{bmatrix} 0 & 0 & 0 & 0\\ 0 & \partial_{x'} v^{x'} & \partial_{y'} v^{y'} & \partial_{x'} v^{z'}\\ 0 & \partial_{y'} v^{x'} & \partial_{y'} v^{y'} & \partial_{y'} v^{z'}\\ 0 & \partial_{z'} v^{x'} & \partial_{z'} v^{y'} & \partial_{z'} v^{z'} \end{bmatrix}, \qquad (2.10)$$

so

$$Q = \frac{1}{2}\left(\left(\partial_{i'} v^{i'}\right)^2 - \partial_{i'} v^{j'} \partial_{j'} v^{i'}\right), \qquad (2.11)$$

where Roman indices run over the spatial coordinates. Therefore, Q measures the relative strength of rotation over strain based on fluid element deformation in the spacelike directions as seen by an inertial observer moving locally with the flow. This is the same interpretation as the original formulation, but involves the four-velocity to account for the possibility of relativistic speeds.

2.3. *Non-relativistic limit*

For consistency, it is required that Eq. (2.8) reduces to Eq. (1.1) in the non-relativistic limit for inertial observers using Cartesian coordinates. The non-relativistic limit applies when the three-velocity is much less than the speed of light and gravity is weak; that is

$$u = \sqrt{u_i u^i} \ll 1 \quad \text{and} \quad g_{\mu\nu} = \eta_{\mu\nu} + h_{\mu\nu}\ , \ |h_{\mu\nu}| \ll 1. \qquad (2.12)$$

Here, the metric tensor has been decomposed into the Minkowski metric, corresponding to a flat spacetime, and a perturbation, $h_{\mu\nu}$. Then, $g_{\mu\nu} = \eta_{\mu\nu} + O(h)$, $v^0 = 1 + O(h) + O(u^2)$, and $v^i = u^i + O(h \cdot u) + O(u^3)$. Equation (2.5) implies that $\Gamma^{\nu}_{\mu\zeta} = O(h)$. The projection tensor in Eq. (2.6) is $P_{\mu\nu} = \mathrm{diag}(0,1,1,1) + O(h) + O(u)$, so that $P^{\mu}{}_{\nu} = \mathrm{diag}(0,1,1,1) + O(h) + O(u)$ as well. Neglecting terms of $O(\max(h, u^2))$ and smaller, the projected velocity gradient tensor is approximately

$$\widehat{\nabla}_{\mu} v^{\nu} \approx \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & \partial_x u^x & \partial_x u^y & \partial_x u^z \\ 0 & \partial_y u^x & \partial_y u^y & \partial_y u^z \\ 0 & \partial_z u^x & \partial_z u^y & \partial_z u^z \end{bmatrix}. \tag{2.13}$$

Finally, inserting Eq. (2.13) into Eq. (2.8) shows that the extended formulation is consistent with Eq. (1.1).

The above approximations also suggest a simplification of Eq. (2.8) for use on non-relativistic flows. In the so-called Newtonian limit, all observers agree on a universal definition of time so that $x^{0'} = x^0 = t$. As a result, the relevant coordinate frame transformations are slightly restricted as compared to the relativistic case. Specifically,

$$x^{0'} = x^0 = t \quad \text{and} \quad x^{i'} = f^{i'}(x^j, t) \tag{2.14}$$

for C^{∞}, bijective functions $f^{i'}$. Note that this set of transformations includes time-dependent rotations such as in Eq. (1.2). Then, define a four-velocity vector as

$$v^{\mu} = \begin{bmatrix} 1 & u^1 & u^2 & u^3 \end{bmatrix}, \tag{2.15}$$

i.e., constant velocity in the time direction and a spatial projection of the velocity that is equal to the ordinary three-velocity. This simple extension of the three-velocity transforms as a tensor under the restricted set of coordinate transformations and $v^0 = 1$ in any such frame of reference. The projection tensor is defined to be the spatial projection tensor

$$P_{\mu\nu} = g_{\mu\nu} + w_{\mu} w_{\nu}, \tag{2.16}$$

where $w_{\mu} = \begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix}$. Note that the components of w_{μ} are invariant under the restricted set of coordinate transformations. In contrast to the relativistic case, this spatial projection applies globally and in any frame, because the spacetime is flat and all observers agree on the definition of time. The projection tensor with one contravariant and one covariant index is simplified as

$$P^{\mu}{}_{\nu} = \delta^{\mu}_{\nu} + w^{\mu} w_{\nu} = \delta^{\mu}_{\nu} + g^{\mu\alpha} w_{\alpha} w_{\nu} = \delta^{\mu}_{\nu} + g^{\mu 0} \delta_{\nu 0}. \tag{2.17}$$

With these specifications, the approximation in Eq. (2.13) for the projected velocity gradient tensor in inertial, Cartesian coordinates becomes an equality. Therefore, the non-relativistic, extended formulation of Q is invariant under very general coordinate frame transformations, including time-dependent rotations, and is equal to the value of Q measured by inertial observers. It has the advantage of being more easily interpreted than the relativistic definition because the ordinary three-velocity is used.

Finally, the non-relativistic formulation demonstrates that the method used to extend Q also applies to any scalar quantity derived from the velocity gradient tensor. Computing the eigenvalues of Eq. (2.13) shows that one eigenvalue is zero, and that the remaining three eigenvalues are equal to those of the ordinary velocity gradient tensor. Equation (2.13) was derived for an inertial observer in a Cartesian frame, but because it is a valid tensor equation, the above conclusion is true in any reference frame.

3. Linear flow examples

Two linear flow examples explicitly illustrate why the extension to four-dimensional spacetime and the covariant derivative are necessary to achieve invariance of Q. Both are two-dimensional flows to reduce the algebraic complexity and retain only the essential features. We also focus on the non-relativistic limit so that the simplified formulation applies. In order to avoid confusion of superscripts with powers, the coordinates are written as $(x^0,\ x^1,\ x^2,\ x^3) = (t,\ x,\ y,\ z)$.

First consider the case of solid-body rotation at a constant rate. In an inertial, Cartesian reference frame where the fluid at the origin is at rest, the four-velocity is given by

$$v^\mu = \begin{bmatrix} 1 & 2y & -2x & 0 \end{bmatrix}. \tag{3.1}$$

The projected velocity gradient tensor is given by Eq. (2.13). Therefore, Eq. (2.8) for Q simplifies to Eq. (1.1), with the result that $Q = 4$. Suppose a second observer rotates with the flow, so that the coordinate transformation from the first frame to the second frame is

$$t' = t,\ \ x' = \cos(2t)x - \sin(2t)y,\ \ y' = \sin(2t)x + \cos(2t)y,\ \ \text{and}\ \ z' = z. \tag{3.2}$$

Then the four-velocity in the second frame of reference calculated from $v^{\mu'} = \partial_\nu x^{\mu'} v^\nu$ has zero spatial projection of velocity, as expected

$$v^{\mu'} = \begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix}. \tag{3.3}$$

The metric tensor in the first frame is simply the Minkowski metric, $\eta_{\mu\nu}$. In the second frame, the metric tensor is calculated from $g_{\mu'\nu'} = \partial_{\mu'} x^\alpha \partial_{\nu'} x^\beta \eta_{\alpha\beta}$ to be

$$g_{\mu'\nu'} = \begin{bmatrix} -1 + 4x'^2 + 4y'^2 & 2y' & -2x' & 0 \\ 2y' & 1 & 0 & 0 \\ -2x' & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}. \tag{3.4}$$

Note that the spacetime is still flat and so the more complex expressions for the tensor components arise due to curvature of the coordinate system in the time direction. The non-zero components of the Christoffel symbol are

$$\Gamma^{1'}_{0'0'} = -4x',\ \ \Gamma^{2'}_{0'0'} = -4y',\ \ \Gamma^{1'}_{0'2'} = \Gamma^{1'}_{2'0'} = 2,\ \ \text{and}\ \ \Gamma^{2'}_{0'1'} = \Gamma^{2'}_{1'0'} = -2. \tag{3.5}$$

Then the velocity gradient tensor is

$$\nabla_{\mu'} v^{\nu'} = \partial_{\mu'} v^{\nu'} + \Gamma^{\nu'}_{\mu'\lambda'} v^{\lambda'} = \Gamma^{\nu'}_{\mu'0'} v^{0'} = \Gamma^{\nu'}_{\mu'0'} = \begin{bmatrix} 0 & -4x' & -4y' & 0 \\ 0 & 0 & -2 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \tag{3.6}$$

The projection tensor in the rotating frame is

$$P^{\mu'}{}_{\nu'} = \delta^{\mu'}_{\nu'} + w^{\mu'} w_{\nu'} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 2y' & 1 & 0 & 0 \\ -2x' & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}. \tag{3.7}$$

The projected velocity gradient tensor is then given by

$$\widehat{\nabla}_{\mu'} v^{\nu'} = \begin{bmatrix} 0 & -4x' & -4y' & 0 \\ 0 & 0 & -2 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \tag{3.8}$$

The fact that only the timelike component of the four-velocity and the Christoffel symbol contribute to the calculation shows that the extension to the four-velocity and the use of the covariant derivative are critical to obtaining a frame-invariant formulation of Q. Finally, applying Eq. (2.8) and following through with the algebra yields $Q = 4$, in agreement with that obtained in the non-rotating frame.

Next, consider the rotating saddle-point flow discussed by Haller *et al.* (2005) and Haller (2016). This is a time-dependent flow with both rotation and strain. The flow field in an inertial, Cartesian reference frame where the flow at the origin is at rest is given by

$$v^{\mu} = \begin{bmatrix} 1 & \sin(4t)x + (2+\cos(4t))y & (-2+\cos(4t))x - \sin(4t)y & 0 \end{bmatrix}. \tag{3.9}$$

At fixed time, a plot of the spatial projection of the velocity has the appearance of an elliptical vortex. Calculation of Q in this reference frame gives $Q = 3$, showing that the bulk rotation dominates the strain. A rotating reference frame given by the coordinate transformation in Eqs. (3.2) reveals a purely straining, saddle-point flow structure corresponding to the velocity field

$$v^{\mu'} = \begin{bmatrix} 1 & y' & x' & 0 \end{bmatrix}. \tag{3.10}$$

The metric tensor, Christoffel symbols, and projection tensor in the rotating frame are the same as given above. The projected velocity gradient tensor is

$$\widehat{\nabla}_{\mu'} v^{\nu'} = \begin{bmatrix} 0 & -6x' & -2y' & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \tag{3.11}$$

Applying Eq. (2.8) gives $Q = 3$ in agreement with the non-rotating frame. Therefore, the extended formulation of Q objectively identifies the dominance of rotation over strain, as would be measured in an inertial frame of reference.

4. Physical significance

The frame-invariant formulation of the Q-criterion is equal in value to Q calculated by inertial observers using Eq. (1.1). Therefore, it includes contributions from local and bulk rotation (e.g., solid-body rotation) of the fluid. In the original formulation of Q, bulk rotational motion was problematic because it could not be distinguished from coordinate frame rotation. Haller (2016) correctly argued that bulk rotation can hide additional flow structure, such as in the rotating saddle-point flow, which may be important for material transport. This spurred the development of alternative vortex identification criteria (Shadden *et al.* 2005; Haller *et al.* 2005; Haller 2016). However, the fact that the invariant formulation of Q objectively identifies local and bulk rotational motion relative to inertial observers is also important. This is exemplified the by the dynamics of inertial particles.

Consider inertial particles dispersed in an incompressible turbulent flow. If the particles are small compared to the flow length scales and the particle density is much larger than the fluid density, then the net force on a particle is accurately predicted by the Stokes drag formula (Maxey & Riley 1983). The particle motion is governed by the following set of ordinary differential equations in an inertial reference frame

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{u}_p \text{ and } \frac{d\mathbf{u}_p}{dt} = \frac{\mathbf{u}(\mathbf{x}_p, t) - \mathbf{u}_p}{St_\eta}. \tag{4.1}$$

Variables in Eqs. (4.1) are made non-dimensional using the Kolmogorov length and timescales, so that St_η is the Stokes number, defined as the ratio of the particle aerodynamic time constant to the Kolmogorov time scale of the turbulence. The subscript p refers to the particle position and velocity.

Inertial particle motion is numerically simulated for Haller's rotating saddle-point flow (Eq. 3.9). Particles are randomly seeded in a circle of unit radius centered at the origin and at the local fluid velocity. Then Eqs. (4.1) are integrated in time using a fourth-order Runge-Kutta scheme. The volume of the particle cloud, or equivalently the number density of particles, is tracked by computing the convex hull of the cloud at each time step. Several Stokes numbers are simulated in the range of zero to 1/2. In this flow, $Q = 3$ globally and the reference time scale is $\tau_\eta = 1/2$.

Figure 2(a) shows the simulated particles for $St_\eta = 0$, or tracer particles. The initially circular cloud is stretched and rotated into an elliptical shape after a time $t/\tau_\eta = 2$. The volume of the cloud remains constant to within an error of less than $2 \cdot 10^{-15}$ due to numerical approximation. Figure 2(b) shows the shape of the particle cloud for $St_\eta = 1/2$ in comparison to the tracer particles and the initial cloud shape. The inertial particle cloud is also stretched by the straining component of the flow, but its volume definitively increases as compared to the tracer particle cloud. Therefore, the number density of inertial particles decreased with time.

The number density evolution has been modeled by solving Eqs. (4.1) and the Navier-Stokes equations in the limit of small St_η (Maxey 1987). If a large number of particles are released in an infinitesimal cloud at $t = 0$ with number density n_o, then the number density of the cloud evolves according to

$$\frac{n(t)}{n_o} = \exp\left(-2St_\eta\tau_\eta \int_0^t Q|_{\mathbf{x}_{p,c}(s)} ds\right) + O(St_\eta^2). \tag{4.2}$$

$Q|_{\mathbf{x}_{p,c}(t)}$ is the Q-criterion from Eq. (1.1) evaluated at the center of mass of the particle cloud at time t. Applying Eq. (4.2) to the rotating saddle-point flow predicts that the number density should decrease exponentially as $n/n_o = \exp(-3St_\eta t)$. Figure 2(c) shows the simulated cloud number density as a function of time with the predicted exponential scaling for several values of St_η. Note that the increasing discrepancy between the theory and simulation results for increasing Stokes number is due to the asymptotic approximations made in deriving Eq. (4.2).

Physically, the simulation results and Eq. (4.2) indicate that particle clouds expand in regions of strong rotation ($Q > 0$) and contract in regions of high strain ($Q < 0$), as expected for the centrifuge mechanism of preferential concentration (Eaton & Fessler 1994; Bragg *et al.* 2015). The net pressure force producing rotational fluid motion is too small to accelerate inertial particles along the same trajectories as fluid elements, so particles are centrifuged out of vortex cores and collect in regions of high strain. The

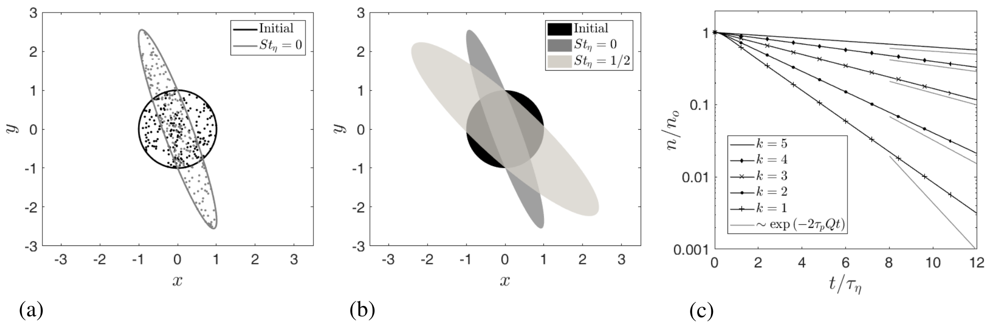

FIGURE 2. Dynamics of inertial particle clouds in the rotating saddle-point flow of Haller *et al.* (2005). (a) Evolution of tracer particle positions initially released within a circle of unit radius. (b) Envelope of tracer and inertial particle positions initially released within a disc of unit radius and at the local fluid velocity. (c) Evolution of the Lagrangian number density of inertial particle clouds for different Stokes numbers given by $St_\eta = 1/2^k$. The analytic exponential decay rate is plotted for comparison: $n/n_o = \exp(-2St_\eta \tau_\eta Qt)$.

rotating saddle-point flow is rotation dominated, so there is a flow of particles away from the origin and the cloud expands.

The simulation results are completely objective; all observers will agree that the cloud expands. However, there is an apparent contradiction in Eq. (4.2). The left-hand side, n/n_o, is also objective, but the right-hand side transforms with the coordinate system (note that Q in Eq. (4.2) uses the original formulation). The problem is that the original formulation of Q is not a scalar, so in an accelerating reference frame one needs to modify Eqs. (4.1) to include fictitious forces due to the acceleration. The radial component of the pressure gradient associated with the bulk rotation of the fluid in an inertial frame, or with balancing the centrifugal acceleration in a rotating frame, is critical for explaining the particle motion relative to the fluid.

The frame-invariant formulation of Q is always equal to the value of Q calculated using Eq. (1.1) in a inertial reference frame, so it correctly predicts the expansion of the particle clouds in any frame of reference when inserted in Eq. (4.2). It encodes the effect of bulk rotational motion, and more fundamentally the corresponding pressure field which is an objective quantity. The geometry of the pressure field does not depend on the frame of reference of the observer. In a rotating reference frame, the inertial forces are captured by the Christoffel symbols included in the covariant derivative.

It is not the intent of the present work to imply that the straining feature of the flow is unimportant. It clearly dictates the detailed shape of the particle cloud. Rather, it is emphasized that the objective formulation of Q, which is consistent with the measurements of inertial observers, captures the rotation of fluid elements associated with measurable forces that lead to preferential concentration.

5. Conclusions

A frame-invariant formulation of the Q-criterion was developed on the basis of concepts from differential geometry and general relativity. Specifically, the four-velocity of a fluid element and the covariant derivative were used to compute the velocity gradient tensor.

The velocity gradient tensor was then projected onto the subspace orthogonal to the four-velocity, which corresponds to the spatial coordinate directions of inertial observers moving with the flow. The use of tensor quantities to define Q eliminated the problem that Q can be zero in one reference frame and non-zero in another. For non-relativistic flows and in an inertial reference frame, the expression for Q simplifies to that originally proposed by Hunt *et al.* (1988) for incompressible flow, and by Chong *et al.* (1990) for compressible flow. The non-relativistic limit was used to identify a simplified version of the formulation. In this case, the timelike component of the four-velocity is equal to unity in any frame of reference, the spacelike components of the four-velocity are the components of the usual three-velocity, and the projection tensor becomes a spatial projection operator. It was also shown that the approach can be used to calculate any scalar quantity derived from the velocity gradient tensor in a frame-invariant way.

The frame-invariant value of Q is equal to that measured by inertial observers. Therefore, Q measures the relative strength of rotation over strain where the associated accelerated motion of fluid elements is produced by net viscous and pressure forces as opposed to apparent forces arising from accelerated reference frames. The importance of this connection to physical forces was demonstrated by the fact that Q calculated from the frame-invariant formulation quantitatively predicts the evolution of the volume of a small cloud of inertial particles when the particle Stokes number is small.

It is important to recognize that explicit knowledge of the frame of reference is required to compute the frame-invariant version of Q (c.f. examples in Section 3). One cannot simply measure the four-velocity and compute partial derivatives; rather, the Christoffel symbols and therefore the metric tensor must be known. However, because the frame-invariant value is equal to that measured by inertial observers, one can in principle determine experimentally whether the current reference frame is inertial or not, and therefore whether the directly measured value of Q is frame-invariant or not. Additionally, the significance of the frame-invariant formulation goes beyond explicit calculations. It demonstrates that Q and other local measures of the flow topology based on the velocity gradient tensor are objective quantities of interest. Previous studies using Q calculated in an inertial frame of reference can also be considered objective in the present context.

Applying the frame-invariant version of Q to vortex identification is still subject to the same issues as the original formulation, specifically, inadequately identifying material coherent vortices and requiring a user-specified threshold (Haller *et al.* 2005; Ouellette 2012; Haller 2016). In achieving objectivity, one is also forced to think of Q with respect to an inertial frame. In strongly rotating turbulent flows, Q will reflect the net pressure forces in the flow and correctly predict that inertial particles are centrifuged away from the center of rotation, but it may be unsuccessful at identifying turbulent eddies riding on top of the bulk fluid rotation. Alternative vortex identification schemes may be useful in such applications (Haller *et al.* 2005; Shadden *et al.* 2005; Haller 2016). Additional avenues of research could also investigate the identification of nested structures with Q, by examining decompositions into a type of mean and fluctuation. Q as a single scalar is also insufficient to completely characterize the local state of the flow. For example, it correctly predicts the expansion of inertial particle clouds due to the dominance of rotation over strain in the rotating saddle-point flow, but it does not provide any information to predict the detailed deformation of the cloud. It does not detect the presence of an unstable critical point (Haller *et al.* 2005). Future work should examine whether other frame-invariant quantities can be derived from the point of view of the spacetime manifold to educe additional flow structure important for Lagrangian transport and mixing.

Finally, the concepts from general relativity were primarily used in this work to motivate the mathematical extension of Q. In doing so, great generality was achieved: invariance under completely arbitrary coordinate transformations, at velocities comparable to the speed of light, and in strongly warped spacetime. Therefore, it may also be of interest in future work to apply Q to relativistic astrophysical flows. This avenue of research would require answers to difficult questions about the significance of coherent structures in the context of relativity. Perhaps most striking is the fact that observers in relative motion to one another will not agree on the simultaneity of events. Broadly throughout the fluid mechanics literature, a coherent structure refers to a volume of fluid undergoing correlated motion throughout a region of space at an instant in time. How should one think of a coherent structure when the concept of now is not universally agreed upon? Q is well defined pointwise, and in small regions of spacetime, discrepancies in simultaneity are not large. Therefore, small enough coherent structures may still be understood in the usual sense. The problem arises when attempting to define coherent structures spanning great spatial distances. A less philosophical problem is that the relationship between Q and the fluid pressure field will be obscured when equations of state are strongly coupled to the fluid motion.

Acknowledgments

This investigation was funded by the Advanced Simulation and Computing (ASC) program of the US Department of Energy's National Nuclear Security Administration via the PSAAP-II Center at Stanford, Grant No. DE-NA0002373. The authors would also like to thank Professor Nicholas Ouellette for insightful conversations during the preparation of this work.

REFERENCES

Adrian, R. J. 2007 Hairpin vortex organization in wall turbulence. *Phys. Fluids* **19**, 041301.

Bermejo-Moreno, I., Pullin, D. I. & Horiuti, K. 2009 Geometry of enstrophy and dissipation, grid resolution effects and proximity issues in turbulence. *J. Fluid Mech.* **620**, 121–166.

Bragg, A. D., Ireland, P. J. & Collins, L. R. 2015 Mechanisms for the clustering of inertial particles in the inertial range of isotropic turbulence. *Phys. Rev. E* **92**, 023029.

Carroll, S. M. 2004 *Spacetime and Geometry: An introduction to general relativity*. Addison Wesley.

Chong, M. S., Perry, A. E. & Cantwell, B. J. 1990 A general classification of three-dimensional flow fields. *Phys. Fluids* **2**, 765–777.

Del Álamo, J. C., Jiménez, J., Zandonade, P. & Moser, R. 2006 Self-similar vortex clusters in the turbulent logarithmic region. *J. Fluid Mech.* **561**, 329–358.

Dubief, Y. & Delcayre, F. 2000 On coherent-vortex identification in turbulence. *J. Turbul.* **1**, 1–22.

Eaton, J. K. & Fessler, J. R. 1994 Preferential concentration of particles by turbulence. *Int. J. of Multiphas. Flow* **20**, 169–209.

Elsinga, G. E., Adrian, R. J., Van Oudheusden, B. W. & Scarano, F. 2010

Three-dimensional vortex organization in a high-Reynolds number supersonic turbulent boundary layer. *J. Fluid Mech.* **644**, 35–60.

Haller, G., Hadjighasem, A., Farazmand, M. & Huhn, F. 2005 An objective definition of a vortex. *J. Fluid Mech.* **525**, 1–26.

Haller, G. 2016 Defining coherent vortices objectively from the vorticity. *J. Fluid Mech.* **795**, 136–173.

Horiuti, K. & Fujisawa, T. 2005 Identification method for vortex sheet structures in turbulent flows. *Phys. Fluids* **17**, 121703.

Hunt, J. C. R., Wray, A. & Moin, P. 1988 Eddies, streams, and convergence zones in turbulent flows. *Proceedings of the Summer Program*, Center for Turbulence Research, Stanford University, pp. 193–208.

Jeong, J. & Hussain, F. 1995 On the identification of a vortex. *J. Fluid Mech.* **285**, 69–94.

Larsson, J., Bermejo-Moreno, I. & Lele, S. K. 2013 Reynolds- and Mach-number effects in canonical shock-turbulence interaction. *J. Fluid Mech.* **717**, 293–321.

Maxey, M. & Riley, J. 1983 Equation of motion for a small rigid sphere in a nonuniform flow. *Phys. Fluids* **26**, 883–889.

Maxey, M. R. 1987 The gravitational settling of aerosol particles in homogeneous turbulence and random flow fields. *J. Fluid Mech.* **174**, 441–465.

Ouellette, N. T. 2012 On the dynamical role of coherent structures in turbulence. *C.R. Phys.* **13**, 866–877.

Pope, S. 2000 *Turbulent Flows*. Cambridge University Press.

Shadden, S. C., Lekien, F. & Marsden, J. E. 2005 Definition and properties of Lagrangian coherent structures from finite-time Lyapunov exponents in two-dimensional aperiodic flows. *Physica D* **212**, 271–304.

Squires, K. D. & Eaton, J. K. 1991 Preferential concentration of particles by turbulence. *Phys. Fluids* **3**, 1169–1178.

Toschi, F. & Bodenschatz, E. 2009 Lagrangian properties of particles in turbulence. *Annu. Rev. Fluid Mech.* **41**, 375–404.

Vanderwel, C. & Tavoularis, S. 2011 Coherent structures in uniformly sheared turbulent flow. *J. Fluid Mech.* **689**, 434–464.

Vanderwel, C. & Tavoularis, S. 2016 Scalar dispersion by coherent structures in uniformly sheared flow generated in a water tunnel. *J. Turbul.* **17**, 633–650.

Wu, X. & Moin, P. 2009 Direct numerical simulation of turbulence in a nominally zero-pressure-gradient flat-plate boundary layer. *J. Fluid Mech.* **630**, 5–41.

Yoshimoto, H. & Goto, S. 2007 Self-similar clustering of inertial particles in homogeneous turbulence. *J. Fluid Mech.* **577**, 275–286.