Equations of atmospheric motion in non-Eulerian vertical coordinates : vector-invariant form and quasi-Hamiltonian formulation

Thomas Dubos * and Marine Tort

École Polytechnique, Laboratoire de Météorologie Dynamique/IPSL, Palaiseau, France

June 4, 2014

Abstract

The curl-form of equations of inviscid atmospheric motion in general non-Eulerian coordinates is obtained. Narrowing down to a general vertical coordinate, a quasi-Hamiltonian form is then obtained in a Lagrangian, isentropic, mass-based or z-based vertical coordinate. In non-Lagrangian vertical coordinates, the conservation of energy by the vertical transport terms results from the invariance of energy under vertical relabelling of fluid parcels. A complete or partial separation between the horizontal and vertical dynamics is achieved, except in the Eulerian case. The horizontal-vertical separation is especially helpful for (quasi-)hydrostatic systems characterized by vanishing vertical momentum. Indeed for such systems vertical momentum balance reduces to a simple statement : total energy is stationary with respect to adiabatic vertical displacements of fluid parcels. From this point of view the

* *Corresponding author address:* Thomas Dubos, École Polytechnique, Route de Saclay, 91128 Palaiseau, France

E-mail: dubos@lmd.polytechnique.fr

purpose of (quasi-)hydrostatic balance is to determine the vertical position of fluid parcels, for which no evolution equation is readily available. This physically appealing formulation significantly extends previous work.

The general formalism is exemplified for the fully compressible Euler equations in a Lagrangian vertical coordinate and a Cartesian (x, z) slice geometry, and the deep-atmosphere quasi-hydrostatic equations in longitude-latitude horizontal coordinates. The latter case especially illuminates how the apparent intricacy of the time-dependent metric terms and of the additional forces can be absorbed into a proper choice of prognostic variables. In both cases it is shown how the quasi-Hamiltonian form leads straightforwardly to the conservation of energy using only integration by parts.

Relation with previous work and implications for stability analysis and the derivation of approximate sets of equations and energy-conserving numerical schemes are discussed.

1. Introduction

Ideal fluid motion obeys many conservation laws (mass, energy, linear/angular momentum, potential vorticity). Certain forms of the equations of motion expose explicitly these conservation properties. Such forms are a good starting point to devise numerical methods that inherit from the continuous equations as many of their conservation properties as possible. For example the flux-form of the equations is the basis of finite volume methods which inherently conserve mass, energy and momentum.

Besides the well-known flux-form of the equations, another form exposing conservation laws of energy and (potential) vorticity is the curl form, also known as the vector-invariant form. The curl form of the equations is the standard starting point to yield numerical methods conserving energy, potential vorticity and/or preserving geostrophic balance (Arakawa 1966; Sadourny et al. 1968; Sadourny 1975; Arakawa and Lamb 1981; Ringler et al. 2010; Gassmann 2013). The existence of the curl form results from Hamilton's principle of least

action with a Lagrangian satisfying the fluid parcel relabelling symmetry (Padhye and Morrison 1996). However it can also be obtained from the usual forms using standard vector calculus, as we shall do here.

For ideal fluid flow, the curl form of the equations of motion is intimately related to their Hamiltonian formulation (Holm et al. 2002, 2009). Instead of focusing on evolution equations for the degrees of freedom (DOFs) of a physical system, the Hamiltonian formulation focuses on the evolution of any quantity that can be expressed in terms of the DOFs. In addition to re-expressing the equations of motion, this approach is particularly suited to the determination of those quantities that *do not* evolve, i.e. the integral invariants such as mass, energy, and angular momentum.

In geophysical fluid dynamics as well as in numerical models of the atmosphere and oceans it is customary to use as an independent vertical coordinate various time-dependent, monotonic functions of the vertical position : pressure, density/potential temperature or combinations thereof (Starr 1945; Kasahara 1974; Laprise 1992). This can be advantageous to cope with bottom orography/topography, to allow for a free-surface upper boundary condition or to reduce the exchange of mass between quasi-horizontal layers and the associated numerical diffusion (Bleck et al. 2009). How to re-write the advective form and the flux-form of the equations in such a coordinate system is well-known (Kasahara 1974; Laprise 1992; Staniforth and Wood 2003). If the vertical coordinate is time-independent, i.e. $z-$based, standard expressions of the curl and grad operators in curvilinear coordinates can be used to re-write the curl form as well. However in the general situation where the vertical coordinate is time-dependent, such a systematic treatment of the curl form is lacking. Moreover, given the close relationship between the curl form and the Hamiltonian formulation, it seems important to investigate how they transform when expressed in a general vertical coordinate, which is the main goal of this work.

Because the conservation of energy is built into the Hamiltonian formulation of the laws of

ideal fluid motion, it has been advocated for some time now that energy-conserving numerical schemes should be obtained by discretizing the Poisson bracket and the energy themselves, rather than the curl-form equations (Salmon 1983, 2004; Gassmann 2013). Furthermore, since conservation laws impose constraints on the admissible flow motions, formalisms that embody the conservation laws are useful also for purely theoretical purposes. An example is the derivation of stability criteria by the energy-Casimir method (Arnold 1965). This provides the two main motivations of our stated goal.

The simplest possible Hamiltonian system is

$$\frac{\mathrm{d}q}{\mathrm{d}t} = \frac{\partial H}{\partial p}, \qquad \frac{\mathrm{d}p}{\mathrm{d}t} = -\frac{\partial H}{\partial q} \qquad \Leftrightarrow \qquad \frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} q \\ p \end{pmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{pmatrix} \partial H/\partial q \\ \partial H/\partial p \end{pmatrix}. \tag{1}$$

When (1) holds, p and q form a pair of canonical conjugate variables. The energy $H(p,q)$ is typically of the form $H = p^2/2m + mV(q)$ where m is the mass of a parcel, q its position, $p = m\mathrm{d}q/\mathrm{d}t$ its linear momentum and $V(q)$ a potential.

More generally, for an abstract dynamical system whose degrees of freedom are subsumed in a state vector $\mathbf{q}$, a Hamiltonian formulation is obtained if the equations of motion, assumed here to be already known, are cast in a form where all tendencies are linear functions of the derivatives of energy $H(\mathbf{q})$ with respect to $\mathbf{q}$:

$$\frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t} = \mathbf{J} \cdot \frac{\partial H}{\partial \mathbf{q}} \tag{2}$$

where the matrix $\mathbf{J}(\mathbf{q})$ is antisymmetric and can depend on the current state $\mathbf{q}$. From the form (2) the evolution equation for an arbitrary quantity $F(\mathbf{q})$ is obtained as :

$$\frac{\mathrm{d}F}{\mathrm{d}t} = \{F, H\}, \qquad \{F, H\} = \left(\frac{\partial F}{\partial \mathbf{q}}\right)^* \cdot \mathbf{J} \cdot \left(\frac{\partial H}{\partial \mathbf{q}}\right) = -\{H, F\} \tag{3}$$

where $()^*$ means the transpose. For fluid flow $\mathbf{q} \in \mathcal{Q}$ where $\mathcal{Q}$ is an infinite-dimensional space, typically a product of spaces of smooth scalar or vector functions over some physical or computational domain with appropriate boundary conditions. $\partial E/\partial \mathbf{q}$ is then a functional

derivative belonging to $\mathcal{Q}^*$, the dual of $\mathcal{Q}$, and $\mathbf{J}$ is an antisymmetric bilinear form on $\mathcal{Q}^* \times \mathcal{Q}^*$. However in practice $\partial E/\partial \mathbf{q}$ can be represented concretely as an element of $\mathcal{Q}$ and $\mathbf{J}$ as a skew-symmetric differential operator $\mathbf{J} : \mathcal{Q} \to \mathcal{Q}$.

Conversely, (2) follows from (3) by considering all linear functionals F. Therefore, (2) and (3) are two equivalent representations of the Hamiltonian formulation. The antisymmetry of $\mathbf{J}$ is equivalent to the antisymmetry of the bracket $\{F, H\} = -\{H, F\}$, from which the conservation of energy $\mathrm{d}H/\mathrm{d}t = \{H, H\} = 0$ follows. In fact, (3) with an antisymmetric bracket is insufficient to define a Hamiltonian system. An additional property is required, the Jacobi identity :

$$\{F, \{G, H\}\} + \{H, \{F, G\}\} + \{G, \{H, F\}\} = 0, \tag{4}$$

for all functionals $F,\ G,\ H$ on $\mathcal{Q}$. Antisymmetric brackets satisfying the Jacobi identity (4) are called Poisson brackets (Morrison 1998). However as long as one is chiefly interested in the conservation of energy, the most important property is the antisymmetry (3). Here no attempt will be made to prove Jacobi identities, and we will describe the systems we obtain as quasi-Hamiltonian. As a consequence the Poisson bracket itself becomes less important. Indeed if the equations of motion can be cast in the form (2), and it is known that energy is conserved, then an underlying antisymmetric bracket must exist. This is the - admittedly restrictive - approach that will be pursued here : starting from known equations of motion, conserving a known energy $E(\mathbf{q})$, the main goal will be to cast the equations of motion in the form (2). For this it will be sufficient to obtain explicit expressions for the functional derivatives $\partial E/\partial \mathbf{q}$, and to express the known time derivatives of the DOFs (i.e. the prognostic fields) in terms of $\partial E/\partial \mathbf{q}$.

The main text is organized as follows. In section 2 the well-established relationship between the curl-form and the quasi-Hamiltonian formulation in Eulerian coordinates is explained in more detail, introducing notation and concepts useful for the sequel. Our starting point is the curl-form equations of atmospheric motion in general curvilinear coordinates as

formulated in Tort and Dubos (2014). This formulation is concise and at the same time captures many approximate sets of equations of motion, hydrostatic or not, assuming or not a spherical geopotential, in a Cartesian, shallow-atmosphere or deep-atmosphere geometry, and also allows sound-proof approximations and arbitrary equations of state. From this starting point the curl-form and Hamiltonian formulation of the equations of motion in a time-dependent general vertical coordinate are obtained in Section 3. The main task there, as in Eulerian coordinates, is to relate the various terms appearing in the equations of motion to functional derivatives of energy. The general result of section 3 is applied in section 4 to specific vertical coordinates, i.e. isentropic, mass-based and $z-$based. Section 5 deals with hydrostatic systems. By 'hydrostatic' we conflate strictly hydrostatic systems (i.e. the shallow-atmosphere primitive equations) and quasi-hydrostatic systems where additional forces, typically the non-traditional Coriolis force and possibly centrifugal acceleration, contribute to vertical momentum balance (White and Bromley 1995; White and Wood 2012; Tort and Dubos 2013a). It is shown in section 5 that hydrostatic balance has a simple and physically appealing quasi-Hamiltonian formulation : energy is stationary with respect to adiabatic vertical displacements of fluid parcels. In section 6 examples applying the previous formalism to specific equations are provided : fully compressible Euler equations in a Lagrangian vertical coordinate and a Cartesian (x, z) slice geometry, and the deep-atmosphere quasi-hydrostatic equations (White and Bromley 1995) in longitude-latitude horizontal coordinates. Section 7 summarizes the results and discusses potential applications.

2. Curl form and Hamiltonian formulation in Eulerian coordinates

The Eulerian coordinates we consider are general curvilinear coordinates $\left(\xi^k\right)$, $k = 1, 2, 3$. We assume that the geopotential Φ is a predefined function of the third coordinate, that is $\xi^3 = cst$ is an equi-geopotential surface (Tort and Dubos 2014). Derivatives with respect to

Eulerian coordinates are noted $\hat{\partial}_t = \hat{\partial}/\hat{\partial}t$ and $\hat{\partial}_k = \hat{\partial}/\hat{\partial}\xi^k$. The notations $\partial/\partial t$, ∂_k will be used later for derivatives with respect to non-Eulerian coordinates. Einstein's convention of summation over repeated indices is used.

a. Kinematics

Independently from the equations of motion under consideration, the transport equations take the form :

$$\begin{aligned} \frac{\hat{\partial} s}{\hat{\partial} t} + \hat{u}^l \hat{\partial}_l s &= 0, \\ \frac{\hat{\partial} \hat{\mu}}{\hat{\partial} t} + \hat{\partial}_l \left(\hat{\mu} \hat{u}^l \right) &= 0, \qquad (5) \\ \frac{\hat{\partial} \left(\hat{\mu} s \right)}{\hat{\partial} t} + \hat{\partial}_l \left(\hat{\mu} s \hat{u}^l \right) &= 0. \qquad (6) \end{aligned}$$

where s is specific entropy, $\hat{\mu}$ is pseudo-density, $\hat{u}^l = D\xi^l/Dt$ are the contravariant components of velocity with D/Dt the Lagrangian (material) derivative. Eulerian variables that change under a change of coordinates, are noted with a hat, e.g. $\hat{\mu}$ and $\hat{u}$. Coordinate-invariant quantities like s and t are left without a hat. In spherical deep-atmosphere geometry with $(\xi^1, \xi^2, \xi^3) = (\lambda, \phi, r)$ one has $(\hat{u}^1, \hat{u}^2, \hat{u}^3) = \left(\dot{\lambda}, \dot{\phi}, \dot{r} \right)$ where the dot stands for the Lagrangian derivative, and $\hat{\mu} = r^2 \cos\phi/\alpha$ with α the specific volume. The Lagrangian derivative considered as an operator acting on a space-time field is

$$\frac{D}{Dt} = \frac{\hat{\partial}}{\hat{\partial} t} + \hat{u}^l \hat{\partial}_l. \qquad (7)$$

For simplicity we will assume rigid boundaries in the main text. A free-surface upper boundary condition with an imposed pressure is considered in Appendix A.

b. Dynamics

The dynamical equations, i.e. the momentum budget, are generated by a Lagrangian density $\hat{L}(\xi^k, \hat{u}^k, \hat{\mu}, s)$ which is specific to each approximate system. Sound-proof approxi-

mations are obtained by introducing a Lagrange multiplier λ as an additional argument of the Lagrangian density $\hat{L}(\xi^k, \hat{u}^k, \hat{\mu}, s, \lambda)$ (see Tort and Dubos 2014). Once the Lagrangian is specified (see section 6 for examples), the equations of motion take one of the three equivalent forms

$$\begin{aligned}
\frac{D\hat{v}_k}{Dt} - \frac{\partial \hat{L}}{\partial \xi^k} - \frac{1}{\hat{\mu}}\hat{\partial}_k\left(\hat{\mu}^2\frac{\partial \hat{L}}{\partial \hat{\mu}}\right) &= 0, &(8)\\
\frac{\hat{\partial}\hat{v}_k}{\hat{\partial}t} + \hat{u}^l\left(\hat{\partial}_l\hat{v}_k - \hat{\partial}_k\hat{v}_l\right) + \hat{\partial}_k\hat{B} + s\hat{\partial}_k T &= 0, &(9)\\
\frac{\hat{\partial}}{\hat{\partial}t}\left(\hat{\mu}\hat{v}_k\right) + \hat{\partial}_l\left(\hat{\mu}\hat{v}_k\hat{u}^l\right) - \hat{\partial}_k\left(\hat{\mu}^2\frac{\partial \hat{L}}{\partial \hat{\mu}}\right) &= \hat{\mu}\frac{\partial \hat{L}}{\partial \xi^k}, &(10)
\end{aligned}$$

where

$$\begin{aligned}
\hat{v}_l &= \frac{\partial \hat{L}}{\partial \hat{u}^l},\\
\hat{B} &= \hat{v}_l\hat{u}^l + s\frac{\partial \hat{L}}{\partial s} - \frac{\partial \hat{L}}{\partial \hat{\mu}}\hat{\mu} - \hat{L},\\
T &= \partial\hat{L}/\partial s,
\end{aligned}$$

Notice that the Eulerian frame is not necessarily inertial. Therefore $\hat{u}^l$ are the contravariant components of velocity relative to the considered Eulerian frame while the conjugate momenta $\hat{v}_l$ are the covariant components of absolute velocity relative to some Galilean reference frame. In spherical coordinates they are related to absolute angular momentum (see subsection 6b). Hydrostatic systems are distinguished by the fact that $\hat{v}_3 = \partial\hat{L}/\partial\hat{u}^3 = 0$. In the case of sound-proof systems, one has in addition the constraint $\partial\hat{L}/\partial\lambda = 0$. Depending on the specific sound-proof equation under consideration, λ is to be interpreted either as the full pressure, or as a non-hydrostatic pressure that comes in addition to a reference pressure.

The energy conserved by (9) is

$$\mathcal{H} = \int \hat{\mu}\left(\hat{u}^k\hat{v}_k - \hat{L}\right)\mathrm{d}\boldsymbol{\xi}. \tag{11}$$

This expression is the standard expression for the energy conserved by the equations of motion resulting from Hamilton's principle of least action with a time-independent Lagrangian.

c. Functional derivatives of energy

(5,6,9) suggests $\hat{\mu}$, $\hat{v}_k$ and mass weighted entropy $\hat{S} = \hat{\mu}s$ as a suitable set of DOFs. Energy becomes a functional $\mathcal{H}\left[\hat{v}_k, \hat{\mu}, \hat{S}\right]$ of those fields whose functional derivatives are defined by :

$$\delta\mathcal{H} = \int \left(\frac{\delta\mathcal{H}}{\delta\hat{v}_k}\delta\hat{v}_k + \frac{\delta\mathcal{H}}{\delta\hat{\mu}}\delta\hat{\mu} + \frac{\delta\mathcal{H}}{\delta\hat{S}}\delta\hat{S} \right) \mathrm{d}^3\boldsymbol{\xi}, \tag{12}$$

where $\delta\mathcal{H}$ is defined for fixed $\delta\hat{v}_k$, $\delta\hat{\mu}$, $\delta\hat{S}$ as

$$\delta\mathcal{H} = \lim_{\varepsilon\to 0} \frac{\mathcal{H}\left[\hat{v}_k + \varepsilon\delta\hat{v}_k,\, \hat{\mu} + \varepsilon\delta\hat{\mu},\, \hat{S} + \varepsilon\delta\hat{S}\right] - \mathcal{H}\left[\hat{v}_k,\, \hat{\mu},\, \hat{S}\right]}{\varepsilon}. \tag{13}$$

(13) defines $\delta\mathcal{H}$ as a linear form over the space of DOFs, $\delta\mathbf{q} = \left(\delta\hat{v}_k,\, \delta\hat{\mu},\, \delta\hat{S}\right) \in \mathcal{Q}$, i.e. $\delta\mathcal{H} \in \mathcal{Q}^*$. (12) represents the linear form $\delta\mathcal{H}$ in concrete terms through the functional derivatives $\left(\frac{\delta\mathcal{H}}{\delta\hat{v}_k}, \frac{\delta\mathcal{H}}{\delta\hat{\mu}}, \frac{\delta\mathcal{H}}{\delta\hat{S}}\right) \in \mathcal{Q}$.

From (12) one obtains $\mathrm{d}\mathcal{H}/\mathrm{d}t$:

$$\frac{\mathrm{d}\mathcal{H}}{\mathrm{d}t} = \int \left(\frac{\delta\mathcal{H}}{\delta\hat{v}_k}\hat{\partial}_t\hat{v}_k + \frac{\delta\mathcal{H}}{\delta\hat{\mu}}\hat{\partial}_t\hat{\mu} + \frac{\delta\mathcal{H}}{\delta\hat{S}}\hat{\partial}_t\hat{S} \right) \mathrm{d}^3\boldsymbol{\xi} \tag{14}$$

In fact (14) can be used as an alternative definition of the functional derivatives, valid independently from the equations of motion. Hence in practice, computing the functional derivatives of energy or an arbitrary integral quantity involves exactly the same algebraic manipulations as computing its time derivative : differentiating under the integral and, as much as necessary, integrating by parts.

In our case time-differentiating (11) yields

$$\begin{aligned} \frac{\mathrm{d}\mathcal{H}}{\mathrm{d}t} &= \int \left[\hat{\mu}\hat{u}^k\hat{\partial}_t\hat{v}_k + \left(\hat{u}^k\hat{v}_k - \hat{L} - \hat{\mu}\frac{\partial\hat{L}}{\partial\hat{\mu}} \right)\hat{\partial}_t\hat{\mu} - \hat{\mu}\frac{\partial\hat{L}}{\partial s}\hat{\partial}_t s \right] \mathrm{d}^3\boldsymbol{\xi} \\ &= \int \left[\hat{\mu}\hat{u}^k\hat{\partial}_t\hat{v}_k + \left(\hat{u}^k\hat{v}_k + s\frac{\partial\hat{L}}{\partial s} - \hat{L} - \hat{\mu}\frac{\partial\hat{L}}{\partial\hat{\mu}} \right)\hat{\partial}_t\hat{\mu} - \frac{\partial\hat{L}}{\partial s}\hat{\partial}_t\hat{S} \right] \mathrm{d}^3\boldsymbol{\xi}. \end{aligned} \tag{15}$$

Comparing (14) and (15) yields the functional derivatives :

$$\frac{\delta\mathcal{H}}{\delta\hat{v}_l} = \hat{\mu}\hat{u}^k, \qquad \frac{\delta\mathcal{H}}{\delta\hat{\mu}} = \hat{B}, \qquad \frac{\delta\mathcal{H}}{\delta\hat{S}} = T. \tag{16}$$

Notice that for hydrostatic systems, the above calculations hold for $k = 1, 2$ only because $\hat{v}_3 = \partial l / \partial \hat{u}^3 = 0$ cannot be a prognostic variable. Furthermore vertical mass flux $\hat{\mu}\hat{u}^3$ cannot be expressed as a functional derivative of energy.

d. Hamiltonian formulation

With (16), the equations of motion and the kinematics can be recast under the desired form, where all tendencies depend linearly on the functional derivatives of energy :

$$\frac{\hat{\partial}\hat{\mu}}{\hat{\partial}t} + \delta_l \frac{\delta \mathcal{H}}{\delta \hat{v}_l} = 0, \tag{17}$$

$$\frac{\hat{\partial}\hat{S}}{\hat{\partial}t} + \delta_l \left(s \frac{\delta \mathcal{H}}{\delta \hat{v}_l} \right) = 0, \tag{18}$$

$$\frac{\hat{\partial}\hat{v}_k}{\hat{\partial}t} + \frac{\hat{\partial}_l \hat{v}_k - \hat{\partial}_k \hat{v}_l}{\hat{\mu}} \frac{\delta \mathcal{H}}{\delta \hat{v}_l} + \hat{\partial}_k \frac{\delta \mathcal{H}}{\delta \hat{\mu}} + s \hat{\partial}_k \frac{\delta \mathcal{H}}{\delta \hat{S}} = 0. \tag{19}$$

Now consider the evolution of another integral quantity $\mathcal{F}\left[\hat{v}_k, \hat{\mu}, \hat{S}\right]$:

$$\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}t} = \int \left(\frac{\delta \mathcal{F}}{\delta \hat{v}_k} \hat{\partial}_t \hat{v}_k + \frac{\delta \mathcal{F}}{\delta \hat{\mu}} \hat{\partial}_t \hat{\mu} + \frac{\delta \mathcal{F}}{\delta \hat{S}} \hat{\partial}_t \hat{S} \right) \mathrm{d}^3 \boldsymbol{\xi}, \tag{20}$$

and inject (17-19) into (20). The result is an integral expression, the bracket $\{\mathcal{F}, \mathcal{H}\}$, which depends bilinearly on the functional derivatives of $\mathcal{F}$ and $\mathcal{H}$. Since $\{\mathcal{F}, \mathcal{H}\}$ must vanish whenever $\mathcal{F} = \mathcal{H}$, the bracket must be antisymmetric. It is usually easy to show directly the antisymmetry, possibly after some integration by parts. It is well-known that the bracket resulting from (17-19) is antisymmetric and satisfies the Jacobi identity (Morrison 1998).

Hydrostatic systems can not be cast in the form (17-19) because $\hat{\mu}\hat{u}^3$ cannot be expressed as a functional derivative of energy. Therefore a different approach is necessary to obtain a (quasi-)Hamiltonian formulation for hydrostatic systems. As will appear in section 5, and already known for specific equation sets, one possible approach is to use a non-Eulerian vertical coordinate (Holm and Long 1989; Roulstone and Brice 1995).

3. Curl form and quasi-Hamiltonian formulation in non-Eulerian vertical coordinates

As stated in the Introduction, we shall only verify that the equations of motion can be written in (linear) terms of the functional derivatives of energy with respect to the prognostic variables. The resulting antisymmetric brackets are given explicitly in Appendix D, but no attempt is made to prove that they satisfy the Jacobi identity (4), therefore qualifying as Poisson brackets.

a. Curl form in non-Eulerian coordinates

KINEMATICS

We now wish to transform the curl-form equations (9) to similar equations using independent coordinates a^k such that the Eulerian coordinates ξ^k depend on a^k and time :

$$\xi^k(a^k, t), \qquad \partial_k = \partial/\partial a^k.$$

We make no further assumption at this point regarding a^k. They are therefore arbitrary Eulerian-Lagrangian coordinates, including the cases of purely Lagrangian coordinates (Lagrangian labels) and purely Eulerian coordinates (time-independent $\xi^k(a^k)$).

Let u^n be the contravariant components of the flow in the new, non-Eulerian coordinate system. i.e

$$D/Dt = \partial/\partial t + u^m \partial_m. \tag{21}$$

Therefore u^m and $\hat{u}^l$ are related by

$$\hat{u}^l = \frac{D\xi^l}{Dt} = \partial_t \xi^l + \partial_m \xi^l \, u^m. \tag{22}$$

In the case of a time-independent change of coordinates $\partial_t \xi^m = 0$, (22) reduces to the transformation rule for contravariant components. For a time-dependent change of coordi-

nates the motion $\partial_t \xi^m$ must be taken into account in $\hat{u}^n$. Corresponding to the Lagrangian derivative (21), the mass budget in the new coordinate system takes the form :

$$\frac{\partial \mu}{\partial t} + \partial_l \left(\mu u^l \right) = 0 \qquad \text{where } \mu = J\hat{\mu}, \qquad J = \det \left[\partial_l \xi^k \right].$$

Dynamics

Let $v_l = \partial_l \xi^k \hat{v}_k$ be the covariant components of absolute velocity in the new coordinate system. Using again the chain rule :

$$\begin{aligned}
\partial_t v_l &= \partial_l \xi^k \left(\hat{\partial}_t \hat{v}_k + \hat{\partial}_m \hat{v}_k \partial_t \xi^m \right) + \partial_{lt} \xi^k \hat{v}_k \\
&= \partial_l \xi^k \left(\hat{\partial}_t \hat{v}_k + \left(\hat{\partial}_m \hat{v}_k - \hat{\partial}_k \hat{v}_m \right) \partial_t \xi^m \right) + \partial_l \xi^k \delta_k \hat{v}_m \partial_t \xi^m + \partial_{lt} \xi^m \hat{v}_m \\
&= \partial_l \xi^k \left(\hat{\partial}_t \hat{v}_k + \left(\hat{\partial}_m \hat{v}_k - \hat{\partial}_k \hat{v}_m \right) \left(\hat{u}^l - \partial_m \xi^l \, u^m \right) \right) + \partial_l \left(\hat{v}_m \partial_t \xi^m \right) \\
&= \partial_l \xi^k \left(\hat{\partial}_t \hat{v}_k + \left(\hat{\partial}_m \hat{v}_k - \hat{\partial}_k \hat{v}_m \right) \hat{u}^l \right) - \left(\partial_m v_k - \partial_k v_m \right) u^m + \partial_l \left(\hat{v}_m \partial_t \xi^m \right)
\end{aligned}$$

Using (9), one obtains the generalized curl-form :

$$\partial_t v_l + \left(\partial_n v_l - \partial_l v_n \right) u^n + \partial_l \left(\hat{B} - \hat{v}_m \partial_t \xi^m \right) + s \partial_l T \;\; = \;\; 0. \tag{23}$$

Notice that for a time-independent change of coordinates, (23) reduces (as expected) to (9) with the covariant and contravariant components corresponding to the new coordinate system. For a time-dependent change of coordinates, the curl-form (23) takes into account $\partial_t \xi^m$.

Having written the equations of motion in curl form in the new, time-dependent coordinates, we now turn to the second step, which is to relate the terms appearing in (23) to the energy. For this a set of prognostic variables must be defined first.

b. Prognostic variables in general vertical coordinates

We now need to distinguish the vertical direction $k = 3$ from the horizontal directions $k = 1, 2$. For this it is implied that the indices i, j span the values $1, 2$ while indices k, l, m

span values $1, 2, 3$ as before. The coordinate a^3 is noted η as usual with hybrid vertical coordinates (Kasahara 1974; Laprise 1992; Staniforth and Wood 2003). The time-dependent change of coordinates to a general vertical coordinate is less general than the one considered in section 3 : $\xi^i = a^i$, $u^i = \hat{u}^i$ and only ξ^3 depends on (ξ^i, η, t). The pseudo-density, covariant components of absolute velocity and vertical contravariant component of relative velocity, mass-weighted entropy and vertical momentum are

$$\mu = \hat{\mu}\partial_\eta \xi^3, \qquad v_i = \hat{v}_i + \hat{v}_3 \partial_i \xi^3, \quad u^3 = \dot{\eta}, \quad S = \mu s, \qquad V_3 = \mu \hat{v}_3. \tag{24}$$

The set of prognostic variables typically depends on the vertical coordinate chosen. For instance while geopotential Φ or equivalently the third coordinate ξ^3 is a prognostic variable if the vertical coordinate is Lagrangian or mass-based, it is not if the vertical coordinate is Eulerian. Pseudo-density μ is a prognostic variable with Eulerian or Lagrangian vertical coordinates, but only column-integrated density is a prognostic variable with a mass-based vertical coordinate. Entropy is not a prognostic variable if the vertical coordinate is isentropic. In order to cover the Lagrangian, isentropic, mass-based and $z-$based coordinates, we consider the set of variables $(\mu, S, \xi^3, v_i, V_3)$. Other choices are possible but this one leads to simple expressions.

We start with a Lagrangian vertical coordinate. From there, a general formulation valid for an arbitrary vertical coordinate is obtained by taking into account vertical transport. In the next section isentropic, mass-based and $z-$based vertical coordinates can then be handled as special cases, corresponding each to the removal of one prognostic variable among μ, S and ξ^3, eliminating the redundancy present in a Lagrangian vertical coordinate (see Appendix B).

c. Lagrangian vertical coordinate

ENERGY

A Lagrangian vertical coordinate is defined by the property $u^3 = \dot{\eta} = 0$. Therefore $\hat{u}^3 = \partial_t \xi^3 + u^i \partial_i \xi^3$ and the Lagrangian is expressed as :

$$L(\xi^k,\, u^i,\, \xi^3_t, \xi^3_k, \mu, s) = \hat{L}\left(\xi^k, u^i, \xi^3_t + u^i \xi^3_i, \mu/\xi^3_\eta, s\right)$$

where ξ^3_t, ξ^3_i, ξ^3_η mean $\partial_t \xi^3$, $\partial_i \xi^3$, $\partial_\eta \xi^3$.

Using (24) energy is expressed in terms of the prognostic variables (μ, S, ξ^3, v_i, V_3) as :

$$\begin{aligned}
\mathcal{H}\left[v_i, \xi^3, V_3, \mu, S\right] &= \int \mu \left(\hat{u}^k \hat{v}_k - \hat{L}\right) \mathrm{d}\xi^1 \mathrm{d}\xi^2 \mathrm{d}\eta \\
&= \int \left(\mu u^i v_i + V_3 \xi^3_t - \mu L\right) \mathrm{d}\xi^1 \mathrm{d}\xi^2 \mathrm{d}\eta. \qquad (25)
\end{aligned}$$

Functional derivatives are obtained by time-differentiating (25) :

$$\begin{aligned}
\frac{\mathrm{d}\mathcal{H}}{\mathrm{d}t} &= \int \left(\mu u^i \partial_t v_i - \frac{\partial L}{\partial s} \partial_t s + \left(u^i v_i - L - \mu \frac{\partial L}{\partial \mu} \right) \partial_t \mu \right. \\
&\quad \left. + \xi^3_t \partial_t V_3 - \mu \frac{\partial L}{\partial \xi^3} \partial_t \xi^3 - \mu v_3 u^i \partial_t \xi^3_i - \mu \frac{\partial L}{\partial \xi^3_3} \partial_t \xi^3_3 \right) \mathrm{d}\xi^1 \mathrm{d}\xi^2 \mathrm{d}\eta \\
&= \int \left(\mu u^i \partial_t v_i - \frac{\partial L}{\partial s} \partial_t S + B \partial_t \mu \right. \\
&\quad \left. + \xi^3_t \partial_t V_3 + \left(\partial_i \left(V_3 u^i\right) - \partial_\eta \left(\hat{\mu}^2 \frac{\partial \hat{L}}{\partial \hat{\mu}} \right) - \mu \frac{\partial L}{\partial \xi^3} \right) \partial_t \xi^3 \right) \mathrm{d}\xi^1 \mathrm{d}\xi^2 \mathrm{d}\eta, \qquad (26)
\end{aligned}$$

where we have used/defined

$$\begin{aligned}
\mu \frac{\partial L}{\partial \xi^3_3} &= -\hat{\mu}^2 \frac{\partial \hat{L}}{\partial \hat{\mu}}, \\
B &= \hat{B} - v_3 \xi^3_t = u^i v_i - L - \mu \frac{\partial L}{\partial \mu} + s \frac{\partial L}{\partial s}.
\end{aligned}$$

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We shall use as prognostic equations for v_i the curl-form (23). Additionally, V_3 is prognosed using the flux-form (10) rewritten in the new coordinate system as :

$$\partial_t V_3 + \partial_i \left(V_3 u^i\right) - \partial_\eta \left(\hat{\mu}^2 \frac{\partial \hat{L}}{\partial \hat{\mu}} \right) = \mu \frac{\partial \hat{L}}{\partial \xi^3}. \qquad (27)$$

Identifying the terms appearing in (23,27) with the functional derivatives explicited by (26) yields the formulation :

$$\partial_t \mu + \partial_i \left(\frac{\delta \mathcal{H}}{\delta v_i} \right) = 0 \tag{28}$$

$$\partial_t S + \partial_i \left(s \frac{\delta \mathcal{H}}{\delta v_i} \right) = 0 \tag{29}$$

$$\partial_t v_i + \frac{\partial_j v_i - \partial_i v_j}{\mu} \frac{\delta \mathcal{H}}{\delta v_j} + \partial_i \left(\frac{\delta \mathcal{H}}{\delta \mu} \right) + s \partial_i \left(\frac{\delta \mathcal{H}}{\delta S} \right) = 0 \tag{30}$$

$$\partial_t V_3 + \frac{\delta \mathcal{H}}{\delta \xi^3} = 0 \tag{31}$$

$$\partial_t \xi^3 - \frac{\delta \mathcal{H}}{\delta V_3} = 0 \tag{32}$$

Equivalently, (28-32) have the form (2), i.e. :

$$\partial_t \begin{pmatrix} \mu \\ S \\ v_1 \\ v_2 \\ \xi^3 \\ V_3 \end{pmatrix} + \mathcal{J} \cdot \begin{pmatrix} \frac{\delta \mathcal{H}}{\delta \mu} \\ \frac{\delta \mathcal{H}}{\delta S} \\ \frac{\delta \mathcal{H}}{\delta v_1} \\ \frac{\delta \mathcal{H}}{\delta v_2} \\ \frac{\delta \mathcal{H}}{\delta \xi^3} \\ \frac{\delta \mathcal{H}}{\delta V_3} \end{pmatrix} = 0$$

where $\mathcal{J}$ is the skew-symmetric 6×6 matrix of differential operators :

$$\mathcal{J} = \begin{pmatrix} & & \partial_1 & \partial_2 & & \\ & & \partial_1 (s \cdot) & \partial_2 (s \cdot) & & \\ \partial_1 & s\partial_1 & & \frac{\partial_2 v_1 - \partial_1 v_2}{\mu} & & \\ \partial_2 & s\partial_2 & \frac{\partial_1 v_2 - \partial_2 v_1}{\mu} & & & \\ & & & & & -1 \\ & & & & 1 & \end{pmatrix}.$$

(28-32) presents a remarkable structure. First, the evolution equations for μ, S, v_i involve only functional derivatives with respect to μ, S, v_i, while the evolution equations for V_3, ξ^3 involve only functional derivatives with respect to V_3, ξ^3. The horizontal dynamics and the vertical dynamics are therefore well separated, and coupled only through energy. Furthermore the evolution equations for μ, S, v_i are identical to the Eulerian equations (17-19), except that they are two-dimensional instead of three-dimensional. This two-dimensional structure presents strong analogies with that of layered models, like the Saint-Venant, Ripa or Green-Naghdi equations. Finally the equations for V_3, ξ^3 are those of a pair of canonical conjugate variables, i.e. (1).

d. General vertical coordinate

We now consider the case of a non-Lagrangian vertical coordinate, i.e. $\dot{\eta} \neq 0$. It must be noted that fields (μ, S, ξ^3, v_i, V_3) do not depend on the vertical coordinate being Lagrangian or otherwise. By this we mean that if one considers the Lagrangian vertical coordinate that coincides at a given instant t with the non-Lagrangian coordinate under consideration, i.e. with the same $\xi^3(\xi^i, \eta)$, then the flow is described by the same (μ, s, v_i, V_3) in both coordinates. As a consequence it is sufficient to add to (28-32) the terms proportional to $\dot{\eta}$ expressing transport across surfaces $\eta = cst$, as well as the correction of the Bernoulli function included in (23). The resulting equations of motion are :

$$
\begin{aligned}
\partial_t \mu + \partial_\eta \left(\mu \dot{\eta}\right) + \partial_i \frac{\delta \mathcal{H}}{\delta v_i} &= 0, \\
\partial_t S + \partial_i \left(s \frac{\delta \mathcal{H}}{\delta v_i} \right) + \partial_\eta \left(S \dot{\eta}\right) &= 0, \\
\partial_t v_i + \left(\partial_\eta v_i - \partial_i v_3\right) \dot{\eta} + \frac{\partial_j v_i - \partial_i v_j}{\mu} \frac{\delta \mathcal{H}}{\delta v_j} + \partial_i \left(\frac{\delta \mathcal{H}}{\delta \mu} + \dot{\eta} v_3 \right) + s \partial_i \left(\frac{\delta \mathcal{H}}{\delta S} \right) &= 0, \\
\partial_t \xi^3 + \dot{\eta} \partial_\eta \xi^3 - \frac{\delta \mathcal{H}}{\delta V_3} &= 0. \\
\partial_t V_3 + \partial_\eta \left(V_3 \dot{\eta}\right) + \frac{\delta \mathcal{H}}{\delta \xi^3} &= 0,
\end{aligned}
$$

i.e. :

$$\partial_t \begin{pmatrix} \mu \\ S \\ v_i \\ \xi^3 \\ V_3 \end{pmatrix} + \mathcal{V}\cdot\dot{\eta} + \mathcal{J}\cdot \begin{pmatrix} \frac{\delta\mathcal{H}}{\delta\mu} \\ \frac{\delta\mathcal{H}}{\delta S} \\ \frac{\delta\mathcal{H}}{\delta v_j} \\ \frac{\delta\mathcal{H}}{\delta\xi^3} \\ \frac{\delta\mathcal{H}}{\delta V_3} \end{pmatrix} = 0 \qquad \text{where } \mathcal{V} : \dot{\eta} \mapsto \begin{pmatrix} \partial_\eta(\dot{\eta}\mu) \\ \partial_\eta(\dot{\eta}S) \\ \dot{\eta}\partial_\eta v_i + v_3\partial_i\dot{\eta} \\ \dot{\eta}\partial_\eta\xi^3 \\ \partial_\eta(\dot{\eta}V_3) \end{pmatrix}. \quad (33)$$

It is shown in Appendix B that variations of the form $\mathcal{V}\cdot\delta\eta$ correspond to an infinitesimal vertical relabelling which does not change the flow, only its description in terms of (μ, S, ξ^3, v_i, V_3). Due to invariance of total energy to such a vertical relabelling :

$$\mathcal{V}^*\cdot \begin{pmatrix} \frac{\delta\mathcal{H}}{\delta\mu} \\ \frac{\delta\mathcal{H}}{\delta S} \\ \frac{\delta\mathcal{H}}{\delta v_j} \\ \frac{\delta\mathcal{H}}{\delta\xi^3} \\ \frac{\delta\mathcal{H}}{\delta V_3} \end{pmatrix} = 0, \quad (34)$$

where $\mathcal{V}^*$ is the adjoint of $\mathcal{V}$:

$$\mathcal{V}^* : (B, T, U^i, \alpha, \beta) \mapsto -\mu\partial_\eta B - S\partial_\eta T + U^i\partial_\eta v_i - v_3\partial_i U^i + \alpha\partial_\eta\xi^3 - V_3\partial_\eta\beta.$$

Using the skew-symmetric character of $\mathcal{J}$ and the above property, one finds that the form (33-34) of the equations of motion implies straightforwardly the conservation of energy.

(33) is not fully in quasi-Hamiltonian form since the vertical transport terms are not expressed in terms of functional derivatives of $\mathcal{H}$. Such an expression requires the specification of the vertical coordinate being used. In the next section we specialize (33-34) for isentropic, mass-based and z-based coordinates.

4. Specific vertical coordinates

a. Isentropic vertical coordinate

An isentropic vertical coordinate is a special case of a Lagrangian vertical coordinate, where furthermore entropy is a prescribed function $s(\eta)$ of the vertical coordinate. As a result S is slaved to μ and ceases to be prognostic. Letting $\mathcal{H}'\left[\mu, v_i, \xi^3, V_3\right] = \mathcal{H}\left[\mu, \mu s,\, v_i, \xi^3, V_3\right]$:

$$\frac{\delta \mathcal{H}'}{\delta \mu} = \frac{\delta \mathcal{H}}{\delta \mu} + s \frac{\delta \mathcal{H}}{\delta S},$$

with the other functional derivatives identical. (33-34) then simplify to :

$$\partial_t \begin{pmatrix} \mu \\ v_1 \\ v_2 \\ \xi^3 \\ V_3 \end{pmatrix} + \mathcal{J}_s \cdot \begin{pmatrix} \dfrac{\delta \mathcal{H}'}{\delta \mu} \\ \dfrac{\delta \mathcal{H}'}{\delta v_1} \\ \dfrac{\delta \mathcal{H}'}{\delta v_2} \\ \dfrac{\delta \mathcal{H}'}{\delta \xi^3} \\ \dfrac{\delta \mathcal{H}'}{\delta V_3} \end{pmatrix} = 0, \qquad \mathcal{J}_s = \begin{pmatrix} & \partial_1 & \partial_2 & & \\ \partial_1 & & \dfrac{\partial_2 v_1 - \partial_1 v_2}{\mu} & & \\ \partial_2 & \dfrac{\partial_1 v_2 - \partial_2 v_1}{\mu} & & & \\ & & & & -1 \\ & & & 1 & \end{pmatrix}.$$

b. Mass-based vertical coordinate

A mass-based vertical coordinate $\eta \in [0, 1]$ is characterized (see Appendix C) by the fact that the pseudo-density μ is related to the column-integrated mass $M(\xi^i, t)$ by :

$$M(\xi^i, t) = \int_0^1 \mu \mathrm{d}\eta \tag{35}$$

$$\mu = A' M + B' \tag{36}$$

where the profiles $A(\eta)$ and $B(\eta)$ are prescribed with $A(0) = 0$, $A(1) = 1$, $B(0) = B(1) = 0$ and $A' = \mathrm{d}A/\mathrm{d}\eta$, $B' = \mathrm{d}B/\mathrm{d}\eta$. (36) expresses the fundamental difference between Lagrangian and mass-based hybrid coordinates : with the former μ is a prognostic variable

while with the latter μ is slaved to M through (36). Therefore energy $\mathcal{H}'$ possesses a functional derivative with respect to M, not μ :

$$\mathcal{H}'\left[v_i, \xi^3, V_3, M, S\right] = \mathcal{H}\left[v_i, \xi^3, V_3, A'M + B', S\right]. \tag{37}$$

From definition (37) derivatives of $\mathcal{H}$ and $\mathcal{H}'$ with respect to prognostic variables other than μ, M are identical. With this in mind, we rewrite equations (33) as well as the kinematic equations in the mass-based coordinate :

$$\partial_t M + \partial_i \int_0^1 \frac{\delta \mathcal{H}'}{\delta v_i} \mathrm{d}\eta = 0, \tag{38}$$

$$\partial_t S + \partial_i \left(s \frac{\delta \mathcal{H}'}{\delta v_i} \right) + \partial_\eta \left(S \dot{\eta} \right) = 0, \tag{39}$$

$$\partial_t v_i + \left(\partial_\eta v_i - \partial_i v_3 \right) \dot{\eta} + \frac{\partial_j v_i - \partial_i v_j}{\mu} \frac{\delta \mathcal{H}'}{\delta v_j} + \partial_i \left(\frac{\delta \mathcal{H}}{\delta \mu} + \dot{\eta} v_3 \right) + s \partial_i \left(\frac{\delta \mathcal{H}'}{\delta S} \right) = 0, \tag{40}$$

$$\partial_t V_3 + \partial_\eta \left(V_3 \dot{\eta} \right) + \frac{\delta \mathcal{H}'}{\delta \xi^3} = 0, \tag{41}$$

$$\partial_t \xi^3 + \dot{\eta} \partial_\eta \xi^3 - \frac{\delta \mathcal{H}'}{\delta V_3} = 0. \tag{42}$$

In (38-42) it is not obvious that all tendencies are linear combinations of derivatives of energy. The problematic terms are $\dot{\eta}$ and the Bernoulli function $\delta \mathcal{H} / \delta \mu$. In fact it is shown in Appendix C using the local mass budget that $\mu \dot{\eta}$ is obtained linearly from $\delta \mathcal{H}' / \delta v_i$. Furthermore $\delta \mathcal{H} / \delta \mu$ is the unique solution of the linear problem :

$$\mu \partial_\eta \frac{\delta \mathcal{H}}{\delta \mu} = \left(\partial_\eta v_i \right) \frac{\delta \mathcal{H}'}{\delta v_i} - \partial_i \left(v_3 \frac{\delta \mathcal{H}'}{\delta v_i} \right) + \left(\partial_\eta \xi^3 \right) \frac{\delta \mathcal{H}'}{\delta \xi^3} - V_3 \partial_\eta \frac{\delta \mathcal{H}'}{\delta V_3} - S \partial_\eta \frac{\delta \mathcal{H}}{\delta S} \tag{43}$$

$$\int_0^1 A' \frac{\delta \mathcal{H}}{\delta \mu} \mathrm{d}\eta = \frac{\delta \mathcal{H}'}{\delta M}. \tag{44}$$

(43) is just (34) and (44) is obtained by varying M in definition (37). Hence both $\dot{\eta}$ and the Bernoulli function are also expressed linearly as a function of the derivatives of $\mathcal{H}'$ and (38-42) is of the desired form where all tendencies are linear in the derivatives of energy.

(38-42) is the quasi-Hamiltonian formulation of the equations of motion in a mass-based vertical coordinate. Horizontal and vertical dynamics are still well separated, although not

as well as in the Lagrangian and isentropic cases due to the horizontal-vertical coupling through vertical transport terms proportional to $\dot{\eta}$ and also through (43-44).

c. *z-based vertical coordinate*

In a $z-$based coordinate, $\xi^3(x_i,\,\eta)$ is prescribed and ceases to be prognostic. The condition $\partial_t \xi^3 = 0$ determines the value taken by $\dot{\eta}$. All terms in the remaining prognostic equations are then fully defined. Strictly speaking, total energy becomes a functional of $(\mu,\,S,\,v_i,\,V_3)$ only so that it has no functional derivative with respect to ξ^3. The relabelling-invariance property then provides a definition of the missing derivative. Performing the substitutions :

$$\begin{aligned}
\dot{\eta} &= \left(\partial_\eta \xi^3\right)^{-1} \frac{\delta \mathcal{H}}{\delta V_3}, \\
\frac{\delta \mathcal{H}}{\delta \xi^3} &= \left(\partial_\eta \xi^3\right)^{-1} \left(\mu \partial_\eta \frac{\delta \mathcal{H}}{\delta \mu} + S \partial_\eta \frac{\delta \mathcal{H}}{\delta S} - \frac{\delta \mathcal{H}}{\delta v_i} \partial_\eta v_i + v_3 \partial_i \frac{\delta \mathcal{H}}{\delta v_i} + V_3 \partial_\eta \frac{\delta \mathcal{H}}{\delta V_3} \right)
\end{aligned}$$

one obtains the quasi-Hamiltonian form :

$$\partial_t \begin{pmatrix} \mu \\ S \\ v_1 \\ v_2 \\ V_3 \end{pmatrix} + \mathcal{J}_z \cdot \begin{pmatrix} \dfrac{\delta \mathcal{H}}{\delta \mu} \\ \dfrac{\delta \mathcal{H}}{\delta S} \\ \dfrac{\delta \mathcal{H}}{\delta v_1} \\ \dfrac{\delta \mathcal{H}}{\delta v_2} \\ \dfrac{\delta \mathcal{H}}{\delta V_3} \end{pmatrix} = 0,$$

$$\mathcal{J}_z = \begin{pmatrix}
 & & \partial_1 & \partial_2 & \partial_\eta \left(\hat{\mu} \cdot\right) \\
 & & \partial_1 \left(s \cdot\right) & \partial_2 \left(s \cdot\right) & \partial_\eta \left(\hat{\mu} s \cdot\right) \\
\partial_1 & s\partial_1 & & \dfrac{\partial_2 v_1 - \partial_1 v_2}{\mu} & \dfrac{\partial_\eta v_1}{\partial_\eta \xi^3} + \partial_1 \left(\dfrac{v_3}{\partial_\eta \xi^3} \cdot \right) \\
\partial_2 & s\partial_2 & \dfrac{\partial_1 v_2 - \partial_2 v_1}{\mu} & & \dfrac{\partial_\eta v_2}{\partial_\eta \xi^3} + \partial_2 \left(\dfrac{v_3}{\partial_\eta \xi^3} \cdot \right) \\
\hat{\mu}\partial_\eta & \hat{\mu} s \partial_\eta & \dfrac{-\partial_\eta v_1 + v_3 \partial_1}{\partial_\eta \xi^3} & \dfrac{-\partial_\eta v_2 + v_3 \partial_2}{\partial_\eta \xi^3} & \dfrac{V_3 \partial_\eta}{\partial_\eta \xi^3} + \partial_\eta \left(\dfrac{V_3}{\partial_\eta \xi^3} \cdot \right)
\end{pmatrix}. \qquad (45)$$

Notice that this formulation is not fundamentally different from the standard Eulerian one (17-19) since it can be derived from it by a time-independent change of coordinates and prognostic variables. Nevertheless (17-19) gives an equal treatment to the three momentum components v_k while (45) treats differently horizontal components v_i (not mass-weighted) and vertical component V_3 (mass-weighted).

5. Hydrostatic systems

Sections 3 and 4 deal with systems for which vertical momentum V_3 is prognostic, i.e. non-hydrostatic systems. In this section we examine the simplifications that arise with hydrostatic systems, which are distinguished by the fact that $\partial \hat{L}/\partial u^3 = 0$, hence $V_3 = 0$.

a. General vertical coordinate

The vertical relabelling invariance property simplifies to :

$$\mu \partial_\eta \frac{\delta \mathcal{H}}{\delta \mu} + S \partial_\eta \frac{\delta \mathcal{H}}{\delta S} - \left(\partial_\eta v_i\right) \frac{\delta \mathcal{H}}{\delta v_i} - \left(\partial_\eta \xi^3\right) \frac{\delta \mathcal{H}}{\delta \xi^3} = 0. \tag{46}$$

Repeating the calculations of subsection 3b without V_3, one finds that the functional derivatives of energy are unchanged. Furthermore the vertical momentum balance (27) remains valid with $V_3 = 0$. Hence :

$$\partial_t \mu + \partial_i \left(\frac{\delta \mathcal{H}}{\delta v_i} \right) + \partial_\eta \left(\mu \dot{\eta} \right) = 0 \tag{47}$$

$$\partial_t S + \partial_i \left(s \frac{\delta \mathcal{H}}{\delta v_i} \right) + \partial_\eta \left(S \dot{\eta} \right) = 0 \tag{48}$$

$$\partial_t v_i + \dot{\eta} \partial_\eta v_i + \frac{\partial_j v_i - \partial_i v_j}{\mu} \frac{\delta \mathcal{H}}{\delta v_j} + \partial_i \left(\frac{\delta \mathcal{H}}{\delta \mu} \right) + s \partial_i \left(\frac{\delta \mathcal{H}}{\delta S} \right) = 0 \tag{49}$$

$$\frac{\delta \mathcal{H}}{\delta \xi^3} = 0. \tag{50}$$

Again, (46-50) imply the conservation of energy for any $\mathcal{H}$. Comparing (47-50) to (28-32), one sees that only the horizontal part of the dynamics remains, while the vertical dynamics have

reduced to hydrostatic balance, expressed concisely in terms of energy as (50). This form is valid for all known hydrostatic systems, since all derive from the Lagrangian considered by Tort and Dubos (2014).

b. Lagrangian vertical coordinate

Hydrostatic balance is often considered as a problem from which one deduces pressure. However, because a prognostic equatiion for ξ^3 is missing from (47-50), it is rather an equation for the vertical position ξ^3 of air parcels. This is consistent with the fact that geopotential $\Phi(\xi^3)$ is a diagnostic quantity for hydrostatic systems formulated in a general vertical coordinate. (50) shows that the hydrostatically-balanced state makes energy stationary with respect to vertical displacements, for given μ, S, v_i. The temporal evolution of a hydrostatic system from time t to $t' = t + \mathrm{d}t$ can therefore be conceptually split into two steps :

- An evolution step where the independent DOFs v_i, μ, S are evolved from time t to t' according to (47-49) with $\dot{\eta} = 0$. The resulting state ($v_i(t')$, $\mu(t')$, $S(t')$, $\xi^3(t)$) is in general not hydrostatically balanced because ξ^3 has not evolved.

- An instantaneous hydrostatic adjustment step during which the fluid parcels are displaced vertically in order to restore hydrostatic balance (50).

Since the adjustment step leaves μ, S unchanged, it is adiabatic : air parcels conserve their mass and entropy. Furthermore since v_i is the same before and after adjustment, absolute vorticity $\partial_j v_i - \partial_i v_j$, hence also potential vorticity, is conserved as well during the adjustment step. Total absolute angular momentum is also conserved since it is a function of v_i and μ (Tort and Dubos 2014).

For finite $\mathrm{d}t$, energy changes during adjustment by :

$$\delta\mathcal{H} = \int \left(\frac{\delta\mathcal{H}}{\delta\xi^3} \left(\xi^3(t) - \xi^3(t') \right) \right) \mathrm{d}\xi^1 \mathrm{d}\xi^2 \mathrm{d}\eta + O\left(\xi^3(t) - \xi^3(t') \right)^2 .$$

But energy changes only by an amount $O\left(\xi^3(t) - \xi^3(t')\right)^2 = O(\mathrm{d}t^2)$ precisely because the adjusted state satisfies the stationarity condition (50) . Hence the adjustment step does conserve energy in the limit $\mathrm{d}t \to 0$.

c. Mass-based vertical coordinate

When a mass-based vertical coordinate is used, the vertical mass flux can be expressed in terms of derivatives of energy in the same way as for non-hydrostatic systems. Indeed this expression results only from the kinematic part of the equations of motion, and remains the same for hydrostatic or non-hydrostatic systems. Therefore the mass-based vertical coordinate possesses the same advantages as the Lagrangian/isentropic vertical coordinate to formulate hydrostatic systems. As in section 3, (46) provides a definition of $\delta\mathcal{H}/\delta\mu$ in terms of the other derivatives of energy, and allows the cancellation of the terms due to vertical transport in the energy budget. This point is exemplified in subsection 6b.

d. z-based vertical coordinate

Section 2 ended with the conclusion that in Eulerian coordinates the vertical mass flux could not be expressed as a functional derivative of energy for hydrostatic systems, which suggested the use of a non-Eulerian vertical coordinate to obtain a quasi-Hamiltonian formulation of such systems. We are now in a position re-examine this conclusion. Starting from where we stood at the end of section 2, the pending issues are the expression of hydrostatic balance in terms of energy and the determination of vertical transport.

Regarding hydrostatic balance, it can now be expressed as $\delta\mathcal{H}/\delta\xi^3 = 0$. One may also wish to formulate it in terms of derivatives of $\mathcal{H}$ with respect to the prognostic fields μ, S, v_i. The relabelling invariance (46) provides the desired formulation :

$$\mu\partial_\eta \frac{\delta\mathcal{H}}{\delta\mu} + S\partial_\eta \frac{\delta\mathcal{H}}{\delta S} - \left(\partial_\eta v_i\right) \frac{\delta\mathcal{H}}{\delta v_i} = 0. \tag{51}$$

When $\xi^3 = \eta$, (51) reduces to (19) with $k = 3$ and $\hat{v}_3 = 0$.

Regarding the determination of $\dot{\eta}$, a linear equation for it can be obtained by time-differentiating (51) and substituting time derivatives using (47-49). It is shown in Appendix E that the resulting equation is :

$$\frac{\delta^2 \mathcal{H}}{\left(\delta \xi^3\right)^2} \left(\partial_\eta \xi^3 \, \dot{\eta}\right) = r.h.s. \tag{52}$$

where $\delta^2 \mathcal{H} / \left(\delta \xi^3\right)^2$ is a self-adjoint vertical differential operator. For the shallow-atmosphere primitive equations, (52) is known as Richardson's equation Richardson (1922); Kasahara (1974). For quasi-hydrostatic systems a more complicated equation is obtained (White et al. 2005).

(52) emphasizes the relation between Richardson's equation and the hydrostatic adjustment process discussed in subsection 4b. Indeed let us again conceptually split the horizontal dynamics from the vertical dynamics while going from time t to t'. We now have a three-step process :

- an evolution step evolving v_i, μ, S from time t to $t' = t + \delta t$ according to (47-49) with $\dot{\eta} = 0$, as in 5b.

- a hydrostatic adjustment step that corrects ξ^3 to restore hydrostatic balance, as in 5b. The correction $\zeta = \xi^3(t') - \xi^3(t)$ satisfies at leading order in δt :

$$\frac{\delta^2 \mathcal{H}}{\left(\delta \xi^3\right)^2} \zeta = -\frac{\delta \mathcal{H}}{\delta \xi^3} \left(v_i(t'),\, \mu(t'),\, S(t'),\, \xi^3(t)\right) \tag{53}$$

  which can be interpreted as one Newton-Raphson iteration to solve $\delta \mathcal{H} / \delta \xi^3 = 0$.

- at the end of the adjustment step ξ^3 has changed. The invariance of the flow with respect to variations of the form

$$\delta\mu = -\partial_\eta \left(\mu \delta\eta\right), \quad \delta S = -\partial_\eta \left(S \delta\eta\right), \qquad \delta v_i = -\partial_\eta v_i \, \delta\eta, \qquad \delta\xi^3 = -\partial_\eta \xi^3 \, \delta\eta. \tag{54}$$

  can be exploited to bring $\xi^3(\xi^i,\, \eta,\, t')$ back to the prescribed value $\xi^3(\xi^i, \eta)$. Adding the above variations does not change the flow (see Appendix B) and cancels the update

(53) of ξ^3 if $\delta\eta$ is chosen appropriately, i.e. $\delta\eta = \zeta/\partial_\eta\xi^3$. It is the role of the vertical transport terms to implement this vertical relabelling (remapping) step. Indeed defining $\dot{\eta}$ by $\zeta = \delta t\, \partial_\eta\xi^3\, \dot{\eta}$ is equivalent to solving Richardson's equation (52).

Therefore a physical interpretation can be given to Richardson's equation (52) : it results from the combination a hydrostatic adjustment step, needed to restore hydrostatic balance, and a vertical relabelling step, needed to maintain a Eulerian vertical coordinate.

6. Examples

In this section the general framework derived in sections 3 to 5 is exemplified with two concrete cases. Assuming an ideal perfect gas, we use potential temperature θ and $\Theta = \mu\theta$ instead of entropy. The following thermodynamic identities will be useful :

$$p = -\frac{\partial e}{\partial \alpha}, \quad \pi = \frac{\partial e}{\partial \theta}, \quad \frac{\partial p}{\partial \theta} = -\frac{\partial \pi}{\partial \alpha}, \quad e + \alpha p - \theta\pi = 0, \quad \theta\frac{\partial p}{\partial \theta} + \alpha\frac{\partial p}{\partial \alpha} = 0. \tag{55}$$

where p is pressure and π is Exner's function. In the first example the non-rotating fully-compressible Euler equations are formulated in a Cartesian (x, z) slice using a Lagrangian vertical coordinate. In the second example the three-dimensional deep-atmosphere hydrostatic equations are formulated in longitude-latitude horizontal coordinates and a mass-based vertical coordinate. In both cases explicit expressions for the derivatives of energy are given, and it is shown how the vector-invariant forms (28-32), (46-50) lead straightforwardly to the conservation of energy.

a. Fully-compressible Euler equations in a Cartesian vertical slice

The domain under consideration here is a vertical slice (x, z) with a bottom $z = z_b(x)$. The Eulerian pseudo-density is the true density $\hat{\mu} = 1/\alpha$. Independent variables are $x = \xi^1$ and η. $\xi^3 = z(x, \eta, t)$ is a dependent, prognostic variable. The Lagrangian pseudo-density is

$\mu = \partial_\eta z/\alpha$. The Lagrangian is :

$$\hat{L}(z, \hat{\mu}, \theta, \dot{x}, \dot{z}) = \frac{\dot{x}^2 + \dot{z}^2}{2} - e\left(\frac{1}{\hat{\mu}}, \theta\right) - gz. \tag{56}$$

Conjugate momenta are simply $\partial\hat{L}/\partial\dot{x} = \dot{x}$ and $\partial\hat{L}/\partial\dot{z} = \dot{z}$. Clearly (8) with definition (56) yields the fully compressible Euler equations.

We consider a Lagrangian vertical coordinate $\dot{\eta} = 0$. The prognostic variables are μ, Θ, z, vertical momentum $V_3 = W = \mu\dot{z}$ and the covariant component $v_1 = u = \dot{x} + \dot{z}\partial_x z$. The energy as a function of the prognostic variables is :

$$\mathcal{H}\left[\mu, \Theta, u, W, z\right] = \int \left(\frac{\left(u - \dfrac{W}{\mu}\partial_x z\right)^2 + \left(\dfrac{W}{\mu}\right)^2}{2} + e\left(\frac{\partial_\eta z}{\mu}, \frac{\Theta}{\mu}\right) + gz \right) \mu \mathrm{d}x\mathrm{d}\eta \tag{57}$$

with $e(\alpha, \theta)$ internal energy. Time-differentiating under the integral, using (55) and

$$\begin{aligned} \frac{u^2}{2} - \left(1 + (\partial_x z)^2\right)\frac{W^2}{2\mu^2} &= \frac{1}{2}\left(\dot{x} + \dot{z}\partial_x z\right)^2 - \frac{1}{2}\left(1 + (\partial_x z)^2\right)\dot{z}^2 \\ &= \frac{\dot{x}^2 - \dot{z}^2}{2} + \dot{z}\dot{x}\partial_x z = \frac{\dot{x}^2 + \dot{z}^2}{2} - \dot{z}\partial_t z \end{aligned}$$

and integrating by parts one finds

$$\frac{\delta\mathcal{H}}{\delta\mu} = \frac{\dot{x}^2 + \dot{z}^2}{2} + gz - \dot{z}\partial_t z \tag{58}$$

$$\frac{\delta\mathcal{H}}{\delta\Theta} = \pi$$

$$\frac{\delta\mathcal{H}}{\delta u} = \mu u - W\partial_x z = \mu\dot{x}$$

$$\frac{\delta\mathcal{H}}{\delta W} = \frac{W}{\mu} - u\partial_x z = \dot{z} - u\partial_x z$$

$$\frac{\delta\mathcal{H}}{\delta z} = \partial_x\left(\dot{x}W\right) + \partial_\eta p + g. \tag{59}$$

Hence (28-32), which simplify here to :

$$\partial_t \mu + \partial_x \frac{\delta \mathcal{H}}{\delta u} = 0 \tag{60}$$

$$\partial_t \Theta + \partial_x \left(\theta \frac{\delta \mathcal{H}}{\delta u} \right) = 0 \tag{61}$$

$$\partial_t u + \partial_x \frac{\delta \mathcal{H}}{\delta \mu} + \theta \partial_x \frac{\delta \mathcal{H}}{\delta \Theta} = 0 \tag{62}$$

$$\partial_t z - \frac{\delta \mathcal{H}}{\delta W} = 0. \tag{63}$$

$$\partial_t W + \frac{\delta \mathcal{H}}{\delta z} = 0 \tag{64}$$

generate indeed the fully compressible Euler equations, formulated here with a Lagrangian vertical coordinate. Furthermore the top and bottom no-normal-flux boundary conditions are expressed as $\delta H / \delta W = 0$. Using (58-59) one can also check explicitly that (43) holds.

We shall now derive the energy budget resulting from (60-64). For this we do not need to know that $\mathcal{H}$ and its derivatives take the specific form (57,58-59). Indeed using only (60-64) and no-flux boundary conditions $\delta \mathcal{H} / \delta u = 0$:

$$\begin{aligned}
\frac{\mathrm{d}\mathcal{H}}{\mathrm{d}t} &= \int \left(\frac{\delta \mathcal{H}}{\delta \mu} \partial_t \mu + \frac{\delta \mathcal{H}}{\delta \Theta} \partial_t \Theta + \frac{\delta \mathcal{H}}{\delta u} \partial_t u + \frac{\delta \mathcal{H}}{\delta W} \partial_t W + \frac{\delta \mathcal{H}}{\delta z} \partial_t z \right) \mathrm{d}x \mathrm{d}\eta \\
&= -\int \left(\frac{\delta \mathcal{H}}{\delta \mu} \partial_x \frac{\delta \mathcal{H}}{\delta u} + \frac{\delta \mathcal{H}}{\delta \Theta} \partial_x \left(\theta \frac{\delta \mathcal{H}}{\delta u} \right) + \frac{\delta \mathcal{H}}{\delta u} \left(\partial_x \frac{\delta \mathcal{H}}{\delta \mu} + \theta \partial_x \frac{\delta \mathcal{H}}{\delta \Theta} \right) + \frac{\delta \mathcal{H}}{\delta W} \frac{\delta \mathcal{H}}{\delta z} - \frac{\delta \mathcal{H}}{\delta z} \frac{\delta \mathcal{H}}{\delta W} \right) \mathrm{d}x \mathrm{d}\eta \\
&= -\int \partial_x \left(\frac{\delta \mathcal{H}}{\delta u} \left(\frac{\delta \mathcal{H}}{\delta \mu} + \theta \frac{\delta \mathcal{H}}{\delta \Theta} \right) \right) \mathrm{d}x \mathrm{d}\eta = 0.
\end{aligned}$$

The above is a particular case of $\mathrm{d}\mathcal{F}/\mathrm{d}t = \{\mathcal{F}, \mathcal{H}\}$ with $\mathcal{F} = \mathcal{H}$, where the bracket $\{\mathcal{F}, \mathcal{H}\}$ is shown in Appendix D to be antisymmetric.

b. Deep-atmosphere quasi-hydrostatic equations

Now the domain under consideration is a fluid volume evolving between the surface of a spherical planet (with a planetary radius a and rotation rate Ω) and a free surface at the top of the atmosphere defined by the pressure $p \mid_{r=r_\infty} = p_\infty$. We consider standard longitude-latitude-radius coordinates $(\lambda, \phi, r) = (\xi^1, \xi^2, \xi^3)$. The elementary volume is

$r^2 \cos\phi \mathrm{d}\lambda \mathrm{d}\phi \mathrm{d}r = \partial_r V \, \mathrm{d}\lambda \mathrm{d}\phi \mathrm{d}r$ with $V(\phi, r) = (1/3)\, r^3 \cos\phi$, so that the Eulerian pseudo-density is $\hat{\mu} = r^2 \cos\phi/\alpha$ with α specific volume. Geopotential is $\Phi(r) = -ga^2/r$ where g is gravity at $r = a$, so that gravity at $r \neq a$ is ga^2/r^2. The dynamical equations of motion (Wood and Staniforth (2003), eqs 2.3-2.5) rewritten in terms of the contravariant velocity components $\dot{\lambda}, \dot{\phi}$ and $\dot{\eta}$ are :

$$\begin{aligned} \frac{D}{Dt}\left(r\cos\phi\dot{\lambda}\right) - r\sin\phi\dot{\lambda}\dot{\phi} + \dot{r}\cos\phi\dot{\lambda} - 2\Omega r\dot{\phi}\sin\phi + 2\Omega\dot{r}\cos\phi & \\ + \frac{r}{\mu}\left(\frac{\partial r}{\partial\eta}\frac{\partial p}{\partial\lambda} - \frac{\partial p}{\partial\eta}\frac{\partial r}{\partial\lambda}\right) &= 0 \quad (65) \\ \frac{D}{Dt}\left(r\dot{\phi}\right) + r\sin\phi\cos\phi\dot{\lambda}^2 + \dot{r}\dot{\phi} + 2\Omega r\dot{\lambda}\cos\phi\sin\phi + \frac{r\cos\phi}{\mu}\left(\frac{\partial r}{\partial\eta}\frac{\partial p}{\partial\phi} - \frac{\partial p}{\partial\eta}\frac{\partial r}{\partial\phi}\right) &= 0 \quad (66) \\ -r\left(\cos^2\phi\dot{\lambda}^2 + \dot{\phi}^2\right) - 2\Omega r\cos^2\phi\dot{\lambda} + \frac{a^2}{r^2}g + \frac{r^2\cos\phi}{\mu}\frac{\partial p}{\partial\eta} &= 0 \quad (67) \end{aligned}$$

One can check that (65-67) are equivalent to (8) with the Lagrangian :

$$\hat{L}\left(\phi, r, \hat{\mu}, \theta, \dot{\lambda}, \dot{\phi}\right) = \frac{r^2}{2}\left(\dot{\phi}^2 + \dot{\lambda}^2\cos^2\phi\right) + \Omega\dot{\lambda}r^2\cos^2\phi - e\left(\frac{r^2\cos\phi}{\hat{\mu}}, \theta\right) - \Phi(r). \quad (68)$$

Conjugate momenta are the covariant components of absolute velocity $v_1 = u = r^2\cos^2\phi\left(\dot{\lambda} + \Omega\right)$, $v_2 = v = r^2\dot{\phi}$ (Roulstone and Brice 1995).

We consider a mass-based vertical coordinate. Independant variables are λ, ϕ, η. $\xi^3 = r(\lambda, \phi, \eta, t)$ is a dependent, diagnostic variable. The non-Eulerian pseudo-density is $\mu = \partial_\eta r\hat{\mu} = r^2\cos\phi\partial_\eta r/\alpha$. Prognostic variables are $M = \int \mu \mathrm{d}\eta$, Θ, u, v. Total energy as a function of the prognostic variables and r, vertical position of the fluid parcels, is :

$$\begin{aligned} \mathcal{H}\left[\mu,\, \Theta,\, u,\, v,\, r\right] &= \int \mu\left(K(u,v,r) + e\left(\frac{r^2\cos\phi\partial_\eta r}{\mu}, \frac{\Theta}{\mu}\right) + \Phi(r)\right)\mathrm{d}\lambda\mathrm{d}\phi\mathrm{d}\eta \quad (69) \\ &\quad + p_\infty \int_{\eta=1} V(\phi,r)\mathrm{d}\lambda\mathrm{d}\phi, \\ \text{where } K(u,v,r) &= \frac{1}{2}\left(\frac{u - \Omega r^2\cos^2\phi}{r\cos\phi}\right)^2 + \frac{1}{2}\left(\frac{v}{r}\right)^2. \quad (70) \end{aligned}$$

481 Let us express the functional derivatives of $\mathcal{H}$. Time-differentiating (69), using (55),

$$\begin{aligned}
\left.\frac{\partial}{\partial\mu}(\mu e)\right|_{\Theta,\, r=cst} &= e+\mu\left(-\frac{r^2\cos\phi\partial_\eta r}{\mu^2}\frac{\partial e}{\partial\alpha}-\frac{\Theta}{\mu^2}\frac{\partial e}{\partial\theta}\right)=0,\\
\mu\left.\frac{\partial e}{\partial r}\right|_{\Theta,\,\mu=cst} &= -p\frac{\partial}{\partial r}\left(r^2\cos\phi\partial_\eta r\right),\\
\frac{\partial K}{\partial r} &= -\frac{2K}{r}-2\Omega\frac{u-\Omega r^2\cos^2\phi}{r},
\end{aligned}$$

482 and integrating by parts one finds :

$$\frac{\delta\mathcal{H}}{\delta r} = \mu\left[-\frac{2K}{r}-2\Omega\frac{u-r^2\cos^2\phi\Omega}{r}+\frac{a^2}{r^2}g\right]+r^2\cos\phi\partial_\eta p \tag{71}$$

$$\frac{\delta\mathcal{H}}{\delta\mu} = K-g\frac{a^2}{r}, \tag{72}$$

$$\frac{\delta\mathcal{H}}{\delta\Theta} = \pi, \tag{73}$$

$$\frac{\delta\mathcal{H}}{\delta u} = \mu\dot{\lambda}, \tag{74}$$

$$\frac{\delta\mathcal{H}}{\delta v} = \mu\dot{\phi}. \tag{75}$$

483 Using :

$$\begin{aligned}
\partial_\eta\frac{\delta\mathcal{H}}{\delta\mu} &= \left[-\frac{2K}{r}-2\Omega\frac{u-\Omega r^2\cos^2\phi}{r}+\frac{a^2}{r^2}g\right]\partial_\eta r+\dot{\lambda}\partial_\eta u+\dot{\phi}\partial_\eta v,\\
\mu\theta\partial_\eta\frac{\delta\mathcal{H}}{\delta\Theta} &= r^2\cos\phi\partial_\eta r\,\partial_\eta p,
\end{aligned}$$

484 one shows explicitly that, in this particular case, (46) holds :

$$\mu\partial_\eta\frac{\delta\mathcal{H}}{\delta\mu}+\mu\theta\partial_\eta\frac{\delta\mathcal{H}}{\delta\Theta}-\partial_\eta u\frac{\delta\mathcal{H}}{\delta u}-\partial_\eta v\frac{\delta\mathcal{H}}{\delta v}-\partial_\eta r\frac{\delta\mathcal{H}}{\delta r}=0. \tag{76}$$

485 (71) shows that $\delta\mathcal{H}/\delta r=0$ is is indeed equivalent to the quasi-hydrostatic balance (67).

486 Assuming a mass-based vertical coordinate, the other dynamical equations, paraphrasing

(49), are :

$$\partial_t M + \partial_\lambda \int_0^1 \frac{\delta \mathcal{H}}{\delta u} \mathrm{d}\eta + \partial_\phi \int_0^1 \frac{\delta \mathcal{H}}{\delta v} \mathrm{d}\eta = 0, \tag{77}$$

$$\partial_t \Theta + \partial_\lambda \left(\theta \frac{\delta \mathcal{H}}{\delta u} \right) + \partial_\phi \left(\theta \frac{\delta \mathcal{H}}{\delta v} \right) + \partial_\eta \left(\Theta \dot{\eta} \right) = 0, \tag{78}$$

$$\partial_t u + \dot{\eta} \partial_\eta u - \frac{\partial_\lambda v - \partial_\phi u}{\mu} \frac{\delta \mathcal{H}}{\delta v} + \partial_\lambda \frac{\delta \mathcal{H}}{\delta \mu} + \theta \partial_\lambda \left(\frac{\delta \mathcal{H}}{\delta \Theta} \right) = 0, \tag{79}$$

$$\partial_t v + \dot{\eta} \partial_\eta v + \frac{\partial_\lambda v - \partial_\phi u}{\mu} \frac{\delta \mathcal{H}}{\delta u} + \partial_\phi \frac{\delta \mathcal{H}}{\delta \mu} + \theta \partial_\phi \left(\frac{\delta \mathcal{H}}{\delta \Theta} \right) = 0. \tag{80}$$

It is straightforward, but somewhat tedious, to show that (79-80) yield (65-66), as obtained by Roulstone and Brice (1995) in an isentropic vertical coordinate. The resulting energy budget is :

$$\begin{aligned} \frac{\mathrm{d}\mathcal{H}}{\mathrm{d}t} &= \int \frac{\delta \mathcal{H}}{\delta M} \partial_t M \mathrm{d}\phi \mathrm{d}\lambda + \int \left(\frac{\delta \mathcal{H}}{\delta \Theta} \partial_t \Theta + \frac{\delta \mathcal{H}}{\delta u} \partial_t u + \frac{\delta \mathcal{H}}{\delta v} \partial_t v + \frac{\delta \mathcal{H}}{\delta r} \partial_t r \right) \mathrm{d}\lambda \mathrm{d}\phi \mathrm{d}\eta \\ &= \int \frac{\delta \mathcal{H}}{\delta M} \partial_t M \mathrm{d}\phi \mathrm{d}\lambda - \int \left[\frac{\delta \mathcal{H}}{\delta \Theta} \partial_\eta \left(\Theta \dot{\eta} \right) + \frac{\delta \mathcal{H}}{\delta u} \left(\dot{\eta} \partial_\eta u + \partial_\lambda \frac{\delta \mathcal{H}}{\delta \mu} \right) + \frac{\delta \mathcal{H}}{\delta v} \left(\dot{\eta} \partial_\eta v + \partial_\phi \frac{\delta \mathcal{H}}{\delta \mu} \right) \right] \mathrm{d}\lambda \mathrm{d}\phi \mathrm{d}\eta \\ &\quad - \int \left(\theta \frac{\delta \mathcal{H}}{\delta u} \partial_\lambda \left(\frac{\delta \mathcal{H}}{\delta \Theta} \right) + \frac{\delta \mathcal{H}}{\delta \Theta} \partial_\lambda \left(\theta \frac{\delta \mathcal{H}}{\delta u} \right) + \theta \frac{\delta \mathcal{H}}{\delta v} \partial_\phi \left(\frac{\delta \mathcal{H}}{\delta \Theta} \right) + \frac{\delta \mathcal{H}}{\delta \Theta} \partial_\phi \left(\theta \frac{\delta \mathcal{H}}{\delta v} \right) \right) \mathrm{d}\lambda \mathrm{d}\phi \mathrm{d}\eta. \end{aligned}$$

Integrating by parts in λ, ϕ, then using $\delta \mathcal{H} / \delta r = 0$ and the mass budget $A' \partial_t M + \partial_\lambda \frac{\delta \mathcal{H}}{\delta u} + \partial_\phi \frac{\delta \mathcal{H}}{\delta v} + \partial_\eta \left(\mu \dot{\eta} \right) = 0$ leaves :

$$\begin{aligned} \frac{\mathrm{d}\mathcal{H}}{\mathrm{d}t} &= \int \frac{\delta \mathcal{H}}{\delta M} \partial_t M \mathrm{d}\phi \mathrm{d}\lambda - \int \frac{\delta \mathcal{H}}{\delta \mu} A' \partial_t M \mathrm{d}\lambda \mathrm{d}\phi \mathrm{d}\eta \\ &\quad - \int \left(\dot{\eta} \left(\frac{\delta \mathcal{H}}{\delta u} \partial_\eta u + \frac{\delta \mathcal{H}}{\delta v} \partial_\eta v \right) + \frac{\delta \mathcal{H}}{\delta \Theta} \partial_\eta \left(\Theta \dot{\eta} \right) + \frac{\delta \mathcal{H}}{\delta \mu} \partial_\eta \left(\mu \dot{\eta} \right) \right) \mathrm{d}\lambda \mathrm{d}\phi \mathrm{d}\eta \end{aligned}$$

which vanishes due to $\frac{\delta \mathcal{H}}{\delta M} = \int_0^1 A' \frac{\delta \mathcal{H}}{\delta \mu} \mathrm{d}\eta$ and (76).

We finally consider a $z-$based vertical coordinate. To obtain Richardson's equation we introduce $\tilde{\partial} / \tilde{\partial} t$, the time-derivative computed as if the vertical coordinate were Lagrangian, i.e. letting $\dot{\eta} = 0$ in (47-50). Applying $\tilde{\partial} / \tilde{\partial} t$ to hydrostatic balance, using (55),

$$\begin{aligned} \frac{\partial}{\partial r} \left(-\frac{2K}{r} - 2\Omega \left(\frac{u}{r} - \Omega r \cos^2 \phi \right) + \frac{a^2}{r^2} g \right) &= 6 \frac{K + \Omega u}{r^2} - 2\Omega^2 \cos^2 \phi - \frac{2a^2}{r^3} g, \\ \frac{\partial}{\partial u} \left(-\frac{2K}{r} - 2\Omega \left(\frac{u}{r} - \Omega r \cos^2 \phi \right) + \frac{a^2}{r^2} g \right) &= -2 \frac{\dot{\lambda} + \Omega}{r}, \end{aligned}$$

and letting $\tilde{\partial} r/\tilde{\partial} t = -\partial_\eta r\,\dot{\eta}$ yields the one-dimensional elliptic equation for $\partial_\eta r\,\dot{\eta}$:

$$\left[\mu\left(6\frac{K+\Omega u}{r^2} - 2\Omega^2\cos^2\phi - \frac{2a^2}{r^3}g\right) + 2r\cos\phi\partial_\eta p\right]\partial_\eta r\,\dot{\eta}$$

$$+r^2\cos\phi\partial_\eta\left(\frac{1}{\mu}\frac{\partial p}{\partial\alpha}\partial_\eta\left(r^2\cos\phi\partial_\eta r\,\dot{\eta}\right)\right) = r^2\cos\phi\partial_\eta\left(\frac{1}{\mu}\frac{\partial p}{\partial\theta}\frac{\tilde{\partial}\Theta}{\tilde{\partial} t}\right) - \frac{2\mu}{r}\left(\left(\dot{\lambda}+\Omega\right)\frac{\tilde{\partial} u}{\tilde{\partial} t} + \dot{\phi}\frac{\tilde{\partial} v}{\tilde{\partial} t}\right)$$
$$+\left[-\frac{2K}{r} - 2\Omega\cos\phi\frac{u - r^2\cos^2\phi\Omega}{r\cos\phi} + \frac{a^2}{r^2}g\right]\frac{\tilde{\partial}\mu}{\tilde{\partial} t}. \quad (81)$$

7. Summary and discussion

a. Main results

In this work, we have established the curl-form of general equations of atmospheric motion in non-Eulerian general coordinates (23). Narrowing down to a general vertical coordinate, the form (33-34) has been obtained. This form is valid for all general vertical coordinates and implies automatically the conservation of energy. A key for this result is the invariance of energy with respect to vertical relabelling transformations, expressed by (34). Notice that the form of the equations of motion depends critically on the prognostic variables being μ, S, ξ^3, v_i, V_3. Incorporating planetary velocity into the prognostic velocity variables and prognosing covariant components is especially important. (33-34) is not quasi-Hamiltonian since vertical transport due to $\dot{\eta}$ is left unspecified, but it serves as a common ancestor to quasi-Hamiltonian formulations in Lagrangian, isentropic, mass-based and z-based coordinates. In Lagrangian, isentropic and mass-based vertical coordinates, a complete or partial separation between the horizontal and vertical dynamics is achieved.

The horizontal-vertical separation is especially helpful for hydrostatic systems characterized by vanishing vertical momentum $\partial\hat{L}/\partial\xi^3 = 0$. Indeed for such systems the formulation (33-34) gracefully reduces to (47-50) while it breaks down for the standard Eulerian formulation (17-19). Vertical momentum balance reduces to the simple statement $\delta\mathcal{H}/\delta\xi^3 = 0$: energy is stationary with respect to adiabatic vertical displacements of fluid parcels. From

this point of view the purpose of hydrostatic balance is to determine the vertical position of fluid parcels, for which no evolution equation is available. The physically appealing formulation $\delta\mathcal{H}/\delta\xi^3 = 0$ is, as far as we know, new. Indeed in Roulstone and Brice (1995), the Hamiltonian formulation of vertical balance is not addressed. On the other hand in Holm and Long (1989) such a formulation is not needed. Indeed due to the Boussinesq approximation the vertical position of fluid parcels is deduced from the pseudo-density field only. Taking into account this kinematic constraint directly into the energy is sufficient to obtain the correct horizontal dynamics. Using the formulation $\delta\mathcal{H}/\delta\xi^3 = 0$ of hydrostatic balance, Richardson's equation for vertical transport in Eulerian coordinates has been shown to take the form (52), interpreted as the combination of a hydrostatic adjustment and a vertical relabelling.

Finally we have exemplified the above general results with the fully compressible Euler equations in a Lagrangian vertical coordinate and a Cartesian (x, z) slice geometry, and the deep-atmosphere quasi-hydrostatic equations in a mass-based vertical coordinate and longitude-latitude horizontal coordinates. The latter case especially illuminates, in our opinion, how the apparent intricacy of the time-dependent metric terms and of the additional forces can be absorbed into a proper choice of prognostic variables (i.e. absolute angular momentum)

b. Stability

Identifying the Hamiltonian formulation of an adiabatic system opens the possibility to study flow stability by energy methods. For this it is useful to identify the Casimir invariants, i.e. the integral quantities that are conserved by (38-42) and (47-50) for any expression of $\mathcal{H}$ (Morrison 1998). It is easy to check that Ertel's potential vorticity

$$q = \frac{1}{\mu}\varepsilon^{klm}\partial_k s\left(\partial_l v_m - \partial_m v_l\right),$$

where ε^{klm} is the totally antisymmetric unit tensor, is conserved for any $\mathcal{H}$. (Tort and Dubos 2013b). Since $Dq/Dt = 0$ and $Ds/Dt = 0$ one finds $Df(s,q)/Dt = 0$ where $f(s,\, q)$ is an arbitrary function, leading to the Casimir invariants of the form :

$$\mathcal{C} = \int \mu f\,(s,\, q)\,\mathrm{d}\xi^1\mathrm{d}\xi^2\mathrm{d}\eta.$$

Notice that this includes total mass as the special case $f(s,\, q) = 1$ but not total axial absolute angular momentum since its conservation depends on the energy being zonally-symmetric. Furthermore $\mathcal{C}$ does not depend on ξ^3.

Because Casimir invariants satisfy $\{\mathcal{F}, \mathcal{C}\} = 0$ for any $\mathcal{F}$, one can replace (assuming f has the unit of specific energy) $\mathcal{H}$ by $\mathcal{H}' = \mathcal{H} + \mathcal{C}$ in the equations of motion, without changing them (Morrison 1998). This also applies to hydrostatic systems since $\delta\mathcal{C}/\delta\xi^3 = 0$. Flows for which the functional derivatives of $\mathcal{H}'$ vanish are therefore necessarily steady-states, and their stability can be studied by examining the convexity of $\mathcal{H}'$ (Arnold 1965; Holm et al. 1985; Holm and Long 1989). Hence our results open the possibility to apply the energy-Casimir stability theory to compressible hydrostatic systems.

c. Approximate models

Generally speaking, a statement or equation which does not depend on the specific forces applied to a mechanical system is of kinematic nature, while those who depend on the forces are of dynamical nature. Therefore our main results summarized above achieve a complete separation between the flow kinematics, expressed by the general forms (38-42) and (47-50), and the flow dynamics, expressed entirely by energy. This opens a route to deriving approximate models, which was a central focus of Tort and Dubos (2014). Tort and Dubos (2014) follow the Hamilton's principle asymptotics approach, whereby approximations are made in the Lagrangian, and the resulting approximate equations follow Holm et al. (2002, 2009). Similarly, it is possible to approximate energy to obtain approximate equations of motion possessing conservation laws for mass, entropy, energy and, subject to zonal invariance of

the energy, angular momentum. For instance letting $r = a$ in the quasi-hydrostatic deep-atmosphere energy yields immediately the hydrostatic primitive equations. This alternative route has the appeal that energy is a physically meaningful quantity, while the Lagrangian is not. Notice that both routes are equivalent, since the Lagrangian corresponding to a given energy can always be recovered by inverting the Legendre transform (11).

d. Energy-conserving numerical schemes

It has been advocated for some time now that energy-conserving numerical schemes should be obtained by discretizing the Poisson bracket and the energy themselves, rather than the curl-form equations (Salmon 1983, 2004). This strategy has been implemented recently to design a global non-hydrostatic dynamical core solving the fully compressible Euler equations in Eulerian coordinates (Gassmann 2013). Our work opens the possibility to do the same in general vertical coordinates by ensuring that the form (33), the skew-symmetric character of the operator $\mathcal{J}$ and, if necessary, the relabelling property (34) hold at the discrete level. For hydrostatic systems one would have to enforce (46) and hydrostasy (50), which is simplest if ξ^3 or equivalently geopotential is an independant field, e.g. in a Lagrangian, isentropic or mass-based vertical coordinate. Most numerical models solving the hydrostatic primitive equations use such a coordinate for convenience, because the calculation of all tendencies is greatly simplified and the necessity to solve Richardson's equation is circumvented. Our results suggest that there is a deeper reason to the suitability of Lagrangian or mass-based coordinates for hydrostatic numerical modeling.

Furthermore the separation between kinematics and dynamics can help designing models solving different sets of equations, by distinguishing those parts of the model that really depend on the equations considered from those parts that are actually kinematic and can be shared among different sets of equations. Finally, comparing (38-42) and (47-50) suggests that a non-hydrostatic solver can cohabit with a hydrostatic solver in a single model and reuse the hydrostatic code to an even greater extent than previously thought (Laprise 1992).

Acknowledgements

We are grateful to three anonymous referees for their careful and constructive remarks. Part of this work was completed during a visit of TD to Isaac Newton Institute's programme "Multiscale Numerics for the Atmosphere and Ocean". MT is supported by a Gaspard Monge PhD fellowship (École Polytechnique).

APPENDIX A

Upper boundary condition

In order to impose a pressure p_{top} instead of altitude at the domain top, it is sufficient to add to energy the work of that pressure force :

$$\mathcal{H}' = \mathcal{H} + p_{top} \int V(\xi^i, \xi^3_{top}) \mathrm{d}\xi^i,$$

where $\xi^3_{top}(\xi^i) = \xi^3(\xi^i, \eta = 1)$ is the vertical position of the domain top and $\int V(\xi^i, \xi^3_{top})\mathrm{d}\xi^i$ the volume of the atmosphere, i.e. the specific volume is $\alpha = \frac{1}{\tilde{\mu}}\partial V/\partial\xi^3 = \frac{1}{\mu}\partial_\eta V(\xi^i, \xi^3)$ (for example, for a deep atmosphere with a flat bottom positioned at $r = a$ using spherical coordinates, $V(\lambda, \phi, r) = \cos\phi\,(r^3 - a^3)/3$). Indeed variations of internal energy contribute a boundary term which vanishes when ξ^3_{top} is prescribed (as assumed in the main text) :

$$\begin{aligned}\delta \int U\left(\frac{1}{\mu}\partial_\eta V(\xi^i, \xi^3),\, \frac{S}{\mu}\right)\mu \mathrm{d}\xi^i \mathrm{d}\eta \;\; &= \;\; \int \left[\left(U + \alpha p - Ts\right)\delta\mu + T\delta S + \partial_\eta p \frac{\partial V}{\partial \xi^3}\delta\xi^3\right]\mathrm{d}\xi^i \mathrm{d}\eta \\ &\quad - \int_{\eta=1} \frac{\partial V}{\partial \xi^3} p \delta\xi^3_{top} \mathrm{d}\xi^i.\end{aligned}$$

Therefore the top boundary condition $p = p_{top}$ becomes simply $\delta\mathcal{H}'/\delta\xi^3_{top} = 0$, where the functional derivative $\delta\mathcal{H}'/\delta\xi^3_{top}$ is defined by :

$$\delta\mathcal{H}' = \int \left[\frac{\delta\mathcal{H}'}{\delta\mu}\delta\mu + \ldots\right]\mathrm{d}\xi^i \mathrm{d}\eta + \int_{\eta=1} \frac{\delta\mathcal{H}'}{\delta\xi^3_{top}}\delta\xi^3_{top}\mathrm{d}\xi^i,$$

the other functional derivatives of $\mathcal{H}'$ being identical to those of $\mathcal{H}$. Replacing $\mathcal{H}$ by $\mathcal{H}'$ in (33) leaves the equations of motion unchanged, while the boundary condition $\delta\mathcal{H}'/\delta\xi^3_{top} = 0$ ensures that $\mathrm{d}\mathcal{H}'/\mathrm{d}t = 0$. $\mathcal{H}'$ is sometimes referrred to as total enthalpy.

APPENDIX B

Vertical relabelling symmetry

The vertically-Lagrangian description of the flow is *redundant*. Indeed one can decide arbitrarily the initial altitudes $\xi^3(\xi^i, \eta, t = 0)$, so that a given flow admits several representations in a vertically-Lagrangian coordinate. This redundancy translates into a symmetry of energy, and more generally any observable quantity, which cannot depend on the arbitrary positions $\xi^3(\xi^i, \eta, t)$. To see this consider two descriptions $(v_i, \xi^3, V_3, \mu, S)$ and $(v'_i, \xi'^3, V'_3, \mu', S')$, assume that the difference between them is infinitesimal, and define $\delta\eta$ from the vertical displacement by

$$\xi'^3(\eta) = \xi^3\left(\eta + \delta\eta\right) \quad \Rightarrow \quad \xi'^3 - \xi^3 = \partial_\eta \xi^3 \, \delta\eta. \tag{B1}$$

If $(v_i, \xi^3, V_3, \mu, S)$ and $(v'_i, \xi'^3, V'_3, \mu', S')$ are to describe the same flow, then (v'_i, V'_3, μ', S') must be related to (v_i, V_3, μ, S) and the vertical displacement, or, equivalently $\delta\eta$. For extensive quantities μ, S, V_3 :

$$\int_{\xi^3_0}^{\xi^3} \hat{\mu}\mathrm{d}\xi^3 = \int_0^{\eta+\delta\eta} \mu \mathrm{d}\eta = \int_0^{\eta} \mu' \mathrm{d}\eta,$$

so that :

$$\mu' - \mu = \partial_\eta \left(\mu \delta\eta\right), \tag{B2}$$

$$S' - S = \partial_\eta \left(S \delta\eta\right), \tag{B3}$$

$$V'_3 - V_3 = \partial_\eta \left(V_3 \delta\eta\right). \tag{B4}$$

Requiring $\hat{v}_i(\eta + \delta\eta) = \hat{v}'_i(\eta)$, yields the rule for v_i :

$$v'_i - v_i = \partial_\eta v_i \delta\eta + v_3 \partial_i \delta\eta. \tag{B5}$$

Hence $\mathcal{H}\left[v_i, \xi^3, V_3, \mu, S\right] = \mathcal{H}\left[v'_i, \xi'^3, V'_3, \mu', S'\right]$ whenever $(v'_i,\, \xi'^3,\, V'_3,\, \mu',\, S') - (v_i,\, \xi^3,\, V_3,\, \mu,\, S) = \mathcal{V} \cdot \delta\eta$ for some infinitesimal $\delta\eta$, where $\mathcal{V}$ has been defined by (33). Integrating by parts with the boundary conditions $\delta\eta = 0$ for $\eta = 0, 1$ yields the relationship (43) between the functional derivatives of $\mathcal{H}$, i.e. $\mathcal{V}^* \cdot \delta\mathcal{H} = 0$.

(43) expresses the invariance of energy with respect to vertical displacements of the surfaces $\eta = cst$, provided the other prognostic variables are adjusted accordingly so that the underlying flow remains the same. It is therefore an instance of the relabelling symmetry, used here only in the vertical direction.

APPENDIX C

Mass budget in a mass-based hybrid coordinate

To define a mass-based vertical coordinate $\eta \in [0, 1]$, the column-integrated mass $M(\xi^i, t)$ is introduced :

$$M(\xi^i, t) \;\; = \;\; \int_{bottom}^{top} \mu \mathrm{d}\eta = \int_{bottom}^{top} \hat{\mu} \mathrm{d}\xi^3. \tag{C1}$$

Given the pseudo-density field $\hat{\mu}(\xi^i, \xi^3)$, the position $\xi^3(\xi^i, \eta)$ is defined uniquely by the condition that :

$$A(\eta) M(\xi^i) + B(\eta) = \int_{\xi_0^3}^{\xi^3(\eta)} \hat{\mu} \mathrm{d}\xi^3, \tag{C2}$$

where $\xi^3(\xi^i, \eta = 0, t) = \xi_0^3(\xi^i)$ is the orography and the profiles $A(\eta)$ and $B(\eta)$ are prescribed with $A(0) = 0$, $A(1) = 1$, $B(0) = B(1) = 0$. Conversely (C2) defines the pseudo-density

$$\mu = A' M + B' \tag{C3}$$

where $A' = \mathrm{d}A/\mathrm{d}\eta$, $B' = \mathrm{d}B/\mathrm{d}\eta$. Notice that the profiles $A(\eta)$, $B(\eta)$ must be chosen such that μ remains always > 0.

(C3) expresses the fundamental difference between Lagrangian and mass-based hybrid coordinates : with the former μ is a prognostic variable while with the latter μ is slaved to M through (C3). Therefore energy should not be considered a functional of $[\mu, S, v_i, \xi^3, V_3]$ but of $[M, S, v_i, \xi^3, V_3]$. In order to make it clear whether energy is considered a functional of $[M, S, v_i, \xi^3, V_3]$ or $[\mu, S, v_i, \xi^3, V_3]$, we let :

$$\mathcal{H}'\left[M, S, v_i, \xi^3, V_3\right] \;=\; \mathcal{H}\left[A'M + B', S, v_i, \xi^3, V_3\right]. \tag{C4}$$

From definition (C4) one obtains that the functional derivatives of $\mathcal{H}'$ and $\mathcal{H}$ with respect to v_i, ξ^3, V_3, S are identical. Especially the horizontal mass flux is still given by $\delta\mathcal{H}/\delta v_i$. The mass budget then reads (recall that $u^3 = Da^3/Dt = \dot{\eta}$) :

$$\partial_t \mu + \partial_i \left(\frac{\delta \mathcal{H}'}{\delta v_i}\right) + \partial_\eta \left(\mu \dot{\eta}\right) = 0. \tag{C5}$$

From (C5) one deduces the prognostic equation for M

$$\frac{\partial M}{\partial t} + \partial_i \left(\int_0^1 \frac{\delta \mathcal{H}}{\delta v_i}\right) \mathrm{d}\eta = 0,$$

then a diagnostic equation from which the vertical mass flux $\mu\dot{\eta}$ is obtained in the form $\mu\dot{\eta} = \mathcal{L} \cdot (\delta\mathcal{H}/\delta v_i)$ where $\mathcal{L}$ is an integro-differential operator :

$$-A'\partial_i \left(\int_0^1 \frac{\delta \mathcal{H}}{\delta v_i} \mathrm{d}\eta\right) + \partial_i \left(\frac{\delta \mathcal{H}'}{\delta v_i}\right) + \partial_\eta W = 0$$

$$\mu\dot{\eta} = \mathcal{L}\frac{\delta \mathcal{H}}{\delta v_i} = A(\eta)\partial_i \left(\int_0^1 \frac{\delta \mathcal{H}}{\delta v_i} \mathrm{d}\eta\right) - \int_0^\eta \partial_i \left(\frac{\delta \mathcal{H}'}{\delta v_i}\right) \mathrm{d}\eta. \tag{C6}$$

Therefore both horizontal and vertical mass fluxes are expressed linearly in terms of functional derivatives of energy. Notice that this holds for hydrostatic systems as well, at contrast with what happens in a Eulerian vertical coordinate.

APPENDIX D

Brackets

In this appendix we derive explicitly the brackets such that :

$$\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}t} = \{\mathcal{F}, \mathcal{H}\}$$

where $\mathcal{F}$ is a functional of the same prognostic fields as $\mathcal{H}$. We show the antisymmetry property $\{\mathcal{F}, \mathcal{H}\} = -\{\mathcal{H}, \mathcal{F}\}$ but not the Jacobi identity (4).

a. Lagrangian vertical coordinate

For non-hydrostatic systems the prognostic variables are μ, S, v^i, ξ^3, V_3 . Using (28-32) and integrating by parts (boundary terms vanish due to boundary conditions satisfied by the mass flux $\delta\mathcal{H}/\delta v^i$) :

$$\begin{aligned}
\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}t} &= -\int \left[\frac{\delta\mathcal{F}}{\delta v_i}\left(\frac{\partial_j v_i - \partial_i v_j}{\mu}\frac{\delta\mathcal{H}}{\delta v_j} + \partial_i\left(\frac{\delta\mathcal{H}}{\delta\mu}\right) + s\partial_i\left(\frac{\delta\mathcal{H}}{\delta S}\right)\right)\right]\mathrm{d}\xi^i\mathrm{d}\eta \\
&\quad -\int \left[\frac{\delta\mathcal{F}}{\delta\mu}\partial_i\frac{\delta\mathcal{H}}{\delta v^i} + \frac{\delta\mathcal{F}}{\delta S}\partial_i\left(s\frac{\delta\mathcal{H}}{\delta v^i}\right) + \frac{\delta\mathcal{F}}{\delta\xi^3}\frac{\delta\mathcal{H}}{\delta V_3} - \frac{\delta\mathcal{F}}{\delta V_3}\frac{\delta\mathcal{H}}{\delta\xi^3}\right]\mathrm{d}\xi^i\mathrm{d}\eta \\
&= \{\mathcal{F}, \mathcal{H}\}^{\mu}_{lag} + \{\mathcal{F}, \mathcal{H}\}^{s}_{lag} + \{\mathcal{F}, \mathcal{H}\}^{\times}_{lag} + \{\mathcal{F}, \mathcal{H}\}^{V}_{lag} \qquad \text{(D1)} \\
\{\mathcal{F}, \mathcal{H}\}^{\mu}_{lag} &= \int \left[\frac{\delta\mathcal{H}}{\delta v^i}\partial_i\frac{\delta\mathcal{F}}{\delta\mu} - \frac{\delta\mathcal{F}}{\delta v^i}\partial_i\frac{\delta\mathcal{H}}{\delta\mu}\right]\mathrm{d}\xi^i\mathrm{d}\eta \\
\{\mathcal{F}, \mathcal{H}\}^{s}_{lag} &= \int s\left[\partial_i\frac{\delta\mathcal{F}}{\delta S}\frac{\delta\mathcal{H}}{\delta v^i} - \frac{\delta\mathcal{F}}{\delta v^i}\partial_i\frac{\delta\mathcal{H}}{\delta S}\right]\mathrm{d}\xi^i\mathrm{d}\eta \\
\{\mathcal{F}, \mathcal{H}\}^{\times}_{lag} &= \int \frac{\partial_j v_i - \partial_i v_j}{\mu}\frac{\delta\mathcal{H}}{\delta v_j}\frac{\delta\mathcal{F}}{\delta v_i}\mathrm{d}\xi^i\mathrm{d}\eta \\
\{\mathcal{F}, \mathcal{H}\}^{V}_{lag} &= \int \left[\frac{\delta\mathcal{F}}{\delta V_3}\frac{\delta\mathcal{H}}{\delta\xi^3} - \frac{\delta\mathcal{F}}{\delta\xi^3}\frac{\delta\mathcal{H}}{\delta V_3}\right]\mathrm{d}\xi^i\mathrm{d}\eta
\end{aligned}$$

Clearly, all the above brackets are antisymmetric and $\mathrm{d}\mathcal{H}/\mathrm{d}t = 0$.

For hydrostatic systems only μ, S, v^i are truly diagnostic and ξ^3 is diagnosed using hydrostatic balance (50). Using (47-49) :

$$\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}t} = \{\mathcal{F}, \mathcal{H}\}^{\mu}_{lag} + \{\mathcal{F}, \mathcal{H}\}^{s}_{lag} + \{\mathcal{F}, \mathcal{H}\}^{\times}_{lag} + \int \frac{\delta\mathcal{F}}{\delta\xi^3}\partial_t\xi^3\mathrm{d}\xi^i\mathrm{d}\eta \qquad \text{(D2)}$$

Notice that (D2) deviates from the standard quasi-Hamiltonian formulation (3). This is a due to ξ^3 being diagnostic instead of prognostic so that an expression for $\partial_t \xi^3$ is lacking. However due to the formulation (50) of hydrostasy, (D2) still guarantees the conservation of energy.

b. Mass-based vertical coordinate

In a mass-based vertical coordinate, non-hydrostatic systems have prognostic variables M, S, v^i, ξ^3, V_3. Using (38-42) :

$$\partial_t M + \partial_i \int_{bottom}^{top} \frac{\delta \mathcal{H}'}{\delta v_i} \mathrm{d}\eta = 0, \quad \text{(D3)}$$

$$\partial_t S + \partial_i \left(s \frac{\delta \mathcal{H}'}{\delta v_i} \right) + \partial_\eta \left(S \dot{\eta} \right) = 0, \quad \text{(D4)}$$

$$\partial_t v_i + \left(\partial_\eta v_i - \partial_i v_3 \right) \dot{\eta} + \frac{\partial_j v_i - \partial_i v_j}{\mu} \frac{\delta \mathcal{H}'}{\delta v_j} + \partial_i \left(\frac{\delta \mathcal{H}}{\delta \mu} + \dot{\eta} v_3 \right) + s \partial_i \left(\frac{\delta \mathcal{H}'}{\delta S} \right) = 0, \quad \text{(D5)}$$

$$\partial_t V_3 + \partial_\eta \left(V_3 \dot{\eta} \right) + \frac{\delta \mathcal{H}'}{\delta \xi^3} = 0, \quad \text{(D6)}$$

$$\partial_t \xi^3 + \dot{\eta} \partial_\eta \xi^3 - \frac{\delta \mathcal{H}'}{\delta V_3} = 0. \quad \text{(D7)}$$

Now for any functional $\mathcal{F}'$

$$\begin{aligned}
&\int \dot{\eta} \left[S \partial_\eta \frac{\delta \mathcal{F}'}{\delta S} + V_3 \partial_\eta \frac{\delta \mathcal{F}'}{\delta V_3} - \frac{\delta \mathcal{F}'}{\delta \xi^3} \partial_\eta \xi^3 \right. \\
&\left. - \left(\partial_\eta v_i - \partial_i v_3 \right) \frac{\delta \mathcal{F}'}{\delta v_i} + v_3 \partial_i \frac{\delta \mathcal{F}'}{\delta v_i} \right] \mathrm{d}\xi^i \mathrm{d}\eta &= \int \frac{\delta \mathcal{F}}{\delta \mu} \partial_\eta \left(\dot{\eta} \mu \right) \mathrm{d}\xi^i \mathrm{d}\eta \\
&&= -\int \frac{\delta \mathcal{F}}{\delta \mu} \left[\partial_i \frac{\delta \mathcal{H}'}{\delta v_i} + A' \partial_t M \right] \mathrm{d}\xi^i \mathrm{d}\eta \\
&&= \int \frac{\delta \mathcal{H}'}{\delta v_i} \partial_i \frac{\delta \mathcal{F}}{\delta \mu} \mathrm{d}\xi^i \mathrm{d}\eta - \int \partial_t M \frac{\delta \mathcal{F}'}{\delta M} \mathrm{d}\xi^i
\end{aligned}$$

hence

$$\begin{aligned}\frac{\mathrm{d}\mathcal{F}'}{\mathrm{d}t} &= \{\mathcal{F}',\mathcal{H}'\}^{s}_{lag}+\{\mathcal{F}',\mathcal{H}'\}^{\times}_{lag}+\{\mathcal{F}',\mathcal{H}'\}^{V}_{lag}\\ &+\int\frac{\delta\mathcal{F}'}{\delta M}\partial_t M\mathrm{d}\xi^i-\int\frac{\delta\mathcal{F}'}{\delta v_i}\partial_i\frac{\delta\mathcal{H}}{\delta\mu}\mathrm{d}\xi^i\mathrm{d}\eta\\ &+\int\dot\eta\left[S\partial_\eta\frac{\delta\mathcal{F}'}{\delta S}+V_3\partial_\eta\frac{\delta\mathcal{F}'}{\delta V_3}-\frac{\delta\mathcal{F}'}{\delta\xi^3}\partial_\eta\xi^3-\left(\partial_\eta v_i-\partial_i v_3\right)\frac{\delta\mathcal{F}'}{\delta v_i}+v_3\partial_i\frac{\delta\mathcal{F}'}{\delta v_i}\right]\mathrm{d}\xi^i\mathrm{d}\eta\\ &= \{\mathcal{F},\mathcal{H}\}^{\mu}_{lag}+\{\mathcal{F}',\mathcal{H}'\}^{s}_{lag}+\{\mathcal{F}',\mathcal{H}'\}^{\times}_{lag}+\{\mathcal{F}',\mathcal{H}'\}^{V}_{lag}.\end{aligned}\tag{D8}$$

Apparently the brackets (D8) and (D1) are identical. However they differ by the meaning of the bracket $\{\mathcal{F},\mathcal{H}\}^{\mu}_{lag}$. Indeed in the case of a Lagrangian coordinate, $\{\mathcal{F},\mathcal{H}\}^{\mu}_{lag}$ is an expression involving functional derivatives with respect to μ and v_i only while in the mass-based case, $\{\mathcal{F},\mathcal{H}\}^{\mu}_{lag}$ is actually an integro-differential expression involving all functional derivatives of $\mathcal{F}',\mathcal{H}'$.

APPENDIX E

Richardson's equation

In this Appendix the problem yielding vertical transport when hydrostatic systems are expressed in a z-based coordinate is obtained and shown to be self-adjoint. First using hydrostatic balance (51) we note that :

$$\begin{aligned}&\partial_\eta\left(\mu\dot\eta\right)\partial_\eta\frac{\delta\mathcal{H}}{\delta\mu}+\partial_\eta\left(S\dot\eta\right)\partial_\eta\frac{\delta\mathcal{H}}{\delta S}-\partial_\eta\left(\dot\eta\partial_\eta v_i\right)\frac{\delta\mathcal{H}}{\delta v_i}\\ &=\partial_\eta\left(\mu\dot\eta\right)\left(\frac{\partial_\eta v_i}{\mu}\frac{\delta\mathcal{H}}{\delta v_i}-s\partial_\eta\frac{\delta\mathcal{H}}{\delta S}\right)+\partial_\eta\left(\mu s\dot\eta\right)\partial_\eta\frac{\delta\mathcal{H}}{\delta S}-\partial_\eta\left(\dot\eta\mu\frac{\partial_\eta v_i}{\mu}\right)\frac{\delta\mathcal{H}}{\delta v_i}\\ &=\left[\partial_\eta s\frac{\delta\mathcal{H}}{\delta S}-\partial_\eta\left(\frac{\partial_\eta v_i}{\mu}\right)\frac{\delta\mathcal{H}}{\delta v_i}\right]\mu\dot\eta.\end{aligned}\tag{E1}$$

In order to time-differentiate (51) we need to define the second functional derivatives. For general functionals, they are distributions rather than regular functions. However because $\mathcal{H}$ is defined as the integral of an energy density depending only on the local values of the

prognostic fields and $\partial_\eta \xi^3$, its second functional derivatives can be defined as differential operators satisfying :

$$\partial_t \frac{\delta \mathcal{H}}{\delta X} = \sum_{Y=\mu,\Theta,v_i,\xi^3} \frac{\delta^2 \mathcal{H}}{\delta X \delta Y} \partial_t Y, \quad X = \mu, \Theta, v_i, \xi^3 \tag{E2}$$

Notice that the order of differentiation matters and that operators $\dfrac{\delta^2 \mathcal{H}}{\delta X \delta Y}$ and $\dfrac{\delta^2 \mathcal{H}}{\delta Y \delta X}$ are mutually adjoint. In fact the only derivatives that appear in the Hamiltonian are $\partial_\eta \xi^3$, and they appear through internal energy only. Therefore $\delta^2 \mathcal{H} / \left(\delta \xi^3\right)^2$ is a second-order self-adjoint differential operator and $\delta^2 \mathcal{H} / \delta \Theta \delta \xi^3$ and $\delta^2 \mathcal{H} / \delta \xi^3 \delta \Theta$ are mutually adjoint first-order differential operators. For an ideal perfect gas and $\Theta = \theta \mu$ as a prognostic variable, $\delta^2 \mathcal{H} / \delta \mu$ has no contribution from internal energy so that $\delta^2 \mathcal{H} / \delta \mu \delta \xi^3$ derives from kinetic and potential energies only, and is scalar. However for a general equation of state $\delta^2 \mathcal{H} / \delta \mu \delta \xi^3$ and $\delta^2 \mathcal{H} / \delta \xi^3 \delta \mu$ are mutually adjoint first-order differential operators as well. All other second functional derivatives are scalar. As an example table 1 summarizes $\delta^2 \mathcal{H} / \delta X \delta Y$ for the deep-atmosphere quasi-hydrostatic equations.

Then, time-differentiating (51) using the equations of motion (47-49) and (E1), we obtain :

$$\left[\partial_\eta s \frac{\delta \mathcal{H}}{\delta S} - \partial_\eta \left(\frac{\partial_\eta v_i}{\mu}\right) \frac{\delta \mathcal{H}}{\delta v_i}\right] \mu \dot{\eta} + \begin{bmatrix} -\mu \partial_\eta \\ -S \partial_\eta \\ \left(\partial_\eta v_i\right) \end{bmatrix}^T \cdot \begin{bmatrix} \dfrac{\delta^2 \mathcal{H}}{\delta \mu^2} & \dfrac{\delta^2 \mathcal{H}}{\delta \mu \delta S} & \dfrac{\delta^2 \mathcal{H}}{\delta \mu \delta v_i} \\ \dfrac{\delta^2 \mathcal{H}}{\delta S \delta \mu} & \dfrac{\delta^2 \mathcal{H}}{\delta S^2} & \dfrac{\delta^2 \mathcal{H}}{\delta S \delta v_i} \\ \dfrac{\delta^2 \mathcal{H}}{\delta v_i \delta \mu} & \dfrac{\delta^2 \mathcal{H}}{\delta v_i \delta S} & \dfrac{\delta^2 \mathcal{H}}{\delta v_i \delta v_j} \end{bmatrix} \cdot \begin{bmatrix} \partial_\eta \left(\mu \dot{\eta}\right) \\ \partial_\eta \left(S \dot{\eta}\right) \\ \dot{\eta} \partial_\eta v_j \end{bmatrix} = r.h.s. \tag{E3}$$

where $r.h.s.$ collects all contributions that do not depend on $\dot{\eta}$ and the bottom and top boundary conditions are $\dot{\eta} = 0$. Richardson's equation (E3) is a self-adjoint linear problem for $\dot{\eta}$. Since the second functional derivatives involved in (E3) are scalars, (E3,E5) is a second-order ODE which can be solved for each atmospheric column separately, an important property from a parallel computing point of view.

(E3) has been written with functional derivatives with respect to the prognostic variables μ only. A more concise form can be obtained if one allows derivatives with respect to ξ^3 to

be taken. Indeed the relabelling symmetry implies :

$$0 = \frac{\delta^2 \mathcal{H}}{\left(\delta \xi^3\right)^2} \delta \xi^3 + \frac{\delta^2 \mathcal{H}}{\delta \xi^3 \delta \mu} \delta \mu + \frac{\delta^2 \mathcal{H}}{\delta \xi^3 \delta S} \delta S + \frac{\delta^2 \mathcal{H}}{\delta \xi^3 \delta v_i} \delta v_i \tag{E4}$$

for variations of the form

$$\delta \mu = \partial_\eta \left(\mu \delta \eta\right), \quad \delta S = \partial_\eta \left(S \dot{\eta}\right), \qquad \delta v_i = \partial_\eta v_i \, \delta \eta, \qquad \delta \xi^3 = \partial_\eta \xi^3 \, \delta \eta.$$

Now time-differentiating hydrostatic balance $\delta \mathcal{H} / \delta \xi^3 = 0$ yields :

$$\frac{\delta^2 \mathcal{H}}{\delta \xi^3 \delta \mu} \partial_\eta \left(\mu \dot{\eta}\right) + \frac{\delta^2 \mathcal{H}}{\delta \xi^3 \delta S} \partial_\eta \left(S \dot{\eta}\right) + \frac{\delta^2 \mathcal{H}}{\delta \xi^3 \delta v_i} \partial_\eta v_i \, \dot{\eta} = r.h.s.$$

Hence, (E4) with $\delta \eta = \partial_\eta \xi^3 \, \dot{\eta}$ yields :

$$\frac{\delta^2 \mathcal{H}}{\left(\delta \xi^3\right)^2} \left(\partial_\eta \xi^3 \, \dot{\eta}\right) = r.h.s. \tag{E5}$$

(E3) and (E5) are equivalent formulations of the same problem.

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List of Tables

1 Second functional derivatives $\delta^2\mathcal{H}/\delta X\delta Y$ of the deep-atmosphere quasi-hydrostatic Hamiltonian (69). $K(u,v,r) = \frac{1}{2}\left(\frac{u-\Omega r^2\cos^2\phi}{r\cos\phi}\right)^2 + \frac{1}{2}\left(\frac{v}{r}\right)^2$, $\alpha = \frac{\cos\phi}{3\mu}\partial_\eta r^3$ is specific volume, $\theta\partial\pi(\alpha,\theta)/\partial\theta = -\alpha\partial\pi(\alpha,\theta)/\partial\alpha$ because π depends on α/θ only. Hence $\partial p/\partial\theta = \frac{p}{\kappa\pi}\partial\pi/\partial\theta = -\partial\pi/\partial\alpha$ (using $\alpha p = \kappa\theta\pi$). 48

	$X=\mu$	$X=\Theta$	$X=u$	$X=v$	$X=r$
$\delta\mathcal{H}/\delta X$	$K-\dfrac{ga^2}{r}$	π	$\mu\dot{\lambda}$	$\mu\dot{\phi}$	$-2\Omega\mu\cos\phi\dfrac{u-r^2\cos^2\phi\Omega}{r\cos\phi}$ $+\mu\left[\dfrac{a^2}{r^2}g-\dfrac{2K}{r}\right]$ $+r^2\cos\phi\partial_\eta p$
$Y=\mu$			$\dot{\lambda}$	$\dot{\phi}$	$-\dfrac{2K}{r}+\dfrac{a^2}{r^2}g$ $-2\Omega\dfrac{u-\Omega r^2\cos^2\phi}{r}$
$Y=\Theta$		$\dfrac{1}{\mu}\dfrac{\partial\pi}{\partial\theta}$			$r^2\cos\phi\partial_\eta\left(\dfrac{1}{\mu}\dfrac{\partial p}{\partial\theta}\cdot\right)$
$Y=u$	$\dot{\lambda}$		$\dfrac{\mu}{r^2\cos^2\phi}$		$-\dfrac{2\mu u}{r^3\cos^2\phi}$
$Y=v$	$\dot{\phi}$			$\dfrac{\mu}{r^2}$	$-\dfrac{2\mu v}{r^3}$
$Y=r$	$-\dfrac{2K}{r}+\dfrac{a^2}{r^2}g$ $-2\Omega\dfrac{u-\Omega r^2\cos^2\phi}{r}$	$\dfrac{\cos\phi}{\mu}\dfrac{\partial\pi}{\partial\alpha}\partial_\eta\left(r^2\cdot\right)$	$-\dfrac{2\mu u}{r^3\cos^2\phi}$	$-\dfrac{2\mu v}{r^3}$	$\mu\left(6\dfrac{K+\Omega u}{r^2}-2\Omega^2\cos^2\phi\right)$ $-\dfrac{2a^2}{r^3}\mu g+2r\cos\phi\partial_\eta p$ $+r^2\cos\phi\partial_\eta\left(\dfrac{\cos\phi}{\mu}\dfrac{\partial p}{\partial\alpha}\partial_\eta\left(r^2\cdot\right)\right)$

TABLE 1. Second functional derivatives $\delta^2\mathcal{H}/\delta X\delta Y$ of the deep-atmosphere quasi-hydrostatic Hamiltonian (69). $K(u,v,r)=\dfrac{1}{2}\left(\dfrac{u-\Omega r^2\cos^2\phi}{r\cos\phi}\right)^2+\dfrac{1}{2}\left(\dfrac{v}{r}\right)^2$, $\alpha=\dfrac{\cos\phi}{3\mu}\partial_\eta r^3$ is specific volume, $\theta\partial\pi(\alpha,\theta)/\partial\theta=-\alpha\partial\pi(\alpha,\theta)/\partial\alpha$ because π depends on α/θ only. Hence $\partial p/\partial\theta=\dfrac{p}{\kappa\pi}\partial\pi/\partial\theta=-\partial\pi/\partial\alpha$ (using $\alpha p=\kappa\theta\pi$).