Rethinking the Reynolds Transport Theorem, Liouville Equation, and Perron-Frobenius and Koopman Operators: Spatial and Generalized Parametric Forms

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Abstract

We exploit a lesser-known connection between the (temporal) Reynolds transport theorem, Reynolds averaging and the Liouville equation for the flow of a conserved quantity, to derive new spatial and parametric forms of these theorems and associated evolution operators, which provide maps between different domains (in various spaces) associated with a conserved quantity in a vector or tensor field. First, for a time-independent continuous flow field described by Eulerian velocity and position coordinates \((u, x)\), we derive spatial analogs of the Reynolds transport theorem and Liouville equation – the latter based on the joint-conditional probability density function \(f(u|x)\) – and spatial analogs of the Perron-Frobenius and Koopman operators. These provide spatial maps between different positions within a velocity gradient field. For intrinsic motion (with a fixed tensorial frame of reference), the spatial mapping is induced by the shear stress tensor field. The analysis is then generalized to derive parametric Reynolds transport theorems and Liouville equations – the latter based either on a probability differential form (using a generalized Lie derivative and other operators) or probability density function – and generalized parametric Perron-Frobenius and Koopman operators. The analyses reveal the existence of multivariate Lie symmetries (in time, space or general parametric coordinates) induced by a vector or tensor field associated with the flow of a conserved quantity. The findings are illustrated by application to a variety of fluid flow and dynamical systems, including turbulent flow, two-point and \(n\)-point correlation, Lagrangian, phase space, spectral and chemical reaction systems.

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I. INTRODUCTION

In the late 19th century, following his earlier success on fluid turbulence [1], Reynolds presented two important contributions to turbulent fluid mechanics [2, 3]. The first, Reynolds decomposition, involves the decomposition of an instantaneous flow quantity into its average and a fluctuating component; for example, the instantaneous Eulerian velocity vector \( \mathbf{u} \) can be decomposed as \( \mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}' \), where the overbar can denote a time average, or more generally a Reynolds average which satisfies a set of mathematical properties [2, 4]. Applying this decomposition to the Navier-Stokes equations, followed by Reynolds averaging, reveals the significance of the mean-fluctuating (Reynolds) stresses in turbulent flow [2]. The second contribution, the Reynolds transport theorem, provides a generalized equation for transport of a conserved physical quantity (such as mass, momentum or energy) by fluid flow through a stationary or moving control volume [3]. Reynolds’ contributions provide the foundation for present-day analyses of fluid turbulence, and for the overwhelming proportion of theoretical and numerical models used by practitioners in fluid mechanics.

In the older field of classical mechanics, Liouville [5] presented a mathematical relation for the derivative of a state function which, when applied by later workers in statistical mechanics, gives an equation for the conservation in time of a local probability density function [5, 6]. The latter is now termed the Liouville equation (noting there are several similar-named equations and interpretations). While often grouped with the Fokker-Planck equation [e.g. 7], the latter includes the effect of stochastic processes or diffusion, and has rather different origins. In the early 20th century, developments in matrix theory [8, 9] led to the formulation of the Perron-Frobenius (or Ruelle-Perron-Frobenius) operator [10] and its dual Koopman operator [11, 12], for the extrapolation of a time-evolving density or observable, respectively, from an initial value. These operators have the advantage that they are linear, enabling the conversion of a nonlinear dynamical system into a linear evolution equation. Over the past decade, there has been considerable interest in the theory and application of these operators, especially for the analysis of dynamical and turbulent flow systems [13–18].

Despite over a century of mathematical generalization, including of the major integral theorems of vector calculus (the gradient, divergence and Stokes’ theorems) to more general fields and spaces, most presentations of the Reynolds transport theorem and Liouville equation remain rigidly formulated for the time evolution of the density of a conserved quantity within a three-dimensional velocity field. Some hints, however, have emerged of more general formulations. Sharma and co-workers [19] introduced both spatial and spatiotemporal Koopman operators for application in fluid mechanics, to exploit underlying symmetries (coherent structures) in the Navier-Stokes equations. The connections between these operators, singular value decomposition (SVD) and dynamic mode decomposition (DMD) were further examined recently by Le Clainche and Vega [20]. From a theoretical perspective, the present study was motivated by an analysis of Flanders [21], who viewed the Reynolds transport theorem as not merely a theorem of fluid mechanics, but a three-dimensional generalization of the Leibniz rule for differentiation of an integral. If so, it could be far more general and powerful than its current usage might suggest. Indeed, Flanders and later workers extended the Reynolds transport theorem to the flow of an \( r \)-dimensional compact submanifold within an \( n \)-dimensional manifold described by a patchwork of local coordinate systems, expressed in the formalism of exterior calculus [21, 22]. However, this still only provides a temporal map induced by a stationary or time-evolving velocity vector field.
The aim of this work is to exploit a lesser-known connection between Reynolds averaging, the Reynolds transport theorem and the Liouville equation, to derive new spatial and parametric forms of these two theorems, which provide a natural mapping between different domains (in various spaces) associated with a continuous vector or tensor field. The analysis also leads to spatial and parametric analogs of the Perron-Frobenius and Koopman operators. An exterior calculus generalization also gives a parametric Reynolds transport theorem and Liouville equation for a probability differential form, as carefully defined herein, which invokes vector generalizations of the Lie derivative and other operators. These analyses reveal the existence of multivariate Lie symmetries (in time, space or general parametric coordinates) induced by a vector or tensor field associated with the flow of a conserved quantity.

This work is set out as follows. First, in §II A, the standard or temporal Reynolds transport theorem, for the density of a conserved quantity in a flow system described by position and time coordinates \((x, t)\), is introduced along with its two standard proofs. This is shown (§II B) to imply the temporal Liouville equation (§II C), if and only if the volumetric average and total derivative operators are commutative. The Liouville equation in turn leads to the temporal Perron-Frobenius and Koopman operators. A new three-dimensional spatial analog of the Reynolds transport theorem, for the density of a conserved quantity in a time-independent flow system described by Eulerian velocity and position coordinates \((u, x)\), is then presented in §III A, along with two separate proofs. If and only if the ensemble average and differential operators are commutative, this gives a new spatial Liouville equation (§III B), which leads naturally to spatial analogs of the Perron-Frobenius and Koopman operators (§III C). For flows with a two-dimensional velocity gradient, the analysis also provides an orthogonal coordinate system and Liouville equation of Hamiltonian form, analogous to those commonly used for potential flow (§III D). Finally, in §IV, generalized parametric versions of the Reynolds transport theorem and Liouville equation are derived, the latter written in terms of a probability differential form (using an extended exterior calculus) or a parametric probability density function, in turn leading to generalized Perron-Frobenius and Koopman operators. The findings are demonstrated by application to a variety of fluid flow and dynamical systems, including turbulent flow, two-point and \(n\)-point correlation, Lagrangian, phase space, spectral and chemical reaction systems.

II. TEMPORAL ANALYSES

A. Temporal Reynolds Transport Theorem

We start from the standard – here termed the temporal – formulation of the Reynolds transport theorem [3]. We adopt Eulerian coordinates, in which each local property of a fluid can be represented as a function of Cartesian position \(x = [x, y, z]^T\) and time \(t\) as the fluid moves past. For fluid transport through an enclosed, moving, smoothly deformable control volume, the temporal Reynolds transport theorem can be written – deliberately using a slightly different notation to that commonly used in fluid mechanics – as:

\[
\frac{d}{dt} \iiint_{\Omega(t)} a \, d^3x = \iiint_{\partial \Omega(t)} \frac{\partial a}{\partial t} \, d^3x + \iiint_{\Omega(t)} a u_{\text{rel}} \cdot d^2x = \iiint_{\Omega(t)} \left[ \frac{\partial a}{\partial t} + \nabla_x \cdot (a u_{\text{rel}}) \right] \, d^3x
\]  

(1)
where $a(x, t)$ is the concentration or density of a conserved property of a fluid (scalar, vector or tensor), expressed per unit volume, $\Omega(t)$ is the deformable and moving domain (control volume), $\partial \Omega(t)$ is the domain boundary (control surface), $u_{rel}(x, t)$ is the relative velocity between the fluid and domain, $d/dt$ is the total derivative (here equivalent to the material or substantial derivative, often written $D/Dt$), $\partial/\partial t$ is the derivative at fixed position, $\nabla = \partial/\partial x, y, z^\top$ is the nabla operator with respect to $x$, $d^3x = dV = dx dy dz$ is an infinitesimal volume element in the domain, and $d^2x = dA = n dA$ is an infinitesimal directed area element at the boundary, where $n$ is the outward unit normal. In fluid mechanics, the domain $\Omega(t)$ on the left-hand side of (1) is commonly interpreted as the fluid volume coincident with the control volume at time $t$.

Proofs of (1) have been given using the tools of continuum mechanics [e.g. 3, 23–27], Lagrangian coordinate transformation [21, 28, 29] and exterior calculus [21, 22]. It is also a special case of the Helmholtz transport theorem [24]. Variants of the first two proofs are presented in Appendix A. The exterior calculus formulation based on differential forms is examined further in §IV.

In (1), we must carefully consider the meaning of the relative velocity $u_{rel}$. In the surface integral form, it expresses the velocity of the fluid relative to the control volume at the boundary, so $u_{rel} \cdot n$ is the volumetric flux normal to and out of the control surface. In the volumetric integral form, $u_{rel}$ expresses the velocity of any point in the fluid relative to the domain. The latter thus invokes – by the divergence theorem of Gauss and Ostrogradsky – the existence of a continuous and continuously differentiable vector field $u_{rel}$ throughout the domain, which by continuity must extend throughout the entire space in which the domain can be present. For consistency, the total or substantial derivative should be defined with respect to this moving frame of reference (see discussion in Appendix A):

$$\frac{da}{dt} = D a := \frac{\partial a}{\partial t} + \nabla_x a \cdot u_{rel}$$

(2)

Combining (2) and the final form of (1) gives a total derivative form of the Reynolds transport theorem [e.g., 28]:

$$\frac{d}{dt} \iiint_{\Omega(t)} a \, d^3x = \iiint_{\Omega(t)} \left[ \frac{da}{dt} + a \nabla_x \cdot u_{rel} \right] d^3x$$

(3)

By kinematics, we further identify $u_{rel} = u - u_{\Omega(t)}$, where $u_{\Omega(t)}$ is the velocity of the domain and $u$ is the intrinsic velocity of the fluid [3, 25, 27]. For a stationary domain $u_{\Omega(t)} = 0$, both (1) and (3) reduce to intrinsic forms of the Reynolds transport theorem, based on the intrinsic velocity field $u$.

B. Temporal Probabilistic Analysis and the Liouville Equation

The connections between the Reynolds transport theorem, Reynolds averaging and the Liouville equation are not widely known, although they have been described by some authors [e.g. 30]. Consider a fluid flow system in which the observables can be described using a multivariate random variable $\mathbf{\Upsilon}_x = [\Upsilon_x, \Upsilon_y, \Upsilon_z]^\top$ with values $x$, and a random

\footnote{In many references, the random variables of observable quantities are denoted by corresponding capital letters [e.g. 31]. Due to clashes with standard symbols used in fluid mechanics, a different notation is used here.}
variable for time $\Upsilon_t$ with values $t$. This gives the instantaneous joint probability of position, at any time:

$$\text{Prob} \left( x \leq \Upsilon_x \leq x + dx, \quad y \leq \Upsilon_y \leq y + dy, \quad z \leq \Upsilon_z \leq z + dz \right| t \leq \Upsilon_t \leq t + dt \right) = p(x|t) \, d^3x = p(x, y, z|t) \, dx \, dy \, dz$$

(4)

based on the probability density function (pdf) $p(x|t)$. The pdf satisfies normalization, for any time $t$:

$$1 = \iiint_{\Omega(t)} p(x|t) \, d^3x$$

(5)

We also define the (time-dependent) volumetric average of an observable $\alpha(x, t)$:

$$\{\alpha\}(t) = \iiint_{\Omega(t)} \alpha(x, t) \, p(x|t) \, d^3x$$

(6)

Substituting $a(x, t) = \alpha(x, t)p(x|t)$, in which $\alpha(x, t)$ is a density of a conserved quantity, into the total derivative form of the temporal Reynolds transport theorem (3), we obtain:

$$\frac{d}{dt} \iiint_{\Omega(t)} \alpha \, d^3x = \iiint_{\Omega(t)} \left[ \frac{d(\alpha p)}{dt} + \alpha p \nabla_x \cdot u_{rel} \right] d^3x$$

(7)

hence using the volumetric expectation notation (6) and total derivative (2):

$$\frac{d}{dt} \{\alpha\} - \{\frac{d\alpha}{dt}\} = \iiint_{\Omega(t)} \alpha \left[ \frac{dp}{dt} + p \nabla_x \cdot u_{rel} \right] d^3x = \iiint_{\Omega(t)} \alpha \left[ \frac{\partial p}{\partial t} + \nabla_x \cdot (p \, u_{rel}) \right] d^3x$$

(8)

We thus see from (8) that for a continuous and differentiable function $\alpha(x, t)$, the volumetric average (6) and total derivative operators will be commutable, i.e.,

$$\frac{d}{dt} \{\alpha\} = \{\frac{d\alpha}{dt}\},$$

(9)

if and only if

$$\frac{\partial p}{\partial t} + \nabla_x \cdot (p \, u_{rel}) = 0$$

(10)

This is the standard or temporal Liouville equation for a fluid flow system, for conservation of the conditional pdf $p(x|t)$ under the relative velocity $u_{rel}$. A proof of the double implication is given in Appendix B. The connections between the above proof and the properties of a Reynolds average are examined further in Appendix C.

We note that the temporal Liouville equation (10) can be obtained directly from the Reynolds transport theorem by taking $a(x, t) = p(x|t)$, whence $d[1]/dt = [d1/dt] = 0$, or equivalently by differentiation of (5). The Liouville equation (10) therefore expresses
The local conservation of the pdf $p(x|t)$, subject to the relative velocity field $u_{rel}$. We also emphasise that the above proof of the Liouville equation (10)-(12) does not apply to discontinuous or non-differentiable $\alpha(x, t)$, and important exceptions may occur, e.g., due to the velocity discontinuity in a shock wave or mixing layer. In such cases, commutativity of the volumetric mean and total derivative (9) may also be violated.

The formulation of the Reynolds transport theorem and its connections to the Liouville equation and evolution operators, examined in this study for the temporal map and in other contexts, are illustrated in Figure 1.

### FIG. 1. Summary diagram of the formulations presented in this study (for definitions of symbols, see text).
C. Temporal Perron-Frobenius and Koopman Operators

The foregoing analyses can be taken a few steps farther. The solution to (10) can be written as the probabilistic evolution equation

\[ p(x|t) = \hat{P}_t p(x|0), \]

where \( \hat{P}_t \) is the Perron-Frobenius operator, and the origin \( t = t_0 = 0 \) is measured in the (relative) coordinate system of \( t \) [32, 33]. Examining a probability product, it is readily verified that this is linear, giving \( \hat{P}_t = \exp(t \hat{L}_t) \), in which \( \hat{L}_t \) is the (multiplicative) temporal Liouville operator defined by

\[ \hat{L}_t p = -\nabla_x \cdot (p u_{rel}). \]

The Koopman operator \( \hat{K}_t \) adjoint to \( \hat{P}_t \) can also be defined by the volumetric mean (6), based on the duality

\[
\alpha(t) = \int_{\Omega(t)} \alpha(x, t) \hat{P}_t p(x|0) d^3x = \int_{\Omega(t)} \hat{K}_t \alpha(x, 0) p(x|t) d^3x
\]

(11)

The Koopman operator provides an evolution equation for the observable \( \alpha(x, t) = \hat{K}_t \alpha(x, 0) \), and can be determined by (complex) spectral decomposition [e.g. 13–18], with close connections to DMD [e.g. 14, 16–18, 34].

D. Further Simplifications

Intrinsic Flows: For a stationary frame of reference \( u_{\Omega(t)} = 0 \), we recover the intrinsic Liouville equation [35]:

\[
\frac{\partial p}{\partial t} + \nabla_x \cdot (p u) = 0
\]

(12)

This expresses the local conservation of \( p \) under its intrinsic motion [35]. This can be compared to the Fokker-Planck equation [7]:

\[
\frac{\partial p}{\partial t} + \nabla_x \cdot (p u) + \nabla^2_x : (D p) = 0
\]

(13)

in which \( \nabla^2_x = \nabla_x (\nabla_x)^\top \) is the second derivative or Hessian operator, \( D \) is a diffusion tensor and \( : \) is the tensor scalar product. Evidently, the Fokker-Planck equation is inconsistent with Reynold’s transport theorem (1), and contains a pdf which is not conserved locally. The distinction between (12) and (13) lies in the fact that in the former, the pdf \( p(x|t) \) is considered to extend over the entire domain \( \Omega(t) \), whilst in the latter, it undergoes the additional process of diffusion into previously unoccupied regions.

From dynamical systems theory, we can consider (12) to be induced by \( dx/dt = u = F(x) \), where \( F \) is the (vector) propagator [36]. For incompressible or solenoidal flow \( \nabla_x \cdot u = 0 \), (12) simplifies further to give

\[
\frac{\partial p}{\partial t} + \nabla_x p \cdot u = \frac{dp}{dt} = 0
\]

(14)

Two-Dimensional Flows: Alternatively, consider the special case of two-dimensional flow with position \( x = [x, y] \) and relative velocity \( u_{rel} = [u_{rel}, v_{rel}] \). If we define a stream function \( \psi \) by the relations \( u_{rel} = \partial \psi / \partial y \) and \( v_{rel} = -\partial \psi / \partial x \) [c.f. 23, 25], substitution in the
general Liouville equation (10), using the rescaled solenoidal condition $\nabla_x \cdot \mathbf{u}_{rel} = 0$, gives the Hamiltonian-like form:

$$\frac{\partial p}{\partial t} + \left( \frac{\partial \psi}{\partial y} \frac{\partial p}{\partial x} - \frac{\partial \psi}{\partial x} \frac{\partial p}{\partial y} \right) = 0$$

(15)

This definition allows for a moving control volume. The stream function $\psi$ will be normal to the relative velocity potential $\varphi$, defined for irrotational flow $\nabla_x \times \mathbf{u}_{rel} = 0$ by $\mathbf{u}_{rel} = \nabla_x \varphi$, hence $u_{rel} = \partial \varphi / \partial x$ and $v_{rel} = \partial \varphi / \partial y$ [23, 25]. For steady flows, these give a "flow net" of curvilinear orthogonal coordinates ($\psi, \varphi$), tangential and normal to the relative velocity vector.

III. THREE-DIMENSIONAL SPATIAL ANALYSES

A. Spatial Reynolds Transport Theorem

We now examine a different class of flow systems, involving three-dimensional, time-independent laminar or turbulent flow of an incompressible fluid described by Eulerian phase space (volumetric and velocimetric) coordinates, in which each fluid property $b(\mathbf{u}, \mathbf{x})$ is represented as a local function of velocity $\mathbf{u} = [u, v, w]^T$ and position $\mathbf{x} = [x, y, z]^T$. This representation encompasses steady (stationary) flow systems, invoking the notion of statistical stationarity. The position coordinates are considered to be independent. For this formulation, the temporal Reynolds transport theorem (1) can be generalized to give a three-dimensional spatial Reynolds transport theorem (more precisely a transformation theorem):

$$d \iiint_{\mathcal{D}(\mathbf{x})} b \, d^3 \mathbf{u} = \iiint_{\mathcal{D}(\mathbf{x})} \nabla_x b \, d^3 \mathbf{u} + \iiint_{\partial \mathcal{D}(\mathbf{x})} b \mathbf{G}_{rel} \cdot d^2 \mathbf{u} \cdot d\mathbf{x}$$

(16)

$$= \iiint_{\mathcal{D}(\mathbf{x})} \left( \nabla_x b + \nabla_{\mathbf{u}} \cdot (b \mathbf{G}_{rel}) \right) d^3 \mathbf{u} \cdot d\mathbf{x}$$

where $b(\mathbf{u}, \mathbf{x})$ is the density of a conserved property of a fluid (scalar, vector or tensor), expressed per unit of velocity volume, $d$ is the differential operator, $d^3 \mathbf{u} = dudvdw$ is an infinitesimal velocimetric element in the domain, $d^2 \mathbf{u}$ is an infinitesimal directed area element at the boundary, $d\mathbf{x} = [dx, dy, dz]^T$ is the differential of (vector) position, $\mathcal{D}(\mathbf{x})$ is the deformable and moving domain in velocity space, $\partial \mathcal{D}(\mathbf{x})$ is the domain boundary (velocity surface), and we use the $\partial(\rightarrow)/\partial(\downarrow)$ convention for vector derivatives, hence $\nabla_x = \partial / \partial \mathbf{x}$ is the spatial gradient operator, $\mathbf{G}_{rel} = \mathbf{G}_{rel}(\mathbf{u}, \mathbf{x})$ is the (relative) velocity gradient tensor field\(^2\) and $\nabla_{\mathbf{u}} = \partial / \partial \mathbf{u}$ is the gradient operator in velocity space. The second form in (16) assumes a continuous and continuously differentiable tensor field $\mathbf{G}_{rel}$, which extends over the entire velocity space within which the domain $\mathcal{D}(\mathbf{x})$ is embedded. For consistency with the vector derivative convention, the vector-tensor dot product in (16) is defined by the matrix operation $\nabla_{\mathbf{u}} \cdot (b \mathbf{G}_{rel}) = \nabla_{\mathbf{u}}^\top (b \mathbf{G}_{rel}^\top)$. Two distinct proofs of (16) are given

\(^2\) In fluid mechanics, the velocity gradient tensor field is commonly written $\partial \mathbf{u} / \partial \mathbf{x}$ or $\nabla_x \mathbf{u}$ with components $\partial u_j / \partial x_i$, but this notation creates a clash between different meanings of $\mathbf{u}$ (see discussion in Appendix D). A separate symbol is used here.
in Appendix D. Moreover, (16) can also be derived from a more general exterior calculus formulation, presented in §IV A and Appendix E.

The formulation (16) bears many similarities to the treatment of molecular systems in position-momentum phase space [e.g. 35, chap. 3] (examined later in §IV C), but here the integrals extend only over the velocity space, following long-standing tradition for the mathematical description of turbulent flow systems [e.g. 4, 37, 38]. The physical interpretation of (16) is analogous to that for the temporal formulation (1): a differential change in the integral of a local quantity \( b(u, x) \) over the velocity space can be subdivided into changes which occur within the velocity domain \( D(x) \), and changes which take place due to (spatial) translations into or out of the domain through the velocity surface \( \partial D(x) \). Using a velocimetric form of the divergence theorem, this is equivalent to the sum of changes within the domain and changes arising from a divergence term (in velocity space). Of course, if the velocity domain is infinite \( (D(x) = \mathbb{R}^3) \), there can be no motion through the velocity boundary, and the surface integral component will vanish.

As with the temporal formulation, we also consider a relative velocity gradient which decomposes into two components:

\[
G_{rel} = G - G_{D(x)}
\]

where \( G \) is the intrinsic field and \( G_{D(x)} \) is an additive term to enable a smoothly-varying tensorial frame of reference. For flow of a compressible Newtonian fluid, the intrinsic velocity gradient can be related (implicitly) to the shear stress tensor field, here defined positive in compression \([39, 40]\)

\[
\tau = -\mu(G + G^\top) - \lambda \delta \Delta
\]

where \( \mu \) is the dynamic viscosity, \( \lambda \) is the second or dilatational viscosity (if needed), \( \delta \) is the Kronecker delta tensor and \( \Delta = \nabla_x \cdot u \) is the divergence of the velocity field.

In consequence, for this category of flow systems expressed using \((u, x)\) coordinates, the velocity gradient tensor field – or equivalently, the shear stress tensor field – provides an intrinsic spatial connection between different velocimetric domains. This is similar to the way in which, for a flow system described by \((x, t)\) coordinates, the velocity field provides an intrinsic temporal connection – a transport equation – between different volumetric domains.

### B. Spatial Probabilistic Analysis and the Liouville Equation

Now consider a probabilistic form of the spatial formulation, based on the three-dimensional random variable for the velocity vector \( \Upsilon_u = [\Upsilon_u, \Upsilon_v, \Upsilon_w]^\top \) with values \( u \), subject to the three-dimensional random variable for position \( \Upsilon_x = [\Upsilon_x, \Upsilon_y, \Upsilon_z]^\top \) with values \( x \). The local joint probability of \( \Upsilon_u \), conditioned on \( \Upsilon_x \), is:

\[
\text{Prob}
\left(
\begin{array}{c}
u \leq \Upsilon_u \leq u + du \\
v \leq \Upsilon_v \leq v + dv \\
w \leq \Upsilon_w \leq w + dw
\end{array}
\right)
\times
\left(
\begin{array}{c}
x \leq \Upsilon_x \leq x + dx \\
y \leq \Upsilon_y \leq y + dy \\
z \leq \Upsilon_z \leq z + dz
\end{array}
\right)
= f(u|x) d^3u = f(u, v, w|x, y, z) dudvdw
\]

where \( f(u|x) \) is a joint conditional pdf. Although not usually written in conditional form, we see that \( f(u|x) \) – more commonly written \( f(u|r) \) as a function of relative position \( r \) –
forms the basis of the Reynolds-averaged Navier-Stokes formulation, and the single-position correlation functions of turbulent fluid mechanics [4, 37, 38, 41].

Taking the domain \( \mathcal{D}(x) \subseteq \mathbb{R}^3 \) of the velocity space to be a function of \( x \), the pdf will be normalized at each position \( x \):

\[
1 = \iiint_{\mathcal{D}(x)} f(u|x) \, d^3u
\]  

(20)

For any local quantity \( \beta(u, x) \) – whether scalar, vector or tensor – we can define the expectation:

\[
\langle \beta \rangle(x) = \iiint_{\mathcal{D}(x)} \beta(u, x) f(u|x) \, d^3u
\]  

(21)

This moment can be interpreted physically as the local ensemble mean of \( \beta(u, x) \), i.e. its average over all values of the instantaneous velocity \( u \in \mathcal{D}(x) \) at position \( x \). In many studies, (21) is assumed equivalent to the local time mean \( \bar{\beta}(x) \). In the present work, we maintain the most general interpretation of (21), without any ergodic hypothesis.

Substitution of \( b(u, x) = \beta(u, x) f(u|x) \), in which \( \beta(u, x) \) is also conserved, into the spatial Reynolds transport theorem (16) gives:

\[
d\langle \beta \rangle = \left[ \iiint_{\mathcal{D}(x)} \left( \nabla_x (\beta f) + \nabla_u (\beta G_{rel}) \right) d^3u \right] \cdot dx
\]

\[
= \left[ \iiint_{\mathcal{D}(x)} f \left( \nabla_x \beta + \nabla_u \beta \cdot G_{rel} \right) d^3u \right] \cdot dx + \left[ \iiint_{\mathcal{D}(x)} \beta (\nabla_x f + \nabla_u \cdot (f G_{rel})) d^3u \right] \cdot dx
\]  

(22)

Using \( u_j \) from \( [u_1, u_2, u_3] = [u, v, w] \) and the expansion

\[
\langle d\beta \rangle = \sum_{i=1}^{3} \left( \frac{\partial \beta}{\partial x_i} \right) dx_i + \sum_{j=1}^{3} \left( \frac{\partial \beta}{\partial u_j} \right) du_j
\]

\[
= \sum_{i=1}^{3} \left[ \left( \frac{\partial \beta}{\partial x_i} \right) + \sum_{j=1}^{3} \left( \frac{\partial \beta}{\partial u_j} \right) G_{rel,ij} \right] dx_i
\]

\[
= \langle \nabla_x \beta + \nabla_u \beta \cdot G_{rel} \rangle \cdot dx
\]  

(23)

where \( G_{rel,ij} = (\partial u_j / \partial x_i)_{rel} \) is the \( ij \)th component of the relative velocity gradient, (22) rearranges to the expectation form

\[
d\langle \beta \rangle - \langle d\beta \rangle = \left[ \iiint_{\mathcal{D}(x)} \beta \left( \nabla_x f + \nabla_u \cdot (f G_{rel}) \right) d^3u \right] \cdot dx
\]  

(24)

Again we see that Reynolds commutativity, in this case expressed by

\[
d\langle \beta \rangle = \langle d\beta \rangle
\]  

(25)
for a continuous and differentiable function $\beta$, is valid if and only if the following three-dimensional spatial Liouville equation is valid:

$$\nabla_x f + \nabla_u \cdot (f G_{rel}) = 0$$ (26)

The meaning of (26) is that each spatial component must independently be equal to zero:

$$\frac{\partial f}{\partial x_i} + \nabla_u \cdot (f G_{rel,i}) = 0, \quad \forall x_i \in [x_1, x_2, x_3] = [x, y, z]$$ (27)

where $G_{rel,i} = \frac{\partial u}{\partial x_i}$ is the $i$th row of the velocity gradient tensor. The proof of the double implication between (25) and (26) is identical, apart from the use of different symbols, to that for the temporal formulation given in Appendix B. The connections between this analysis and the Reynolds average are examined in Appendix C.

We note that the spatial Liouville equation (26) can be obtained directly from the Reynolds transport theorem by taking $\beta = 1$, or by differentiation of (20). We also again emphasise that if the velocity gradient is not continuous or continuously differentiable, the spatial Liouville equation (26)-(27) may be invalid, e.g., due to a discontinuity in the velocity gradient. In such cases, commutativity of the differential and ensemble mean operators may also be invalid.

Note that – despite an extensive search – we have been unable to identify any previous report of a spatial Liouville equation (26)-(27) in the fluid mechanics or physics literature, or even in the probability literature. A contributing factor may be that in the traditional Liouville equation derived by Gibbs [42], based on the pdf $f(q, \dot{q}|t)$ in $6N$-dimensional phase space (where $q$ and $\dot{q}$ are the position and momentum vectors), all parameters are functions of time, leading exclusively to a temporal Liouville equation [e.g. 43, 44] (we analyse this system in §IV C(4)). As shown in §IV, spatial Liouville equations are also accessible using the apparatus of exterior calculus, but we have not found any previous study to do so (noting that this requires a multiparameter Lie derivative, divorcing this operator from the concept of physical time).

C. Spatial Perron-Frobenius and Koopman Operators

We can again take the foregoing analysis a few steps farther. The solution to (26) is $f(u|x) = \hat{P}_x f(u|0)$, using a three-dimensional spatial Perron-Frobenius operator $\hat{P}_x$, and in which the origin $x = x_0 = 0$ is measured in the (relative) coordinate system of $x$. Again it can be verified that this is linear, giving $\hat{P}_x = \exp(x \cdot \hat{L}_x)$, in which $\hat{L}_x$ is a vector spatial Liouville operator defined by $\hat{L}_x f = -\nabla_u \cdot (f G_{rel})$. The adjoint three-dimensional spatial Koopman operator $\hat{K}_x$, defined by the duality

$$\langle \beta \rangle (x) = \iiint_{D(x)} \beta(u, x) \hat{P}_x f(u|0) \, d^3u = \iiint_{D(x)} \hat{K}_x \beta(u, 0) f(u|x) \, d^3u$$ (28)

gives the spatial evolution equation $\beta(u, x) = \hat{K}_x \beta(u, 0)$. We note the connection between $\hat{K}_x$ and Koopman operators derived for other partial derivative equations, under different contexts [45].
In consequence, if one has local information on a time-independent flow system at one position, either in probabilistic form or in the form of a conserved observable property, it is possible to extrapolate this information using the spatial Perron-Frobenius and Koopman operators to all positions within the velocity gradient field. These operators therefore provide new tools for the analysis of time-independent dynamical systems.

D. Further Simplifications

Intrinsic Velocity Gradients: For a fixed velocity gradient frame of reference $G_\mathcal{D}(x) = 0$, we obtain the intrinsic spatial Liouville equation:

$$\nabla_x f + \nabla_u \cdot (f G) = 0$$

(29)

expressing the natural variation of $f$ with $x$. We can consider (29) to be induced by $G = \Xi(u)$, a system of spatial partial differential equations with tensor operator $\Xi$.

For incompressible or solenoidal flow $\nabla_x \cdot u = 0$ of a Newtonian fluid with a symmetric shear stress tensor, reduction of (18) to the explicit relation $G = -\tau/2\mu$ gives the simplified spatial Liouville equation:

$$\nabla_x f - \tau/2\mu \cdot \nabla_u f = 0$$

(30)

or if the shear stress tensor is homogenous in velocity space:

$$\nabla_x f - \tau/2\mu \cdot \nabla_u f = 0$$

(31)

One-Dimensional Geometries: For flows with a one-directional velocity gradient aligned with one $x_i$ from $[x_1, x_2, x_3]$, for example plane parallel flow in the zone of established flow, the above analysis will reduce to a one-dimensional spatial Reynolds theorem, which can be written as the total derivative:

$$\frac{d}{dx_i} \int \int \int b \, d^3u = \int \int \int \frac{\partial b}{\partial x_i} \, d^3u + \int \int \int b \, G_{rel,i} \cdot d^2u = \int \int \int \left[ \frac{\partial b}{\partial x_i} + \nabla_u \cdot (b \, G_{rel,i}) \right] d^3u$$

(32)

Substituting $b = \beta f$, Reynolds commutativity $d\langle\beta\rangle/dx_i = \langle d\beta/dx_i \rangle$ then gives a single one-dimensional Liouville equation of the form expressed in (27).

Two-Dimensional Velocity Gradients: A special case involves a two-dimensional velocity vector $u = [u, v]^\top$ with gradients in a single direction $x_i$, leading to a velocity gradient vector $(du/dx_i)_{rel} = [(du/dx_i)_{rel}, (dv/dx_i)_{rel}]^\top$ (here reverting to traditional notation). If this is also subject to the no-divergence condition $\nabla_u \cdot (du/dx_i)_{rel} = 0$, we can define a spatial stream function or “velocity gradient function” $\gamma$ by $(du/dx_i)_{rel} = [\partial\gamma/\partial v, -\partial\gamma/\partial u]^\top$. Substitution into the one-dimensional spatial Liouville equation (27) gives the Hamiltonian form:

$$\frac{\partial f}{\partial x_i} + \left( \frac{\partial\gamma}{\partial v} \frac{\partial f}{\partial u} - \frac{\partial\gamma}{\partial u} \frac{\partial f}{\partial v} \right) = 0$$

(33)

As with the temporal formulation, for a curl-free gradient $\nabla_u \times (du/dx_i)_{rel} = 0$, the function $\gamma$ will be normal to a “velocity gradient potential” $\zeta$ defined by $(du/dx_i)_{rel} = \nabla_u \zeta = [\partial\zeta/\partial u, \partial\zeta/\partial v]^\top$. For constant gradients these give a “gradient net” of curvilinear orthogonal coordinates $(\gamma, \zeta)$, tangential and normal to the velocity gradient vector.
IV. GENERAL FORMULATIONS

A. Exterior Calculus Formulation

The foregoing analyses can be further generalized to the analysis of differential forms. Let $V$ be a smooth vector or tensor field on an $n$-dimensional manifold $M^n \subseteq \mathbb{R}^n$, in which there is an $r$-dimensional oriented compact submanifold $\Omega^r \subset M^n$. If the field trajectories (tangent bundles) are independent of the $m$-dimensional parameter vector $C$ (which could include time $t$), they will generate the “flow” $\phi^C : M^n \to M^n$, which will map the submanifold to $\Omega^r(C) = \phi^C \Omega^r(0)$ at $C$. For this we can construct a generalized Reynolds transport theorem (more precisely, a transformation theorem) for a field of $r$-forms $\omega^r$ in $\Omega^r$, based on parametric versions of differential operators:

$$d \int_{\Omega(C)} \omega^r = \left[ \int_{\Omega(C)} L_V^{(C)} \omega^r \right] \cdot dC = \left[ \int_{\Omega(C)} i_{V}^{(C)} d\omega^r + \oint_{\partial \Omega(C)} i_{V}^{(C)} \omega^r \right] \cdot dC = \left[ \int_{\Omega(C)} i_{V}^{(C)} d\omega^r + d(i_{V}^{(C)} \omega^r) \right] \cdot dC$$

(34)

where $d$ is the exterior derivative, $\partial \Omega(C)$ is the submanifold boundary, $L_V^{(C)}$ is a multi-parameter Lie derivative with respect to $V$ over parameters $C$, $i_{V}^{(C)}$ is a multi-parameter interior product with respect to $V$ over parameters $C$, and “." is the usual vector scalar product (dot product). The multiparameter operators used in (34), and its proof, are given in Appendix E.

For each point in the manifold, we then define the expected value of the function (0-form) $\beta = \beta_C$ on the submanifold by:

$$\mathcal{J}(\beta)(C) = \int_{\Omega(C)} \beta \rho^r \quad \text{with} \quad \rho^r \geq 0 \quad \text{and} \quad \int_{\Omega(C)} \rho^r = 1$$

(35)

where $\rho^r = \rho_C$ is the underlying probability $r$-form at each point conditioned on $C$, making a field of probability $r$-forms. Substituting $\omega^r = \beta \rho^r$ in (34), there will be commutativity $d[\beta] = [d \beta]$ if and only if the generalized Liouville equation is satisfied:

$$L_V^{(C)} \rho^r = i_{V}^{(C)} d\rho^r + d(i_{V}^{(C)} \rho^r) = 0$$

(36)

This expresses the local conservation of the probability $r$-form $\rho^r$ under the (intrinsic) variation of its conditions.

Finally, the solution to (36) can be written as $\rho^r_C = \hat{P}_C \rho^r_0$, which defines an exterior Perron-Frobenius operator $\hat{P}_C$. From the moment (35), this will have an adjoint exterior Koopman operator $\hat{K}_C$ defined by the observable map $\beta_C = \hat{K}_C \beta_0$.

Examining the previous literature, multiparameter Lie groups and transformations have been explored in recent times [e.g., 46–49], but neither the full multiparameter transformation equation (34) nor its associated Liouville equation (36) appear to have been reported previously. The coordinate augmentation method used for previous analyses of time-dependent flows [e.g. 22, eqs. 0.50 and 4.42], based on an augmented Lie derivative, is rather
different to the treatment here, although it serves a similar purpose. For one-parameter flows $C = t$, (34) reduces to the exterior calculus formulation of the temporal Reynolds transport theorem [e.g., 22, eqs. 0.49 and 4.33-4.34]. A temporal Liouville equation has also been written for an arbitrary conserved $r$-form in terms of the standard Lie derivative [e.g., 50], but not (we believe) in terms of a probability $r$-form. The inherent subtleties in the definition of a probability form are discussed further in Appendix F.

B. Parametric Formulation

If $\omega^n$ is a top-level $n$-dimensional compact material form based on the density $b(X, C)$ in the $n$-dimensional space described by the global coordinates $X$, and is a function of the $m$-dimensional “flow” parameter $C$, (34) reduces to a generalized parametric Reynolds transport theorem:

\[
\frac{d}{\Omega(C)} \int b^n d^n X = \left[ \frac{\Omega(C)}{\Omega(C)} \nabla_C b^n d^n X + \int b V \cdot d^{n-1} X \right] \cdot dC
\]

\[
\quad = \left[ \frac{\Omega(C)}{\Omega(C)} \left[ \nabla_C b + \nabla_X \cdot (b V) \right] d^n X \right] \cdot dC
\]

(37)

in which $V = \nabla_C X$ is the tensor field created by the $C$-gradient of $X$, and vector operators are extended naturally to their $n$- and $m$-dimensional variants. For consistency with the $\partial(\to)/\partial(\downarrow)$ convention, the vector-tensor dot product in (37) is again defined by $\nabla_X \cdot (b V) = \nabla^T_X (b V^T)$.

Substituting $b(X, C) = \beta(X, C) \hat{p}(X|C)$ based on pdf $\hat{p}(X|C)$, and defining the moment $\langle \beta \rangle(C) = \int_{\Omega(C)} \beta(X, C) \hat{p}(X|C) d^n X$, then from (37), the commutativity relation $d \langle \beta \rangle = \langle d \beta \rangle$ will be valid if and only if the parametric Liouville equation applies:

\[
\nabla_C \hat{p} + \nabla_X \cdot (\hat{p} V) = 0
\]

(38)

This expresses the conservation of the pdf $\hat{p}(X|C)$ under the (intrinsic) variation of its parameters $C$.

Finally, we note that (38) is induced by the dynamical system $V = \mathcal{F}(X)$ with operator $\mathcal{F}$. Its solution can be written $\hat{p}(X|C) = \hat{P}_C \hat{p}(X|0)$ using a linear parametric Perron-Frobenius operator $\hat{P}_C = \exp(C \cdot \hat{L}_C)$, in which the origin $C = C_0 = 0$ is measured in the (relative) coordinate system of $C$. Here $\hat{L}_C$ is a parametric Liouville operator defined by $\hat{L}_C \hat{p} = -\nabla_X \cdot (\hat{p} V)$. The adjoint parametric Koopman operator $\hat{K}_C$, defined via the moment $\langle \beta \rangle$, gives the observable equation $\beta(X, C) = \hat{K}_C \beta(X, 0)$.

C. Applications

We now have an apparatus to construct multidimensional parametric Liouville equations for a variety of physical systems. Several example applications are listed, in intrinsic form, below.
(1) **Spatiotemporal fluid flow systems** with spatially and time-varying flow described by \( \tilde{p}(u(x,t)|x,t) \), which gives joint spatial and temporal Liouville equations:

\[
\begin{align*}
\nabla_x \tilde{p} + \nabla u \cdot (\tilde{p} \mathbf{G}) &= 0 \\
\frac{\partial \tilde{p}}{\partial t} + \nabla u \cdot (\tilde{p} \mathbf{u}) &= 0
\end{align*}
\]

(39)

with \( \mathbf{u} = \partial u/\partial t \). Using the four-dimensional operator \( \nabla_x = [\partial/\partial x, \partial/\partial y, \partial/\partial z, \partial/\partial t]^\top \) and tensor-vector field \( \mathbf{G} = [G, \mathbf{u}]^\top = \nabla_x \mathbf{u} \), this can be simplified to

\[
\nabla_x \tilde{p} + \nabla u \cdot (\tilde{p} \mathbf{G}) = 0
\]

(40)

This can be considered to be induced by the system \( \tilde{G} = \mathbf{F}(u) \). The Liouville equation (40) and moment (41) then give the spatiotemporal maps \( \tilde{p}(u|x,t) = \tilde{P}_{x,t} \), to \( \tilde{p}(u|0,0) = \beta(u) \), and \( \beta(u,x,t) = K_{x,t} \beta(u,0,0) \), invoking spatiotemporal Perron-Frobenius, Liouville and Koopman operators, respectively \( \tilde{P}_{x,t} = \exp([x,t] \tilde{L}_{x,t}) \), \( \tilde{L}_{x,t} \tilde{p} = -\nabla_u \cdot (\tilde{p} \tilde{G}) = -\nabla_u \cdot (\tilde{p} \mathbf{F}(u)) \) and \( K_{x,t} \). The connections between these operators and those examined recently in the literature \([19, 20]\) warrant further examination.

We note that time-dependent flows have been treated somewhat differently in previous exterior calculus formulations, by augmentation of the manifold \( M^n \) to include the time coordinate \([e.g. \, 22, \, eqs. \, 0.50 \, and \, 4.42]\). Here, we use a multidimensional "flow" \( \phi^{x,t} \), bringing additional conditions into the probability form or pdf.

(2) **Spatiotemporal fluid flow systems with pairwise correlations**: these invoke the pairwise pdf \( \tilde{p}(u_1(x_1,t), u_2(x_2,t)|x_1, x_2, t) \) \([e.g. \, 4, \, 37, \, 38]\), whence:

\[
\begin{align*}
\nabla_{x_i} \tilde{p} + \nabla u_i \cdot (\tilde{p} \mathbf{G}_i) &= 0 \\
\frac{\partial \tilde{p}}{\partial t} + \nabla u_i \cdot (\tilde{p} \mathbf{u}_i) &= 0
\end{align*}
\]

(41)

where \( \nabla_{x_i} \) is based on \( x_i \), \( \mathbf{u}_i = \partial u_i/\partial t \) and \( \mathbf{G}_i = \nabla_{x_i} \mathbf{u}_i \). This expresses the dynamical system \( \nabla_{x_1,x_2} \mathbf{u}_1, \mathbf{u}_2 = \mathbf{F}(\mathbf{u}_1, \mathbf{u}_2) \). Previous fluid mechanics workers give only the temporal equation \([e.g. \, 51]\). The Liouville equation (41) and two-point moments \( \langle \beta \rangle(x_1, x_2, t) \) then give the pairwise maps \( \tilde{p}(u_1, u_2|x_1, x_2, t) = \tilde{P}_{x_1,x_2,t} \tilde{p}(u_1, u_2|0,0,t) \) and \( \beta(u_1, u_2, x_1, x_2, t) = K_{x_1,x_2,t} \beta(u_1, u_2, 0, 0, 0) \), invoking the pairwise Perron-Frobenius, Liouville and Koopman operators, respectively \( \tilde{P}_{x_1,x_2,t} = \exp([x_1, x_2, t] \tilde{L}_{x_1,x_2,t}) \), \( \tilde{L}_{x_1,x_2,t} \tilde{p} = -\nabla_{u_1} \cdot (\tilde{p} \tilde{G}_1) \) and \( K_{x_1,x_2,t} \). For homogenous turbulence \( x_1 \mapsto x, \, x_2 \mapsto x + r, \, u_1 \mapsto u_0, \, u_2 \mapsto u_r \), the pdf reduces to \( \tilde{p}(u_0(t), u_r(t)|r, t) \) \([4, \, 37]\), transforming (41):

\[
\begin{align*}
\nabla_r \tilde{p} + \nabla u_r \cdot (\tilde{p} \mathbf{G}_r) &= 0 \\
\frac{\partial \tilde{p}}{\partial t} + \nabla u_0 \cdot (\tilde{p} \mathbf{u}_0) + \nabla u_r \cdot (\tilde{p} \mathbf{u}_r) &= 0
\end{align*}
\]

(42)

using \( \mathbf{G}_0 = \nabla_x u_0 = 0 \) and \( \mathbf{G}_r = \nabla_r u_r \). This is induced by the dynamical system \( \nabla_r \mathbf{u}_0, \mathbf{u}_r = \mathbf{F}(\mathbf{u}_0, \mathbf{u}_r) \), and gives maps with simplified homogeneous operators \( \tilde{P}_{r,t} = \exp([r,t] \tilde{L}_{r,t}) \), \( \tilde{L}_{r,t} \tilde{p} = -\nabla_{u_0,u_r} \cdot (\tilde{p} \mathbf{F}(\mathbf{u}_0, \mathbf{u}_r)) \) and \( K_{r,t} \). In isotropic flow, the velocity gradient is constant in all directions \( \mathbf{G}_r = \delta \mathbf{d}|\mathbf{u}_r|/dr = -\tau \mathbf{\delta}/\mu \), allowing further simplification.
(3) **Spatiotemporal fluid flow systems with n-wise correlations**: the previous system can indeed be extended to examine triadic, quartic or n-wise correlations, based on the pdf \( \hat{p}(\mathbf{u}_1(x_1, t), \ldots, \mathbf{u}_n(x_n, t) | \mathbf{x}_1, \ldots, \mathbf{x}_n, t) \) [4, 37, 38]. The Liouville system is then:

\[
\nabla_x \hat{p} + \nabla_{\mathbf{u}_i} \cdot (\hat{p} \mathbf{G}_i) = 0, \quad \forall i \in \{1, \ldots, n\}
\]

The dynamical system can be written as \( \nabla_{x, 1} \ldots x_n, t}[\mathbf{u}_1^T, \ldots, \mathbf{u}_n^T] = \mathbf{F}(\mathbf{u}_1, \ldots, \mathbf{u}_n) \). The Liouville system (43) and n-point moments then give the maps \( \hat{p} = \hat{P}_{x_1, \ldots, x_n, t} \hat{p}_0 \) and \( \beta = \hat{K}_{x_1, \ldots, x_n, t} \beta_0 \), based on multipoint operators \( \hat{P}_{x_1, \ldots, x_n, t} = \exp([\mathbf{x}_1, \ldots, \mathbf{x}_n, t] L_{x_1, \ldots, x_n, t}) \), \( \hat{L}_{x_1, \ldots, x_n, t} \hat{p} = -\nabla_{u_1, \ldots, u_n} \cdot (\hat{p} \mathbf{F}(\mathbf{u}_1, \ldots, \mathbf{u}_n)) \) and \( \hat{K}_{x_1, \ldots, x_n, t} \).

(4) **Phase space systems** (including molecular gases) described by \( \hat{p}(\mathbf{u}(t), \mathbf{x}(t)|t) \), with \( \mathbf{u} \) and \( \mathbf{x} \) now defined as 6N-vectors to represent \( N \) particles, giving the combined Liouville equation (here reverting to traditional notation):

\[
\frac{\partial \hat{p}}{\partial t} + \nabla_{\mathbf{x}} \cdot \left( \hat{p} \frac{d\mathbf{x}}{dt} \right) + \nabla_{\mathbf{u}} \cdot \left( \hat{p} \frac{d\mathbf{u}}{dt} \right) = 0
\]

This expresses the dynamical system \( d[\mathbf{u}, \mathbf{x}]^T / dt = \mathbf{F}(\mathbf{u}, \mathbf{x}) \). Indeed, the Boltzmann equation (usually written with \( \mathbf{x} \mapsto \mathbf{q} \) and \( \mathbf{u} \mapsto \mathbf{q} \) for positions \( \mathbf{q} \) and momenta \( \mathbf{q} \)) can be written in this form [52, 53]. The Liouville equation (44) and moment \( \langle \beta \rangle \) then give the phase space maps \( \hat{p}(\mathbf{u}, \mathbf{x}|t) = \hat{P}_t \hat{p}(\mathbf{u}, \mathbf{x}|0) \) and \( \beta(\mathbf{u}, \mathbf{x}, t) = \hat{K}_t \beta(\mathbf{u}, \mathbf{x}, 0) \), invoking temporal forms of the Perron-Frobenius and Koopman operators (§II C), in this case with Liouville operator \( \hat{L}_t \hat{p} = -\nabla_{\mathbf{u}, \mathbf{x}} \cdot (\hat{p} \mathbf{F}(\mathbf{u}, \mathbf{x})) \).

Making the further assumption of zero divergence, incompressible or non-dissipative flow \( \nabla_{x, u} \hat{p} \hat{x}, \hat{u} = 0 \) [54, 55] gives Liouville’s theorem as written by Gibbs [42, 52]:

\[
\frac{d\hat{p}}{dt} = \frac{\partial \hat{p}}{\partial t} + \left( \nabla_x \hat{p} \cdot \frac{d\mathbf{x}}{dt} + \nabla_u \hat{p} \cdot \frac{d\mathbf{u}}{dt} \right) = 0
\]

This is the oft-quoted statement of “conservation of phase”, a special case of the more general result (44). Introducing the Hamiltonian relations:

\[
\frac{d\mathbf{x}}{dt} = \frac{\partial H}{\partial \mathbf{u}}, \quad \frac{d\mathbf{u}}{dt} = -\frac{\partial H}{\partial \mathbf{x}}
\]

this reduces to the Hamiltonian form [35, 43, 52]:

\[
\frac{d\hat{p}}{dt} = \frac{\partial \hat{p}}{\partial t} + \left( \nabla_x \hat{p} \cdot \frac{\partial H}{\partial \mathbf{u}} - \nabla_u \hat{p} \cdot \frac{\partial H}{\partial \mathbf{x}} \right) = 0
\]

It is readily verified that the Hamiltonian form (46) satisfies zero divergence [55].

(5) **Lagrangian fluid flow systems** described by \( \hat{p}(\mathbf{x}|\mathbf{x}_0, t) \) based on the initial position \( \mathbf{x}_0 \) [4, 29]. These have the joint spatial and temporal Liouville equations:

\[
\begin{cases}
\nabla_{\mathbf{x}_0} \hat{p} + \nabla_x \cdot (\hat{p} \mathbf{J}) = 0 \\
\frac{\partial \hat{p}}{\partial t} + \nabla_x \cdot (\hat{p} \mathbf{u}) = 0
\end{cases}
\]
where $\nabla_{x_0}$ is based on $x_0$ and $J = \nabla_{x_0} x$. This can be summarised by

$$\nabla_{x_0} \dot{p} + \nabla_x \cdot (\dot{p} \tilde{J}) = 0$$

(49)

where $\tilde{J} = \nabla_{x_0} x$. This is induced by the system $\tilde{J} = F(x)$. The Liouville equation (49) and moment $\langle \beta \rangle$ then give the Lagrangian maps $\dot{p}(x|x_0,t) = P_{x_0,t} \dot{p}(x|0,0)$ and $\beta(x,x_0,t) = \dot{K}_{x_0,t} \beta(x,0,0)$, invoking Lagrangian variants of the Perron-Frobenius, Liouville and Koopman operators $P_{x_0,t} = \exp([x_0,t] \cdot L_{x_0,t})$, $L_{x_0,t} \dot{p} = -\nabla_x \cdot (\dot{p} \tilde{J})$ and $\dot{K}_{x_0,t}$.

(6) **Spectral flow systems** with observables $\beta(\dot{u}, \kappa, t)$ and pdf $\dot{p}(\dot{u}|\kappa, t)$, where $\dot{u}$ is the modal amplitude vector and $\kappa$ the wavenumber vector [e.g. 38]. This gives the joint Liouville equations:

$$\begin{cases}
\nabla_k \dot{p} + \nabla_u \cdot (\dot{p} \Gamma) = 0 \\
\frac{\partial \dot{p}}{\partial t} + \nabla_u \cdot (\dot{p} \dot{u}) = 0
\end{cases}$$

(50)

using $\Gamma = \nabla_k \dot{u}$ and $\dot{u} = \partial \dot{u} / \partial t$. This is induced by the system $\tilde{\Gamma} = \nabla_k \dot{u} = F(\dot{u})$.

Eq. (50) and the spectral moment $\langle \beta \rangle$ then give the maps $\dot{p}(\dot{u}|\kappa, t) = \dot{P}_{k,t} \dot{p}(\dot{u}|0,0)$ and $\beta(\dot{u}, \kappa, t) = \dot{K}_{k,t} \beta(\dot{u}, 0, 0)$, invoking spectral Perron-Frobenius, Liouville and Koopman operators, respectively $\dot{P}_{k,t} = \exp([k,t] \dot{L}_{k,t})$, $\dot{L}_{k,t} \dot{p} = -\nabla_u \cdot (\dot{p} F(\dot{u}))$ and $\dot{K}_{k,t}$. Many other Fourier transform dynamical systems in space and/or time can also be analysed in a similar manner.

(7) **Chemical reaction and flow systems** described by $\dot{p}(m, u|x,t)$, where $m$ is the vector of mass (or molar) concentrations of different species, with joint Liouville equations:

$$\begin{cases}
\nabla_m \dot{p} + \nabla_m \cdot (\dot{p} M) + \nabla_u \cdot (\dot{p} G) = 0 \\
\frac{\partial \dot{p}}{\partial t} + \nabla_m \cdot (\dot{p} \dot{m}) + \nabla_u \cdot (\dot{p} \dot{u}) = 0
\end{cases}$$

(51)

using $\nabla_m = \partial / \partial m$ and $M = \nabla_x m$, hence $\nabla_x [m,u] = F(m,u)$. These in turn give the maps $\dot{p}(m,u|x,t) = \dot{P}_{x,t} \dot{p}(m,u|0,0)$ and $\beta(m,u,x,t) = \dot{K}_{x,t} \beta(m,u,0,0)$, invoking spatiotemporal Perron-Frobenius and Koopman operators similar to those in part (1), now with Liouville operator $\dot{L}_{x,t} \dot{p} = -\nabla_{m,u} \cdot (\dot{p} F(m,u))$. These relations give a very different approach for the probabilistic analysis of reactive dynamical systems [e.g. 56].

(8) **Chemical reaction-dependent flow systems**, in general described by the $r$-form $\rho^{(r)}_{x,m,t}$, a function of local velocity $u$ conditioned on $x$, $m$ and $t$, giving the Liouville equation system:

$$\mathcal{L}_{u}^{(x,m,t)} \rho^{r} = \int_{u}^{(x,m,t)} d\rho^{r} + d \int_{u}^{(x,m,t)} \rho^{r} = 0$$

(52)

For global velocity coordinates these reduce to (39) and $\nabla_m \dot{p} + \nabla_u \cdot (\dot{p} K) = 0$ with $K = \nabla_m u$ for variations in chemical species, induced by the system $[\nabla_x, \nabla_m, \partial / \partial t] \cdot u = \nabla_x m u = F(u)$. These in turn give the spatiochemicalotemporal maps $\dot{p}(u|x,m,t) = \dot{P}_{x,m,t} \dot{p}(u|0,0,0)$ and $\beta(u,x,m,t) = \dot{K}_{x,m,t} \beta(u,0,0,0)$, invoking spatiochemicalotemporal Perron-Frobenius, Liouville and Koopman operators $\dot{P}_{x,m,t} = \exp([x,m,t] \dot{L}_{x,m,t})$, $\dot{L}_{x,m,t} \dot{p} = -\nabla_u \cdot (\dot{p} F(u))$ and $\dot{K}_{x,m,t}$.
V. CONCLUSIONS

This study draws on the connections between the Reynolds transport theorem, Reynolds averaging and the Liouville equation, for a flow system described by position and time coordinates \((\mathbf{x}, t)\), to derive generalized versions of these theorems and associated evolution operators for a variety of flow or dynamical systems, as illustrated in Figure 1.

The standard or temporal Reynolds transport theorem for systems described by position and time coordinates \((\mathbf{x}, t)\) is first analysed, and shown to give the temporal Liouville equation if and only if the volumetric average and total derivative operators are commutative. A new three-dimensional spatial analog of the Reynolds transport theorem, for a time-independent flow system described by Eulerian velocity and position coordinates \((\mathbf{u}, \mathbf{x})\), is then given along with two separate proofs. For intrinsic motion (based on a fixed tensorial frame of reference), the spatial connection is shown to be induced by the shear stress tensor field. The spatial Reynolds transport theorem also gives a new spatial Liouville equation, if and only if the ensemble average and differential operators are commutative; this in turn gives spatial analogs of the Perron-Frobenius and Koopman operators. For flows with a two-dimensional velocity gradient, subject to divergence-free and curl-free assumptions in velocity space, the analysis furnishes an orthogonal coordinate system and Liouville equation of Hamiltonian form, analogous to the stream function and velocity potential representation commonly used for potential flow.

The analysis is then generalized to give a parametric Reynolds transport theorem and Liouville equation for a conditional probability \(r\)-form, using a generalized vector Lie derivative and other operators of exterior calculus, which in turn give generalized parametric Perron-Frobenius and Koopman operators. For systems described by a global coordinate system, these simplify to give parametric equations based on a conditional parametric pdf. The findings are demonstrated by application to a variety of fluid flow and dynamical systems, including turbulent flow, two-point and \(n\)-point correlation, Lagrangian, phase space, spectral and chemical reaction systems.

This study opens a number of important avenues for further research. The new spatial Reynolds transport (or transformation) theorem, Liouville equation, and Perron-Frobenius and Koopman operators enable new analyses of spatial maps in time-stationary flows, while the parametric formulations enable applications to a diverse range of other dynamical systems governed by a conservation equation. The role of the conditions to the pdf or probability differential form (such as time, position or parametric space) – especially the effects of fluctuations or stochastic phenomena on their “stationarity” – demand further study. Furthermore, the extended exterior calculus formulation reveals the existence of generalized Lie symmetries in a wide range of dynamical systems governed by a conservation equation, induced by any vector or tensor field; these symmetries are not restricted to the temporal map associated with a velocity vector field. Such symmetries could be exploited to develop new methods for the solution of partial differential equations, including the Navier-Stokes equations – and indeed may have started to be exploited [e.g. 19, 20]. The connections between the extended Lie symmetries and other diffeomorphisms, such as those previously associated with the Perron-Frobenius and Koopman operators [e.g. 57, 58], warrant further examination.
VI. ACKNOWLEDGMENTS

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Appendix A: Proof of the Reynolds Transport Theorem

We here give two proofs of the standard Reynolds transport theorem (1), based respectively on continuum mechanics [modified after 3, 23–27] and a Lagrangian coordinate transformation [e.g. 21, 28, 29].

Proof 1: Continuum Mechanics

For the first proof, we adopt the continuum assumption and Eulerian description of fluid flow, in which each conserved fluid property $a(x, t)$ can be represented as a local function of Cartesian position $x = [x, y, z]^T$ and time $t$ within a prescribed domain (control volume) as the fluid moves past. We also consider the Lagrangian or material description of fluid flow, in which each fluid element is assigned a characteristic label, for example its position vector $x_0$ at time $t_0$. The position of each fluid element at time $t$ is then $x(x_0, t)$, giving the fluid element velocity $u^L(x_0, t) = \partial x(x_0, t)/\partial t$. The two descriptions can be united by the equivalence of the material and Eulerian velocities [29, 59]:

\[
\frac{\partial x(x_0, t)}{\partial t} = u^L(x_0, t) = u(x, t) \tag{A1}
\]

For the present analysis, we also incorporate a moving and smoothly deforming domain with local velocity field $u_{\Omega(t)}$, so the fluid velocity field relative to the domain is $u_{rel} = u - u_{\Omega(t)}$. 

FIG. 2. Schematic diagrams of (a) a velocity field for fluid flow through a geometric domain, and (b) a volume element on the boundary induced by the flow.
A schematic diagram of several streamlines of this relative velocity field moving through the domain is given in Figure 2(a). The two descriptions in (A1) also establish the equivalence of the substantial and total derivatives (2), based on the moving frame of reference:

\[
\frac{Da(x, t)}{Dt} = \frac{\partial a}{\partial t} + \nabla_x a \cdot \mathbf{u}_{rel}(x, t) = \frac{\partial a}{\partial t} + \nabla_x a \cdot \frac{\partial x(x_0, t)}{\partial t} = \frac{da(x, t)}{dt}
\]  

(A2)

Now consider the volumetric integral of a conserved quantity \(a(x, t)\), given by:

\[
\hat{a}(t) = \iiint_{\Omega(t)} a(x, t) \, dV
\]  

(A3)

where \(dV = d^3x = dx dy dz\) is an infinitesimal volume element and \(\Omega(t)\) is the time-varying volumetric domain. Since \(\hat{a}(t)\) is a function only of time, it is possible to write its total derivative as:

\[
\frac{d\hat{a}(t)}{dt} = \frac{d}{dt} \iiint_{\Omega(t)} a(x, t) \, dV = \lim_{\Delta t \to 0} \frac{1}{\Delta t} \left[ \iiint_{\Omega(t+\Delta t)} a(x, t+\Delta t) \, dV - \iiint_{\Omega(t)} a(x, t) \, dV \right]
\]  

(A4)

The second form follows by definition of the derivative, with \(\Omega(t + \Delta t)\) interpreted as the fluid volume (relative to the moving domain) at time \(t + \Delta t\). By a Taylor expansion [24]:

\[
a(x, t + \Delta t) = a(x, t) + \frac{\partial a(x, t)}{\partial t} \Delta t + \frac{1}{2} \frac{\partial^2 a(x, t)}{\partial t^2} (\Delta t)^2 + ...
\]  

(A5)

Substitution into (A4) gives

\[
\frac{d\hat{a}(t)}{dt} = \lim_{\Delta t \to 0} \frac{1}{\Delta t} \left[ \iiint_{\Omega(t+\Delta t)} \left( a(x, t) + \frac{\partial a(x, t)}{\partial t} \Delta t + \frac{1}{2} \frac{\partial^2 a(x, t)}{\partial t^2} (\Delta t)^2 + ... \right) \, dV - \iiint_{\Omega(t)} a(x, t) \, dV \right]
\]

\[
= \lim_{\Delta t \to 0} \frac{1}{\Delta t} \iiint_{\Omega(t+\Delta t)} \frac{\partial a(x, t)}{\partial t} \Delta t \, dV + \frac{1}{\Delta t} \left[ \iiint_{\Omega(t+\Delta t)} a(x, t) \, dV - \iiint_{\Omega(t)} a(x, t) \, dV \right]
\]

\[
= \iiint_{\Omega(t)} \frac{\partial a(x, t)}{\partial t} \, dV + \lim_{\Delta t \to 0} \frac{1}{\Delta t} \iiint_{\Omega(t+\Delta t)-\Omega(t)} a(x, t) \, dV
\]  

(A6)

Note the second-order and higher derivatives vanish in the limit.

We see that the second integral reduces to that of a thin domain (of variable sign) adjacent to the boundary, created by motion of the fluid (relative to the domain) between \(t\) and \(t + \Delta t\). To examine this, consider a volume element \(dV\) in this boundary region, illustrated schematically in Figure 2(b) [after 23–27, 60]. At time \(t\), the rate of change of fluid position relative to the boundary is \(d\mathbf{x}(x_0, t)/dt = \mathbf{u}_{rel}\). In time \(\Delta t\), this will induce the displacement \(\mathbf{u}_{rel}\Delta t\) in the direction of \(\mathbf{u}_{rel}\). The volumetric element \(dV\) is therefore the inclined cylinder formed by projection of the boundary element \(dA\) over the inclined distance \(\mathbf{u}_{rel}\Delta t\). Accounting for its height in the direction of the outward unit normal \(\mathbf{n}\),
this gives the intrinsic length \( d\ell = u_{rel} \Delta t \cdot n \), hence \( dV = d\ell dA = u_{rel} \Delta t \cdot n \, dA \) (in principle, of either sign). Thus (A6) reduces to

\[
\frac{d\hat{a}(t)}{dt} = \iiint_{\Omega(t)} \frac{\partial a(x,t)}{\partial t} \, dV + \lim_{\Delta t \to 0} \frac{1}{\Delta t} \iiint_{\partial \Omega(t)} a(x,t) \, u_{rel} \Delta t \cdot n \, dA
\]

\[
= \iiint_{\Omega(t)} \frac{\partial a(x,t)}{\partial t} \, dV + \iiint_{\partial \Omega(t)} a(x,t) \, u_{rel} \cdot n \, dA
\]  

(A7)

where \( \partial \Omega(t) \) is the domain boundary. This gives the first form of the Reynolds transport theorem in (1). The second form in (1) is obtained by the divergence theorem. \( \square \)

**Proof 2: Lagrangian Coordinate Transformation**

For the second proof, we follow [21, 29] and consider Lagrangian coordinates \( x_0 = [x_0, y_0, z_0]^T \) with the fixed original domain \( \Omega(t_0) \). Rewriting the first two parts of (A4) in Lagrangian coordinates gives

\[
\frac{d\hat{a}(t)}{dt} = \frac{d}{dt} \iiint_{\Omega(t)} a(x,t) \, dV = \frac{d}{dt} \iiint_{\partial \Omega(t_0)} a(x_0(t),t) \left| \frac{\partial x}{\partial x_0} \right| \, dV_0
\]  

(A8)

where \( V_0 = dx_0 dy_0 dz_0 \) and \( \left| \frac{\partial x}{\partial x_0} \right| \) is the determinant of the Jacobian matrix of Eulerian with respect to Lagrangian coordinates. The domain in the last part of (A8) is now independent of time, so the derivative can be brought inside the integral. Furthermore, since fluid elements are unique and indivisible, the Jacobian \( \frac{\partial x}{\partial x_0} \) will be non-singular and its determinant everywhere non-zero. The derivative of the determinant, in the moving frame of reference, is [21, 61]:

\[
\frac{d}{dt} \left| \frac{\partial x}{\partial x_0} \right| = \left| \frac{\partial x}{\partial x_0} \right| \nabla_x \cdot \left( \frac{\partial x}{\partial t} \right)_{rel} = \left| \frac{\partial x}{\partial x_0} \right| \nabla_x \cdot u_{rel}
\]  

(A9)

Expanding (A8) using (A2) and (A9), and then reverting back to the variable domain, gives:

\[
\frac{d\hat{a}(t)}{dt} = \iiint_{\Omega(t)} \left[ \left( \frac{\partial a}{\partial t} + (\nabla_x a) \cdot u_{rel} \right) \left| \frac{\partial x}{\partial x_0} \right| + a \left| \frac{\partial x}{\partial x_0} \right| \nabla_x \cdot u_{rel} \right] \, dV_0
\]

\[
= \iiint_{\Omega(t)} \left[ \frac{\partial a}{\partial t} + (\nabla_x a) \cdot u_{rel} + a \nabla_x \cdot u_{rel} \right] \, dV
\]  

(A10)

This is identical to the second form of the Reynolds transport theorem in (1). The first form is then obtained by the divergence theorem. \( \square \)
Appendix B: Proof of Double Implication

We first examine the forward implication ($\Rightarrow$) between Reynolds commutativity (9) and the Liouville equation (10). Setting $\frac{d[J\alpha]}{dt} = \frac{d\alpha}{dt}$ gives

$$0 = \iiint_{\Omega(t)} \alpha \left( \frac{\partial p}{\partial t} + \nabla_x \cdot (p u_{rel}) \right) d^3x$$

(B1)

Since the differential $d^3x$ is in principle non-zero, and invoking the fundamental lemma of the calculus of variations – thus for continuous and continuously differentiable functions $\alpha(x,t)$ – the square bracketed term must vanish, giving the Liouville equation (10). The reverse implication ($\Leftarrow$) follows directly from substitution of $\partial p/\partial t + \nabla_x \cdot (p u_{rel}) = 0$ into (8). $\Box$

Appendix C: Reynolds Averages and the Liouville Equation

As defined by Reynolds [2, 3] and later workers [e.g. 4], the Reynolds average of a set of observables $\{a_1, a_2, \ldots\}$, often denoted with an overbar $\bar{a}$, is a statistical (probabilistic) measure of central tendency which satisfies the following conditions or axioms [4]:

$$a + b = \bar{a} + \bar{b}, \quad ka = k\bar{a}, \quad \left( \frac{\partial a}{\partial s} \right) = \frac{\partial \bar{a}}{\partial s}, \quad \bar{ab} = \bar{a}\bar{b}$$

(C1)

where $a$ and $b$ refer to two compatible groups of observables, $k$ is a constant and $s$ is a parameter. Other equivalent choices of axioms are also possible [e.g 4]. For observables with multivariate dependencies, we could rewrite the third condition in terms of the differential:

$$\bar{a} + \bar{b} = \bar{a} + \bar{b}, \quad ka = k\bar{a}, \quad da = d\bar{a}, \quad \bar{ab} = \bar{a}\bar{b}$$

(C2)

Commonly, $\bar{a}$ or $\bar{b}$ are interpreted as time averages. However, for an infinite domain of integration, it is clear that any probabilistic expectation will also satisfy the Reynolds conditions (C1)-(C2), for example the volumetric mean defined in (6) as a function of time, or the ensemble mean defined in (21) as a function of three-dimensional position.

For non-infinite, functionally dependent domains of integration, the consistency between an expectation and the third Reynolds condition in (C1) or (C2) might be thought to be problematic. However, from the analyses in §II B and §III B, in particular from (8)-(9) and (24)-(25), we can conclude that even in these circumstances, expected values can satisfy the properties of a Reynolds average, provided the observable is continuous and continuously differentiable. Furthermore, the existence of a Reynolds average is then equivalent to the existence of a Liouville equation for the underlying joint-conditional probability density function for the system.

Appendix D: Proofs of the Spatial Reynolds Transport Theorem

We now provide two proofs of the spatial Reynolds transport theorem (16) for time-independent flows, based respectively on arguments from continuum mechanics and a coordinate transformation method. These follow the essential details of the temporal proofs in Appendix A.
Proof 1: Continuum Mechanics (Steady Flow)

FIG. 3. Schematic diagrams showing the $i$th component of (a) a velocity gradient field for steady flow in a velocimetric domain, and (b) a velocity volume element on the domain boundary induced by the tensor field.

For the first proof we again make the continuum assumption, and consider an Eulerian phase space (volumetric and velocimetric) description of fluid flow, in which each conserved fluid property $b(u, x)$ can be represented as a local function of velocity $u = \begin{bmatrix} u, v, w \end{bmatrix}^\top$ and position $x = \begin{bmatrix} x, y, z \end{bmatrix}^\top$. This representation assumes time-independent flow, for example a steady velocity field, although in the probabilistic formulation this can be relaxed to consider statistical rather than strict stationarity. We also consider an alternative description in which the velocity at each point $u^R(u_0, x)$ is a function of the velocity $u_0$ at some reference location $x_0$, while the spatial coordinates $x$ are independent variables. The two descriptions are united by the equivalence of the velocity gradient tensor:

$$\frac{\partial u^R}{\partial x}(u_0, x) = G(u, x) \quad (D1)$$

As with the temporal analysis, we also incorporate a spatially varying velocimetric domain $D(x)$ which undergoes a changing reference velocity gradient $G_D(x)$, giving the relative gradient $G_{rel} = G - G_D(x)$. A set of field lines for such a system - for example in one spatial coordinate of the tensor - is illustrated schematically in Figure 3(a).

Consider the integral of the conserved local quantity $b(u, x)$, a function of both velocity and position, over the velocity domain:

$$\hat{b}(x) = \iiint_{D(x)} b(u, x) \, dU \quad (D2)$$

where $dU = d^3u = du \, dv \, dw$ is the velocity volume element. Since $\hat{b}(x)$ is multivariate, it is not possible to define the total derivative, but we can directly consider its differential:

$$\hat{d}b(x) = \sum_{i=1}^{3} \frac{\partial \hat{b}(x)}{\partial x_i} \, dx_i = \sum_{i=1}^{3} \frac{\partial}{\partial x_i} \left[ \iiint_{D(x)} b(u, x) \, dU \right] \, dx_i \quad (D3)$$
where \( x_i \in [x_1, x_2, x_3] \). Each partial derivative is, by definition:

\[
\frac{\partial \tilde{b}(\mathbf{x})}{\partial x_i} = \lim_{\Delta x_i \to 0} \frac{1}{\Delta x_i} \left[ \iint_{\mathcal{D}(x + \Delta x_i)} b(\mathbf{u}, \mathbf{x} + \Delta x_i) dU - \iint_{\mathcal{D}(x)} b(\mathbf{u}, \mathbf{x}) dU \right]
\]  

(D4)

where we use the notation \((x + \Delta x)\) to indicate \((x + \Delta x, y, z), (x, y + \Delta y, z)\) or \((x, y, z + \Delta z)\) respectively for \( x_i \in [x_1, x_2, x_3] \). \( \mathcal{D}(\mathbf{x} + \Delta x_i) \) is then interpreted as the velocity domain shifted to position \( \mathbf{x} + \Delta x_i \). By a one-dimensional Taylor expansion – or a multi-dimensional expansion with non-zero translation in only one coordinate – we obtain [24]:

\[
b(\mathbf{u}, \mathbf{x} + \Delta x_i) = b(\mathbf{u}, \mathbf{x}) + \frac{\partial b(\mathbf{u}, \mathbf{x})}{\partial x_i} \Delta x_i + \frac{1}{2} \frac{\partial^2 b(\mathbf{u}, \mathbf{x})}{\partial x_i^2} (\Delta x_i)^2 + ...
\]

(D5)

Substitution into (D4) gives

\[
\frac{\partial \tilde{b}(\mathbf{x})}{\partial x_i} = \lim_{\Delta x_i \to 0} \frac{1}{\Delta x_i} \left[ \iint_{\mathcal{D}(x + \Delta x_i)} \left( b(\mathbf{u}, \mathbf{x}) + \frac{\partial b(\mathbf{u}, \mathbf{x})}{\partial x_i} \Delta x_i + \frac{1}{2} \frac{\partial^2 b(\mathbf{u}, \mathbf{x})}{\partial x_i^2} (\Delta x_i)^2 + ... \right) dU - \iint_{\mathcal{D}(x)} b(\mathbf{u}, \mathbf{x}) dU \right]
\]

\[
= \lim_{\Delta x_i \to 0} \frac{1}{\Delta x_i} \left[ \iint_{\mathcal{D}(x + \Delta x_i)} \frac{\partial b(\mathbf{u}, \mathbf{x})}{\partial x_i} dU + \lim_{\Delta x_i \to 0} \frac{1}{\Delta x_i} \left[ \iint_{\mathcal{D}(x + \Delta x_i)} b(\mathbf{u}, \mathbf{x}) dU - \iint_{\mathcal{D}(x)} b(\mathbf{u}, \mathbf{x}) dU \right] \right]
\]

\[
= \iint_{\mathcal{D}(x)} \frac{\partial b(\mathbf{u}, \mathbf{x})}{\partial x_i} dU + \lim_{\Delta x_i \to 0} \frac{1}{\Delta x_i} \left[ \iint_{\mathcal{D}(x + \Delta x_i) - \mathcal{D}(x)} b(\mathbf{u}, \mathbf{x}) dU \right]
\]

(D6)

where again the second-order and higher derivatives vanish in the limit.

We again see that the second integral reduces to that of a thin domain (of variable sign) in velocimetric space adjacent to the boundary, created by translation of the field (relative to the domain) between \( \mathbf{x} \) and \( \mathbf{x} + \Delta x_i \). Consider a velocimetric element \( dU \) in this boundary region, illustrated schematically in Figure 3(b), with spatial displacement in only one component \( x_i \in [x_1, x_2, x_3] \). At position \( \mathbf{x} \), the velocity gradient relative to the boundary \( \partial \mathcal{D} \) is \( \mathbf{G}_{rel,i} \). Over the distance \( \Delta x_i \), this will induce the change in velocity \( \mathbf{G}_{rel,i} \Delta x_i \) in the direction described by \( \mathbf{G}_{rel,i} \). The velocimetric element \( dU \) is therefore the inclined cylinder formed by projection of the boundary element \( dS \) over the inclined distance \( \mathbf{G}_{rel,i} \Delta x_i \). Accounting for its height in the direction of the outward unit normal \( \mathbf{n}_S \), this gives the intrinsic length \( d\ell_S = \mathbf{G}_{rel,i} \Delta x_i \cdot \mathbf{n}_S \), hence \( dU = d\ell_S dS = \mathbf{G}_{rel,i} \Delta x_i \cdot \mathbf{n}_S dS \) (in principle, of either sign). Thus (D6) reduces to

\[
\frac{\partial \tilde{b}(\mathbf{x})}{\partial x_i} = \iint_{\mathcal{D}(x)} \frac{\partial b(\mathbf{u}, \mathbf{x})}{\partial x_i} dU + \lim_{\Delta x_i \to 0} \frac{1}{\Delta x_i} \left[ \iint_{\partial \mathcal{D}(x)} b(\mathbf{u}, \mathbf{x}) \mathbf{G}_{rel,i} \Delta x_i \cdot \mathbf{n}_S dS \right]
\]

(D7)

Assembling these into (D3), we obtain the differential

\[
d\tilde{b}(\mathbf{x}) = \sum_{i=1}^{3} \left[ \iint_{\partial \mathcal{D}(x)} \frac{\partial b(\mathbf{u}, \mathbf{x})}{\partial x_i} dU + \iint_{\partial \mathcal{D}(x)} b(\mathbf{u}, \mathbf{x}) \mathbf{G}_{rel,i} \cdot \mathbf{n}_S dS \right] dx_i
\]

(D8)
The divergence theorem can be extended (strictly, in the form of Stokes’ theorem) to any
metric space [e.g. 62]. Applying its three-dimensional velocimetric formulation then gives:

\[ \begin{aligned}
\vec{d}\vec{b}(\vec{x}) = \sum_{i=1}^{3} \left[ \int_{\partial D(\vec{x})} \left( \frac{\partial b(u, \vec{x})}{\partial x_i} + \nabla u \cdot (b(u, \vec{x}) \mathbf{G}_{rel,i}) \right) dU \right] dx_i
\end{aligned} \] (D9)

Reverting to \( d^2 \mathbf{u} = dU, \ d^2 \mathbf{u} = \mathbf{n}_S \cdot dS \) and adopting vector and tensor notation, based
on the gradient convention used herein, eqs. (D8)-(D9) give the spatial Reynolds transport
theorem in (16). □

**Alternative proof:** A more direct proof is to recognise \( \vec{d}\vec{b}(\vec{x}) \) in (D3) as the directional
derivative \( D_r \vec{b}(\vec{x}) = \nabla_\vec{x} \vec{b}(\vec{x}) \cdot \vec{r} \), in the direction of the differential vector \( \vec{r} = d\vec{x} \). By
definition:

\[ \begin{aligned}
D_{dx} \vec{b}(\vec{x}) = \lim_{h \to 0} \frac{\vec{b}(\vec{x} + h \vec{d}\vec{x}) - \vec{b}(\vec{x})}{h} = \lim_{h \to 0} \frac{1}{h} \left[ \int_{\partial D(\vec{x}+h \vec{d}\vec{x})} b(u, \vec{x} + h \vec{d}\vec{x}) dU - \int_{\partial D(\vec{x})} b(u, \vec{x}) dU \right]
\end{aligned} \] (D10)

Using a multidimensional Taylor expansion:

\[ \begin{aligned}
b(u, \vec{x} + h \vec{d}\vec{x}) = b(u, \vec{x}) + h \vec{d}\vec{x} \cdot \nabla \vec{x} b(u, \vec{x}) + \frac{h^2}{2} \vec{d}\vec{x} \cdot \nabla_x^2 b(u, \vec{x}) d\vec{x} + ...
\end{aligned} \] (D11)

where \( \nabla_x^2 = \nabla \vec{x} (\nabla \vec{x})^\top \) is the second derivative or Hessian operator, we obtain:

\[ \begin{aligned}
D_{dx} \vec{b}(\vec{x}) &= \lim_{h \to 0} \frac{1}{h} \left[ \int_{\partial D(\vec{x}+h \vec{d}\vec{x})} \left( b(u, \vec{x}) + h \vec{d}\vec{x} \cdot \nabla \vec{x} b(u, \vec{x}) + \frac{h^2}{2} \vec{d}\vec{x} \cdot \nabla_x^2 b(u, \vec{x}) d\vec{x} + ... \right) dU \right] \\
&\quad - \int_{\partial D(\vec{x})} b(u, \vec{x}) dU \\
&= \lim_{h \to 0} \frac{1}{h} \left[ \int_{\partial D(\vec{x}+h \vec{d}\vec{x})} h \vec{d}\vec{x} \cdot \nabla \vec{x} b(u, \vec{x}) dU + \frac{1}{h} \left[ \int_{\partial D(\vec{x}+h \vec{d}\vec{x})} b(u, \vec{x}) dU - \int_{\partial D(\vec{x})} b(u, \vec{x}) dU \right] \right] \\
&\quad + \int_{\partial D(\vec{x})} b(u, \vec{x}) dU \\
&= \int_{\partial D(\vec{x})} \vec{d}\vec{x} \cdot \nabla \vec{x} b(u, \vec{x}) dU + \lim_{h \to 0} \frac{1}{h} \left[ \int_{\partial D(\vec{x}+h \vec{d}\vec{x})} b(u, \vec{x}) dU - \int_{\partial D(\vec{x})} b(u, \vec{x}) dU \right]
\end{aligned} \] (D12)

where again the second and higher derivatives vanish. The analysis uses the same directional
argument as before, now in resultant form \( dU = h \vec{d}\vec{x} \cdot \mathbf{G}_{rel} \cdot \mathbf{n}_S dS \), giving the limit

\[ \begin{aligned}
\vec{d}\vec{b}(\vec{x}) = D_{dx} \vec{b}(\vec{x}) = \int_{\partial D(\vec{x})} \vec{d}\vec{x} \cdot \nabla \vec{x} b(u, \vec{x}) dU + \int_{\partial D(\vec{x})} b(u, \vec{x}) \vec{d}\vec{x} \cdot \mathbf{G}_{rel} \cdot \mathbf{n}_S dS
\end{aligned} \] (D13)

This is identical to (D8) and the first part of (16). □
Proof 2: Reference Velocity Coordinate Transformation

For the second proof, we consider the alternative description based on a reference set of velocity coordinates \( \mathbf{u}_0 = [u_0, v_0, w_0]^\top \) in a spatially fixed velocity domain \( D(x_0) \). Rewriting the left hand side of (D3) gives

\[
\hat{b}(x) = \sum_{i=1}^{3} \frac{\partial}{\partial x_i} \left[ \iiint_{D(x)} b(\mathbf{u}, x) \, dU \right] \, dx_i = \sum_{i=1}^{3} \frac{\partial}{\partial x_i} \left[ \iiint_{D(x_0)} b(\mathbf{u}(\mathbf{u}_0, x), x) \, \left| \frac{\partial \mathbf{u}}{\partial \mathbf{u}_0} \right| \, dU \right] \, dx_i \tag{D14}
\]

where \( dU_0 = du_0 \, dv_0 \, dw_0 \) and \( \left| \frac{\partial \mathbf{u}}{\partial \mathbf{u}_0} \right| \) is the Jacobian determinant for this coordinate transformation. For the class of time-independent flow systems examined here, we consider the Jacobian \( \frac{\partial \mathbf{u}}{\partial \mathbf{u}_0} \) to be non-singular. Using the velocity analog of the relation (A9) for independent spatial coordinates \( x \):

\[
\frac{\partial}{\partial x_i} \left| \frac{\partial \mathbf{u}}{\partial \mathbf{u}_0} \right| = \left| \frac{\partial \mathbf{u}}{\partial \mathbf{u}_0} \right| \nabla \mathbf{u} \cdot \mathbf{G}_{\text{rel,i}} \tag{D15}
\]

then from (D14)

\[
\hat{b}(x) = \sum_{i=1}^{3} \left[ \iiint_{D(x_0)} \left\{ \left( \frac{\partial b}{\partial x_i} + (\nabla \mathbf{u} b) \cdot \mathbf{G}_{\text{rel,i}} \right) \left| \frac{\partial \mathbf{u}}{\partial \mathbf{u}_0} \right| + b \left| \frac{\partial \mathbf{u}}{\partial \mathbf{u}_0} \right| \nabla \mathbf{u} \cdot \mathbf{G}_{\text{rel,i}} \right\} dU_0 \right] \, dx_i \tag{D16}
\]

This gives the second form of the spatial Reynolds transport theorem in (16), with the first form obtained by Gauss’ divergence theorem in velocity space. \( \square \)

Appendix E: Definitions and Proof of the Multiparameter Reynolds Transport Theorem in Exterior Calculus

We now prove the multiparameter Reynolds Transport Theorem for differential forms (34), based on multiparameter extensions of exterior calculus operators and the proof of the one-parameter case [e.g., 21; 22, eqs. 0.49 and 4.33-4.34]. Excellent reviews of the tools of existing (one-parameter) exterior calculus are available in a number of monographs [e.g. 22, 63–68].

Consider an \( n \)-dimensional differentiable manifold \( M^n \subseteq \mathbb{R}^n \), described using local coordinates \( \mathbf{X} = [X_1, \ldots, X_n]^\top \) defined in some neighbourhood \( N(s) \) of each point \( s \in M^n \). Let \( \mathbf{V} \) be a vector or tensor field on the manifold, which is independent of the \( m \)-dimensional vector of parameters \( \mathbf{C} = [C_1, \ldots, C_m]^\top \) (which could include time \( t \)). This field will create the \( m \)-parameter “flow” within the manifold, defined by the map [compare 63, chap. 1; 64, §3.3; 66, §2.1; 22, §1.4];

\[
\phi : M^n \times \mathbb{R}^m \rightarrow M^n \times \mathbb{R}^m \tag{E1}
\]
such that, respectively in vector form (using the $\partial(\rightarrow)/\partial(\downarrow)$ convention) or in terms of the components $s_i \in s$ and $C_c \in C$:

$$
\left( \frac{\partial \phi(s, C)}{\partial C} \right)^\top = V(s) \quad \text{and} \quad \frac{\partial \phi(s, C_c)}{\partial C_c} = V_{ic}
$$

Since (by construction) the flow is independent of $C$, $\phi$ will satisfy the following properties for all $s \in M^n$ and all $B, C \in \mathbb{R}^m$ [c.f. 63; 66; 22]:

$$
\phi(s, 0) = s \\
\phi(\phi(s, C), B) = \phi(s, B + C)
$$

By previous custom for the one-parameter case, we write this as the bijection (diffeomorphism) [c.f. 63; 66; 22];

$$
\phi^C : M^n \rightarrow M^n, \quad \phi^C(s) = \phi(s, C)
$$

which is therefore invertible, and operates linearly $\phi^{C+B} = \phi^{C} \circ \phi^{B} = \phi^{B} \circ \phi^{C}$. Thus if the manifold contains an $r$-dimensional oriented compact submanifold $\Omega^r \subset M^n$, each point in the submanifold at $C$ can be mapped to that at $C = 0$ by $\Omega^r(C) = \phi^C \Omega^r(0)$, and vice versa $\Omega^r(0) = \phi^{-C} \Omega^r(C)$. Informally, we might describe $\Omega^r(C)$ as a “moving domain” and the map $\phi^C$ as a “movement”, although they each involve a transformation in the parameter vector $C$ (such as in spatial coordinates) – reflecting the symmetries of the vector or tensor field – rather than necessarily in physical time.

Now consider the $r$-form $\omega^r$, a linear function defined on the cotangent space of the manifold $M^n$. This can be written as [e.g., 63, chap. 1; 64, §1.1; 65, §A.3]4:

$$
\omega^r = \sum_{j_1 < \ldots < j_r} w_{j_1 \ldots j_r} \ dX_{j_1} \wedge \ldots \wedge dX_{j_r}
$$

where $w_{j_1 \ldots j_r}$ are scalars (possibly functions of $X$), $\wedge$ is the exterior or wedge product and the $dX_{j_k}$ are an ordered selection of $r$ terms from the vectors $dX = [dX_1, \ldots, dX_n]^\top$, with the sum taken over all increasing combinations of the $dX_{j_k}$. Physically, the wedge product $dX_{j_1} \wedge \ldots \wedge dX_{j_r}$ is the oriented volume of an infinitesimal $r$-dimensional parallelepiped.

Integration of $\omega^r$ over the submanifold $\Omega(C) \subset M^n$:

$$
W(C) = \int_{\Omega(C)} \omega^r
$$

therefore gives the total oriented quantity $W(C)$ in the submanifold, as a function of its parameters $C$. The $r$-form formalism thus extends standard multivariate calculus to the analysis of oriented areas and volumes on manifolds, using a patchwork of local coordinate systems.

For a smooth (infinitely differentiable) map $f : M^n \rightarrow N^\ell$ between smooth manifolds $M^n$ and $N^\ell$ (for $\ell, n \in \mathbb{N}$), there exists an important theorem that a smooth $r$-form $\omega^r$ on $N^\ell$

---

3 For tensor fields, it may be convenient to represent the manifold using higher-order coordinates $s \in \mathbb{R}^{n_1} \times \ldots \times \mathbb{R}^{n_k}$. For example, the shear stress tensor $\tau$, represented with second order elements $\tau_{ij} \in M^{3 \times 3} \subseteq \mathbb{R}^{3 \times 3}$, can be used to define the third-order tensor field $\partial \tau / \partial C$ with elements $V_{ijr} = \partial \tau_{ij} / \partial C_r$.

4 Note many references adopt the implied summation convention for this and subsequent equations; we do not do so here.
can be mapped to a smooth $r$-form $f^*\omega^r$ on $M^n$, where $f^*$ is known as the pullback [e.g., 22, §2.7]. In consequence, assuming smoothness, the multiparametric diffeomorphism $\phi^C$ defined in (E4) can be used to define a vector pullback $\phi^C$, providing an invertible coordinate transformation between $M^n$ and itself in the $C$ direction (with inverse $\phi^{-C}$, known as the pushforward). Formally, we define [compare 65, §5.5; 22, §0j and §2.7; 68, §3.2]:

$$\phi^C \omega^r = \sum_{j_1<\ldots<j_r} (w_{j_1<\ldots<j_r} \cdot \phi^C) \frac{d\phi^C_{j_1}}{\partial} \ldots \frac{d\phi^C_{j_r}}{\partial}$$ (E7)

$$= \sum_{j_1<\ldots<j_r} \sum_{k_1<\ldots<k_r} (w_{j_1\ldots j_r} \cdot \phi^C) \left( \frac{\partial(\phi^C_{j_1}, \ldots, \phi^C_{j_r})}{\partial(X_{k_1}, \ldots, X_{k_r})} \right) \frac{dX_{k_1}}{\partial} \ldots \frac{dX_{k_r}}{\partial}$$ (E8)

where $|\partial(\phi^C_{j_1}, \ldots, \phi^C_{j_r})/\partial(X_{k_1}, \ldots, X_{k_r})|$ is the determinant of the Jacobian matrix between the two coordinate systems, without change of sign. We see that the pullback $\phi^C$ satisfies linearity, and enables an $r$-form at $C$ to be mapped back to $C = 0$, or vice versa using the pushforward $\phi^C$.

We next consider the exterior derivative, which when applied to an $r$-form gives [e.g., 63, chap. 1; 64, §3.2; 65, §A.3; 22, §2.6]:

$$d\omega^r = \sum_{j_1<\ldots<j_r} dw_{j_1\ldots j_r} \cdot dX_{j_1} \ldots dX_{j_r}$$ (E9)

Since the integral (E6) is a 0-form, its exterior derivative is its differential:

$$dW(C) = \sum_{c=1}^m \frac{\partial W}{\partial C_c} \bigg|_{C_k \neq C_c} dC_c = \frac{\partial W}{\partial C} \cdot dC = \frac{\partial(\int_{\Omega(0)} \phi^C \omega^r)}{\partial C} \cdot dC$$ (E10)

which indicates the terms $C_k$, for all $k \neq c$, are held constant in each partial derivative, and which uses the standard dot product. To simplify, the variable domain of integration can be converted to a fixed domain via the pullback:

$$dW(C) = \frac{\partial(\int_{\Omega(0)} \phi^C \omega^r)}{\partial C} \cdot dC = \sum_{c=1}^m \frac{\partial(\int_{\Omega(0)} \phi^C \omega^r)}{\partial C_c} \bigg|_{C_k \neq C_c} dC_c$$ (E11)

using the reference position $C = 0$, in the (relative) coordinate system chosen for $C$. For each component in (E11), from the definition of the partial derivative and the linearity of the pullback (E8):

$$\frac{\partial}{\partial C_c} \int_{\Omega(0)} \phi^C \omega^r = \lim_{h \to 0} \frac{\int_{\Omega(0)} \phi^C(C_c+h) \omega^r - \int_{\Omega(0)} \phi^C \omega^r}{h}$$

$$= \lim_{h \to 0} \int_{\Omega(0)} \phi^C(C_c) \frac{\omega^r - \omega^r}{h}$$

$$= \int_{\Omega(C_c)} \left\{ \lim_{h \to 0} \frac{(\phi^C(C_c) \omega^r - \omega^r)}{h} \right\}$$ (E12)

where the last step converts back to a variable domain using the pushforward $\phi^C_{C_c}$. The term in braces is the Lie derivative $L_{V_c}$ with respect to the column vector field $V_c \in V$.
associated with the flow $\phi^{C_c} \in \phi^{C}$, based on the increment $h$ in the one-dimensional flow parameter $C_c$ [66, §2.2; 22, §4.3a]. Taking a cue from the directional derivative (see Appendix D), this could equivalently be defined in terms of the pullback $\phi^{\cdot h d C_c}$ and written as $\mathcal{L}_{V}^{(C_c)}$, to explicitly identify the direction $C_c$. In consequence, we can define an $m$-dimensional multiparameter Lie derivative of an $r$-form with respect to $V$ over parameter $C$ by:

$$\mathcal{L}_{V}^{(C)} \omega^r = [\mathcal{L}_{V}^{(C_1)}, ..., \mathcal{L}_{V}^{(C_m)}]^\top \omega^r = \lim_{h \to 0} \left[ \frac{\phi^{\cdot h d C_1} \omega^r - \omega^r}{h}, ..., \frac{\phi^{\cdot h d C_m} \omega^r - \omega^r}{h} \right]^\top$$

(E13)

Assembling (E6)-(E13) then gives:

$$dW(C) = d \int_{\Omega(C)} \omega^r = \left[ \int_{\Omega(C)} \mathcal{L}_{V}^{(C)} \omega^r \right] \cdot dC$$

(E14)

This is the first part of (34).

Finally, we consider the one-parameter interior product, which effects the contraction of an $r$-form to an $(r-1)$-form, given by [e.g., 63, chap. 1; 65, §A.3; 22, §2.9]:

$$i_U \omega^r = \sum_{j_2 < ... < j_r} \sum_k U_k w_{k,j_2...j_r} dX_{j_2} \wedge ... \wedge dX_{j_r}$$

(E15)

based on components $U_k$ of a one-parameter vector field $U$ with implicit parameter $t$. This was shown by Cartan to satisfy the equation $\mathcal{L}_U \omega^r = i_U d\omega^r + d(i_U \omega^r)$ [e.g., 64, §5.8; 65, §A.3; 22, §4.2b]. By component-wise extension, it is possible to define a multiparameter interior product based on the field $V$ with parameters $C$:

$$i_V^{(C)} \omega^r = \left[ i_V^{(C_1)} \omega^r, ..., i_V^{(C_m)} \omega^r \right]^\top = \sum_{j_2 < ... < j_r} \sum_k V_k^\top w_{k,j_2...j_r} dX_{j_2} \wedge ... \wedge dX_{j_r}$$

(E16)

based on row vectors $V_k \in V$. By construction, this satisfies a multiparameter Cartan equation $\mathcal{L}_V^{(C)} \omega^r = i_V^{(C)} d\omega^r + d(i_V^{(C)} \omega^r)$. Using this result, and the exterior calculus expression of Stokes’ theorem $\int_{\Omega(C)} d\omega^r = \oint_{\partial \Omega(C)} \omega^r$ [e.g., 65, §5.5; 67, §6.2; 22, §3.3b], we obtain the third and fourth terms in (34). □

The above proof invokes $m$-parameter vector extensions of “flow” (E1)-(E4), the pullback (E8) and pushforward, the Lie derivative (E13) and the interior product (E16), which follow naturally from their one-parameter definitions. The $r$-form, exterior derivative and dot product are unchanged. The proof also extends naturally to higher-order tensor fields and to vector- or tensor-valued differential forms, by component-wise application of operators, in the same manner as does the traditional Reynolds transport theorem (1). It also can be extended to a parametric condition tensor $C$, if desired, using an element-wise (Hadamard) tensor product, or alternatively by the use of trace or higher-order diagonal operators on matrix products (such as in the Frobenius inner product). The parametric formulation of the Reynolds transport theorem (37) is obtained from (34) by substitution of vector operators, or can be derived directly using multidimensional extensions of the analyses in Appendices A and D.
Appendix F: Probability $r$-forms

There is a complication in the definition of probability $r$-forms, due to the question of orientation [e.g. 69, §11.4; 70]. We here adopt the definition:

$$\rho^r = \sum_{j_1 < \ldots < j_r} b_{j_1 \ldots j_r} dX_{j_1} \wedge \ldots \wedge dX_{j_r}$$  \hspace{1cm} (F1)

where $b_{j_1 \ldots j_r}$ are scalars and the $dX_{j_k}$ are an ordered selection of $r$ vectors from $[dX_1, \ldots, dX_n]^\top$. This definition is made subject to local and global constraints, respectively:

$$\rho^r \geq 0, \quad \forall s \in M^n$$

$$\int_{\Omega(C)} \rho^r = 1, \quad \forall \Omega(C) \in M^n$$  \hspace{1cm} (F2)

To satisfy these constraints, we define (F1)-(F2) only for an oriented compact submanifold $\Omega(C)$ within an orientable manifold $M^n$, and preclude non-orientable manifolds [69]. Furthermore, the choices of the $b_{j_1 \ldots j_r}$ terms and/or the combinations of $dX_{j_k}$ may need to be restricted with respect to the orientation of the submanifold $\Omega(C)$ to satisfy the constraints. The $b_{j_1 \ldots j_r}$ terms can then be interpreted as connected segments or portions of a joint-conditional pdf $\hat{p}(s|C)$ defined over all points $s \in \Omega(C)$ in the submanifold, with local coordinate system $X(s)$, subject to the conditions $C$.

The nonnegativity constraint in (F2) can be achieved in several ways: a brute force method would be to take $\rho^r$ as the absolute and normalised value of some $r$-form $\nu^r$ defined over the manifold. A broader method would be to impose equivalence of signs $\text{sign}(b_{j_1 \ldots j_r}) = \text{sign}(dX_{j_1} \wedge \ldots \wedge dX_{j_r})$, ensuring non-negative terms in the sum. An even broader method would be to allow negative local terms $b_{j_1 \ldots j_r} < 0$ and oriented volume elements $dX_{j_1} \wedge \ldots \wedge dX_{j_r} < 0$, so long as the constraints (F2) are satisfied in the sum (F1).

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