Vorticity and symplecticity in Lagrangian fluid dynamics

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The relationship between potential vorticity (PV) and the symplectic form for the Lagrangian form of the shallow water equations and its implications are considered. Starting with the symplectic form, the PV is found by the pull-back operation to the reference space. At first sight, the encoding of PV in the symplectic form appears to be independent of the particle relabelling symmetry. We carry the analysis a step further in two ways. Using the conservation of symplecticity as a starting point, the fluxes of symplecticity are differential forms, and a complete pull-back of the flux forms leads to a geometric description of PV conservation. Secondly we use symmetry methods to give a rigorous connection between particle relabelling, symplecticity and PV conservation. Generalisations of these issues to semi-geostrophic flow and three-dimensional Lagrangian fluid flows, and the connection with Ertel's theorem are also discussed.

Keywords: geophysical fluid dynamics, potential vorticity, multisymplectic, particle relabelling, symmetry

1. Introduction

In Lagrangian fluid dynamics, the 1-form $\boldsymbol{\alpha} = \langle \mathbf{u}, \mathrm{d}\mathbf{x}\rangle = u_1 \mathrm{d}x_1 + u_2 \mathrm{d}x_2 + u_3 \mathrm{d}x_3$ plays the dual role of a circulation density and the generator for a canonical symplectic structure. This elementary observation can easily be seen using the equations governing incompressible Lagrangian fluid dynamics in two space dimensions

$$\begin{aligned} \frac{\partial x_1}{\partial t} &= u_1\,, \qquad \frac{\partial u_1}{\partial t} = -\frac{\partial x_2}{\partial m_2}\frac{\partial p}{\partial m_1} + \frac{\partial x_2}{\partial m_1}\frac{\partial p}{\partial m_2}\,, \\ \frac{\partial x_2}{\partial t} &= u_2\,, \qquad \frac{\partial u_2}{\partial t} = \frac{\partial x_1}{\partial m_2}\frac{\partial p}{\partial m_1} - \frac{\partial x_1}{\partial m_1}\frac{\partial p}{\partial m_2}\,. \end{aligned}$$

Here $x_1 = m_1$ and $x_2 = m_2$ at $t = 0$, where $\mathbf{m} = (m_1, m_2)$ are Lagrangian mass coordinates, p is the pressure, and the incompressibility constraint is

$$\det(\mathbf{x_m}) = 1, \qquad \text{where} \quad \mathbf{x_m} = \begin{bmatrix} \frac{\partial x_1}{\partial m_1} & \frac{\partial x_1}{\partial m_2} \\ \frac{\partial x_2}{\partial m_1} & \frac{\partial x_2}{\partial m_2} \end{bmatrix}.$$

This system is a constrained Hamiltonian system with the Hamiltonian function

$$H(\mathbf{x}, \mathbf{u}, p) = \int S \,\mathrm{d}\mathbf{m}\,, \qquad \text{where} \quad S = \tfrac{1}{2}\langle \mathbf{u}, \mathbf{u}\rangle + (1 - \det(\mathbf{x_m}))\, p\,, \tag{1.1}$$

and the canonical representation is

$$\begin{bmatrix} 0 & -\mathbf{I} & 0 \\ \mathbf{I} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{pmatrix} \mathbf{x} \\ \mathbf{u} \\ p \end{pmatrix}_{,t} = \begin{pmatrix} \delta H/\delta \mathbf{x} \\ \delta H/\delta \mathbf{u} \\ \delta H/\delta p \end{pmatrix} . \tag{1.2}$$

The symplectic form for this system is the integral of the exterior derivative of the circulation 1-form

$$\overline{\boldsymbol{\omega}} = \int \mathrm{d}\boldsymbol{\alpha}\, \mathrm{d}\mathbf{m} = \int \mathrm{d}\mathbf{u} \wedge \mathrm{d}\mathbf{x}\, \mathrm{d}\mathbf{m} = \int (\, \mathrm{d}u_1 \wedge \mathrm{d}x_1 + \mathrm{d}u_2 \wedge \mathrm{d}x_2\,)\, \mathrm{d}\mathbf{m}\,, \tag{1.3}$$

where the line over $\boldsymbol{\omega}$ signifies that it is integrated over $\mathbf{m}$-space.

On the other hand, in the classical description, the circulation is obtained by integrating the 1-form $\boldsymbol{\alpha}$ along a loop in the $(\mathbf{x}, \mathbf{u})-$space, and by Stokes Theorem, the circulation can be related to a surface integral of the vorticity (cf. Batchelor 1967, p. 93). Comparing this classical observation with (1.3) suggests that it is natural to expect some connection between vorticity and symplecticity.

When stripped of the integral, the *density of the symplectic form*, $\boldsymbol{\omega} = \mathrm{d}\boldsymbol{\alpha}$, has the following precise relation with vorticity,

$$\psi^* \boldsymbol{\omega} = \Omega\, dm_1 \wedge dm_2\,. \tag{1.4}$$

Here Ω is the vorticity in Lagrangian coordinates,

$$\Omega \;=\; \frac{\partial x_1}{\partial m_2}\frac{\partial u_1}{\partial m_1} - \frac{\partial x_1}{\partial m_1}\frac{\partial u_1}{\partial m_2} + \frac{\partial x_2}{\partial m_2}\frac{\partial u_2}{\partial m_1} - \frac{\partial x_2}{\partial m_1}\frac{\partial u_2}{\partial m_2}\,,$$

and ψ^* is the *pull-back* mapping which is obtained by restricting the phase space coordinates $\mathbf{x}, \mathbf{u}$ to the label space $\mathbf{m}$, i.e., $\mathbf{x} = \mathbf{x}(m_1, m_2)$, $\mathbf{u} = \mathbf{u}(m_1, m_2)$. Hence the pull-back is defined by

$$\psi^*(\mathrm{d}\mathbf{x}) = \frac{\partial \mathbf{x}}{\partial m_1}\mathrm{d}m_1 + \frac{\partial \mathbf{x}}{\partial m_2}\mathrm{d}m_2\,, \qquad \psi^*(\mathrm{d}\mathbf{u}) = \frac{\partial \mathbf{u}}{\partial m_1}\mathrm{d}m_1 + \frac{\partial \mathbf{u}}{\partial m_2}\mathrm{d}m_2\,.$$

The generalization to higher dimensions and to other functions and forms is obvious (cf. Cartan (1983, p. 28)). The proof of (1.4) is therefore

$$\begin{aligned} \psi^* \boldsymbol{\omega} &= \psi^*(\mathrm{d}\mathbf{u} \wedge \mathrm{d}\mathbf{x}) = \psi^*(\mathrm{d}\mathbf{u}) \wedge \psi^*(\mathrm{d}\mathbf{x}) \\ &= \left(\frac{\partial \mathbf{u}}{\partial m_1}\mathrm{d}m_1 + \frac{\partial \mathbf{u}}{\partial m_2}\mathrm{d}m_2\right) \wedge \left(\frac{\partial \mathbf{x}}{\partial m_1}\mathrm{d}m_1 + \frac{\partial \mathbf{x}}{\partial m_2}\mathrm{d}m_2\right) \\ &= \sum_{i=1}^{2} \left\{ \left(\frac{\partial u_i}{\partial m_1}\mathrm{d}m_1 + \frac{\partial u_i}{\partial m_2}\mathrm{d}m_2\right) \wedge \left(\frac{\partial x_i}{\partial m_1}\mathrm{d}m_1 + \frac{\partial x_i}{\partial m_2}\mathrm{d}m_2\right) \right\} \\ &= \Omega\, dm_1 \wedge dm_2\,. \end{aligned}$$

A similar argument applied to the shallow water equations in geophysical fluid dynamics shows that the pull-back of the symplectic form density there results in the potential vorticity. The details of this construction are given in §2. The only place in the literature that we have seen the connection between potential vorticity and symplecticity discussed is in the work of Abarbanel & Holm (1987) (see equation

(81) on page 3375). There it is mentioned in passing that the pullback of the density of the symplectic form results in the potential vorticity, but the consequences of this observation are not studied. ARNOLD & KHESIN (1998) emphasize that the vorticity can be characterized by a two form (see pages 22 and 46), but the connection between vorticity and symplecticity is not explored.

While the above examples and the work of ABARBANEL & HOLM show a connection between vorticity or potential vorticity and symplecticity, there are several unanswered questions. The phase space variables $\mathbf{x}, \mathbf{u}$ depend on (m_1, m_2, t). Why pull back to the label space $\mathbf{m} = (m_1, m_2)$? Why not pull back to the full reference space (m_1, m_2, t)? Indeed, this more general pull-back leads to both vorticity conservation and energy conservation. Generalisations to $(\mathbf{m}, t) \in \mathbb{R}^4$ are also considered and lead to a symplectic derivation of Ertel's Theorem.

Further geometry is obtained by stripping away the integral in the 2-form which defines the symplectic structure, leading to a conservation law which can be generated on the reference space, a *conservation law for symplecticity*. This conservation law arises in a natural way when the equations governing Lagrangian fluid dynamics and geophysical fluid dynamics are formulated in a multisymplectic setting. For the purposes of this paper a multisymplectic PDE is a system of PDEs of the form

$$\mathbf{K}\boldsymbol{z}_{,t} + \mathbf{L}\boldsymbol{z}_{,1} + \mathbf{M}\boldsymbol{z}_{,2} = \boldsymbol{\nabla}_{\boldsymbol{z}} S_M(\boldsymbol{z}) \,, \quad \boldsymbol{z} \in \mathbb{R}^n \,, \tag{1.5}$$

where $\mathbf{K}$, $\mathbf{L}$ and $\mathbf{M}$ are skew-symmetric matrices and $S_M : \mathbb{R}^n \to \mathbb{R}$ is a smooth function. Equivalently, such PDEs can be characterized as Lagrangian PDEs with the Lagrangian functional in the canonical form

$$\mathscr{L} = \int_{\mathscr{V}} \left\{ \tfrac{1}{2}\langle \boldsymbol{z}, \mathbf{M}\boldsymbol{z}_{,t}\rangle + \tfrac{1}{2}\langle \boldsymbol{z}, \mathbf{K}\boldsymbol{z}_{,1}\rangle + \tfrac{1}{2}\langle \boldsymbol{z}, \mathbf{L}\boldsymbol{z}_{,2}\rangle - S_M(\boldsymbol{z}) \right\} \mathrm{d}t\,\mathrm{d}x_1\mathrm{d}x_2 \,,$$

where $\langle \cdot, \cdot \rangle$ is a standard inner product on $\mathbb{R}^n$, and $\int_{\mathscr{V}}$ is a volume integral. See BRIDGES (1997a,1997b) for general properties of such systems.

In the multisymplectic setting, the fluxes of symplecticity arise as 2-forms. The symplectic 2-form then satisfies a conservation law of the form

$$\frac{\partial}{\partial t}\boldsymbol{\omega} + \frac{\partial}{\partial m_1}\boldsymbol{\kappa}_1 + \frac{\partial}{\partial m_2}\boldsymbol{\kappa}_2 = 0 \,, \tag{1.6}$$

where $\boldsymbol{\kappa}_1$ and $\boldsymbol{\kappa}_2$ are a pair of 2-forms that represent the flux of symplecticity. Pulling back this equation to the label space, $\mathbf{m}$, leads to

$$\frac{\partial}{\partial t}\psi^*\boldsymbol{\omega} + \frac{\partial}{\partial m_1}\psi^*\boldsymbol{\kappa}_1 + \frac{\partial}{\partial m_2}\psi^*\boldsymbol{\kappa}_2 = 0 \,, \tag{1.7}$$

where $\psi^*\boldsymbol{\kappa}_1$ and $\psi^*\boldsymbol{\kappa}_2$ are 2-forms on the label space that represent the flux of potential vorticity.

It is in the investigation of the fluxes in the symplectic conservation law that the importance of particle relabelling and the homentropic nature of the fluid arises. For example, this formulation leads to the result that potential vorticity (or vorticity) is conserved on particle paths if and only if the divergence of the pull-back of the flux 2-forms to the label space vanish identically, that is if

$$\mathrm{div}(\psi^*\boldsymbol{\kappa}_l, \psi^*\boldsymbol{\kappa}_2) = \boldsymbol{\nabla}_{\mathbf{m}} \cdot \psi^*\boldsymbol{\kappa} = 0 \,, \qquad \boldsymbol{\kappa} = (\boldsymbol{\kappa}_1, \boldsymbol{\kappa}_2)^T \,. \tag{1.8}$$

We will show that a *sufficient* condition for (1.8) to be satisfied is the the Hamiltonian function is invariant under particle relabelling (homentropic). Note that this derivation of PV conservation is fundamentally different from the ones typically given in fluid dynamics (compare, for example, SALMON (1998, p. 302)).

In §2, the Lagrangian form of the shallow water equations is treated in detail, and the following features are treated in turn: the encoding of PV in symplecticity, the multisymplectic structure that leads to a geometric form of PV conservation, the pull-back as a generator of PV and energy conservation, and the use of symmetry methods to establish rigorously the connection between particle relabelling and PV conservation.

One of the motivations of this paper is understand the geometric structure of Lagrangian fluid dynamics in order to incorporate it into numerical methods. In §4 we show how the ideas in this paper can influence the design of numerical methods.

The ideas generalize in a straightforward way to other systems in Lagrangian fluid dynamics, and it §4 we briefly consider the semi-geostrophic equations and three-dimensional Lagrangian incompressible fluid dynamics.

2. Multisymplectic GFD: shallow water equations

In this section, the shallow water equations will be considered in the Lagrangian particle-path representation. The connection between potential vorticity and symplecticity will be established, as will conditions for conservation of potential vorticity along particle paths, by constructing the flux 2-forms associated with conservation of symplecticity.

As in the introduction, let $\mathbf{x} \in \mathbb{R}^2$, $\mathbf{u} \in \mathbb{R}^2$ represent the position and velocity of the fluid particles, parametrized by Lagrangian mass coordinates $\mathbf{m} = (m_1, m_2)$, and let $h \in \mathbb{R}$ represent the fluid depth. The system is rotating at constant angular velocity $f/2$.

Henceforth, we use Latin indices to denote components of $\mathbf{x}$ and $\mathbf{u}$, and Greek indices to denote components of $\mathbf{m}$; the usual summation convention is adopted. Total derivatives with respect to t or m_α, for which all variables are regarded as functions of (m_1, m_2, t), are denoted by the subscript t or α after a comma. For example,

$$x_{i,\alpha} = \frac{\partial x_i(\mathbf{m}, t)}{\partial m_\alpha}, \qquad x_{i,\alpha t} = \frac{\partial^2 x_i(\mathbf{m}, t)}{\partial m_\alpha \partial t}, \qquad \text{etc.}$$

Partial derivatives with respect to any other variable are written in full.

Define the Jacobian matrix

$$\mathbf{x_m} = \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix} \qquad \text{where} \qquad x_{i\alpha} \equiv x_{i,\alpha}.$$

Conservation of mass reduces to $h\tau = 1$ where $\tau = \det(\mathbf{x_m}) = x_{11}x_{22} - x_{12}x_{21}$. The governing equations for $\mathbf{u}$ and $\mathbf{x}$ are

$$u_{1,t} = -(x_{22} \cdot p)_{,1} + (x_{21} \cdot p)_{,2} + f u_2, \tag{2.1}$$

$$u_{2,t} = (x_{12} \cdot p)_{,1} - (x_{11} \cdot p)_{,2} - f u_1, \tag{2.2}$$

$$x_{1,t} = u_1, \tag{2.3}$$

$$x_{2,t} = u_2. \tag{2.4}$$

The pressure is defined by $p = -e'(\tau)$ where $e(\tau)$ is the *specific internal energy*, in homentropic form. The classical shallow-water equations are recovered by taking $e(\tau) = g/(2\tau)$.

In terms of $e(\tau)$, the equations of motion amount to

$$u_{1,t} - f x_{2,t} = \left(\frac{\partial e(\tau)}{\partial x_{11}}\right)_{,1} + \left(\frac{\partial e(\tau)}{\partial x_{12}}\right)_{,2}, \tag{2.5}$$

$$u_{2,t} + f x_{1,t} = \left(\frac{\partial e(\tau)}{\partial x_{21}}\right)_{,1} + \left(\frac{\partial e(\tau)}{\partial x_{22}}\right)_{,2}, \tag{2.6}$$

$$x_{1,t} = u_1, \tag{2.7}$$

$$x_{2,t} = u_2. \tag{2.8}$$

This system has a Hamiltonian representation with canonical coordinates $(\mathbf{x}, \mathbf{u})$:

$$\begin{bmatrix} -f\mathbf{J} & -\mathbf{I} \\ \mathbf{I} & \mathbf{0} \end{bmatrix} \begin{pmatrix} \mathbf{x} \\ \mathbf{u} \end{pmatrix}_t = \begin{pmatrix} \delta H/\delta \mathbf{x} \\ \delta H/\delta \mathbf{u} \end{pmatrix}, \qquad \mathbf{J} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},$$

where

$$H(\mathbf{x}, \mathbf{u}) = \int S \, \mathrm{d}\mathbf{m}, \qquad S = \tfrac{1}{2}\langle \mathbf{u}, \mathbf{u} \rangle + e(\tau). \tag{2.9}$$

The symplectic form for this system is

$$\overline{\boldsymbol{\omega}} = \int \boldsymbol{\omega} \, \mathrm{d}\mathbf{m}, \qquad \boldsymbol{\omega} \mathrm{d}u_1 \wedge \mathrm{d}x_1 + \mathrm{d}u_2 \wedge \mathrm{d}x_2 + f \mathrm{d}x_1 \wedge \mathrm{d}x_2 .$$

We will prove that $\psi^* \boldsymbol{\omega} = q \, \mathrm{d}m_1 \wedge \mathrm{d}m_2$, where q is the potential vorticity. However, we first recast the system into a multisymplectic formulation in order to deduce further information.

(*a*) *A multisymplectic formulation*

Introduce the additional variables

$$w_{i\alpha} \equiv -\frac{\partial S}{\partial x_{i\alpha}} = -\frac{\partial e(\tau)}{\partial x_{i\alpha}} = -e'(\tau)\frac{\partial \tau}{\partial x_{i\alpha}} = p(\tau)\frac{\partial \tau}{\partial x_{i\alpha}},$$

and the extended set of dependent variables

$$\boldsymbol{z} = (x_1, x_2, u_1, u_2, w_{11}, w_{12}, w_{21}, w_{22}, x_{11}, x_{12}, x_{21}, x_{22})^T, \tag{2.10}$$

so that $\boldsymbol{z} \in \mathbb{R}^{12}$. Then (2.5)-(2.8) can be written as the following system of first-order PDEs:

$$\begin{aligned}
-u_{1,t} + f x_{2,t} - w_{11,1} - w_{12,2} &= 0, \\
-u_{2,t} - f x_{1,t} - w_{21,1} - w_{22,2} &= 0, \\
x_{i,t} &= u_i, && i = 1, 2, \\
x_{i,\alpha} &= x_{i\alpha}, && i = 1, 2, \quad \alpha = 1, 2, \\
0 &= \frac{\partial e(\tau)}{\partial x_{i\alpha}} + w_{i\alpha}, && i = 1, 2, \quad \alpha = 1, 2.
\end{aligned}$$

This system is of the form (1.5) with

$$S_M(\boldsymbol{z}) = S + x_{i\alpha} w_{i\alpha} = \tfrac{1}{2}\langle \mathbf{u}, \mathbf{u}\rangle + e(\tau) + x_{i\alpha} w_{i\alpha}\,. \tag{2.11}$$

Here $\mathbf{K}, \mathbf{L}, \mathbf{M} \in \mathbb{R}^{12\times 12}$ are skew-symmetric matrices with nonzero entries

$$\begin{gathered} K_{1,2} = f,\ \ K_{1,3} = -1,\ \ K_{2,1} = -f,\ \ K_{2,4} = -1,\ \ K_{3,1} = 1,\ \ K_{4,2} = 1, \\ L_{1,5} = -1,\ \ L_{2,7} = -1,\ \ L_{5,1} = 1,\ \ L_{7,2} = 1, \\ M_{1,6} = -1,\ \ M_{2,8} = -1,\ \ M_{6,1} = 1,\ \ M_{8,2} = 1. \end{gathered}$$

Note that $S_M(\boldsymbol{z})$ in (2.11) is defined locally (for it involves no integrals), and it differs from the classical Hamiltonian function density S by the third term. The following identities hold:

$$x_{i\alpha}\frac{\partial \tau}{\partial x_{i\beta}} = \tau\delta_{\alpha\beta}\,, \qquad x_{i\alpha}\frac{\partial \tau}{\partial x_{j\alpha}} = \tau\delta_{ij}\,,$$

where δ is the Kronecker delta. Therefore

$$x_{i\alpha} w_{i\beta} = -\tau e'(\tau)\delta_{\alpha\beta}\,, \qquad x_{i\alpha} w_{j\alpha} = -\tau e'(\tau)\delta_{ij}\,, \tag{2.12}$$

and so the multisymplectic density S_M can be reduced to the form

$$S_M(\boldsymbol{z}) = \tfrac{1}{2}\langle \mathbf{u}, \mathbf{u}\rangle + e(\tau) - 2\tau e'(\tau). \tag{2.13}$$

However, in order for (1.5) to yield the multisymplectic shallow water equations, $S_M(\boldsymbol{z})$ must be expressed in terms of the multisymplectic coordinates, i.e. in the form (2.11).

The abstract formulation (1.5) gives rise to a conservation law of symplecticity (Bridges, 1997b)

$$(\mathrm{d}\boldsymbol{z}\wedge\mathbf{K}\mathrm{d}\boldsymbol{z})_{,t} + (\mathrm{d}\boldsymbol{z}\wedge\mathbf{L}\mathrm{d}\boldsymbol{z})_{,1} + (\mathrm{d}\boldsymbol{z}\wedge\mathbf{M}\mathrm{d}\boldsymbol{z})_{,2} = 0, \tag{2.14}$$

which, for the present system, amounts to

$$\boldsymbol{\omega}_{,t} + \boldsymbol{\kappa}_{\alpha,\alpha} = 0\,, \tag{2.15}$$

where

$$\boldsymbol{\omega} = \mathrm{d}u_i\wedge\mathrm{d}x_i + f\,\mathrm{d}x_1\wedge\mathrm{d}x_2 \quad\text{and}\quad \boldsymbol{\kappa}_\alpha = \mathrm{d}w_{i\alpha}\wedge\mathrm{d}x_i\,, \qquad \alpha = 1,2.$$

(*b*) *Pullback and the geometry of conservation laws*

In this section, we explore in detail the connection between conservation of symplecticity, the pull-back operation, and conservation laws, in the setting of the shallow water equations.

The potential vorticity for the shallow water system is

$$q = h^{-1}\left(f + \frac{\partial u_2}{\partial x_1} - \frac{\partial u_1}{\partial x_2}\right) = f\tau + x_{i2}u_{i,1} - x_{i1}u_{i,2}\,,$$

where the second expression is in Lagrangian mass coordinates satisfying $\tau h = 1$. Let Ψ^* represent the pull-back operation from the phase space to the full reference space, $(\mathbf{m}, t)$. Application to the symplectic 2-form results in

$$\begin{aligned}
\Psi^*\boldsymbol{\omega} &= (u_{i,t}\,\mathrm{d}t + u_{i,\beta}\,\mathrm{d}m_\beta) \wedge (x_{i,t}\,\mathrm{d}t + x_{i\gamma}\,\mathrm{d}m_\gamma) \\
&+ f\,(x_{1,t}\,\mathrm{d}t + x_{1\beta}\,\mathrm{d}m_\beta) \wedge (x_{2,t}\,\mathrm{d}t + x_{2\gamma}\,\mathrm{d}m_\gamma) \\
&= \{x_{i,t}u_{i,\beta} - x_{i\beta}u_{i,t} + f(x_{1\beta}x_{2,t} - x_{1,t}x_{2\beta})\}\,\mathrm{d}m_\beta \wedge \mathrm{d}t \\
&\quad + \{x_{i2}u_{i,1} - x_{i1}u_{i,2} + f(x_{11}x_{22} - x_{12}x_{21})\}\,\mathrm{d}m_1 \wedge \mathrm{d}m_2 \\
&= \{x_{i,t}u_{i,\beta} - x_{i\beta}u_{i,t} + f(x_{1\beta}x_{2,t} - x_{1,t}x_{2\beta})\}\,\mathrm{d}m_\beta \wedge \mathrm{d}t + q\,\mathrm{d}m_1 \wedge \mathrm{d}m_2\,,
\end{aligned}$$

and

$$\begin{aligned}
\Psi^*\boldsymbol{\kappa}_\alpha &= (w_{i\alpha,t}\,\mathrm{d}t + w_{i\alpha,\beta}\,\mathrm{d}m_\beta) \wedge (x_{i,t}\,\mathrm{d}t + x_{i\gamma}\,\mathrm{d}m_\gamma) \\
&= \{x_{i,t}w_{i\alpha,\beta} - x_{i\beta}w_{i\alpha,t}\}\,\mathrm{d}m_\beta \wedge \mathrm{d}t + \{x_{i2}w_{i\alpha,1} - x_{i1}w_{i\alpha,2}\}\,\mathrm{d}m_1 \wedge \mathrm{d}m_2\,.
\end{aligned}$$

Evaluating $(\Psi^*\boldsymbol{\omega}, \Psi^*\boldsymbol{\kappa}_\alpha)$ on the set of solutions of the shallow water equations, and taking (2.12) into account, we finally obtain

$$\begin{aligned}
\Psi^*\boldsymbol{\omega} &= \{u_i u_{i,\beta} + x_{i\beta}w_{i\gamma,\gamma}\}\,\mathrm{d}m_\beta \wedge \mathrm{d}t + q\,\mathrm{d}m_1 \wedge \mathrm{d}m_2 \\
&= \{u_i u_{i,\beta} + (x_{i\beta}w_{i\gamma})_{,\gamma} - x_{i,\beta\gamma}w_{i\gamma}\}\,\mathrm{d}m_\beta \wedge \mathrm{d}t + q\,\mathrm{d}m_1 \wedge \mathrm{d}m_2 \\
&= \left\{\tfrac{1}{2}\langle\mathbf{u},\mathbf{u}\rangle - \tau e'(\tau) + e(\tau)\right\}_{,\beta}\,\mathrm{d}m_\beta \wedge \mathrm{d}t + q\,\mathrm{d}m_1 \wedge \mathrm{d}m_2\,,
\end{aligned}$$

and

$$\begin{aligned}
\Psi^*\boldsymbol{\kappa}_\alpha &= \{(u_i w_{i\alpha})_{,\beta} - (x_{i\beta}w_{i\alpha})_{,t}\}\,\mathrm{d}m_\beta \wedge \mathrm{d}t \\
&\qquad + \{(x_{i2}w_{i\alpha})_{,1} - (x_{i1}w_{i\alpha})_{,2}\}\,\mathrm{d}m_1 \wedge \mathrm{d}m_2 \\
&= \left\{(u_i w_{i\alpha})_{,\beta} + \delta_{\alpha\beta}\,(\tau e'(\tau))_{,t}\right\}\,\mathrm{d}m_\beta \wedge \mathrm{d}t \\
&\qquad + \left\{\delta_{\alpha 1}\,(\tau e'(\tau))_{,2} - \delta_{\alpha 2}\,(\tau e'(\tau))_{,1}\right\}\,\mathrm{d}m_1 \wedge \mathrm{d}m_2\,.
\end{aligned}$$

The pull-back operator Ψ^* commutes with total differentiation with respect to t, m_1, or m_2. Consequently

$$\Psi^*\boldsymbol{\kappa}_{\alpha,\alpha} = \left\{(u_i w_{i\alpha})_{,\alpha\beta} + (\tau e'(\tau))_{,t\beta}\right\}\,\mathrm{d}m_\beta \wedge \mathrm{d}t\,;$$

note that the $\mathrm{d}m_1 \wedge \mathrm{d}m_2$ component is zero. Therefore the multisymplectic conservation law (2.15) is pulled back to

$$\begin{aligned}
0 = \Psi^*(\boldsymbol{\omega}_{,t} + \boldsymbol{\kappa}_{\alpha,\alpha}) &= q_{,t}\,\mathrm{d}m_1 \wedge \mathrm{d}m_2 \\
&+ \left\{\left(\tfrac{1}{2}\langle\mathbf{u},\mathbf{u}\rangle + e(\tau)\right)_{,t} + (u_i w_{i\alpha})_{,\alpha}\right\}_{,\beta}\,\mathrm{d}m_\beta \wedge \mathrm{d}t\,.
\end{aligned}$$

Separating this conservation law into its three components, we obtain

$$q_{,t} = 0, \tag{2.16}$$

$$\left\{\left(\tfrac{1}{2}\langle\mathbf{u},\mathbf{u}\rangle + e(\tau)\right)_{,t} + (u_i w_{i\alpha})_{,\alpha}\right\}_{,\beta} = 0, \qquad \beta = 1, 2. \tag{2.17}$$

The $\mathrm{d}m_1 \wedge \mathrm{d}m_2$ component (2.16) encapsulates the conservation of potential vorticity on particle paths. Note that the label-space divergence of the flux of potential vorticity is zero. In the next subsection, the geometry of this material conservation of PV will be examined in more detail.

The other conservation laws generated automatically by the pull-back in (2.17) are label-space derivatives of the local energy conservation law:

$$\left(\tfrac{1}{2}\langle \mathbf{u}, \mathbf{u}\rangle + e(\tau)\right)_{,t} + (u_i w_{i\alpha})_{,\alpha} = 0\,. \tag{2.18}$$

This conservation law implies that the total energy $\mathcal{E}$ is conserved, i.e.,

$$\partial_t \mathcal{E} = \partial_t \int \tfrac{1}{2}\langle \mathbf{u}, \mathbf{u}\rangle + e(\tau)\,\mathrm{d}\mathbf{m} = 0,$$

provided that appropriate boundary conditions are given.

(c) *The origin of conservation laws obtained by pull-back*

The idea of pulling back conservation laws to the reference space can be put on a more general footing. Hydon (2002) shows that for *any* multisymplectic system of PDEs (1.5), the 2-form conservation laws are obtained by differentiating conservation laws that correspond to translational symmetry in each independent variable.

For the multisymplectic shallow-water equations, translations in t produce energy conservation (2.18). Translations in label-space produce the following interesting conservation laws:

$$(u_i x_{i1} + f x_1 x_{21})_{,t} + \left(e(\tau) - \tfrac{1}{2}u_i u_i - f x_1 u_2 + x_{i1} w_{i1}\right)_{,1} + (x_{i1} w_{i2})_{,2} = 0; \tag{2.19}$$

$$(u_i x_{i2} + f x_1 x_{22})_{,t} + (x_{i2} w_{i1})_{,1} + \left(e(\tau) - \tfrac{1}{2}u_i u_i - f x_1 u_2 + x_{i2} w_{i2}\right)_{,2} = 0. \tag{2.20}$$

These can be regarded as expressing conservation of Lagrangian momentum. They are not connected with the ordinary (Eulerian) momentum conservation law, which corresponds to translations in $\mathbf{x}$. We have already seen that (2.17) are obtained as label-space derivatives of (2.18). It is easy to verify that the potential vorticity conservation law (2.16) is a differential consequence of (2.19) and (2.20). Specifically, (2.16) is the m_1-derivative of (2.20) minus the m_2-derivative of (2.19). Hence from the Lagrangian viewpoint, (2.19) and (2.20) are more fundamental than (2.16); unlike potential vorticity, however, they are strictly Lagrangian and cannot be written solely in Eulerian variables.

(d) *Symmetries and multisymplectic conservation laws*

If a system of equations stems from a variational principle, Noether's theorem links conservation laws with symmetries of the Lagrangian form (which are called variational symmetries). Noether's theorem has been extended to Hamiltonian systems (see Olver 1993), and is applied to particle relabelling symmetries in Egger (1994), Padhye & Morrison (1996), Padhye (1998) and Albert (1997a,1997b). Indeed, Padhye & Morrison (1996) write down the generalized

form of the relabelling symmetry, and identify all known symmetries of the Lagrangian and Euler-Lagrange map. The corresponding conserved quantities of the ideal fluid were summarized in both Lagrangian and Hamiltonian frameworks by Padyhe (1998).

The shallow water equations (2.5)-(2.8) possess various point symmetries, which can be found systematically using the approach pioneered by Lie (see HYDON, 2000, for a simple introduction). BILA (2002) gives the most complete study of the symmetries and conservation laws of the shallow water equations. However, the approach here, based on the multisymplectic formulation leads to a connection between the *fluxes* of the conservation law and symmetry. A restricted form of Noether's theorem for multisymplectic systems was first derived in (cf. BRIDGES, 1997a, App. C). A general form of Noether's Theorem for multisymplectic systems can be found in HYDON (2002).

The simplest symmetries of the shallow water equations are the invariance under translations $\mathbf{x} \mapsto \mathbf{x} + \varepsilon$ for any $\varepsilon \in \mathbb{R}^2$. These symmetries lead to the unremarkable conservation laws (2.5) and (2.6).

The symmetries that lead to conservation of potential vorticity and total energy are particle relabelling and time-translation respectively. It can be shown that these are the only symmetries that have no effect upon (and are independent of) the variables $\mathbf{x}$ and $\mathbf{u}$.

The implication of relabelling symmetry seems to have been first pointed out by NEWCOMB (1967), who discovered a relabelling symmetry for incompressible ideal fluid without internal energy. The connection between the conservation of potential vorticity and a Lagrangian (variational) symmetry was first pointed out by RIPA (1981) in the context of incompressible stratified flows, and SALMON (1982) notes the connection as well. NEWCOMB (1967) and BRETHERTON (1970) have also related relabeling symmetry to Kelvin's circulation theorem.

In this section, we demonstrate that the relabelling and time-translation symmetries are encoded in the multisymplectic conservation law, explaining why the pull-back of this law produces conservation of total energy and potential vorticity.

A particle relabelling transformation is a diffeomorphism of the label space:

$$\Gamma : (m_1, m_2) \mapsto (\hat{m}_1(m_1, m_2),\, \hat{m}_2(m_1, m_2))\,.$$

Neither $\mathbf{x}$ nor $\mathbf{u}$ are affected by any such transformation. However, the Hamiltonian density S depends on an arbitrary function $e(\tau)$, so the transformation is a symmetry for every $e(\tau)$ only if τ is invariant. (It is easy to verify that this necessary condition is also sufficient.) By definition,

$$\tau = \det(\mathbf{x_m}) = \det(\mathbf{x}_{\hat{\mathbf{m}}}) \det(\hat{\mathbf{m}}_\mathbf{m}) \quad \text{where} \quad \det(\hat{\mathbf{m}}_\mathbf{m}) = \hat{m}_{1,1}\hat{m}_{2,2} - \hat{m}_{1,2}\hat{m}_{2,1}\,.$$

Therefore τ is invariant if and only if

$$\det(\hat{\mathbf{m}}_\mathbf{m}) = 1, \tag{2.21}$$

so that Γ is an area-preserving transformation. The set of all particle relabelling symmetries is an infinite-dimensional Lie (pseudo-) group. Every one-parameter Lie subgroup of this group has a generator of the form

$$X = \phi_{,2}\frac{\partial}{\partial m_1} - \phi_{,1}\frac{\partial}{\partial m_2}\,,$$

for some smooth function $\phi(\mathbf{m})$. A function $F(\mathbf{m}, t, \mathbf{x}, \mathbf{u})$ is invariant under the subgroup generated by X if and only if $XF = 0$. If F also depends upon derivatives of $\mathbf{x}$ and $\mathbf{u}$, the same condition for invariance applies once X has been prolonged to take account of the group action on derivatives. For example, τ is a function of the first derivatives $x_{i\alpha}$. The prolongation of the generator to these derivatives is

$$X^{(1)} = \phi_{,2}\frac{\partial}{\partial m_1} - \phi_{,1}\frac{\partial}{\partial m_2} + \{x_{i2}\phi_{,1\alpha} - x_{i1}\phi_{,2\alpha}\}\frac{\partial}{\partial x_{i\alpha}}\,, \tag{2.22}$$

and therefore

$$\begin{aligned} X^{(1)}\tau \;=\;& x_{22}(x_{12}\phi_{,11} - x_{11}\phi_{,21}) - x_{21}(x_{12}\phi_{,12} - x_{11}\phi_{,22}) \\ & -x_{12}(x_{22}\phi_{,11} - x_{21}\phi_{,21}) + x_{11}(x_{22}\phi_{,12} - x_{21}\phi_{,22}) = 0\,, \end{aligned}$$

which is to be expected, because we obtained the relabelling symmetries by requiring that τ is invariant.

Before we examine the link between the particle relabelling symmetries and conservation of potential vorticity within the multisymplectic framework, it is instructive to seek generalizations of the Hamiltonian density S that retain the particle relabelling symmetries. We restrict attention to densities of the form

$$\tilde{S} = \tilde{S}(t, \mathbf{x}, \mathbf{u}, \mathbf{x_m}),$$

so that the resulting Hamiltonian system can be recast as a multisymplectic system, using the matrices $\mathbf{K}, \mathbf{L}, \mathbf{M}$ that were defined in §2(a). Consequently, the conservation law (2.15) holds for the same 2-forms $\boldsymbol{\omega}$ and $\boldsymbol{\kappa}_\alpha$ that were used earlier, bearing in mind that the auxiliary variables $w_{i\alpha}$ are now defined as follows:

$$w_{i\alpha} = -\frac{\partial \tilde{S}}{\partial x_{i\alpha}}\,.$$

If $\tilde{S}$ has no explicit dependence on t, it is invariant under translations in time. The density $\tilde{S}$ is invariant under the particle relabelling symmetries generated by X if and only if

$$X^{(1)}\tilde{S} \equiv \left(X^{(1)}t\right)\frac{\partial \tilde{S}}{\partial t} + \left(X^{(1)}x_i\right)\frac{\partial \tilde{S}}{\partial x_i} + \left(X^{(1)}u_i\right)\frac{\partial \tilde{S}}{\partial u_i} + \left(X^{(1)}x_{i\alpha}\right)\frac{\partial \tilde{S}}{\partial x_{i\alpha}} = 0.$$

But

$$X^{(1)}t = X^{(1)}x_i = X^{(1)}u_i = 0,$$

so $\tilde{S}$ can depend arbitrarily on t, $\mathbf{x}$, and $\mathbf{u}$. Given any smooth function $F(\mathbf{x_m})$,

$$\begin{aligned} X^{(1)}F(\mathbf{x_m}) \;&=\; \{x_{i2}\phi_{,1\alpha} - x_{i1}\phi_{,2\alpha}\}\frac{\partial F(\mathbf{x_m})}{\partial x_{i\alpha}} \\ &=\; \phi_{,11}x_{i2}\frac{\partial F(\mathbf{x_m})}{\partial x_{i1}} + \phi_{,12}\left(x_{i2}\frac{\partial F(\mathbf{x_m})}{\partial x_{i2}} - x_{i1}\frac{\partial F(\mathbf{x_m})}{\partial x_{i1}}\right) \\ &\qquad -\phi_{,22}x_{i1}\frac{\partial F(\mathbf{x_m})}{\partial x_{i2}}\,, \end{aligned}$$

so for $F(\mathbf{x_m})$ to be invariant under arbitrary particle relabelling transformations, the following conditions must hold:

$$x_{i2}\frac{\partial F(\mathbf{x_m})}{\partial x_{i1}} = 0, \qquad x_{i2}\frac{\partial F(\mathbf{x_m})}{\partial x_{i2}} - x_{i1}\frac{\partial F(\mathbf{x_m})}{\partial x_{i1}} = 0, \qquad x_{i1}\frac{\partial F(\mathbf{x_m})}{\partial x_{i2}} = 0.$$

By using the method of characteristics, it is easy to show that F is invariant if and only if it is a function of τ alone. Therefore $\tilde{S}$ admits the group of particle relabelling symmetries provided that it is a function of t, $\mathbf{x}, \mathbf{u}$, and τ only. Note that this result is based solely on mathematical considerations. There may be good physical reasons for restricting the class of allowable functions still further. For example, the governing equations include

$$x_{i,t} = \frac{\partial \tilde{S}}{\partial u_i}\,,$$

so if $\mathbf{u}$ is to represent the particle velocity, the most general form that $\tilde{S}$ can take is

$$\tilde{S} = \tfrac{1}{2}\langle \mathbf{u}, \mathbf{u}\rangle + \sigma(t, \mathbf{x}, \tau)\,,$$

for some function σ.

Our main observation is that *whatever functional form $\tilde{S}(t, \mathbf{x}, \mathbf{u}, \tau)$ takes, potential vorticity is conserved on the solutions of the system* (1.5), where now

$$S_M = \tilde{S} + x_{i\alpha} w_{i\alpha}\,.$$

This PV conservation can be seen by substituting (1.5) into

$$\begin{aligned}
\Psi^*\boldsymbol{\omega} &= \{x_{i,t}u_{i,\beta} - x_{i\beta}u_{i,t} + f(x_{1\beta}x_{2,t} - x_{1,t}x_{2\beta})\}\,\mathrm{d}m_\beta \wedge \mathrm{d}t + q\,\mathrm{d}m_1 \wedge \mathrm{d}m_2\,,\\
\Psi^*\boldsymbol{\kappa}_\alpha &= \{x_{i,t}w_{i\alpha,\beta} - x_{i\beta}w_{i\alpha,t}\}\,\mathrm{d}m_\beta \wedge \mathrm{d}t + \{x_{i2}w_{i\alpha,1} - x_{i1}w_{i\alpha,2}\}\,\mathrm{d}m_1 \wedge \mathrm{d}m_2\,,
\end{aligned}$$

and rearranging terms in the same way as in the previous section. After a slightly messy calculation, we obtain

$$\Psi^*\boldsymbol{\omega} = \left\{\tilde{S} - \tau\frac{\partial \tilde{S}}{\partial \tau}\right\}_{,\beta} \mathrm{d}m_\beta \wedge \mathrm{d}t + q\,\mathrm{d}m_1 \wedge \mathrm{d}m_2\,,$$

$$\begin{aligned}
\Psi^*\boldsymbol{\kappa}_\alpha &= \left\{(u_i w_{i\alpha})_{,\beta} + \delta_{\alpha\beta}\left(\tau\frac{\partial \tilde{S}}{\partial \tau}\right)_{,t}\right\}\mathrm{d}m_\beta \wedge \mathrm{d}t\\
&\quad + \left\{\delta_{\alpha 1}\left(\tau\frac{\partial \tilde{S}}{\partial \tau}\right)_{,2} - \delta_{\alpha 2}\left(\tau\frac{\partial \tilde{S}}{\partial \tau}\right)_{,1}\right\}\mathrm{d}m_1 \wedge \mathrm{d}m_2\,.
\end{aligned}$$

Therefore the pull-back of the multisymplectic conservation law is

$$\Psi^*(\boldsymbol{\omega}_{,t} + \boldsymbol{\kappa}_{\alpha,\alpha}) = \left\{\tilde{S}_{,t} + (u_i w_{i\alpha})_{,\alpha}\right\}_{,\beta} \mathrm{d}m_\beta \wedge \mathrm{d}t + q_{,t}\,\mathrm{d}m_1 \wedge \mathrm{d}m_2 = 0.$$

Hence if the Hamiltonian density is invariant under arbitrary area-preserving particle relabelling transformations, potential vorticity is conserved. Furthermore, the remaining components of the conservation law lead to the result

$$\Psi^* \left(\tilde{S}_{,t} + (u_i w_{i\alpha})_{,\alpha} \right) = f(t),$$

for some function f. From the equations of motion, we obtain

$$f(t) = \Psi^* \left(\frac{\partial \tilde{S}}{\partial t} \right),$$

so $f(t) = 0$ if $\tilde{S}$ is invariant under translations in time. For the shallow water equations, this leads to the local energy conservation law (2.18).

How is the conservation of potential vorticity encoded in the multisymplectic 2-forms? To answer this question, it is sufficient to restrict attention to the $\mathrm{d}m_1 \wedge \mathrm{d}m_2$ component. First note that

$$\boldsymbol{\omega} = \mathrm{d}u_i \wedge \mathrm{d}x_i + f \, \mathrm{d}x_1 \wedge \mathrm{d}x_2 \tag{2.23}$$

is invariant under particle relabelling symmetries, because x_i and u_i are invariant and the exterior derivative d is essentially coordinate-invariant. Neither of the flux 2-forms $\boldsymbol{\kappa}_\alpha$ is invariant; however, we have shown that if the Hamiltonian density is invariant under particle relabelling then the $\mathrm{d}m_1 \wedge \mathrm{d}m_2$ component of $\Psi^* \boldsymbol{\kappa}_{\alpha,\alpha}$ vanishes. Finally, the pull-back of $\boldsymbol{\omega}$ to label space is the product of the potential vorticity and the 2-form $\mathrm{d}m_1 \wedge \mathrm{d}m_2$ (which is itself invariant under the relabelling symmetries). Consequently $q_{,t} = 0$.

3. Particle methods and conservation of potential vorticity

In this section, we discuss symplecticity and conservation of PV for a Lagrangian particle discretization of the shallow-water equations. Particle methods, such as smoothed particle hydrodynamics (SPH) (cf. Monaghan (1992), are based on an approximation of the layer-depth of type

$$h(\mathbf{x}, t) = \sum_{k=1}^{N} m_k \psi(\|\mathbf{x} - \mathbf{X}_k(t)\|), \tag{3.1}$$

where $\psi(r) \geq 0$ is an appropriate shape function and $\mathbf{X}_k(t)$ are Lagrangian particles with mass m_k following the fluid flow. Let us assume for a moment that $h(\mathbf{x}, t)$ is given (or has been computed). Then each particle position $\mathbf{x}(\mathbf{m}, t)$ satisfies the following time-dependent Hamiltonian ODE:

$$\mathbf{x}_t = \mathbf{u}, \qquad \mathbf{u}_t = -f\mathbf{J}\mathbf{u} - g\nabla_{\mathbf{x}} h(\mathbf{x}, t). \tag{3.2}$$

It is obvious that the symplectic 2-form $\boldsymbol{\omega}$, defined by (2.23), is conserved along solutions and, as pointed out before, this gives rise to conservation of PV. In fact, this observation gives a new interpretation of the statement made by Abarbanel & Holm (1987) (see equation (81) on page 3375) in the context of the primitive unapproximated fluid equations.

It is worth carrying this thought experiment a step further. Following this point of view – taking h as given – conservation of PV can be shown for the induced two degrees-of-freedom Hamiltonian system of the above form (3.2) with h any arbitrary (possibly time-dependent) potential energy function. The restriction of the associated symplectic 2-form $\boldsymbol{\omega}$ is to be taken in the following sense. Consider a family of solutions $(\mathbf{x}(\mathbf{m},t),\mathbf{u}(\mathbf{m},t)) \in \mathbb{R}^4$ parameterized by their initial positions $\mathbf{m} = \boldsymbol{x}(0)$, then the pull-back described in §1 leads to conservation of PV.

Of course, the above point of view is not equivalent to the multi-symplectic approach where the layer-depth h is also treated as a dynamical variable and where $\boldsymbol{\omega}$ is no longer constant along solutions of the full fluid equations of motion. We will come back to this point below.

Another standard result (e.g., Frank & Reich (2003)) states that the layer-depth approximation (3.1) satisfies a continuity equation

$$h_t = -\nabla_{\mathbf{x}}(h\bar{\mathbf{u}})$$

with the velocity field $\bar{\mathbf{u}}(\mathbf{x},t)$ appropriately defined. Hence the energy of each particle in the flow changes according to

$$\frac{d}{dt}\left(\frac{1}{2}\|\mathbf{u}(t)\|^2 + gh(\mathbf{x}(t),t)\right) = -g\nabla_{\mathbf{x}}(h\bar{\mathbf{u}}).$$

So far we have assumed the discrete particle paths $\mathbf{X}_k(t)$, $k = 1,\ldots,N$, in (3.1) as given. Hence the next step is to set up a closed system of equations for $\{\mathbf{X}_k\}_{k=1,\ldots,N}$. In smoothed particle hydrodynamics these equations are given by

$$\frac{d^2}{dt^2}\mathbf{X}_k = -f\mathbf{J}\frac{d}{dt}\mathbf{X}_k - g\nabla_{\mathbf{X}_k}h(\mathbf{X}_k,\{\mathbf{X}_l\})$$

with

$$h(\mathbf{X}_k,\{\mathbf{X}_l\}) = \sum_{l=1}^{N} m_l\psi(\|\mathbf{X}_k - \mathbf{X}_l\|).$$

Again, we can associate a symplectic form with each particle $\mathbf{X}_k$. Let us denote this form by $\boldsymbol{\omega}_k$. While we had $\frac{d}{dt}\boldsymbol{\omega}_k = 0$ along solutions $\mathbf{x}(\mathbf{m}_k,t) = \mathbf{X}_k(t)$ of (3.2), we now treat h as a dynamic variable and obtain

$$\frac{d}{dt}\boldsymbol{\omega}_k = -g\sum_{l=1}^{N} \mathrm{d}\mathbf{X}_k \wedge m_l D_{\mathbf{X}_k\mathbf{X}_l}\psi(\|\mathbf{X}_k - \mathbf{X}_l\|)\,\mathrm{d}\mathbf{X}_l,$$

which can be viewed as a discretization of the multi-symplectic conservation law (2.15). Since the label space has been replaced by N point labels $\mathbf{m}_k$, a pull-back of the symplectic conservation law to label space is no longer possible. Hence conservation of PV holds for particle methods only in the sense of a single two degrees-of-freedom Hamiltonian ODE (3.2) with a continuous set of initial data. This "continuum" interpretation of particle methods is the backbone of the argument suggested by Frank & Reich (2003) to prove conservation of circulation for the discretized system.

4. Symplecticity and vorticity for other ideal-fluid models

In this section, we briefly describe the implications of the constructions in §2 based on conservation of symplecticity for other models in Lagrangian fluid dynamics. For three-dimensional Lagrangian fluid dynamics the main result is that the pull-back to the reference space of the symplectic form leads to Ertel's Theorem.

(a) *Semi-geostrophic shallow water equations*

In the semi-geostrophic approximation (cf. Salmon (1988), Roulstone & Norbury (1994), Roulstone & Sewell (1997)), the shallow water equations (2.5)-(2.8) are replaced by

$$u_{1,t} - f x_{2,t} = \left(\frac{\partial e(\tau)}{\partial x_{11}}\right)_{,1} + \left(\frac{\partial e(\tau)}{\partial x_{12}}\right)_{,2}, \tag{4.1}$$

$$u_{2,t} + f x_{1,t} = \left(\frac{\partial e(\tau)}{\partial x_{21}}\right)_{,1} + \left(\frac{\partial e(\tau)}{\partial x_{22}}\right)_{,2}, \tag{4.2}$$

$$0 = f u_1 - \left(\frac{\partial e(\tau)}{\partial x_{21}}\right)_{,1} - \left(\frac{\partial e(\tau)}{\partial x_{22}}\right)_{,2}, \tag{4.3}$$

$$0 = f u_2 + \left(\frac{\partial e(\tau)}{\partial x_{11}}\right)_{,1} + \left(\frac{\partial e(\tau)}{\partial x_{12}}\right)_{,2}, \tag{4.4}$$

where

$$e(\tau) = \frac{g}{2\tau}. \tag{4.5}$$

Here $\mathbf{u}$ is the geostrophic velocity, not the particle velocity (which is $\mathbf{x}_{,t}$). This system of equations is equivalent to the following Hamiltonian system:

$$\begin{bmatrix} -f\mathbf{J} & -\mathbf{I} \\ \mathbf{I} & -f^{-1}\mathbf{J} \end{bmatrix} \begin{pmatrix} \mathbf{x} \\ \mathbf{u} \end{pmatrix}_t = \begin{pmatrix} \delta H/\delta \mathbf{x} \\ \delta H/\delta \mathbf{u} \end{pmatrix}, \qquad \mathbf{J} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \tag{4.6}$$

where

$$H(\mathbf{x}, \mathbf{u}) = \int S \, \mathrm{d}\mathbf{m}, \qquad S = \tfrac{1}{2}\langle \mathbf{u}, \mathbf{u} \rangle + e(\tau). \tag{4.7}$$

The skew-symmetric operator on the left-hand side of (4.6) is not invertible. This degeneracy reflects the constraints in the semi-geostrophic formulation. In other words, the gradient of H is required to be in the range of the skew-symmetric operator; this solvability condition imposes the constraints. A closed but degenerate two-form is called a *pre-symplectic form*, and for this system the pre-symplectic form is

$$\overline{\boldsymbol{\omega}} = \int \boldsymbol{\omega} \, \mathrm{d}\mathbf{m}, \quad \boldsymbol{\omega} = \mathrm{d}u_1 \wedge \mathrm{d}x_1 + \mathrm{d}u_2 \wedge \mathrm{d}x_2 + f \mathrm{d}x_1 \wedge \mathrm{d}x_2 + f^{-1} \mathrm{d}u_1 \wedge \mathrm{d}u_2 .$$

This two-form differs from the symplectic form for the standard shallow-water equations by the last term only. In the multisymplectic formulation, the analysis of §2 goes through with the following minor changes.

1. The skew-symmetric matrix $\boldsymbol{K}$ has two extra nonzero components:
$$K_{3,4} = f^{-1}, \qquad K_{4,3} = -f^{-1}.$$

2. The potential vorticity is
$$q = f^{-1}\left\{ (u_1 - fx_2)_{,1}\,(u_2 + fx_1)_{,2} \;-\; (u_1 - fx_2)_{,2}\,(u_2 + fx_1)_{,1} \right\}.$$
(As before, the potential vorticity is the $\mathrm{d}m_1 \wedge \mathrm{d}m_2$ component of $\Psi^*\boldsymbol{\omega}$; the corresponding component of $\Psi^*\boldsymbol{\kappa}_{\alpha,\alpha}$ is zero on solutions, so q is conserved on particle paths.)

3. The energy conservation law, which can be deduced from the $\mathrm{d}m_\alpha \wedge \mathrm{d}t$ components of the pull-back of the symplectic conservation law, is
$$S_{,t} + \left(x_{i,t} w_{i\alpha}\right)_{,\alpha} = 0.$$

(*b*) *Three-dimensional ideal fluid dynamics*

The Euler equations for incompressible fluid dynamics in three dimensions, written in terms of the Lagrangian mass coordinates $\mathbf{m} = (m_1, m_2, m_3)$, are
$$x_{i,t} = u_i\,, \qquad x_{i,\alpha} u_{i,t} = -p_{,\alpha}\,, \qquad \det(\mathbf{x_m}) = 1.$$
Here $\mathbf{x_m}$ is the Jacobian matrix, so the incompressibility condition amounts to
$$\tau \equiv \varepsilon_{\alpha\beta\gamma}\, x_{1\alpha}\, x_{2\beta}\, x_{3\gamma} = 1,$$
where $\varepsilon_{\alpha\beta\gamma}$ is the alternating tensor and $x_{i\alpha} = x_{i,\alpha}$.

The Euler equations have the same Hamiltonian formulation (1.2) in two and three dimensions. From (1.1), the Hamiltonian density is
$$S = \tfrac{1}{2}\langle \mathbf{u}, \mathbf{u} \rangle + (1 - \det(\mathbf{x_m}))\, p\,.$$
As usual, we construct the multisymplectic formulation by defining the auxiliary variables
$$w_{i\alpha} = -\frac{\partial S}{\partial x_{i\alpha}}\,.$$
Then the Euler equations can be rewritten as
$$\begin{aligned} -u_{i,t} - w_{i\alpha,\alpha} &= 0, \\ x_{i,t} &= u_i\,, \\ x_{i,\alpha} &= x_{i\alpha}\,, \\ 0 &= \frac{\partial S}{\partial x_{i\alpha}} + w_{i\alpha}\,, \\ 0 &= 1 - \tau. \end{aligned}$$
Let $\mathbf{z} = (x_i, u_i, w_{i\alpha}, x_{i\alpha}, p)^{\mathrm{T}}$, where the variables are ordered by the value of i (and, where there are two subscripts, by the value of α for each i). Then the Euler equations amount to
$$\mathbf{K}\boldsymbol{z}_{,t} + \mathbf{L}^\alpha \boldsymbol{z}_{,\alpha} = \boldsymbol{\nabla}_{\boldsymbol{z}} S_M(\boldsymbol{z}),$$

where $\mathbf{K}, \mathbf{L}^1, \mathbf{L}^2, \mathbf{L}^3$ are skew-symmetric matrices whose only nonzero components are

$$\begin{aligned}
K_{1,4} &= K_{2,5} = K_{3,6} = -1, & K_{4,1} &= K_{5,2} = K_{6,3} = 1,\\
L^1_{1,7} &= L^1_{2,10} = L^1_{3,13} = -1, & L^1_{7,1} &= L^1_{10,2} = L^1_{13,3} = 1,\\
L^2_{1,8} &= L^2_{2,11} = L^2_{3,14} = -1, & L^2_{8,1} &= L^2_{11,2} = L^2_{14,3} = 1,\\
L^3_{1,9} &= L^3_{2,12} = L^3_{3,15} = -1, & L^3_{9,1} &= L^3_{12,2} = L^3_{15,3} = 1,
\end{aligned}$$

and where $S_M = S + x_{i\alpha} w_{i\alpha}$. The conservation law of symplecticity is

$$\boldsymbol{\omega}_{,t} + \boldsymbol{\kappa}_{\alpha,\alpha} = 0,$$

where

$$\boldsymbol{\omega} = \mathrm{d}\boldsymbol{z} \wedge \mathbf{K}\mathrm{d}\boldsymbol{z} = \mathrm{d}u_i \wedge \mathrm{d}x_i \quad \text{and} \quad \boldsymbol{\kappa}_\alpha = \mathrm{d}\boldsymbol{z} \wedge \mathbf{L}^\alpha \mathrm{d}\boldsymbol{z} = \mathrm{d}w_{i\alpha} \wedge \mathrm{d}x_i\,.$$

The pull-back of the multisymplectic conservation law to $(\mathbf{m}, t)$ space is

$$\begin{aligned}
0 = \Psi^* \left(\boldsymbol{\omega}_{,t} + \boldsymbol{\kappa}_{\alpha,\alpha}\right) &= \varepsilon_{\alpha\beta\gamma}\, \Omega_{\gamma,t}\, \mathrm{d}m_\alpha \wedge \mathrm{d}m_\beta \\
&+ \left\{ \left(\tfrac{1}{2}\langle \mathbf{u}, \mathbf{u}\rangle\right)_{,t} + (u_i w_{i\beta})_{,\beta} \right\}_{,\alpha} \mathrm{d}m_\alpha \wedge \mathrm{d}t\,,
\end{aligned}$$

where

$$\Omega_\gamma = \varepsilon_{\lambda\mu\gamma}\, x_{i\mu}\, u_{i,\lambda} = \varepsilon_{\lambda\mu\gamma}\, \left(x_{i\mu} u_i\right)_{,\lambda}\,. \tag{4.8}$$

(This result derived in essentially the same way as the conservation laws in §2; details are omitted for the sake of brevity.) Thus the pull-back leads to conservation of total energy,

$$\left(\tfrac{1}{2}\langle \mathbf{u}, \mathbf{u}\rangle\right)_{,t} + (u_i w_{i\beta})_{,\beta} = 0,$$

and conservation of $\boldsymbol{\Omega} = (\Omega_1, \Omega_2, \Omega_3)^{\mathrm{T}}$:

$$\boldsymbol{\Omega}_{,t} = 0\,.$$

Now, from (4.8),

$$\Omega_\gamma = \varepsilon_{\lambda\mu\gamma}\, x_{i\mu} x_{j\lambda} \frac{\partial u_i}{\partial x_j}\,,$$

which can be written in the form

$$\boldsymbol{\Omega} = -\mathbf{x}_{\mathbf{m}}^{-1} (\boldsymbol{\nabla}_{\mathbf{x}} \times \mathbf{u}). \tag{4.9}$$

In contrast to corresponding result for the two-dimensional Euler equations (cf. §1), $\boldsymbol{\Omega}$ is not the vorticity. Ertel's theorem (cf. MÜLLER 1995, SALMON 1982) is an immediate consequence of (4.9). Let θ be any materially conserved quantity, so that $\theta_{,t} = 0$. Then the vector product

$$Q = \Omega_\gamma \theta_{,\gamma}$$

is also materially conserved: $Q_{,t} = 0$. Unlike $\mathbf{\Omega}$, the quantity Q has a representation in terms of the Eulerian variables $\mathbf{x}$ and $\mathbf{u}$ only:

$$Q = -\langle \boldsymbol{\nabla}_{\mathbf{x}}\theta, \boldsymbol{\nabla}_{\mathbf{x}} \times \mathbf{u}\rangle.$$

For compressible homentropic fluids, the only significant modification is to replace (4.9) by $\mathbf{\Omega} = -\tau \mathbf{x}_{\mathbf{m}}^{-1}(\boldsymbol{\nabla}_{\mathbf{x}} \times \mathbf{u})$; then

$$Q = \frac{-\langle \boldsymbol{\nabla}_{\mathbf{x}}\theta, (\boldsymbol{\nabla}_{\mathbf{x}} \times \mathbf{u})\rangle}{\rho},$$

where $\rho = 1/\tau$ the density of the fluid.

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