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RESEARCH ARTICLE

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Hamilton's principle with phase changes and conservation principles for moist potential vorticity

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Abstract

Many definitions of moist potential vorticity (PV) have been proposed to extend the dry theory of Ertel PV. None of the moist PV definitions seem to have all of the desirable properties of the dry Ertel PV. For instance, dry PV is not only a globally conserved quantity, but also a material invariant that is conserved along fluid parcel trajectories. Therefore, an open question remains: Is there a moist PV that is a material invariant, if clouds and phase changes of water are present? In prior studies, definitions of moist PV have been proposed based on physical and mathematical intuition. Here, a systematic approach is used. In particular, a particle relabeling symmetry is devised for a moist atmosphere and then Noether's theorem is employed to arrive at the associated conservation laws for a moist PV. A priori, it is not clear whether this systematic approach will be viable, since it relies on variational derivatives in Hamilton's principle, and phase changes introduce singularities that could potentially prevent derivatives at the cloud edge. However, it is shown that the energy and the Lagrangian density are sufficiently smooth to allow variational derivatives, in a moist Boussinesq system with reversible phase transitions between water vapor and liquid cloud water. From the particle relabeling symmetry, a moist Kelvin circulation theorem is found, along with a moist PV conservation law that applies not for each individual parcel but for parcel-integrated PV, integrated over certain local volumes.

KEYWORDS

clouds, Ertel potential vorticity, Hamiltonian formulation, Kelvin's circulation theorem, moist atmospheric flows, particle relabeling symmetry

1 | INTRODUCTION

Potential vorticity (PV) is one of the fundamental conserved quantities of geophysical fluid dynamics. Conservation of PV was recognized long ago by Rossby (1939) and Ertel (1942). One important property of PV is that it is a material invariant, meaning that it is conserved along fluid particle trajectories; this allows it to function as a tracer of fluid particles. This material invariance property is exploited in isentropic PV maps, which have

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been used extensively as an operational diagnostic tool in the development of midlatitude synoptic weather systems (Hoskins *et al.*, 1985; Thorpe, 1985; Hoskins and Berrisford, 1988; Hoskins, 1991). Another important property is its invertibility: the instantaneous global distribution of PV with appropriate boundary conditions can be used to recover the balanced parts of the wind and temperature fields.

Though the concept of PV is well established for a dry atmosphere, the concept of PV is less clear for a moist atmosphere with clouds, phase changes, and latent heating. Several definitions of moist PV have been proposed, but a moist counterpart that retains all of the desirable properties of a dry PV has been elusive. For example, one moist PV definition (here called PV_{y}) is defined in terms of the virtual potential temperature $\theta_{\rm v}$, and it was shown to possess an invertibility principle that produces certain velocity and temperature fields (Schubert et al., 2001). However, Wetzel et al. (2020) have shown that the evolution equation for PV_v is coupled with inertia-gravity waves due to latent heating, and therefore PV_v is not balanced, and inversion of PV_v does not recover the balanced velocity and temperature fields. Although PV_v is not balanced, it is a conserved quantity in unsaturated regions and, therefore, can be used to monitor and diagnose latent heating in the atmosphere (Davis and Emanuel, 1991; Lackmann, 2002; Gao et al., 2004; Brennan and Lackmann, 2005; Brennan et al., 2008; Lackmann, 2011; Martin, 2013; Madonna et al., 2014; Büeler and Pfahl, 2017). Another widely used PV (here called PV_e) is based on the equivalent potential temperature θ_{e} (Bennetts and Hoskins, 1979; Emanuel, 1979). One criticism of PVe is that it fails to possess an invertibility principle in the presence of phase changes (Cao and Cho, 1995; Schubert et al., 2001). However, taking advantage of one or more additional balanced quantities M involving water, extended PV-M inversion can indeed be used to solve for the balanced moist flow using PVe (Smith and Stechmann, 2017; Wetzel et al., 2019, 2020). As a general principle, for a moist system, a single moist PV variable by itself is not sufficient information to find the balanced flow components, and additional moisture variables M need to be retained (Smith and Stechmann, 2017).

Furthermore, the moist PV quantities that have been proposed are lacking the fundamental conservation property of dry PV: conservation along fluid parcel trajectories. Some moist PV quantities are conserved in one phase (either inside a cloud or outside a cloud) but none are conserved along fluid parcel trajectories in the presence of clouds and phase changes. Hence, there remains an open question: For a moist system with clouds and phase changes, is there a moist PV quantity that is a material invariant? Though past definitions of moist PV have been proposed based on physical and mathematical intuition, there is, in fact, a systematic approach to identifying conservation principles. In Hamiltonian mechanics and Lagrangian mechanics, conservation principles are related to symmetries in the action, via Noether's theorem (Noether, 1918; Hill, 1951; Olver, 2000). Therefore, as a systematic route to identifying a moist PV conservation law, one can first write the moist atmospheric equations in a Hamiltonian or Lagrangian formulation and then look for symmetries in the action or the Lagrangian density.

The goal of the present paper is to take the systematic approach described above. To first define a Hamiltonian or Lagrangian formulation, we use the piecewise-quadratic energy that was recently identified for the moist Boussinesq equations with phase changes (Marsico *et al.*, 2019). As the symmetry of interest for moist PV, we will seek a moist analog of the symmetry associated with dry PV conservation: particle relabeling symmetry (Bretherton, 1970; Ripa, 1981; Salmon, 1988; Shepherd, 1990; Müller, 1995).

This article is another contribution of the use of the Lagrangian or Hamiltonian formulation for geophysical fluid dynamics. For example, in other applications, by attaching additional constraints to the Lagrangian/Hamiltonian, the Lagrangian/Hamiltonian formulation provides a systematic way of deriving approximate dynamical equations that retain analogs of exact conservation laws (Holm et al., 1998; Salmon, 1998; Cotter and Holm, 2014). Well-known examples of such approximate models are the quasi-geostrophic, shallow water, Korteweg-de Vries, and Green-Naghdi equations (see Salmon, 1988, and references therein). Additionally, the Hamiltonian formulation is useful in nonlinear stability theory (Salmon, 1988). Other applications include data assimilation (Cotter, 2013; Hastermann et al., 2021), statistical analysis (Abramov et al., 2003; Majda et al., 2019; Moore et al., 2020), and stochastic partial differential equations for fluid dynamics from a stochastic variational principle (Holm, 2015). It has also been used in the development of numerical methods (Pavlov et al., 2011).

In Section 2, we provide background about the governing moist Boussinesq equations and their conservation of energy principle. Next, in Section 3, we show that the energy is differentiable, allowing for a formulation of the dynamics from the perspective of Lagrangian mechanics. We further demonstrate that Hamilton's principle leads to Euler–Lagrange equations that are equivalent to the original equations. Section 4 explains how to adapt particle-relabeling symmetry to the moist system with phase changes, and thereby derive moist analogs of Kelvin's circulation theorem and conservation of PV. Conclusions are given in Section 5.

2 | BACKGROUND

As background, we describe the model equations in Section 2.1 and the conserved energy in Section 2.2. The energy will be used later to suggest the form of a Hamiltonian and a Lagrangian.

2.1 | Governing equations

We start by presenting the model equations, which are moist Boussinesq equations with phase changes. This type of model has been used for many purposes and with varying degrees of idealization (e.g., Kuo, 1961; Sommeria, 1976; Bretherton, 1987; Cuijpers and Duynkerke, 1993; Spyksma et al., 2006; Pauluis and Schumacher, 2010; Marsico et al., 2019; Zhang et al., 2021a,b). Though a Boussinesq framework is used here, one would suspect that similar results could be obtained for an anelastic or compressible system, although such cases are beyond the scope of this article. A Boussinesq framework is used here instead of an anelastic or compressible framework because it allows for some calculations to be in simpler form and because it allows use of an energy function (Section 2.2) that has a simple piecewise quadratic form (Marsico et al., 2019).

When the two thermodynamic variables are chosen to be θ_e and q_t , the equations take the form

$$\frac{D\vec{u}}{Dt} = -\nabla\phi + b\hat{k},\tag{1}$$

$$\frac{D\theta_{\rm e}}{Dt} + \frac{d\tilde{\theta_{\rm e}}}{dz}w = 0, \tag{2}$$

$$\frac{Dq_{\rm t}}{Dt} + \frac{d\tilde{q}_{\rm t}}{dz}w = 0, \tag{3}$$

$$\nabla \cdot \vec{u} = 0, \tag{4}$$

where $\vec{x} = (x, y, z)$ is the position vector, \hat{k} is the unit vector in the *z*-direction, $\vec{u} = (u, v, w)$ is the velocity vector, $D/Dt = \partial/\partial t + \vec{u} \cdot \nabla$ is the material derivative, $\phi = p'/\rho_0$, p' is the pressure anomaly, ρ_0 is a constant background density, θ_e is the equivalent potential temperature anomaly, and q_t is the anomalous total water mixing ratio. Every thermodynamic variable considered here has been decomposed into a background function of height *z* and an anomalous part. For example, $\theta_e^{\text{tot}} = \tilde{\theta}_e(z) + \theta_e(\vec{x}, t)$ and $q_t^{\text{tot}} = \tilde{q}_t(z) + q_t(\vec{x}, t)$. The background vertical gradients, $d\tilde{\theta}_e/dz$ and $d\tilde{q}_t/dz$, will be assumed to be constants, in analogy with a common set-up of the Boussinesq equations in the dry case (e.g., Majda, 2003). The buoyancy *b* is influenced by phase changes of water, and *b* can be expressed as a function of θ_e , q_t , and *z*. To do this, one can start from a definition of

$$b = g\left(\frac{\theta}{\theta_0} + R_{\rm vd}q_{\rm v} - q_{\rm l}\right),\tag{5}$$

where $\theta_0 \approx 300 \text{ K}$ is the constant background potential temperature, $g \approx 9.8 \text{ m} \cdot \text{s}^{-2}$ is the acceleration due to gravity and $R_{\text{vd}} = (R_{\text{v}}/R_{\text{d}}) - 1 \approx 0.61$, where R_{d} is the gas constant for dry air and R_{v} is the gas constant for water vapor. The three variables in this buoyancy expression are potential temperature θ , water vapor mixing ratio q_{v} , and liquid water mixing ratio q_{l} , and they can be related to q_{t} and θ_{e} as described in the following.

The set of variables (θ, q_v, q_l) can be related to the set of variables (θ_e, q_t) in the following way. The total water q_t is defined as the sum of water vapor q_v and liquid water q_l :

$$q_{\rm t} = q_{\rm v} + q_{\rm l}.\tag{6}$$

The second variable, equivalent potential temperature θ_{e} , is defined here in linearized form as

$$\theta_{\rm e} = \theta + \frac{L_{\rm v}}{c_p} q_{\rm v},\tag{7}$$

where the latent heat is a constant with value $L_v \approx 2.5 \times 10^6 \text{ J} \cdot \text{kg}^{-1}$ and specific heat is a constant with value $c_p \approx 10^3 \text{ J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$. From these definitions in Equations (6) and (7), one can find the variables (θ_e, q_t) if given the variables (θ, q_v, q_l).

For the opposite direction, if given q_t , one can partition it into its vapor (q_v) and liquid (q_l) components by using the saturation mixing ratio q_{vs} , which acts as a threshold. The saturation mixing ratio will be assumed to be a function of only z by making the assumption that T^{tot} and p^{tot} are close to the background states $\tilde{p}(z)$ and $\tilde{T}(z)$, which in turn depend only on the height, in which case $q_{vs}^{\text{tot}}(T^{\text{tot}}, p^{\text{tot}}) \approx q_{vs}^{\text{tot}}(\tilde{T}(z), \tilde{p}(z))$ (see, e.g., the appendix of Hernandez-Duenas et al., 2013). Two cases are possible, depending on whether q_t is below the threshold ($q_t < q_{vs}$) or above the threshold ($q_t > q_{vs}$). If q_t is below the threshold ($q_t < q_{vs}$), then no liquid water is present (i.e., $q_1 = 0$), and the water is all in the form of vapor: $q_t = q_y$. On the other hand, if q_t is above the threshold $(q_t > q_{vs})$, then the water vapor is at its saturation value (i.e., $q_v = q_{vs}$), and the remaining water is liquid water: $q_1 = q_t - q_{vs}$. To encompass both of these cases in a unified way, the formulas for q_v and q_l can be written as

$$q_{\rm v} = \min(q_{\rm t}, q_{\rm vs}),\tag{8}$$

$$q_{\rm l} = \max(0, q_{\rm t} - q_{\rm vs}).$$
 (9)

The two cases will be called the unsaturated phase (if $q_v < q_{vs}$) and the saturated phase (if $q_v = q_{vs}$).

If θ_e and q_t are both given, then one can also see that

$$\theta = \theta_{\rm e} - \frac{L_{\rm v}}{c_p} \min(q_{\rm t}, q_{\rm vs}). \tag{10}$$

This expression follows from Equations (7) and (8). Together, the three expressions in Equations (8)–(10) give a specification of the variables (θ, q_v, q_l) if given the variables (θ_e, q_t) .

Note that many of the aforementioned expressions have been written in terms of anomalies, such as θ_e , rather than the total expressions, such as $\theta_e^{\text{tot}} = \tilde{\theta}_e(z) + \theta_e(\vec{x}, t)$, which include background states. In particular, notice that the fundamental condition for saturation should be $q_t^{\text{tot}} = q_{\text{vs}}^{\text{tot}}$. Nevertheless, one can choose the background state to be unsaturated with $\tilde{q}_t(z) = \tilde{q}_v(z)$, and one can also break $q_{\text{vs}}^{\text{tot}}$ into background and anomaly as $q_{\text{vs}}^{\text{tot}} = \tilde{q}_{\text{vs}} + q_{\text{vs}}$, with the choice of $\tilde{q}_{\text{vs}}(z) = \tilde{q}_v(z)$. With these choices of $\tilde{q}_t(z) = \tilde{q}_{\text{vs}}(z) = \tilde{q}_{\text{vs}}(z)$, it follows that the saturation condition $q_t^{\text{tot}} = q_{\text{vs}}^{\text{tot}}$ can be written in terms of anomalies in a simple way, as $q_t = q_{\text{vs}}$.

It is convenient to rewrite these equations by replacing the thermodynamic variables, θ_e and q_t , with the unsaturated and saturated buoyancy variables, b_u and b_s . The variables b_u and b_s are defined so that the buoyancy *b* can be written simply as

$$b = b_{\rm u}H_{\rm u} + b_{\rm s}H_{\rm s},\tag{11}$$

where H_u and H_s are Heaviside functions that are indicators of the unsaturated and saturated regions, respectively:

$$H_{\rm u} = \begin{cases} 1 & \text{if } q_{\rm t} < q_{\rm vs}(z) \\ 0 & \text{if } q_{\rm t} \ge q_{\rm vs}(z), \end{cases} \qquad H_{\rm s} = 1 - H_{\rm u}.$$
(12)

To define b_u and b_s , the buoyancy definition in Equation (5) is rewritten in terms of equivalent potential temperature θ_e , total water q_t , and prescribed saturation mixing ratio q_{vs} , using Equations (6)–(10), which yields

$$b_{\rm u} = g \left[\frac{\theta_{\rm e}}{\theta_0} + \left(R_{\rm vd} - \frac{L_{\rm v}}{c_p \theta_0} \right) q_{\rm t} \right], \tag{13}$$

$$b_{\rm s} = g \left[\frac{\theta_{\rm e}}{\theta_0} + \left(R_{\rm vd} - \frac{L_{\rm v}}{c_p \theta_0} + 1 \right) q_{\rm vs} - q_{\rm t} \right].$$
(14)

These types of unsaturated and saturated buoyancy variables have also been used in other work on moist convection (e.g., Kuo, 1961; Bretherton, 1987; Pauluis and Schumacher, 2010; Smith and Stechmann, 2017) and are sometimes called the dry and moist buoyancy variables.

Notice that $b = b_u$ in unsaturated regions and $b = b_s$ in saturated regions, but the variables b_u and b_s are defined and exist everywhere, since they are defined as functions of θ_e , q_t , and q_{vs} .

The governing equations in terms of b_u and b_s are

$$\frac{D\vec{u}}{Dt} = -\nabla\phi + (b_{\rm u}H_{\rm u} + b_{\rm s}H_{\rm s})\hat{k}$$
(15)

$$\frac{Db_{\rm u}}{Dt} + N_{\rm u}^2 w = 0 \tag{16}$$

$$\frac{Db_{\rm s}}{Dt} + N_{\rm s}^2 w = 0, \tag{17}$$

$$\nabla \cdot \vec{u} = 0, \tag{18}$$

where the unsaturated and saturated buoyancy frequencies N_{μ}^2 and N_s^2 are constants given by

$$N_{\rm u}^2 = g \frac{d}{dz} \left[\frac{\tilde{\theta}_{\rm e}}{\theta_0} + \left(R_{\rm vd} - \frac{L_{\rm v}}{c_p \theta_0} \right) \tilde{q}_{\rm t} \right], \tag{19}$$

$$N_{\rm s}^2 = g \frac{d}{dz} \left[\frac{\tilde{\theta}_{\rm e}}{\theta_0} - \left(R_{\rm vd} - \frac{L_{\rm v}}{c_p \theta_0} \right) q_{\rm vs}(z) - \tilde{q}_{\rm t} \right].$$
(20)

The evolution equations for b_u and b_s in Equations (16) and (17) follow from the evolution equations for θ_e and q_t in Equations (2) and (3), using the definitions of b_u and b_s in Equations (13) and (14); and the definitions of N_u^2 and N_s^2 in Equations (19) and (20) also follow from this derivation. Finally, the indicator functions in Equation (12) can be written as

$$H_{\rm u} = \begin{cases} 1 & \text{if } b_{\rm u} > b_{\rm s} \\ 0 & \text{if } b_{\rm u} \le b_{\rm s}, \end{cases} \qquad H_{\rm s} = 1 - H_{\rm u}.$$
(21)

With this reformulation of the equations in terms of buoyancy variables, many aspects of the subsequent discussion will be simplified.

2.2 | Piecewise quadratic energy

In subsequent sections, to explore a possible particle-relabeling symmetry of the Lagrangian, it will first be necessary to define a suitable Lagrangian functional. To help motivate the form of a Lagrangian functional for the model in Equations (1)–(4), we now describe an energy function that was recently derived (Marsico *et al.*, 2019).

The model in Equations (1)-(4) or Equations (15)-(18) has an associated energy that is given by

$$E = \mathcal{K} + \mathcal{V}$$

= $\frac{1}{2}\vec{u}\cdot\vec{u} + \frac{1}{2}\frac{b_{u}^{2}}{N_{u}^{2}}H_{u} + \frac{1}{2}\frac{b_{s}^{2}}{N_{s}^{2}}H_{s} + \frac{1}{2}\frac{N_{u}^{2}N_{s}^{2}}{N_{u}^{2} - N_{s}^{2}}M^{2}H_{u}$ (22)

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and evolves according to

$$\frac{\partial E}{\partial t} + \nabla \cdot \left[\vec{u}(E + \phi) \right] = 0, \tag{23}$$

so that the domain-integrated energy is conserved (Marsico *et al.*, 2019). In the energy definition in Equation (22), the first term is the kinetic energy \mathcal{K} and the latter three terms are the potential energy \mathcal{V} . The b_u^2 and b_s^2 terms are the buoyant potential energy terms in the unsaturated and saturated phases, respectively. The new variable Mthat appears in the potential energy is actually related to b_u and b_s via

$$M = \frac{b_{\rm u}}{N_{\rm u}^2} - \frac{b_{\rm s}}{N_{\rm s}^2},$$
 (24)

and it is a material invariant; that is:

$$\frac{DM}{Dt} = 0,$$
(25)

which can be seen from Equations (16), (17), and (24). This variable M is associated with the additional eigenmode that is present in moist systems as opposed to dry systems (Hernandez-Duenas *et al.*, 2015; Smith and Stechmann, 2017). The M^2 term in the potential energy in Equation (22) is a moist energy term that accounts for the latent heat released during change of phase. Notice that each potential energy term is multiplied by either H_u or H_s , so the form of the potential energy will be different in different phases. In this way, the energy in Equation (22) is piecewise quadratic, as opposed to the quadratic energy that arises in the dry case.

Since the energy in Equation (22) is piecewisequadratic, it is positive if the coefficients N_u^2 , N_s^2 , and $N_u^2 - N_s^2$ are positive. Each of N_u^2 and N_s^2 will be positive if the fluid is stably stratified in the dry and moist sense, according to Equations (19) and (20). For simpler expressions of N_u^2 and N_s^2 , approximate forms of Equations (19) and (20) are

$$N_{\rm u}^2 \approx \frac{g}{\theta_0} \frac{d\tilde{\theta}}{dz}, \qquad N_{\rm s}^2 \approx \frac{g}{\theta_0} \frac{d\tilde{\theta}_{\rm e}}{dz},$$
 (26)

which indicate that N_u^2 and N_s^2 will be positive if the background vertical gradients of θ and θ_e are positive. In this case, the difference $N_u^2 - N_s^2$ will be positive if $d\tilde{q}_v/dz$ is negative, as can be seen from (7) and (26).

Though the energy in Equation (22) is piecewisedefined in terms of Heaviside functions, it was shown by Marsico *et al.* (2019) that the energy is continuous across phase boundaries. In other words, the potential energy in the unsaturated phase,

$$\frac{1}{2}\frac{b_{\rm u}^2}{N_{\rm u}^2} + \frac{1}{2}\frac{N_{\rm u}^2N_{\rm s}^2}{N_{\rm u}^2 - N_{\rm s}^2}M^2,$$
(27)

and the potential energy in the saturated phase,

$$\frac{1}{2}\frac{b_{\rm s}^2}{N_{\rm s}^2},$$
 (28)

will be equal at the phase interface. To see this, recall from Equation (21) that the phase interface can be defined as locations where $b_u = b_s$. Consequently, at the phase interface, one can rewrite the potential energy from the unsaturated phase as

$$\frac{1}{2}\frac{b_{u}^{2}}{N_{u}^{2}} + \frac{1}{2}\frac{N_{u}^{2}N_{s}^{2}}{N_{u}^{2} - N_{s}^{2}}M^{2}$$
$$= \frac{1}{2}\frac{b_{u}^{2}}{N_{u}^{2}} + \frac{1}{2}\frac{N_{u}^{2}N_{s}^{2}}{N_{u}^{2} - N_{s}^{2}}\left(\frac{b_{u}}{N_{u}^{2}} - \frac{b_{s}}{N_{s}^{2}}\right)^{2}$$
(29)

$$= \frac{1}{2}\frac{b_{\rm u}^2}{N_{\rm u}^2} + \frac{1}{2}\frac{N_{\rm u}^2N_{\rm s}^2}{N_{\rm u}^2 - N_{\rm s}^2} \left(\frac{b_{\rm u}^2}{N_{\rm u}^4} - \frac{2b_{\rm u}b_{\rm s}}{N_{\rm u}^2N_{\rm s}^2} + \frac{b_{\rm s}^2}{N_{\rm s}^4}\right) \qquad (30)$$

$$= \frac{1}{2} \frac{b_s^2}{N_u^2} + \frac{1}{2} \frac{N_u^2 N_s^2}{N_u^2 - N_s^2} \left(\frac{b_s^2}{N_u^4} - \frac{2b_s^2}{N_u^2 N_s^2} + \frac{b_s^2}{N_s^4} \right)$$
(31)

$$=\frac{1}{2}\frac{b_{\rm s}^2}{N_{\rm s}^2},\tag{32}$$

so that Equations (27) and (28) are equal at the phase interface, where the definition of M from Equation (24) was also used in the calculation. Intuitively, the buoyant energy b_u^2/N_u^2 should be smaller than b_s^2/N_s^2 at the phase interface, since N_u^2 is typically larger than N_s^2 ; the moist energy M^2 then compensates for the difference and ensures continuity of potential energy.

Beyond this earlier demonstration of continuity, we will show that the energy is also continuously differentiable, which allows us to take derivatives, which are needed for using the energy in a Hamiltonian or Lagrangian formulation.

3 | LAGRANGIAN FORMULATION AND EULER-LAGRANGE EQUATIONS

The goal of this section is to present a Lagrangian formulation of the model in Equations (1)-(4) or Equations (15)-(18). Then, in Section 4, the Lagrangian

formulation can be used to investigate PV and particle-relabeling symmetry of the Lagrangian.

3.1 | Lagrangian density and its regularity at cloud edge

The piecewise-quadratic energy in (22) can be used to construct a Lagrangian density ℓ for our system as the difference between kinetic \mathcal{K} and potential \mathcal{V} energy terms:

$$\ell = \mathcal{K} - \mathcal{V}$$

= $\frac{1}{2}\vec{u} \cdot \vec{u} - \left(\frac{1}{2}\frac{b_{u}^{2}}{N_{u}^{2}}H_{u} + \frac{1}{2}\frac{b_{s}^{2}}{N_{s}^{2}}H_{s} + \frac{1}{2}\frac{N_{u}^{2}N_{s}^{2}}{N_{u}^{2} - N_{s}^{2}}M^{2}H_{u}\right),$
(33)

where the potential energy \mathcal{V} was discussed in Section 2.2. For instance, though \mathcal{V} is defined in a piecewise manner in unsaturated and saturated phases, it is nevertheless a continuous function.

In order to proceed with a Lagrangian formulation of the dynamics including phase changes, it is necessary to demonstrate that the density ℓ given by Equation (33) is differentiable at phase boundaries, which are indicated by the Heaviside functions H_u and H_s . Thus, we proceed to compute derivatives in the unsaturated ($b_u > b_s$) and saturated ($b_u < b_s$) phases separately, and then to show equality of their one-sided limits as the phase boundary ($b_u = b_s$) is approached.

Let us fist consider Equation (33) in an unsaturated flow region with $H_u = 1$ and $H_s = 0$, and denote q as a placeholder for x, y, z or t. A derivative with respect to q of Equation (33) in the unsaturated phase gives

$$\frac{\partial \ell}{\partial q} = \vec{u} \cdot \frac{\partial \vec{u}}{\partial q} - \frac{b_{\rm u}}{N_{\rm u}^2} \frac{\partial b_{\rm u}}{\partial q} - \frac{N_{\rm u}^2 N_{\rm s}^2}{N_{\rm u}^2 - N_{\rm s}^2} M \frac{\partial M}{\partial q}$$
(34)

$$= \vec{u} \cdot \frac{\partial \vec{u}}{\partial q} - \frac{b_{\rm u}}{N_{\rm u}^2} \frac{\partial b_{\rm u}}{\partial q} - \frac{1}{N_{\rm u}^2 - N_{\rm s}^2} \\ \times \left(b_{\rm u} \frac{N_{\rm s}^2}{N_{\rm u}^2} \frac{\partial b_{\rm u}}{\partial q} - b_{\rm u} \frac{\partial b_{\rm s}}{\partial q} + b_{\rm s} \frac{N_{\rm u}^2}{N_{\rm s}^2} \frac{\partial b_{\rm s}}{\partial q} - b_{\rm s} \frac{\partial b_{\rm u}}{\partial q} \right), \quad (35)$$

where we have used the definition of M given by Equation (24). As the phase interface is approached from the unsaturated side, b_u tends to b_s from above, and therefore

$$\lim_{b_{u}-b_{s}\to0^{+}}\frac{\partial\ell}{\partial q}$$

$$=\lim_{b_{u}-b_{s}\to0^{+}}\left(\vec{u}\cdot\frac{\partial\vec{u}}{\partial q}-\left\{\frac{[(N_{u}^{2}-N_{s}^{2})+N_{s}^{2}]b_{u}-N_{u}^{2}b_{s}}{N_{u}^{2}(N_{u}^{2}-N_{s}^{2})}\right\}$$

$$\times\frac{\partial b_{u}}{\partial q}-\left[\frac{b_{s}N_{u}^{2}-b_{u}N_{s}^{2}}{N_{s}^{2}(N_{u}^{2}-N_{s}^{2})}\right]\frac{\partial b_{s}}{\partial q}\right)$$
(36)

$$= \vec{u} \cdot \frac{\partial \vec{u}}{\partial q} - \frac{b_{\rm s}}{N_{\rm s}^2} \frac{\partial b_{\rm s}}{\partial q}.$$
 (37)

Starting again from Equation (33), but now in a saturated region, the derivative of ℓ with respect to q is

$$\frac{\partial \ell}{\partial q} = \vec{u} \cdot \frac{\partial \vec{u}}{\partial q} - \frac{b_{\rm s}}{N_{\rm s}^2} \frac{\partial b_{\rm s}}{\partial q}.$$
(38)

From Equations (37) and (38), one can see that

$$\lim_{b_{u}-b_{s}\to 0^{+}}\frac{\partial\ell}{\partial q} = \lim_{b_{s}-b_{u}\to 0^{-}}\frac{\partial\ell}{\partial q} = \vec{u}\cdot\frac{\partial\vec{u}}{\partial q} - \frac{b_{s}}{N_{s}^{2}}\frac{\partial b_{s}}{\partial q},\qquad(39)$$

which establishes differentiability of the Lagrangian density ℓ at phase boundaries where $b_u = b_s$. Note that in these calculations we are only considering the possibility of non-smoothness that may have been introduced into the Lagrangian density in Equation (33) by the Heaviside functions. A further issue is that the regularity of this Lagrangian density also depends on the smoothness of the velocity field, buoyancy variables b_u and b_s , and so on, which we assume here to be sufficiently smooth. Establishing the regularity of solutions to moist dynamics would require a detailed mathematical analysis, and this has been carried out for some related systems (Majda and Souganidis, 2010; Zelati and Temam, 2012; Zelati *et al.*, 2013; Bousquet *et al.*, 2014; Zelati *et al.*, 2015; Li and Titi, 2016; Hittmeir *et al.*, 2017; Cao *et al.*, 2018; Hittmeir *et al.*, 2020).

Also note that, though the derivatives in Equations (35) and (38) were calculated by restricting attention to unsaturated and saturated regions, respectively, one might further desire a derivative formula that is valid throughout the entire domain. In this direction, and for a generic scenario, consider a piecewise-defined function g(q) given by

$$g(q) = g_u(q)H_u + g_s(q)H_s.$$
 (40)

For example, the Lagrangian density in Equation (33) is of this form. Then its derivative can be formally calculated as

$$\frac{dg}{dq} = \frac{d}{dq} \left[g_{\rm u}(q)H_{\rm u} + g_{\rm s}(q)H_{\rm s} \right] \tag{41}$$

$$= g'_{\rm u}(q)H_{\rm u} + g'_{\rm s}(q)H_{\rm s} + g_{\rm u}(q)\frac{dH_{\rm u}}{dq} + g_{\rm s}(q)\frac{dH_{\rm s}}{dq} \qquad (42)$$

$$= g'_{u}(q)H_{u} + g'_{s}(q)H_{s} + g_{u}(q)\frac{dH_{u}}{dq} + g_{s}(q)\frac{d}{dq}(1 - H_{u})$$
(43)

$$=g'_{\rm u}(q)H_{\rm u}+g'_{\rm s}(q)H_{\rm s}+[g_{\rm u}(q)-g_{\rm s}(q)]\frac{dH_{\rm u}}{dq} \tag{44}$$

$$= g'_{\rm u}(q)H_{\rm u} + g'_{\rm s}(q)H_{\rm s}, \tag{45}$$

where the last equality follows from an additional assumption that *g* is continuous, which implies that $g_u(q) - g_s(q) = 0$ at the phase interface, so that the coefficient of the Dirac-delta dH_u/dq is zero at the phase interface. (Note that these formal derivatives can be formulated as weak derivatives; see the Supporting Information for details.) Consequently, in calculating the derivative of a piecewise-defined function as in Equation (40), if the function is also continuous, then one can simply use

$$\frac{dg}{dq} = g'_{\rm u}(q)H_{\rm u} + g'_{\rm s}(q)H_{\rm s},\tag{46}$$

by differentiating the coefficients of H_u and H_s , without needing to consider derivatives of H_u and H_s themselves. We will use this result in Section 3.2.

3.2 | Hamilton's principle and the Euler-Lagrange equations

The ℓ defined in Equation (33) is a candidate for a Lagrangian density, which can potentially be used to define an associated set of Euler–Lagrange equations, via a variational principle – that is, the principle of least action, or Hamilton's principle. A priori, it is not immediately clear whether this will work here, owing to complications of phase changes. In Section 3.1 we established that, at the very least, ℓ is differentiable, so it is at least possible to take variational derivatives of ℓ . Now we investigate whether a variational principle, using ℓ as the Lagrangian density, will lead to the model in Equations (1)–(4) or Equations (15)–(18) as the associated Euler–Lagrange equations.

Hamilton's principle states that the dynamics of a system are determined according to a variational statement, and for fluid systems the variational statement may be expressed in either the Lagrangian¹ description or the Eulerian description (Hill, 1951; Bretherton, 1970; Salmon, 1982, 1988, 1998; Cotter and Holm, 2014). Our goal is to derive the model in Equations (15)–(18), which is written in the Eulerian description. Nevertheless, for clarity, and for further use later herein, we shall start now from the Lagrangian description and then briefly recall the steps in the transformation from the Lagrangian to the Eulerian description. In the Lagrangian description, one considers variations $\delta \vec{x}$ in the particle trajectories $\vec{x} = \vec{x}(\vec{a}, t)$ corresponding to particles labeled by \vec{a} . In the

Eulerian description, the system is described by the velocity \vec{u} at fixed locations, and thus one must use the inverse flow map $\vec{a} = \vec{a}(\vec{x}, t)$ (assumed one-to-one) to transform the variational statement accordingly. As in the previous sections, it will be convenient to work in Cartesian coordinates for simplicity.

Following fluid particles labeled by \vec{a} , the Lagrangian \mathcal{L} for the system is given by

$$\mathcal{L}(t) = \iiint dV_a \,\ell(\vec{x}(\vec{a},t),\vec{x}_t(\vec{a},t),\vec{a}) = \iiint dV_a \,\frac{1}{2} \left(\vec{x}_t \cdot \vec{x}_t - \frac{b_u^2}{N_u^2} H_u - \frac{b_s^2}{N_s^2} H_s - \frac{N_u^2 N_s^2}{N_u^2 - N_s^2} M^2 H_u\right),$$
(47)

where \vec{a} is chosen such that dV_a represents a differential mass element dm in particle-label space. For example, \vec{a} can be chosen as the initial position \vec{x}_0 . We make use of a different such choice of \vec{a} in later sections. The notation \vec{x}_t means the derivative of \vec{x} with respect to time t, keeping particle label \vec{a} fixed. Hamilton's principle is stated in terms of the action A:

$$\delta \mathcal{A} = 0, \quad \mathcal{A} = \int_{t_1}^{t_2} dt \mathcal{L}(t), \tag{48}$$

for variations $\delta \vec{x}(\vec{a}, t)$ that vanish outside the range $t \in [t_1, t_2]$. These variations must also tend to zero as \vec{x} tends to infinity, or satisfy no flow through the domain boundary (see e.g., Bretherton, 1970). To transform Equation (48) to the Eulerian description, one must change variables in the volume element using

$$dV_a = \mathcal{J}dV_x = \frac{\partial(\vec{a})}{\partial(\vec{x})}dV_x,\tag{49}$$

where dV_x is the volume element in physical space and \mathcal{J} is the Jacobian determinant, and we adopt the notation $\mathcal{J} \equiv \partial(\vec{a})/\partial(\vec{x})$ as in some of the previous literature. In Cartesian coordinates, \mathcal{J} is the determinant of the matrix $\partial a_i/\partial x_j$. For labeling coordinates chosen such that equal volumes in \vec{a} -space have equal masses, $\partial(\vec{a})/\partial(\vec{x})$ is the mass density ρ . Here, we wish to describe incompressible Boussinesq dynamics, and thus we take the constant $\rho = 1$. Using the Eulerian notation $\vec{u} = \vec{x}_t$, Hamilton's principle Equation (48) becomes

$$\delta \mathcal{A} = 0, \quad \mathcal{A} = \int_{t_1}^{t_2} dt \iiint dV_x \frac{1}{2} \left(\vec{u} \cdot \vec{u} - \frac{b_u^2}{N_u^2} H_u - \frac{b_s^2}{N_s^2} H_s - \frac{N_u^2 N_s^2}{N_u^2 - N_s^2} M^2 H_u \right),$$
(50)

¹Note that the adjective "Lagrangian" is sometimes used in the sense of Lagrangian versus Eulerian description of fluid dynamics, and sometimes in the sense of Lagrangian versus Hamiltonian formulation of classical mechanics. The different uses here should be clear from the context.

where now the action \mathcal{A} must be stationary with respect to arbitrary variations $\delta \vec{a}$. Thus, one must express the integrand as $\ell = \ell(\vec{a}(\vec{x}, t), \dots, \vec{x})$, where the \dots means derivatives of \vec{a} with respect to \vec{x} and/or *t*.

For example, let us consider how to express the velocity \vec{u} in Equation (50) as first derivatives of \vec{a} with respect to \vec{x} and *t*. The latter can be achieved from conservation of label \vec{a} following fluid particles:

$$\frac{D}{Dt}\vec{a} = \vec{a}_t + \vec{u} \cdot \nabla \vec{a} = 0, \qquad (51)$$

by solving Equation (51) as a 3×3 system for \vec{u} (Salmon, 1988), and we note that the ∇ without a subscript is the gradient operator $\nabla = (\partial_x, \partial_y, \partial_z)$. Alternatively, an equivalent variational statement is found by appending Equation (51) to Equation (50) as constraints (the Lin constraints), and then considering independent variations $\delta \vec{u}$ and $\delta \vec{a}$ (Bretherton, 1970; Salmon, 1988). In addition to the Lin constraints, a constraint is required to enforce the incompressibility condition $\nabla \cdot \vec{u} = 0$, thus leading to

$$\mathcal{A} = \int dt \iiint dV_{x} \left[\frac{1}{2} \vec{u} \cdot \vec{u} - \frac{1}{2} \frac{b_{u}^{2}}{N_{u}^{2}} H_{u} - \frac{1}{2} \frac{b_{s}^{2}}{N_{s}^{2}} H_{s} - \frac{1}{2} \frac{N_{u}^{2} N_{s}^{2}}{N_{u}^{2} - N_{s}^{2}} M^{2} H_{u} - \vec{\alpha} \cdot \frac{D\vec{a}}{Dt} - \lambda (\nabla \cdot \vec{u}) \right],$$
(52)

where λ and $\vec{\alpha} = (\alpha, \beta, \gamma)$ are Lagrange multipliers. As will be shown later, the multiplier λ contributes to the pressure. Next, the potential energy in the integrand can be rewritten in terms of the material invariants $b_u^{\text{tot}} = b_u^{\text{tot}}(\vec{a})$ and $b_s^{\text{tot}} = b_s^{\text{tot}}(\vec{a})$ using the relations

$$b_{\rm u} = b_{\rm u}^{\rm tot} - N_{\rm u}^2 z, \quad b_{\rm s} = b_{\rm s}^{\rm tot} - N_{\rm s}^2 z.$$
 (53)

One can verify that b_u^{tot} and b_s^{tot} are invariant following fluid particles according to the conservation equations

$$\frac{D}{Dt}b_{u}^{\text{tot}} = \frac{D}{Dt}b_{s}^{\text{tot}} = 0, \quad \frac{D}{Dt} = \frac{\partial}{\partial t} + \vec{u} \cdot \nabla.$$
 (54)

Using Equation (53), one can also rewrite H_u , H_s , and M in the potential energy to be functions of b_u^{tot} and b_s^{tot} , based on their definitions in Equations (21) and (24). Notice that, via Equation (53), the height z now appears explicitly in the potential energy terms, along with b_u^{tot} and b_s^{tot} . However, the explicit z-dependence does not have an influence on variations $\delta \vec{a}$ for the Lagrangian density $\ell = \ell(\vec{a}(\vec{x}, t), \dots, \vec{x})$, since the explicit z-dependence is part of the explicit \vec{x} -dependence in $\ell = \ell(\vec{a}(\vec{x}, t), \dots, \vec{x})$ and is separate from the *implicit* \vec{x} -dependence of the $\vec{a}(\vec{x}, t)$ -dependence of ℓ . As some physical connection, note that the potential energy is now considered as a function of

the three variables b_{u}^{tot} , b_{s}^{tot} , and z, and the presence of these three variables is analogous to the presence of three thermodynamic variables θ_{e}^{tot} , q_{t}^{tot} , and z or s^{tot} , q_{t}^{tot} , and p that are needed to describe the thermodynamic state of a moist system. The quantities b_u^{tot} and b_s^{tot} are material invariants that play the same type of role as the material invariants of entropy s^{tot} and total water mixing ratio q_t^{tot} , and z plays the role of pressure p in Boussinesq and anelastic systems (Pauluis, 2008). We continue to write the potential energy in terms of $b_{\rm u}$, $b_{\rm s}$, and M for simplicity of the expression; however, the transformation to the variables b_{μ}^{tot} , b_{s}^{tot} , and z is henceforth implied. Finally, we can exploit the material invariance of the buoyancy variables b_{u}^{tot} and b_{s}^{tot} by assigning them as two of the particle labels: $\vec{a} = (a, b, c) =$ $(a, b_{\mu}^{\text{tot}}, b_{s}^{\text{tot}})$, thereby allowing for independent variations δb_{u}^{tot} and δb_{s}^{tot} . Using the new labels, and integration by parts in the incompressibility constraint, we arrive at

$$\mathcal{A} = \int dt \iiint dV_x \left(\frac{1}{2} \vec{u} \cdot \vec{u} - \frac{1}{2} \frac{b_u^2}{N_u^2} H_u - \frac{1}{2} \frac{b_s^2}{N_s^2} H_s - \frac{1}{2} \frac{N_u^2 N_s^2}{N_u^2 - N_s^2} M^2 H_u - \alpha \frac{Da}{Dt} - \beta \frac{Db_u^{\text{tot}}}{Dt} - \gamma \frac{Db_s^{\text{tot}}}{Dt} - \vec{u} \cdot \nabla \lambda \right).$$
(55)

After all of the preceding transformations, Hamilton's principle requires that the A be stationary with respect to variations in $\vec{u}(\vec{x}, t)$, $a(\vec{x}, t)$, $b_u^{\text{tot}}(\vec{x}, t)$, $b_s^{\text{tot}}(\vec{x}, t)$, $\alpha(\vec{x}, t)$, $\beta(\vec{x}, t)$, $\gamma(\vec{x}, t)$, and $\lambda(\vec{x}, t)$. These variations result in the following:

$$\delta u: \quad \vec{u} - \alpha \nabla a - \beta \nabla b_{\rm u}^{\rm tot} - \gamma \nabla b_{\rm s}^{\rm tot} - \nabla \lambda = 0, \tag{56}$$

$$\delta \alpha: \quad \frac{Da}{Dt} = 0, \tag{57}$$

$$\delta a: \quad \frac{D\alpha}{Dt} = 0, \tag{58}$$

$$\delta\beta: \quad \frac{Db_{\rm u}^{\rm tot}}{Dt} = 0, \tag{59}$$

$$\delta b_{\rm u}^{\rm tot}: \quad \frac{D\beta}{Dt} - \frac{b_{\rm u}}{N_{\rm u}^2} H_{\rm u} - \frac{N_{\rm s}^2}{N_{\rm u}^2 - N_{\rm s}^2} M H_{\rm u} = 0, \tag{60}$$

$$\delta\gamma: \quad \frac{Db_{\rm s}^{\rm tot}}{Dt} = 0, \tag{61}$$

$$\delta b_{\rm s}^{\rm tot}: \quad \frac{D\gamma}{Dt} - \frac{b_{\rm s}}{N_{\rm s}^2} H_{\rm s} + \frac{N_{\rm u}^2}{N_{\rm u}^2 - N_{\rm s}^2} M H_{\rm u} = 0, \tag{62}$$

$$\delta \lambda: \quad \nabla \cdot \vec{u} = 0, \tag{63}$$

where we have used Equation (46). To obtain the momentum equation, one can compute $D\vec{u}/Dt$ using Equation (56), and then substitute from the remaining

equations in Equations (57)-(63) to obtain

$$\frac{D\vec{u}}{Dt} = \frac{D}{Dt} (\alpha \nabla a + \beta \nabla b_{u}^{tot} + \gamma \nabla b_{s}^{tot} + \nabla \lambda)
= \frac{\partial}{\partial t} (\alpha \nabla a + \beta \nabla b_{u}^{tot} + \gamma \nabla b_{s}^{tot} + \nabla \lambda) + \vec{u} \cdot \nabla \vec{u}$$
(64)

$$= \alpha \frac{\partial \nabla a}{\partial t} + \beta \frac{\partial \nabla b_{u}^{\text{tot}}}{\partial t} + \gamma \frac{\partial \nabla b_{s}^{\text{tot}}}{\partial t} + \frac{\partial \nabla \lambda}{\partial t} + \nabla a \frac{\partial \alpha}{\partial t} + \nabla b_{u}^{\text{tot}} \frac{\partial \beta}{\partial t} + \nabla b_{s}^{\text{tot}} \frac{\partial \gamma}{\partial t} + \vec{u} \cdot \nabla \vec{u}$$
(65)

$$= -[\alpha \nabla (\vec{u} \cdot \nabla \alpha) + \beta \nabla (\vec{u} \cdot \nabla b_{u}^{\text{tot}}) + \gamma \nabla (\vec{u} \cdot \nabla b_{s}^{\text{tot}}) + \nabla (\vec{u} \cdot \nabla \lambda)] + \nabla \left(\vec{u} \cdot \nabla \lambda + \frac{\partial \lambda}{\partial t} \right) + H_{u} \frac{b_{u}}{N_{u}^{2}} \nabla b_{u}^{\text{tot}} + H_{u} \frac{N_{s}^{2}}{N_{u}^{2} - N_{s}^{2}} M \nabla b_{u}^{\text{tot}} + H_{s} \frac{b_{s}}{N_{s}^{2}} \nabla b_{s}^{\text{tot}} - H_{u} \frac{N_{u}^{2}}{N_{u}^{2} - N_{s}^{2}} M \nabla b_{s}^{\text{tot}} + \vec{u} \cdot \nabla \vec{u} - [\nabla a (\vec{u} \cdot \nabla \alpha) + \nabla b_{u}^{\text{tot}} (\vec{u} \cdot \nabla \beta) + \nabla b_{s}^{\text{tot}} (\vec{u} \cdot \nabla \gamma)]$$
(66)

$$= -[\alpha \nabla (\vec{u} \cdot \nabla a) + \beta \nabla (\vec{u} \cdot \nabla b_{u}^{tot}) + \gamma \nabla (\vec{u} \cdot \nabla b_{s}^{tot}) + \nabla (\vec{u} \cdot \nabla \lambda)] - \nabla \left(-\vec{u} \cdot \nabla \lambda - \frac{\partial \lambda}{\partial t} - \frac{1}{2} \frac{(b_{u})^{2}}{N_{u}^{2}} H_{u} - \frac{1}{2} \frac{(b_{s})^{2}}{N_{s}^{2}} H_{s} - \frac{1}{2} \frac{N_{u}^{2} N_{s}^{2}}{N_{u}^{2} - N_{s}^{2}} M^{2} H_{u} \right) + (b_{u} H_{u} + b_{s} H_{s}) \hat{k} + \vec{u} \cdot \nabla \vec{u} - [\nabla a (\vec{u} \cdot \nabla \alpha) + \nabla b_{u}^{tot} (\vec{u} \cdot \nabla \beta) + \nabla b_{s}^{tot} (\vec{u} \cdot \nabla \gamma)].$$
(67)

In moving from Equation (65) to Equation (66), the term $\nabla(\vec{u} \cdot \nabla \lambda)$ was added and subtracted, and several of the relations from Equations (57)–(63) were used to replace $\partial/\partial t$ terms. Then, in moving from Equation (66) to Equation (67), the term ∇b_u^{tot} was split into contributions from b_u and $N_u^2 z$, using the definition in Equation (53), and similarly for ∇b_s^{tot} , leading to the buoyancy term $(b_u H_u + b_s H_s)\hat{k}$ in Equation (67). Also used in moving from Equation (66) to Equation (67) are Equations (24), (39), and (46). To proceed further, the main challenge is to identify and collect gradient terms so as to determine an effective pressure to recover the requisite governing equations. With that goal, we use the identity

$$\alpha \nabla (\vec{u} \cdot \nabla a) + \nabla a (\vec{u} \cdot \nabla \alpha) = \nabla [\vec{u} \cdot (\alpha \nabla a)] + \vec{u} \cdot \nabla (\alpha \nabla a) - [\nabla (\alpha \nabla a)]^{\mathrm{T}} \vec{u}$$
(68)

where $[\nabla(\alpha \nabla a)]^{\mathrm{T}}\vec{u}$ is a matrix–vector multiplication that can be written in index notation as $u_j \partial_{x_i}(\alpha \partial_{x_j}a)$, with summation over repeated indices. Using this identity in Equation (67), we obtain

$$\frac{D\vec{u}}{Dt} = -\nabla p + (b_{\rm u}H_{\rm u} + b_{\rm s}H_{\rm s})\hat{k},\tag{69}$$

where the pressure *p* is related to the Lagrange multiplier λ via

$$p = \left(\frac{1}{2}|\vec{u}|^2 - \vec{u} \cdot \nabla \lambda - \frac{\partial \lambda}{\partial t} - \frac{1}{2}\frac{(b_{\rm u})^2}{N_{\rm u}^2}H_{\rm u} - \frac{1}{2}\frac{(b_{\rm s})^2}{N_{\rm s}^2}H_{\rm s} - \frac{1}{2}\frac{N_{\rm u}^2N_{\rm s}^2}{N_{\rm u}^2 - N_{\rm s}^2}M^2H_{\rm u}\right)$$
(70)

$$= \left(\ell - \vec{u} \cdot \nabla \lambda - \frac{\partial \lambda}{\partial t}\right). \tag{71}$$

Therefore, we have demonstrated that the governing equations, Equations (59), (61), (63), and (69), are obtained using Hamilton's principle, starting from the Lagrangian density in Equation (33) – compare with Equations (15)–(18) and use Equation (53).

4 | CIRCULATION AND PV IN MOIST SYSTEMS

Using the Lagrangian formulation from Section 3, we can now investigate PV from the perspective of particle-relabeling symmetry of the Lagrangian. In this section, a moist version of particle-relabeling symmetry is studied, and it is used to identify various versions of PV conservation.

4.1 | Background on Noether's theorem and possible outcomes

As a systematic approach to seeking conservation laws, one could identify symmetries of the Lagrangian function and apply Noether's theorem to arrive at a corresponding conservation law (Noether, 1918). For conservation of PV and Kelvin's circulation theorem, the symmetry of interest for dry dynamics is the particle-relabeling symmetry (e.g., Bretherton, 1970; Salmon, 1988; Padhye and Morrison, 1996). Here, we now seek a particle-relabeling symmetry that is valid for moist dynamics with phase changes. By taking such a systematic approach, we can discover statements for conservation of circulation and moist PV in a system with phase changes.

Before considering particle-relabeling symmetry and the systematic approach itself, it is worthwhile to consider what the possible outcomes may be. As examples, consider other known symmetries and their associated conservation laws. One well-known symmetry is translation

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invariance, whereby the action is invariant under translations of the \vec{x} coordinates. The corresponding conservation law is conservation of momentum. A second symmetry is the particle-relabeling symmetry, which, for a dry atmosphere, is known to correspond with conservation of PV. As examples of conservation laws, these two examples differ in that it is the total (or global) momentum, integrated over all fluid parcels that is conserved, whereas the PV is conserved for each individual fluid parcel. A priori, for the moist case of this article, either scenario is possible. In other words, it is possible that moist PV will be conserved for each individual fluid parcel, or that moist PV is globally conserved (upon integrating over all fluid parcels), or some other type of conservation law. By finding the moist particle-relabeling symmetry and applying Noether's theorem, we will discover the corresponding conservation law that arises.

4.2 | Particle-relabeling symmetry and PV

In this section, our goal is to find a particle-relabeling symmetry for the action \mathcal{A} defined in Equations (47) and (48), whose Euler–Lagrange equations are the moist system in Equations (15)–(18) with phase changes. The action for our system may be written as

$$\mathcal{A} = \int dt \iiint dV_a \,\ell(\vec{x}(\vec{a},t),\vec{x}_t(\vec{a},t),\vec{a})$$

=
$$\int dt \iiint dV_a \,\frac{1}{2}\vec{x}_t \cdot \vec{x}_t - \mathcal{V}(b_u^{\text{tot}}(\vec{a}),b_s^{\text{tot}}(\vec{a}),z) \quad (72)$$

where $\vec{x} = \vec{x}(\vec{a}, t)$ is the particle path, $\vec{x}_t = \vec{x}_t(\vec{a}, t)$ is the fluid velocity following fluid particles, and b_u^{tot} and b_s^{tot} are the total buoyancies specified by Equations (53) and (54). Henceforth, it is understood that the limits of integration and boundary conditions are appropriately defined, as mentioned in Section 3.2 and discussed by Bretherton (1970).

To achieve the goal of deriving conservation statements for the moist system with phase changes, we consider here a particle relabeling $\vec{a}' = \vec{a} + \delta \vec{a}(\vec{a}, t)$ that does not change the particle paths, such that $\vec{x}'(\vec{a}', t) = \vec{x}(\vec{a}, t)$. Furthermore, the relabeling should not change the mass, such that

$$dV_a = \frac{\partial(\vec{a})}{\partial(\vec{a}')} dV'_a = dV'_a, \tag{73}$$

and hence we must have $\partial(\vec{a})/\partial(\vec{a}') = 1$, from which it follows that the label variation $\delta \vec{a}$ satisfies a divergence-free constraint (see the Supporting Information or

Salmon (1998) for details):

$$\frac{\partial \delta a}{\partial a} + \frac{\partial \delta b}{\partial b} + \frac{\partial \delta c}{\partial c} = 0.$$
(74)

In addition, we restrict the relabeling to those that do not alter the potential energy density \mathcal{V} itself. To achieve invariance of potential energy, based on its form $\mathcal{V}(b_u^{tot}, b_s^{tot}, z)$, we see that we should consider variations $\delta \vec{a}$ along curves of constant b_u^{tot} and constant b_s^{tot} , where a schematic of such curves is shown in Figure 1. These are curves at the intersection of two surfaces: one with constant b_u^{tot} and the other with constant b_s^{tot} . Since surfaces of constant b_u^{tot} and surfaces of constant b_s^{tot} are both material invariant, it follows that their intersection is also material invariant. Mathematically, in any label coordinate system \vec{a} , we require the infinitesimal particle label variation $\delta \vec{a}$ to satisfy

$$\delta \vec{a} \cdot \nabla_a b_{\rm u}^{\rm tot} = 0, \tag{75}$$

$$\delta \vec{a} \cdot \nabla_a b_{\rm s}^{\rm tot} = 0, \tag{76}$$

$$\nabla_a \cdot \delta \vec{a} = 0, \tag{77}$$

where the operator $\nabla_a = (\frac{\partial}{\partial a}, \frac{\partial}{\partial b}, \frac{\partial}{\partial c})$. For example, the label coordinate system \vec{a} can be taken to be the position of the particles at t = 0.

To satisfy the conditions in Equations (75)–(77), one can take $\delta \vec{a}$ to be of the form

$$\delta \vec{a} = \delta f(b_{\rm u}^{\rm tot}, b_{\rm s}^{\rm tot}, t) (\nabla_a b_{\rm u}^{\rm tot} \times \nabla_a b_{\rm s}^{\rm tot}).$$
(78)

Here, $\delta f(b_u^{\text{tot}}, b_s^{\text{tot}}, t)$ is an arbitrary smooth scalar function of b_u^{tot} , b_s^{tot} , and t (with an additional constraint specified later; see discussion after (89)). The cross-product term $(\nabla_a b_u^{\text{tot}} \times \nabla_a b_s^{\text{tot}})$ ensures that Equations (75) and (76) are satisfied, and one can see that Equation (77) is satisfied because of the restriction that the function δf depends only on b_u^{tot} , b_s^{tot} , and t:

$$\nabla_{a} \cdot (\delta f(b_{u}^{\text{tot}}, b_{s}^{\text{tot}}, t)(\nabla_{a}b_{u}^{\text{tot}} \times \nabla_{a}b_{s}^{\text{tot}})) = \nabla_{a} \cdot (\delta f(b_{u}^{\text{tot}}, b_{s}^{\text{tot}}, t)\nabla_{a} \times (b_{u}^{\text{tot}} \nabla_{a}b_{s}^{\text{tot}})),$$
(79)

$$= [\nabla_a \delta f(b_u^{\text{tot}}, b_s^{\text{tot}}, t)] \cdot [\nabla_a \times (b_u^{\text{tot}} \nabla_a b_s^{\text{tot}})], \tag{80}$$

$$= \left(\frac{\partial \delta f}{\partial b_{u}^{\text{tot}}} \nabla_{a} b_{u}^{\text{tot}} + \frac{\partial \delta f}{\partial b_{s}^{\text{tot}}} \nabla_{a} b_{s}^{\text{tot}}\right) \cdot (\nabla_{a} b_{u}^{\text{tot}} \times \nabla_{a} b_{s}^{\text{tot}}),$$
(81)

$$= 0.$$
 (82)

The form of the variation in Equation (78) therefore ensures a mass-conserving particle relabeling. Intuitively,





FIGURE 1 Left: Schematic diagram showing the particle labels, $\vec{a} = (a, b_u^{tot}, b_s^{tot})$. Right: Schematic diagram showing level sets of b_s^{tot} on a surface of constant b_u^{tot} , assuming that b_s^{tot} and b_u^{tot} are smooth functions. [Colour figure can be viewed at wileyonlinelibrary.com]

the relabeling in Equation (78) is a uniform shift on level sets of constant b_u^{tot} and b_s^{tot} because $\delta f(b_u^{tot}, b_s^{tot}, t)$ depends only on b_u^{tot} and b_s^{tot} .

In the derivation of the circulation theorem that follows, it will be desirable to restrict attention to the vicinity of a single closed curve. To do so, one can make a slight modification of Equation (78) in order to localize the variation in certain regions of the domain:

$$\delta \vec{a} = \delta f(b_{\rm u}^{\rm tot}, b_{\rm s}^{\rm tot}, t) (\nabla_a b_{\rm u}^{\rm tot} \times \nabla_a b_{\rm s}^{\rm tot}) \chi_D(\vec{a}), \qquad (83)$$

where a new factor of $\chi_D(\vec{a})$ has been included, where $\chi_D(\vec{a})$ is a smooth cut-off function for an appropriately chosen region of interest *D*. Note that the conditions in Equations (75)–(77) are still satisfied if the region of non-zero δf values is contained in the region where $\chi_D = 1$.

By adopting variations of the form in Equation (83), we now proceed to enforce $\delta A = 0$, where δA arises from variations $\delta \vec{x}_t$ in the kinetic energy,

$$\delta \mathcal{A} = \int dt \iiint dV_a \frac{\partial \vec{x}}{\partial t} \cdot \delta \frac{\partial \vec{x}}{\partial t}$$
$$= \int dt \iiint dV_a \, \vec{x}_t \cdot \delta \vec{x}_t = 0, \qquad (84)$$

with the eventual aim of relating the result to conservation of PV. We remind the reader that \vec{x}_t means the derivative of $\vec{x}(\vec{a}, t)$ with respect to time *t*, keeping \vec{a} fixed. In what follows, the steps in the rather lengthy calculation are (i) express $\delta \vec{x}_t$ in terms of $(\delta \vec{a})_t$, (ii) substitute Equation (83) for $\delta \vec{a}$, (iii) specify region *D* of interest and transform to buoyancy-based label coordinates, (iv) rearrange the ordering of terms in the integral, and (v) simplify the integral and interpret the result in physical terms. An expression for $\delta \vec{x}_t$ in terms of $(\delta \vec{a})_t$ follows from calculus and takes the form

$$\delta \frac{\partial \vec{x}}{\partial t} \sim -\left(\left. \frac{\partial \vec{x}}{\partial a} \left. \frac{\partial \delta a}{\partial t} \right|_{\vec{a}} + \frac{\partial \vec{x}}{\partial b} \left. \frac{\partial \delta b}{\partial t} \right|_{\vec{a}} + \frac{\partial \vec{x}}{\partial c} \left. \frac{\partial \delta c}{\partial t} \right|_{\vec{a}} \right) \tag{85}$$

(see the Supporting Information for details of the calculation). Using Equation (85) in Equation (84), we arrive at

$$\int dt \iiint dV_a \left(\frac{\partial x_i}{\partial t} \frac{\partial x_i}{\partial a_j} \frac{\partial \delta a_j}{\partial t} \right) = 0.$$
 (86)

Now, by integration by parts in time *t*, we have

$$\int dt \iiint dV_a \frac{\partial \vec{A}}{\partial t} \cdot \delta \vec{a} = 0, \qquad (87)$$

where

$$A_j = \frac{\partial x_i}{\partial t} \frac{\partial x_i}{\partial a_j}.$$
(88)

Therefore,

$$\int dt \iiint dV_a \frac{\partial \vec{A}}{\partial t} \\ \times \delta f(b_u^{\text{tot}}, b_s^{\text{tot}}) (\nabla_a b_u^{\text{tot}} \times \nabla_a b_s^{\text{tot}}) \chi_D(\vec{a}) = 0.$$
(89)

At this point, it is helpful to identify a particular closed curve of interest, on which b_u^{tot} and b_s^{tot} have constant values. The region *D*, associated with the cut-off function χ_D , is chosen to encompass the neighborhood of the closed curve of interest, so that, in region *D*, a buoyancy-based label coordinate system can be used. More specifically, in region *D* there exists a smooth invertible map from initial-position-based label coordinates \vec{a} to buoyancy-based label coordinates $(a'', b_u^{tot}, b_s^{tot})$. The purpose of defining region *D* is to ensure that the buoyancy-based label coordinates are valid and a given pair (b_u^{tot}, b_s^{tot}) identifies at most one simple closed curve (see the Appendix for a detailed discussion of this mapping). To proceed with the integral in Equation (89), before the change in label coordinates, the region *D* is divided into two disjoint regions D_1 and D_2 such that D_1 is the region where $\chi_D(\vec{a}) = 1$ and $D_2 = D \setminus D_1$, where the cut-off function smoothly approaches zero. By constraining $\delta f(b_u^{tot}, b_s^{tot}, t)$ to be zero on D_2 , the second integral in the aforementioned expression vanishes, and we have

$$\int dt \iiint_{D_1} dV_a \frac{\partial \vec{A}}{\partial t} \cdot \delta f(b_u^{\text{tot}}, b_s^{\text{tot}}, t) (\nabla_a b_u^{\text{tot}} \times \nabla_a b_s^{\text{tot}}) = 0.$$
(90)

It is now convenient to transform from the general label coordinates \vec{a} to the buoyancy-based label coordinates $\vec{a''} = (a'', b'', c'') = (a'', b_u^{tot}, b_s^{tot})$ as shown in Figure 2 (see the Appendix for an explicit construction starting from initial-position labels). In the buoyancy-based label coordinates, the label variation in Equation (78) has the simple form of $\delta \vec{a}'' = (\delta f(b'', c'', t), 0, 0) = (\delta f(b_u^{tot}, b_s^{tot}, t), 0, 0)$. After dropping the primes to simplify notation, Equation (90) becomes, in the new coordinate system,

$$\int dt \iiint_{D_1} da \ db \ dc \ \frac{\partial}{\partial t} \left(\frac{\partial \vec{x}}{\partial t} \cdot \frac{\partial \vec{x}}{\partial a} \right) \delta f(b, c, t)$$
$$= \int dt \iint db \ dc \ \delta f(b, c, t) \int da \ \frac{\partial}{\partial t} \left(\frac{\partial \vec{x}}{\partial t} \cdot \frac{\partial \vec{x}}{\partial a} \right) = 0.$$
(91)



FIGURE 2 Schematic diagram showing level sets of b_s^{tot} on a surface of constant b_u^{tot} , assuming that b_s^{tot} and b_u^{tot} are smooth functions. Also shown is the local buoyancy-based label coordinate system in an appropriately chosen region *D*. [Colour figure can be viewed at wileyonlinelibrary.com]

Since $\delta f(b, c, t)$ is arbitrary, it follows that

$$\int da \, \frac{\partial}{\partial t} \left(\frac{\partial \vec{x}}{\partial t} \cdot \frac{\partial \vec{x}}{\partial a} \right) = 0. \tag{92}$$

Note that $\partial/\partial t$ can be brought outside the integral, since it is a time derivative with the label coordinates $\vec{a} = (a, b, c)$ held fixed. Also note that $\partial \vec{x}/\partial t$ is the velocity \vec{u} , and consequently we arrive at

$$\frac{d}{dt}\int \vec{u}\cdot\frac{\partial\vec{x}}{\partial a}\,da=0.$$
(93)

According to our definition of labels, *a* parametrizes closed simple curves of constant (b_u^{tot}, b_s^{tot}) ; see Figure 1. Therefore, returning from label space to \vec{x} -space and considering closed curves $C(b_u^{tot}, b_s^{tot}, t)$ of constant (b_u^{tot}, b_s^{tot}) , the result Equation (93) may be restated as

$$\frac{D}{Dt} \oint_{C(b_u^{\text{tot}}, b_s^{\text{tot}}, t)} \vec{u} \cdot d\vec{x} = 0, \qquad (94)$$

where $d\vec{x}$ is the line element tangent to the curve $C(b_u^{\text{tot}}, b_s^{\text{tot}}, t)$. The statement in Equation (94) is the moist circulation theorem for the system of Equations (15)–(18) with phase changes. It is the moist analogue of the Kelvin or Bjerknes circulation theorems from the dry case (e.g., Majda and Bertozzi, 2002; Thorpe *et al.*, 2003; Cotter and Holm, 2014).

Furthermore, it is possible to obtain conservation principles for PV. In this direction, using Stokes' theorem, we may rewrite the moist Kelvin circulation theorem in Equation (94) to obtain a conservation law for vorticity, $\vec{\omega} = \nabla \times \vec{u}$, on a material surface patch $S(\vec{x}, t)$:

$$\frac{D}{Dt} \iint_{S(\vec{x},t)} \vec{\omega} \cdot d\vec{S} = 0, \tag{95}$$

where the boundary of the patch is the closed curve $C(b_u^{\text{tot}}, b_s^{\text{tot}}, t)$. For the special case where $S(\vec{x}, t)$ is on a surface of constant b_u^{tot} , we find

$$\frac{D}{Dt} \iint_{S(\vec{x},t)} \vec{\omega} \cdot \frac{\nabla b_u^{\text{tot}}}{\|\nabla b_u^{\text{tot}}\|} dS = 0.$$
(96)

To then move toward a volumetric integral, take an additional integral with respect to b_u^{tot} to yield

$$\int_{C_1}^{C_2} \frac{D}{Dt} \iint_{S(\vec{x},t)} \vec{\omega} \cdot \frac{\nabla b_u^{\text{tot}}}{\|\nabla b_u^{\text{tot}}\|} dS \ db_u^{\text{tot}} = 0.$$
(97)

Since b_u^{tot} is a label coordinate, and the material derivative D/Dt is a time derivative holding labels fixed, we may



FIGURE 3 "Pancake"-like local material volume for parcel-integrated potential vorticity. [Colour figure can be viewed at wileyonlinelibrary.com]

rewrite Equation (97) as

$$\frac{D}{Dt} \int \iint_{S(\vec{x},t)} \vec{\omega} \cdot \frac{\nabla b_{u}^{\text{tot}}}{\|\nabla b_{u}^{\text{tot}}\|} dS \ db_{u}^{\text{tot}} = \frac{D}{Dt} \int \iint_{S(\vec{x},t)} \vec{\omega}$$
$$\cdot \frac{\nabla b_{u}^{\text{tot}}}{\|\nabla b_{u}^{\text{tot}}\|} dS \ \left(\|\nabla b_{u}^{\text{tot}}\| d\sigma\right) = 0, \tag{98}$$

where σ is the arc length along curves in the direction of ∇b_u^{tot} (Figure 3). Simplifying, we find conservation of a volume-integrated moist PV $\int PV_u$ for a material volume that looks like a distorted cylinder or pill-box or pancake as in Figure 3:

$$\frac{D}{Dt} \iiint_{V(\vec{x},t)} dV \ \mathrm{PV}_{\mathrm{u}} = \frac{D}{Dt} \iiint_{V(\vec{x},t)} dV \ \vec{\omega} \cdot \nabla b_{\mathrm{u}}^{\mathrm{tot}} = 0.$$
(99)

In Equation (99), the base and lid of the cylinder are surfaces of constant b_u^{tot} , connected by gradient lines of b_u^{tot} . Moreover, the cylinder can be viewed as a stack of patches, where each patch is on a different surface of constant b_u^{tot} , and the boundary of each patch is a curve of constant b_s^{tot} . In this way, the b_s^{tot} values on the sides of the cylinder can be written as functions $b_s^{tot}(b_u^{tot})$. In the Supporting Information, we also show that the conservation statement can be extended to a volume with sides given by any arbitrary function $b_s^{tot}(b_u^{tot})$.

Similarly, one can also arrive at conservation of volume-integrated moist PV / PV_s :

$$\frac{D}{Dt} \iiint_{V(\vec{x},t)} dV \ \mathrm{PV}_{\mathrm{s}} = \frac{D}{Dt} \iiint_{V(\vec{x},t)} dV \ \vec{\omega} \cdot \nabla b_{\mathrm{s}}^{\mathrm{tot}} = 0,$$
(100)

where the material volume in Equation (100) has base and lid which are surfaces of constant b_s^{tot} , connected by sides given by any arbitrary function $b_u^{tot}(b_s^{tot})$.

For the moist Boussinesq system in Equations (15)–(18), Equations (99) and (100) are the strongest type of conservation statement for PV. When phase changes are present, conservation applies following local volumes

of PV, enclosed by special surfaces defined in terms of (b_u^{tot}, b_s^{tot}) , rather than following individual fluid particles as in the dry system.

Now that the systematic procedure has produced the form of the circulation theorem and the conservation principle for PV, it is possible to derive these results directly from the moist Boussinesq evolution equations in Equations (15)–(18). In the Supporting Information, we present direct derivations for the circulation theorem, globally integrated PV_u , and parcel-integrated PV_u and PV_s . The direct derivations provide an independent confirmation of these conservation principles. The Supporting Information also includes special variations of the action leading to global conservation of PV_u and PV_s .

5 | DISCUSSION AND CONCLUSIONS

Here, we have shown that Hamilton's principle can be used to derive the moist Boussinesq dynamics, Equations (1)-(4), including phase changes between water vapor and liquid water. The Hamiltonian formulation is not obvious a priori because the buoyancy is piecewise, changing its functional form at interfaces between unsaturated and cloudy air. A key observation is that the piecewise potential energy associated with buoyancy is both continuous and differentiable.

After the Hamiltonian formulation was established, we were then able to investigate particle-relabeling symmetry for the action associated with the moist dynamics, and thereby provide a systematic derivation of conservation statements for moist PV. The conservation statements derived herein had not previously been found from other approaches. Furthermore, the symmetry analysis naturally links the moist versions of Kelvin's circulation theorem and conservation of PV.

Using particle-relabeling symmetry, we uncover a fundamental difference between the dry and moist conservation statements for PV, following directly from the requirement that potential energy must remain invariant under the relabeling. In the dry case, it is necessary to restrict relabeling to constant entropy, leading to material invariance of dry PV on constant-entropy surfaces. In the moist case with phase changes, the relabeling is restricted to fluid parcels situated on curves of constant b_{u}^{tot} and constant b_s^{tot}. These curves are not restricted to the unsaturated or saturated regimes since b_u and b_s are globally defined quantities as in Equations (13) and (14). Ultimately, the stronger constraint leads to a weaker conservation law; namely, material invariance of parcel-integrated moist PV, where the local volumes have special surfaces defined in terms of $(b_{u}^{\text{tot}}, b_{s}^{\text{tot}})$, as in Figure 3, for example. Table 1

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TABLE 1 Summary of potential vorticity (PV) conservation principles for various regimes.

-	-	
Feature	Dry case (non-isentropic)	Moist Boussinesq case
Particle-relabeling symmetry	On level surfaces $S_s(t)$ of entropy <i>s</i> .	On curves $C_b(t)$ of constant b_u^{tot} and b_s^{tot}
Circulation theorem: $\oint_{C(t)} \vec{u} \cdot d\vec{x} = 0$	C(t): Any curve on $S_s(t)$	C(t): Special curves $C_b(t)$
PV definition	$\frac{1}{ ho}\vec{\omega}\cdot\nabla s$	$PV_{u} = \vec{\omega} \cdot \nabla b_{u}^{tot}; PV_{s} = \vec{\omega} \cdot \nabla b_{s}^{tot}$
Conserved quantity	Individual parcel PV	Parcel-integrated PV

summarizes the dry and moist results, with respective definitions for PV. Note that one could restate the moist results in terms of any two material invariants for the system in Equations (1)–(4); for example, total potential temperature θ_{e}^{tot} and total water q_{t}^{tot} .

In previous work (Marsico et al., 2019), we established conservation of a piecewise-quadratic energy for the moist Boussinesq dynamics. Here, we expand our knowledge of the relevant conservation laws to include a moist Kelvin circulation theorem and conservation of parcel-integrated moist PV, as well as their relationship to each other. Thus, we now have moist analogs for some of the most important theorems for dry Boussinesq dynamics. Future work will explore how these results can be applied to analyze observations and numerical simulations of atmospheric flows. It is straightforward to include the effects of rotation (e.g., Cotter and Holm, 2014), which were omitted here for simplicity. In addition, we have already generalized the statement for conservation of PV and Kelvin's circulation theorem to the case of compressible moist flows in work that is presented elsewhere (Kooloth et al., 2022). Note: After the present article was accepted for publication, the authors became aware of a paper by Bannon 2003 that describes a circulation theorem for binary fluids although not a parcel-integrated conservation law for potential vorticity.

AUTHOR CONTRIBUTIONS

Parvathi Kooloth: conceptualization; investigation; methodology; supervision; validation; writing – review and editing. **Leslie M. Smith:** conceptualization; investigation; methodology; supervision; validation; writing – review and editing. **Samuel N. Stechmann:** conceptualization; investigation; methodology; supervision; validation; writing – review and editing.

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CONFLICT OF INTEREST STATEMENT

The authors declare no conflict of interest.

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APPENDIX A. PARTICLE LABEL DEFINITION

We can define the particle label \vec{a} as follows:

$$\vec{a} = (a, b, c) = (a, b_{\rm u}^{\rm tot}, b_{\rm s}^{\rm tot}),$$
 (A.1)

where the first component *a* should be such that it locates particles on curves of constant (b_u^{tot}, b_s^{tot}) . In addition, we require that $dV_a = da \ db_u^{tot} \ db_s^{tot}$ represents a mass element in physical space with $dV_a = [\partial(\vec{a})/\partial(\vec{x})] \ dV_x = \rho \ dV_x$. Keeping in mind that the initial position vector \vec{x}_0 is a mass-conserving label with $\partial(\vec{x}_0)/\partial(\vec{x}) = \rho$, we therefore choose the first component *a* in Equation (A.1) such that $\partial(\vec{a})/\partial(\vec{x}_0) = 1$. A third requirement is for *a* to be material invariant with Da/Dt = 0. In the following, we show an explicit construction for \vec{a} satisfying all the aforementioned three restrictions.

In order to concretely define the label *a*, start by drawing a parallelepiped in terms of *a*, b_u^{tot} , b_s^{tot} , where the direction of *a* is determined by the cross product $\nabla_0 b_u^{tot} \times \nabla_0 b_s^{tot}$, and where ∇_0 is a gradient with respect to the initial position vector \vec{x}_0 at time t = 0. To enforce Equation (49), and using the chain rule, the magnitude of *a* is determined by $\partial(\vec{a})/\partial(\vec{x}_0) = |\nabla_0 a \nabla_0 b_u^{tot} \nabla_0 b_s^{tot}| = 1$, where $\nabla_0 a$ and so on are column vectors. Therefore, the label *a* is chosen to



FIGURE A.1 Schematic to illustrate the computation of the label $a(\vec{x}_0)$ in terms of initial position labels \vec{x}_0 , where *a* is the first coordinate of $\vec{a} = (a, b_u^{\text{tot}}, b_s^{\text{tot}})$. [Colour figure can be viewed at wileyonlinelibrary.com]



FIGURE A.2 Schematic to illustrate cases for which the label coordinate mapping is not one-to-one globally. Left: Level surfaces of b_u^{tot} and b_s^{tot} coincide. Right: Intersection of level surfaces of b_u^{tot} and b_s^{tot} results in multiple distinct closed curves. [Colour figure can be viewed at wileyonlinelibrary.com]

satisfy the condition $|\nabla_0 a \nabla_0 b_u^{tot} \nabla_0 b_s^{tot}| = 1$, which can be restated in terms of a scalar triple product as

$$(\nabla_0 b_u^{\text{tot}} \times \nabla_0 b_s^{\text{tot}}) \cdot \nabla_0 a = 1.$$
 (A.2)

The relation in Equation (A.2) will be true if we define

$$\nabla_0 a = \frac{\nabla_0 b_u^{\text{tot}} \times \nabla_0 b_s^{\text{tot}}}{|\nabla_0 b_u^{\text{tot}} \times \nabla_0 b_s^{\text{tot}}|^2}.$$
 (A.3)

Then, integrating along a material curve *C* of constant $(b_u^{\text{tot}}, b_s^{\text{tot}})$, the particle label *a* is given by

$$a(\vec{x}_0) = \int_C \frac{\nabla_{x_0} b_u^{\text{tot}} \times \nabla_{x_0} b_s^{\text{tot}}}{|\nabla_{x_0} b_u^{\text{tot}} \times \nabla_{x_0} b_s^{\text{tot}}|^2} \cdot d\vec{x}_0', \qquad (A.4)$$

where the integration is from reference point \vec{x}_0^r to initial point \vec{x}_0 . Equivalently, we may write

$$a(\vec{x}_0) = \int_0^\sigma \frac{d\sigma'}{|\nabla_{x_0} b_u^{\text{tot}} \times \nabla_{x_0} b_s^{\text{tot}}|},$$
(A.5)

where σ is the arc length along the curve *C* (see Figure A.1). Finally, notice that since *a* is completely determined by \vec{x}_0 , then Da/Dt = 0 by the chain rule, and therefore *a* is material invariant as required.

Note that this label coordinate system will apply in many scenarios but will have issues in some special cases, such as at points where the gradient $\nabla_0 b_u^{\text{tot}}$ is in the same direction as $\nabla_0 b_s^{\text{tot}}$ and when a fixed value of $(b_u^{\text{tot}}, b_s^{\text{tot}})$ corresponds to multiple closed curves. Schematics of these two scenarios are shown in Figure A.2.