INSTITUTE OF PHYSICS PUBLISHING NONLINEARITY

Nonlinearity **18** (2005) R1–R16 doi:10.1088/0951-7715/18/5/R01

INVITED ARTICLE

A general method for conserving quantities related to potential vorticity in numerical models

Rick Salmon

Scripps Institution of Oceanography, University of California, San Diego, La Jolla, CA 92093-0213, USA

E-mail: rsalmon@ucsd.edu

Received 14 March 2005, in final form 10 May 2005
Published 6 June 2005
Online at stacks.iop.org/Non/18/R1

Recommended by K Ohkitani

Abstract

Nambu proposed a generalization of Hamiltonian dynamics in the form $\mathrm{d}F/\mathrm{d}t = \{F, H, Z\}$, which conserves H and Z because the Nambu bracket $\{F, H, Z\}$ is completely antisymmetric. The equations of fluid dynamics fit Nambu's form with H the energy and Z a quantity related to potential vorticity. This formulation makes it easy, in principle, to construct numerical fluid-models that conserve analogues of H and Z; one need only discretize the Nambu bracket in such a way that the antisymmetry property is preserved. In practice, the bracket may contain apparent singularities that are cancelled by the functional derivatives of Z. Then the discretization must be carried out in such a way that the cancellation is maintained. Following this strategy, we derive numerical models of the shallow-water equations and the equations for incompressible flow in two and three dimensions. The models conserve the energy and an arbitrary moment of the potential vorticity. The conservation of potential enstrophy—the second moment of potential vorticity—is thought to be especially important because it prevents the spurious cascade of energy into high wavenumbers.

Mathematics Subject Classification: 65P10

1. Introduction

The equations of fluid dynamics fit the Hamiltonian form

$$\frac{\mathrm{d}F}{\mathrm{d}t} = \{F, H\}, \tag{1.1}$$

where F is an arbitrary functional of the fields representing the state of the fluid; H is the Hamiltonian functional; and $\{\,,\}$ is the Poisson bracket, an antisymmetric, bilinear operator that obeys the Jacobi identity (5.3). For example, the equations for two-dimensional, incompressible flow may be written in the form

$$\frac{\partial \zeta}{\partial t} = J(\zeta, \psi), \tag{1.2}$$

where

$$\zeta = \nabla^2 \psi \tag{1.3}$$

is the vorticity of the fluid; $\psi(x, y, t)$ is the stream function; $(u, v) = (-\psi_y, \psi_x)$ is the velocity in the (x, y) direction; and

$$J(A, B) \equiv \frac{\partial(A, B)}{\partial(x, y)} \tag{1.4}$$

is the Jacobian operator in two dimensions. For simplicity, we consider only periodic boundary conditions. The dynamics (1.2) and (1.3) fits the form (1.1) with

$$\{F, H\} \equiv \iint \mathrm{d}\boldsymbol{x}\, \zeta\, J(F_\zeta, H_\zeta), \tag{1.5}$$

where $F_\zeta \equiv \delta F/\delta\zeta$ denotes the functional derivative,

$$H[\zeta(x, y)] = \frac{1}{2} \iint \mathrm{d}\boldsymbol{x}\, \nabla\psi \cdot \nabla\psi \tag{1.6}$$

and ψ and ζ are related by (1.3) and the periodic boundary conditions. We note that $\delta H/\delta\zeta = -\psi$ and $\delta H/\delta\psi = -\zeta$.

Nambu (1973) proposed a generalization of Hamiltonian dynamics in the form

$$\frac{\mathrm{d}F}{\mathrm{d}t} = \{F, H, Z\}, \tag{1.7}$$

where $\{F, H, Z\}$ is a *trilinear* antisymmetric bracket, and H and Z are a *pair* of Hamiltonians. Since $\{F, H\}$ represents the contraction of $\{F, H, Z\}$ with Z, the second Hamiltonian Z is always a *Casimir* of the original Poisson bracket. That is, $\{F, Z\} = 0$ for any F. Nambu noted that the Euler equations for a rigid rotator fit the form of (1.7) with Hamiltonians equal to the kinetic energy and to the square of the angular momentum.

Nevir and Blender (1993; see also Guha (2004)) found that two-dimensional Euler dynamics (1.2) and (1.3) fits the form of (1.7) with H given by (1.6),

$$Z[\zeta] = \frac{1}{2} \iint \mathrm{d}\boldsymbol{x}\, \zeta^2 \tag{1.8}$$

and

$$\{F, H, Z\} \equiv \iint \mathrm{d}\boldsymbol{x}\, J(F_\zeta, H_\zeta) Z_\zeta. \tag{1.9}$$

The antisymmetry of (1.9) follows from the antisymmetry of (1.4) and the periodic boundary conditions. Thus the dynamics (1.2) and (1.3) takes the Nambu form with the second Hamiltonian equal to the enstrophy (1.8).

The formulation (1.7)–(1.9) has practical consequences for the construction of numerical algorithms. By the antisymmetry property of (1.9) we may rewrite it as

$$\begin{aligned} \{F, H, Z\} &= \frac{1}{3} \iint \mathrm{d}\boldsymbol{x}[J(F_\zeta, H_\zeta)Z_\zeta + J(H_\zeta, Z_\zeta)F_\zeta + J(Z_\zeta, F_\zeta)H_\zeta] \\ &\equiv \frac{1}{3} \iint \mathrm{d}\boldsymbol{x}[J(F_\zeta, H_\zeta)Z_\zeta + \mathrm{cyc}\,(F, H, Z)], \end{aligned} \tag{1.10}$$

where cyc denotes cyclic permutations of the three functionals F, H and Z. Imagine that the three integrals in (1.10) are replaced by discrete (e.g. finite-difference) approximations in precisely the same way, and in such a way that the discrete approximation to $J(\ ,\ )$ is antisymmetric. Then the resulting discrete approximation to (1.9) retains the antisymmetry property of the exact bracket and therefore vanishes whenever two of its arguments are equal. Consequently, the discrete dynamics obtained by replacing the right-hand side (rhs) of (1.7) by this discrete bracket, and by introducing arbitrary discrete approximations to the energy (1.6) and enstrophy (1.8), automatically conserves that energy and enstrophy. Thus, the existence of an exact, antisymmetric bracket (1.9) involving H and Z leads to a general method for constructing discrete numerical approximations that exactly conserve discrete analogues of H and Z.

In claiming 'exact conservation' of H and Z, we ignore the effects of replacing the time derivative in (1.7) by a discrete approximation. That is, our claim actually only applies to the system of coupled ordinary differential equations obtained by discretizing the rhs of (1.7) in the manner described above. However, experience shows that the errors introduced by discretizing the time step have a negligible effect on conservation properties. On the other hand, the destruction of conservation laws by discrete approximations to the spatial derivatives has a well known and very deleterious effect on numerical calculations. In particular, numerical analogues of (1.2) and (1.3) that do not conserve an analogue of the enstrophy (1.8) typically allow too much energy to reach the smallest resolved spatial scales, where it must inevitably be removed by sub-grid-scale dissipation. That is, models that, in the inviscid limit, conserve energy but *not* enstrophy must dissipate spuriously large amounts of energy when an eddy viscosity is added to the model, as is always necessary in practice. This connection between the conservation of enstrophy (or potential enstrophy) and the dissipation of energy has been understood for at least 30 years; see, for example, Sadourny (1975). However, virtually none of the models now used to compute large-scale flow in the atmosphere or ocean conserve a form of potential enstrophy in the inviscid limit. The need for models with such a conservation property was a primary practical motivation for this work.

We stress that the method by which (1.10) is discretized—whether by finite differences, finite elements, spectral representations or any combination of these—is completely arbitrary. This gives the method great flexibility. The accuracy too is arbitrary; more accurate approximations to the integral in (1.10) correspond to more accurate discrete analogues of (1.2) and (1.3). It only matters that the discrete triple bracket retain the antisymmetry property of its continuous counterpart, and this is assured if the discretization of (1.10) maintains the antisymmetry of $J(,)$. In fact, even this trivial restriction can be avoided. Let FHZ denote a completely arbitrary discrete approximation to (1.9). In particular, FHZ need not be antisymmetric. However, the discrete bracket defined by

$$\{F, H, Z\} = \tfrac{1}{6}(FHZ + HZF + ZFH - HFZ - FZH - ZHF) \tag{1.11}$$

has the same accuracy as FHZ and is, moreover, completely antisymmetric. The 'antisymmetrization' (1.11) takes all even permutations with positive sign, and all odd permutations with negative sign, in the manner familiar from quantum mechanics.

Arakawa's (1966) second-order Jacobian corresponds to the approximation

$$\iint \mathrm{d}\boldsymbol{x}\, J\left(F_\zeta, H_\zeta\right) Z_\zeta \to \sum_{\text{gridboxes}} \frac{1}{8}\left(\frac{\partial Z}{\partial \zeta_1} + \frac{\partial Z}{\partial \zeta_2} + \frac{\partial Z}{\partial \zeta_3} + \frac{\partial Z}{\partial \zeta_4}\right) \times \left[\left(\frac{\partial F}{\partial \zeta_3} - \frac{\partial F}{\partial \zeta_1}\right)\left(\frac{\partial H}{\partial \zeta_4} - \frac{\partial H}{\partial \zeta_2}\right) - \left(\frac{\partial H}{\partial \zeta_3} - \frac{\partial H}{\partial \zeta_1}\right)\left(\frac{\partial F}{\partial \zeta_4} - \frac{\partial F}{\partial \zeta_2}\right)\right] \tag{1.12}$$

in which the sum runs over square gridboxes, and the integer subscripts refer to the corners of each gridbox, as shown in figure 1. The resulting finite-difference analogue of (1.2) is

$$\frac{\mathrm{d}\zeta_{ij}}{\mathrm{d}t} = \Delta^{-2}\{\zeta_{ij}, H, Z\}, \tag{1.13}$$

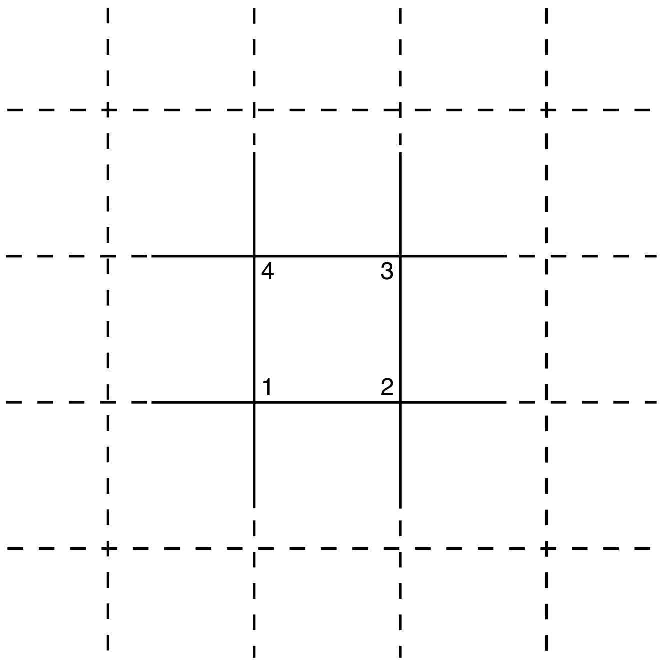

Figure 1. A single gridbox with the corners numbered as in (1.12), (2.4) and (2.5).

where ζ_{ij} is ζ at the *ij*th gridpoint, Δ is the grid spacing, $\{ , , \}$ is the discrete bracket formed from (1.10) by use of (1.12) and H and Z are arbitrary finite-difference analogues of (1.6) and (1.8). The discrete form of (1.3) is determined by the discrete form of H and by the definition

$$\psi_{ij} = -\frac{\partial H}{\partial \zeta_{ij}}. \tag{1.14}$$

The approximation (1.12) is very closely related to the method of Salmon and Talley (1989), who did not make the connection with Nambu brackets. However, it is this connection that raises the possibility that the method underlying Arakawa's Jacobian might be generalized to arbitrary fluid systems. As the preceding discussion shows, all that is really required is the exact form of a Nambu bracket corresponding to the desired dynamics. If the appropriate Nambu bracket can be found, the problem of constructing conservative numerical algorithms seems largely solved.

Nevir and Blender (1993) give a second, stunning example that greatly encourages the hope that useful Nambu brackets abound. They note that the equations for the three-dimensional incompressible flow are equivalent to

$$\frac{dF}{dt} = \{F, H, \Omega\}, \tag{1.15}$$

where

$$H[\omega] = \frac{1}{2}\iiint d\boldsymbol{x}\, \boldsymbol{u}\cdot\boldsymbol{u} \tag{1.16}$$

is the energy of the fluid with velocity $\boldsymbol{u}$ and vorticity $\boldsymbol{\omega} = \nabla \times \boldsymbol{u}$;

$$\Omega[\omega] = \frac{1}{2}\iiint d\boldsymbol{x}\, \boldsymbol{u}\cdot\boldsymbol{\omega} \tag{1.17}$$

is the helicity; and

$$\{F, H, \Omega\} = \iiint \mathrm{d}\boldsymbol{x} (\nabla \times F_\omega) \times (\nabla \times H_\omega) \cdot (\nabla \times \Omega_\omega), \tag{1.18}$$

where $F_\omega = \delta F/\delta \boldsymbol{\omega} = (\delta F/\delta\omega_x, \delta F/\delta\omega_y, \delta F/\delta\omega_z)$. The existence of the antisymmetric triple-bracket formulation (1.18) means that the same trick used to construct the Arakawa Jacobian can be extended to the three-dimensional flow. That is, by handling (1.18) in the same way as (1.9), we easily construct discrete approximations—of arbitrarily high accuracy—to the three-dimensional Euler equations that exactly conserve discrete analogues of the energy and helicity.

In this paper we show that the method based on (1.9) and (1.18) appears to be a general one. Although we offer no completely general method for obtaining Nambu brackets, we present numerous examples to support the conjecture that every Hamiltonian fluid system possessing Casimirs—that is, quantities like helicity or potential enstrophy that correspond to null vectors of the Poisson bracket—has a family of Nambu-bracket formulations in which each Casimir plays the role of the second Hamiltonian. In fact, our examples show that the Nambu-bracket formulation corresponding to a particular Casimir is not unique. Thus, it seems generally possible to find exact Nambu brackets corresponding to any Casimir whose conservation is desired. However, the step of discretizing the exact Nambu bracket frequently encounters a significant challenge: the exact Nambu bracket may contain *apparent* singularities that are cancelled by the functional derivatives of the Casimir. Unless the corresponding discrete bracket maintains an analogue of this cancellation property, the discrete dynamics will contain an unphysical singularity. We begin our series of examples.

2. Generalizations of Arakawa's Jacobian

The two-dimensional incompressible flow governed by (1.2) and (1.3) conserves every moment

$$Z_n = \frac{1}{(2+n)} \iint \mathrm{d}\boldsymbol{x}\, \zeta^{2+n} \tag{2.1}$$

of the vorticity ζ. The enstrophy (1.8) corresponds to $n = 0$. The two-dimensional Euler dynamics (1.2) and (1.3) is equivalent to

$$\frac{\mathrm{d}F}{\mathrm{d}t} = \{F, H, Z_n\}_n, \tag{2.2}$$

where

$$\{F, H, Z_n\}_n \equiv \frac{1}{(3+2n)} \iint \mathrm{d}\boldsymbol{x}\, \zeta^{-n} [J(F_\zeta, H_\zeta)(Z_n)_\zeta + \mathrm{cyc}(F, H, Z_n)]. \tag{2.3}$$

When $n = 0$ (2.3) reduces to (1.9). However, the more general formulation (2.2) and (2.3) allows us to construct numerical analogues of (1.2) and (1.3) that exactly conserve analogues of the energy (1.6) and any single moment of the vorticity. As an example, we generalize Arakawa's (1966) classic algorithm.

The Arakawa algorithm corresponding to (1.7), (1.10) and (1.12) is

$$\frac{\mathrm{d}F}{\mathrm{d}t} = \frac{1}{12\Delta^2} \sum_{\text{gridboxes}} \left[\frac{\partial(F, H, Z)}{\partial(\zeta_1, \zeta_2, \zeta_3)} + \frac{\partial(F, H, Z)}{\partial(\zeta_1, \zeta_2, \zeta_4)} + \frac{\partial(F, H, Z)}{\partial(\zeta_1, \zeta_3, \zeta_4)} + \frac{\partial(F, H, Z)}{\partial(\zeta_2, \zeta_3, \zeta_4)} \right], \tag{2.4}$$

where Δ is the grid spacing, and the subscripts refer to the local numbering system in figure 1. Setting $F = \zeta_{ij}$ in (2.4), where ζ_{ij} is the vorticity at gridpoint ij, we obtain Arakawa's evolution equation for vorticity. However, the form (2.4) displays the conservation properties at a glance.

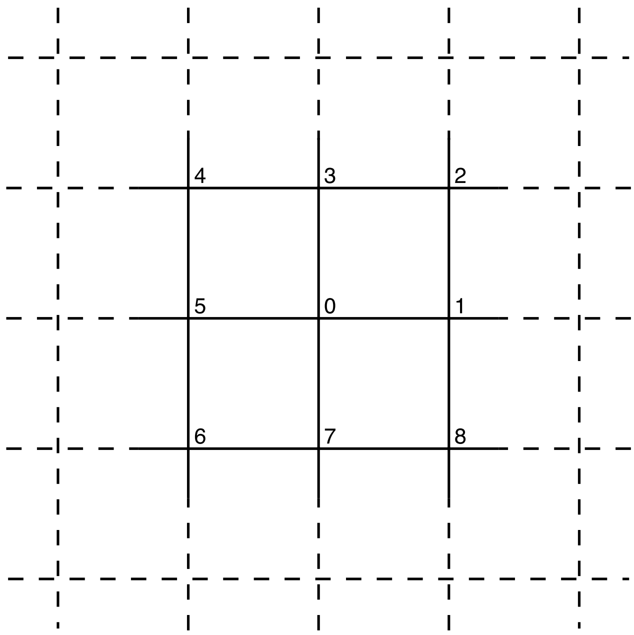

Figure 2. Four neighbouring gridboxes with the corners numbered as in (2.6).

To obtain a numerical algorithm that conserves energy and Z_n, we use (2.3) instead of (1.9), obtaining the generalization

$$\frac{\mathrm{d}F}{\mathrm{d}t} = \frac{1}{4(3+2n)\Delta^2} \times \sum_{\text{gridboxes}} \zeta_{1234}^{-n} \left[\frac{\partial(F,H,Z_n)}{\partial(\zeta_1,\zeta_2,\zeta_3)} + \frac{\partial(F,H,Z_n)}{\partial(\zeta_1,\zeta_2,\zeta_4)} + \frac{\partial(F,H,Z_n)}{\partial(\zeta_1,\zeta_3,\zeta_4)} + \frac{\partial(F,H,Z_n)}{\partial(\zeta_2,\zeta_3,\zeta_4)} \right] \tag{2.5}$$

of (2.4), where ζ_{1234}^{-n} is an arbitrary approximation to ζ^{-n} on the gridbox with corners numbered $1, 2, 3, 4$. Once again, the conservation properties are manifest in the form (2.5). Let the gridpoint corresponding to *ij* be labelled 0; then the contributions to the rhs of (2.5) arise from the surrounding four gridboxes as shown in figure 2. Setting $F = \zeta_0$ and carrying out the sum in (2.5), we obtain the discrete vorticity equation

$$\begin{aligned} 4(3+2n)\Delta^2 \frac{\mathrm{d}\zeta_0}{\mathrm{d}t} = {} & \zeta_{0123}^{-n} \left[\frac{\partial(H,Z_n)}{\partial(\zeta_1,\zeta_2)} + \frac{\partial(H,Z_n)}{\partial(\zeta_1,\zeta_3)} + \frac{\partial(H,Z_n)}{\partial(\zeta_2,\zeta_3)} \right] \\ & + \zeta_{0345}^{-n} \left[\frac{\partial(H,Z_n)}{\partial(\zeta_3,\zeta_4)} + \frac{\partial(H,Z_n)}{\partial(\zeta_3,\zeta_5)} + \frac{\partial(H,Z_n)}{\partial(\zeta_4,\zeta_5)} \right] \\ & + \zeta_{0567}^{-n} \left[\frac{\partial(H,Z_n)}{\partial(\zeta_5,\zeta_6)} + \frac{\partial(H,Z_n)}{\partial(\zeta_5,\zeta_7)} + \frac{\partial(H,Z_n)}{\partial(\zeta_6,\zeta_7)} \right] \\ & + \zeta_{0781}^{-n} \left[\frac{\partial(H,Z_n)}{\partial(\zeta_7,\zeta_8)} + \frac{\partial(H,Z_n)}{\partial(\zeta_7,\zeta_1)} + \frac{\partial(H,Z_n)}{\partial(\zeta_8,\zeta_1)} \right], \end{aligned} \tag{2.6}$$

where the subscripts correspond to figure 2. The four terms on the rhs of (2.6) correspond to the contributions of the four gridboxes surrounding gridpoint 0 in figure 2. Only H, Z_n and ζ_{abcd}^{-n}, as functions of the gridpoint values of vorticity, remain to be defined.

We are primarily interested in cases in which n is a positive integer[1]. For such cases the terms ζ_{abcd}^{-n} represent apparent singularities in (2.6). In the exact bracket (2.3), these singularities are cancelled by the functional derivative Z_ζ. In the discrete case, the terms ζ_{abcd}^{-n} must be carefully chosen to ensure the cancellation. Suppose that

$$Z_n = \frac{1}{(2+n)} \sum_{ij} \zeta_{ij}^{2+n}. \tag{2.7}$$

Then $\partial Z_n / \partial \zeta_{ij} = \zeta_{ij}^{1+n}$, and, defining

$$\psi_{ij} = -\frac{\partial H}{\partial \zeta_{ij}}, \tag{2.8}$$

we find that the first term on the rhs of (2.6) takes the form

$$\zeta_{0123}^{-n}[(\psi_2+\psi_3)\zeta_1^{1+n} + (\psi_3-\psi_1)\zeta_2^{1+n} - (\psi_1+\psi_2)\zeta_3^{1+n}]. \tag{2.9}$$

If n is a positive *even* integer, then the choice

$$\zeta_{0123}^{-n} = \frac{4}{(\zeta_0^n+\zeta_1^n+\zeta_2^n+\zeta_3^n)} \tag{2.10}$$

avoids the singularity, because (2.10) blows up only if all of $\zeta_0, \zeta_1, \zeta_2, \zeta_3$ vanish, in which case the square-bracket term in (2.9) also vanishes. If n is a positive *odd* integer, we let $n = m - 1$; then the choice

$$\zeta_{0123}^{-n} = \frac{(\zeta_0+\zeta_1+\zeta_2+\zeta_3)}{(\zeta_0^m+\zeta_1^m+\zeta_2^m+\zeta_3^m)} \tag{2.11}$$

yields a well-behaved result. We encounter the problem of apparent singularities again in the next section, but there the problem is more serious because the singularities involve the derivatives of the dependent variables.

3. Shallow-water equations

The shallow-water equations may be written in the form

$$\frac{\partial u}{\partial t} = qhv - \Phi_x, \qquad \frac{\partial v}{\partial t} = -qhu - \Phi_y, \qquad \frac{\partial h}{\partial t} = -(hu)_x - (hv)_y, \tag{3.1}$$

where $q = (v_x - u_y)/h$ is the potential vorticity, and $\Phi = \frac{1}{2}u^2 + \frac{1}{2}v^2 + gh$. The dynamics (3.1) takes the Hamiltonian form (1.1) with

$$\{F, H\} = \iint \mathrm{d}\boldsymbol{x}(q(F_u H_v - H_u F_v) - F_{\boldsymbol{u}} \cdot \nabla H_h + H_{\boldsymbol{u}} \cdot \nabla F_h) \tag{3.2}$$

and

$$H[u, v, h] = \frac{1}{2} \iint \mathrm{d}\boldsymbol{x}(hu^2 + hv^2 + gh^2). \tag{3.3}$$

In (3.2), $F_u = \delta F/\delta u$ and $F_{\boldsymbol{u}} = \delta F/\delta \boldsymbol{u} = (F_u, F_v)$. For present purposes, it seems advantageous to abandon (u, v, h) in favour of the new dependent variables (ζ, μ, h), where

$$\zeta = v_x - u_y \tag{3.4}$$

is the relative vorticity, and

$$\mu = u_x + v_y \tag{3.5}$$

[1] Negative and fractional powers of ζ correspond to pathological integrals of the form (2.1) if the vorticity vanishes over a finite area. The case $n = -1$ is uninteresting because Z_{-1} is conserved by the dynamics corresponding to $n = 0$, namely (2.4).

is the divergence. Invoking the chain rule for functional derivatives, we have

$$\begin{aligned} F_u &= \partial_y F_\zeta - \partial_x F_\mu, \\ F_v &= -\partial_x F_\zeta - \partial_y F_\mu, \\ F_h &= F_h, \end{aligned} \tag{3.6}$$

where $F[u, v, h] = F[\zeta, \mu, h]$ is an arbitrary functional. Then substituting (3.6) into (3.2) we obtain the shallow-water Poisson bracket in the form

$$\{F, H\} = \{F, H\}_{\mu\mu} + \{F, H\}_{\zeta\zeta} + \{F, H\}_{\zeta\mu h}, \tag{3.7}$$

where

$$\{F, H\}_{\mu\mu} = \iint \mathrm{d}\boldsymbol{x}\, q J(F_\mu, H_\mu), \tag{3.8}$$

$$\{F, H\}_{\zeta\zeta} = \iint \mathrm{d}\boldsymbol{x}\, q J(F_\zeta, H_\zeta) \tag{3.9}$$

and

$$\{F, H\}_{\zeta\mu h} = \iint \mathrm{d}\boldsymbol{x}\, (q(\nabla F_\mu \cdot \nabla H_\zeta - \nabla H_\mu \cdot \nabla F_\zeta) + (\nabla F_\mu \cdot \nabla H_h - \nabla H_\mu \cdot \nabla F_h)). \tag{3.10}$$

To close the dynamics based on (3.7)–(3.10), we must express the Hamiltonian (3.3) as a functional, $H[\zeta, \mu, h]$, of the new variables. This requires the definitions (3.4) and (3.5), and the use of the periodic boundary conditions.

Each of the three brackets (3.8)–(3.10) is antisymmetric in its two arguments, and each bracket has the same general Casimir functional

$$\iint \mathrm{d}\boldsymbol{x}\, hG(q) \tag{3.11}$$

as (3.2), where $G(q)$ is an arbitrary function. Once again, we are primarily interested in the moments

$$Z_n = \frac{1}{(2+n)} \iint \mathrm{d}\boldsymbol{x}\, hq^{2+n} = \frac{1}{(2+n)} \iint \mathrm{d}\boldsymbol{x} \frac{\zeta^{2+n}}{h^{1+n}}. \tag{3.12}$$

As in section 2, potential enstrophy corresponds to the case $n = 0$. Each of (3.8)–(3.10) vanishes when F or H is replaced by Z_n. For (3.8) this is trivial, because $(Z_n)_\mu = 0$. For (3.9) it follows from the property

$$(Z_n)_\zeta = q^{1+n} \tag{3.13}$$

in exactly the same way as for the two-dimensional incompressible flow. For (3.10) it follows from (3.13) and

$$(Z_n)_h = -\frac{(1+n)}{(2+n)} q^{2+n}. \tag{3.14}$$

We seek a discrete analogue of the shallow-water equations that conserves discrete analogues of H and Z_n. First we note that *any* discretization of the $\mu\mu$-bracket (3.8) conserves H and Z_n provided that the discrete analogue of Z_n does not depend on μ. We choose

$$Z_n = \frac{1}{(2+n)} \sum_{ij} h_{ij} q_{ij}^{2+n} = \frac{1}{(2+n)} \sum_{ij} \frac{\zeta_{ij}^{2+n}}{h_{ij}^{1+n}}, \tag{3.15}$$

where $h_{ij}, q_{ij}, \zeta_{ij}$ denote the values at gridpoint *ij*.

Next, the $\zeta\zeta$-bracket (3.9) may be written in a form

$$\{F, H\}_{\zeta\zeta} = \{F, H, Z_n\}_{\zeta\zeta\zeta} = \frac{1}{(3+2n)} \iint \mathrm{d}\boldsymbol{x}\, q^{-n}[J(F_\zeta, H_\zeta)(Z_n)_\zeta + \mathrm{cyc}(F, H, Z_n)] \tag{3.16}$$

that is virtually identical to the Nambu bracket (2.3) for the two-dimensional Euler flow; the q^{-n} in (3.16) replaces ζ^{-n} in (2.3). To obtain a conservative dynamics that avoids the apparent singularity in (3.16), we proceed as in section 2, obtaining a formula analogous to (2.6) but with q replacing ζ in (2.10) or (2.11).

Only (3.10) remains to be considered. The $\zeta\mu h$-bracket (3.10) takes the Nambu form

$$\begin{aligned}\{F,H\}_{\zeta\mu h} &= \{F,H,Z_n\}_{\zeta\mu h}\\ &= -\iint \mathrm{d}\boldsymbol{x}\frac{q^{-n}}{(1+n)q_x}[(\partial_x F_\mu\partial_x H_\zeta - \partial_x H_\mu\partial_x F_\zeta)\partial_x(Z_n)_h + \mathrm{cyc}(F,H,Z_n)]\\ &\quad -\iint \mathrm{d}\boldsymbol{x}\frac{q^{-n}}{(1+n)q_y}[(\partial_y F_\mu\partial_y H_\zeta - \partial_y H_\mu\partial_y F_\zeta)\partial_y(Z_n)_h + \mathrm{cyc}(F,H,Z_n)].\end{aligned} \tag{3.17}$$

Note that each of the two integrals in (3.17) involves derivatives in only one direction. This greatly simplifies the problem of finding discretizations that avoid the apparent singularities in (3.17). For example, the finite-difference approximation

$$\begin{aligned}&\frac{1}{(2\Delta)^2}\frac{1}{(1+n)}\sum_i \frac{1}{q_{i-1}-q_{i+1}}\frac{2}{(q_{i-1}^n+q_{i+1}^n)}\left[\left(\frac{\partial F}{\partial\mu_{i+1}}-\frac{\partial F}{\partial\mu_{i-1}}\right)\left(\frac{\partial H}{\partial\zeta_{i+1}}-\frac{\partial H}{\partial\zeta_{i-1}}\right)\right.\\ &\qquad\left.-\left(\frac{\partial H}{\partial\mu_{i+1}}-\frac{\partial H}{\partial\mu_{i-1}}\right)\left(\frac{\partial F}{\partial\zeta_{i+1}}-\frac{\partial F}{\partial\zeta_{i-1}}\right)\right]\left(\frac{\partial Z_n}{\partial h_{i+1}}-\frac{\partial Z_n}{\partial h_{i-1}}\right)+\mathrm{cyc}(F,H,Z_n)\end{aligned} \tag{3.18}$$

applied to each of the integrals in (3.17) yields a finite-difference approximation to (3.10) that is free of singularities after substitution of (3.15). Suppose, for example, that $n = 2$. Then substituting (3.15) into (3.18), and making use of

$$q_{i+1}^4 - q_{i-1}^4 = (q_{i+1}-q_{i-1})(q_{i+1}+q_{i-1})(q_{i+1}^2+q_{i-1}^2) \tag{3.19}$$

and

$$q_{i+1}^3 - q_{i-1}^3 = (q_{i+1}-q_{i-1})(q_{i+1}^2+q_{i+1}q_{i-1}+q_{i-1}^2) \tag{3.20}$$

we obtain the finite-difference approximation

$$\begin{aligned}&\frac{1}{(2\Delta)^2}\sum_i\left\{\frac{1}{2}(q_{i-1}+q_{i+1})\left[\left(\frac{\partial F}{\partial\mu_{i+1}}-\frac{\partial F}{\partial\mu_{i-1}}\right)\left(\frac{\partial H}{\partial\zeta_{i+1}}-\frac{\partial H}{\partial\zeta_{i-1}}\right)\right.\right.\\ &\qquad\left.-\left(\frac{\partial H}{\partial\mu_{i+1}}-\frac{\partial H}{\partial\mu_{i-1}}\right)\left(\frac{\partial F}{\partial\zeta_{i+1}}-\frac{\partial F}{\partial\zeta_{i-1}}\right)\right]\\ &\qquad+\frac{2}{3}\frac{(q_{i-1}^2+q_{i-1}q_{i+1}+q_{i+1}^2)}{(q_{i-1}^2+q_{i+1}^2)}\left[\left(\frac{\partial F}{\partial\mu_{i+1}}-\frac{\partial F}{\partial\mu_{i-1}}\right)\left(\frac{\partial H}{\partial h_{i+1}}-\frac{\partial H}{\partial h_{i-1}}\right)\right.\\ &\qquad\left.\left.-\left(\frac{\partial H}{\partial\mu_{i+1}}-\frac{\partial H}{\partial\mu_{i-1}}\right)\left(\frac{\partial F}{\partial h_{i+1}}-\frac{\partial F}{\partial h_{i-1}}\right)\right]\right\}\end{aligned} \tag{3.21}$$

to (3.10) (in each direction). The approximation (3.21) conserves energy by its manifest antisymmetry with respect to F and H. It conserves Z_2, the fourth moment of potential vorticity, by the fact that (3.21) vanishes when either F or H is replaced by Z_2. This latter property is not immediately obvious from the form of (3.21), but it is manifest from (3.18), which is antisymmetric with respect to F, H and Z_2. These results easily extend to arbitrary n by the generalization

$$\begin{aligned}q_{i+1}^n - q_{i-1}^n &= (q_{i+1}-q_{i-1})(q_{i+1}+q_{i-1})(q_{i+1}^{n/2-1}+q_{i+1}^{n/2-2}q_{i-1}+q_{i+1}^{n/2-3}q_{i-1}^2+q_{i+1}^{n/2-4}q_{i-1}^3+\cdots)\\ &\quad\times(q_{i+1}^{n/2-1}-q_{i+1}^{n/2-2}q_{i-1}+q_{i+1}^{n/2-3}q_{i-1}^2-q_{i+1}^{n/2-4}q_{i-1}^3+\cdots)\end{aligned} \tag{3.22}$$

of (3.19) and by the corresponding generalization of (3.20).

The complete Nambu bracket for shallow-water dynamics comprises the triple brackets (3.16) and (3.17) corresponding to (3.9) and (3.10), respectively, plus a third triple bracket corresponding to (3.8). Since Z_n does not depend on the divergence μ, the latter may be taken as

$$\{F, H, Z_n\}_{\mu\mu\zeta} = \iint \mathrm{d}\boldsymbol{x}\, q\, J(F_\mu, H_\mu)\, q^{-1-n} (Z_n)_\zeta + \mathrm{cyc}(F, H, Z_n). \tag{3.23}$$

Recall (3.13). However, one could take instead

$$\{F, H, Z_n\}_{\mu\mu\zeta} = \iint \mathrm{d}\boldsymbol{x}\, q\, J(F_\mu, H_\mu) \partial_x (Z_n)_\zeta ((1+n) q^n q_x)^{-1} + \mathrm{cyc}(F, H, Z_n) \tag{3.24}$$

as one of the many alternatives. This example demonstrates, in an admittedly trivial way, the general non-uniqueness of Nambu brackets. That is, although the Poisson bracket is unique up to a transformation of the variables, each Poisson bracket corresponds to an infinite number of *distinct* Nambu brackets. (Although the brackets (3.23) and (3.24) yield the same Poisson bracket upon substitution of (3.13), they are distinct in the sense that they yield non-identical values upon substitution of three *arbitrary* functional arguments.) This non-uniqueness extends, not surprisingly, to the discrete case as well; discrete Poisson brackets generally correspond to more than one distinct, discrete Nambu bracket. The non-uniqueness of Nambu brackets adds scope, but also complexity, to the search for conservative numerical schemes.

Once again, the Nambu-bracket formulation based on (3.8)–(3.10) requires the functional derivatives of H with respect to the variables ζ, μ and h. However, H is most naturally expressed in the form (3.3) as a functional of u, v and h. The functional derivative H_h is the same in both systems because holding (u, v) fixed is the same as holding (ζ, μ) fixed. To compute H_ζ and H_μ, we set $h\boldsymbol{u} = (-\chi_y + \gamma_x, +\chi_x + \gamma_y)$. Then $H_\zeta = -\chi$ and $H_\mu = -\gamma$. The fields χ and γ can be determined from ζ, μ, h by solving

$$\nabla \cdot (h^{-1} \nabla \chi) + J(h^{-1}, \gamma) = \zeta, \tag{3.25a}$$

$$\nabla \cdot (h^{-1} \nabla \gamma) + J(\chi, h^{-1}) = \mu. \tag{3.25b}$$

The precise manner in which this process is discretized does not affect the conservation properties of the resulting algorithm. The conservation properties depend only on the antisymmetry property of the Nambu bracket.

Of course, it is distasteful to pose shallow-water dynamics in a form that requires the solution of elliptic equations because the basic equations (3.1) are entirely prognostic. Moreover, Arakawa and Lamb (1981)—hereafter AL—discovered a finite-difference analogue of (3.1) that conserves discrete analogues of the energy and potential enstrophy. Salmon (2004)—hereafter S04—showed that the AL algorithm corresponds to the discrete Poisson bracket

$$\begin{aligned}
\{F, H\} = \sum_{ij} & \frac{1}{24}(q_{i-1,j-1} + 2q_{i-1,j+1} + 2q_{i+1,j-1} + q_{i+1,j+1}) \frac{\partial(F, H)}{\partial(u_{i-1,j}, v_{i,j-1})} \\
& + \frac{1}{24}(2q_{i-1,j-1} + q_{i-1,j+1} + q_{i+1,j-1} + 2q_{i+1,j+1}) \frac{\partial(F, H)}{\partial(u_{i+1,j}, v_{i,j-1})} \\
& + \frac{1}{24}(2q_{i-1,j-1} + q_{i-1,j+1} + q_{i+1,j-1} + 2q_{i+1,j+1}) \frac{\partial(F, H)}{\partial(u_{i-1,j}, v_{i,j+1})} \\
& + \frac{1}{24}(q_{i-1,j-1} + 2q_{i-1,j+1} + 2q_{i+1,j-1} + q_{i+1,j+1}) \frac{\partial(F, H)}{\partial(u_{i+1,j}, v_{i,j+1})} \\
& + \frac{1}{24}(q_{i-1,j-1} - q_{i-1,j+1} + q_{i+1,j-1} - q_{i+1,j+1}) \frac{\partial(F, H)}{\partial(u_{i-1,j}, u_{i+1,j})}
\end{aligned}$$

$$+\frac{1}{24}(-q_{i-1,j-1}-q_{i-1,j+1}+q_{i+1,j-1}+q_{i+1,j+1})\frac{\partial(F,H)}{\partial(v_{i,j-1},v_{i,j+1})}$$
$$+\frac{1}{2\Delta}\left(\frac{\partial(F,H)}{\partial(h_{ij},u_{i-1,j})}-\frac{\partial(F,H)}{\partial(h_{ij},u_{i+1,j})}+\frac{\partial(F,H)}{\partial(h_{ij},v_{i,j-1})}-\frac{\partial(F,H)}{\partial(h_{ij},v_{i,j+1})}\right) \quad (3.26)$$

and that (3.26) is the simplest member of a large family of discrete Poisson brackets that conserve arbitrary energy H and potential enstrophy in the form

$$Z=\frac{1}{2}\sum_{ij}\frac{1}{4}(h_{i+1,j+1}+h_{i+1,j-1}+h_{i-1,j+1}+h_{i-1,j-1})\,q_{ij}^2, \quad (3.27)$$

where

$$q_{ij}\equiv\frac{(v_{i+1,j}-v_{i-1,j}+u_{i,j-1}-u_{i,j+1})/2\Delta}{\frac{1}{4}(h_{i+1,j+1}+h_{i+1,j-1}+h_{i-1,j+1}+h_{i-1,j-1})}. \quad (3.28)$$

The AL bracket (3.26) vanishes when either F or H is replaced by (3.27).

The basic shallow-water dynamics (3.1) has the exact Nambu-bracket formulation

$$\{F,H,Z\}=\iint \mathrm{d}\mathbf{x}\left\{\frac{\delta(F,H)}{\delta(u,v)}\left[-\frac{1}{2q_x}\partial_x Z_h-\frac{1}{2q_y}\partial_y Z_h\right]-\frac{1}{3q^2}J\left(\frac{q^{3/2}}{q_y}F_u,\frac{q^{3/2}}{q_y}H_u\right)Z_h\right.$$
$$\left.-\frac{1}{3q^2}J\left(\frac{q^{3/2}}{q_x}F_v,\frac{q^{3/2}}{q_x}H_v\right)Z_h+\mathrm{cyc}(F,H,Z)\right\}, \quad (3.29)$$

where $Z = Z_0$ is the potential enstrophy, and all the functional derivatives are taken with respect to the basic variables u, v and h. The fractional powers in (3.29) disappear upon expansion of the terms. The Nambu bracket (3.29) is not unique, and in fact is not equivalent to the Nambu bracket constructed from (3.7). This is obvious from the fact that every triplet in (3.29) involves one functional derivative with respect to h, whereas (3.16) and (3.23) contain no h-derivatives. The bracket (3.29) can be generalized to arbitrary moments Z_n of the potential enstrophy, and in fact all the exact Nambu brackets presented here can be further generalized to cover the general shallow-water Casimir (3.11). However, the discrete form (3.29) seems very closely related to the AL bracket (3.26), and the conjecture is offered that a finite-difference approximation to (3.29) yields (3.26) after substitution of (3.27). This conjecture has been proved for the case of one space dimension, but, despite very persistent effort, no two-dimensional discretization of (3.29) corresponding to (3.26) has been found. More generally, it seems very difficult to defeat the problem of apparent singularities that arises in the discretization of (3.29). Thus, despite the examples provided by AL and S04, and despite the burden of solving elliptic problems, the Nambu formulation in terms of ζ, μ and h seems to be the most convenient vehicle for constructing conservative shallow-water algorithms. The analogous statement seems especially true of the primitive equations, where elliptic problems are anyway unavoidable.

4. Primitive equations

The shallow-water equations are closely analogous to the hydrostatic primitive equations in isentropic coordinates; see, for example, Salmon (1998, pp 105–7). Because of this analogy, all the results of the preceding section apply at once to the hydrostatic primitive equations, provided that one is willing to accommodate the outcrop of isentropes at boundaries by a device related to the concept of ‘massless layers’. See, for example, Hsu and Arakawa (1990).

In this section we consider the *non-hydrostatic* primitive equations in the form

$$\frac{D\boldsymbol{v}}{Dt} = -\nabla\phi + \theta\boldsymbol{k}, \tag{4.1a}$$

$$\nabla\cdot\boldsymbol{v} = 0, \tag{4.1b}$$

$$\frac{D\theta}{Dt} = 0, \tag{4.1c}$$

where $\boldsymbol{v} = (u, v, w)$ is the three-dimensional velocity, θ is the buoyancy and all variables are considered functions of (x, y, z). The dynamics (4.1) is equivalent to

$$\frac{D\boldsymbol{\omega}}{Dt} = \boldsymbol{\omega}\cdot\nabla\boldsymbol{v} + (\theta_y, -\theta_x, 0), \tag{4.2a}$$

$$\frac{D\theta}{Dt} = 0 \tag{4.2b}$$

with

$$\boldsymbol{\omega} = \nabla\times\boldsymbol{v} \tag{4.3}$$

and $\boldsymbol{v}$ determined from $\boldsymbol{\omega}$ by (4.3), (4.1*b*) and the periodic boundary conditions; see, for example, Batchelor (1970, pp 84–7). The dynamics (4.2) takes the Hamiltonian form (1.1) with

$$\{F, H\} = \iiint \mathrm{d}\boldsymbol{x}\{\boldsymbol{\omega}\cdot[(\nabla\times F_{\boldsymbol{\omega}})\times(\nabla\times H_{\boldsymbol{\omega}})] + \nabla\theta\cdot[(\nabla\times F_{\boldsymbol{\omega}})H_\theta - (\nabla\times H_{\boldsymbol{\omega}})F_\theta]\} \tag{4.4}$$

and

$$H = \iiint \mathrm{d}\boldsymbol{x}\left(\frac{1}{2}\boldsymbol{v}\cdot\boldsymbol{v} - z\theta\right). \tag{4.5}$$

As in section 2, the connection between $\boldsymbol{v}$ and $\boldsymbol{\omega}$ is required only to compute the functional derivatives of H. The conservation laws depend only on the Poisson bracket (4.4), which has the general Casimir

$$Z_G = \iiint \mathrm{d}\boldsymbol{x}\, G(q, \theta), \tag{4.6}$$

where $q = \boldsymbol{\omega}\cdot\nabla\theta$ is the potential vorticity and G is an arbitrary function of two variables.

We seek a Nambu bracket corresponding to (4.4) that will serve as the basis for an energy- and potential-enstrophy-conserving model of the non-hydrostatic primitive equations. Following the same general strategy as in section 2, we switch from $\boldsymbol{\omega}$ and θ to new variables q, θ, and

$$\boldsymbol{s} = \boldsymbol{\omega}\times\nabla\theta. \tag{4.7}$$

We note that $\boldsymbol{s}$ has no component in the direction of $\nabla\theta$, and that the mapping from $(\boldsymbol{\omega}, \theta)$ to $(q, \theta, \boldsymbol{s})$ is one-to-one. By the chain rule for functional derivatives, we have

$$F_{\boldsymbol{\omega}} = F_q\nabla\theta + \nabla\theta\times F_{\boldsymbol{s}} \tag{4.8}$$

and

$$F_\theta|_{\boldsymbol{\omega}} = F_\theta|_{\boldsymbol{s},q} - \boldsymbol{\omega}\cdot\nabla F_q + \nabla\cdot(\boldsymbol{\omega}\times F_{\boldsymbol{s}}). \tag{4.9}$$

Substituting (4.8) and (4.9) into (4.4), invoking vector identities and making use of the periodic boundary conditions, we obtain the Poisson bracket in the form

$$\{F, H\} = \{F, H\}_{qq} + \{F, H\}_{qs} + \{F, H\}_{\theta s} + \{F, H\}_{ss}, \tag{4.10}$$

where

$$\{F, H\}_{qq} = -\iiint \mathrm{d}\boldsymbol{x}\, \theta(\nabla F_q \times \nabla H_q)\cdot\nabla q, \tag{4.11}$$

$$\{F, H\}_{qs} = \iiint \mathrm{d}\boldsymbol{x}[(\nabla q \times \nabla F_q)\cdot(\nabla\theta \times \boldsymbol{H_s}) - (\nabla q \times \nabla H_q)\cdot(\nabla\theta \times \boldsymbol{F_s})], \tag{4.12}$$

$$\{F, H\}_{\theta s} = \iiint \mathrm{d}\boldsymbol{x}[(\nabla\theta \times \nabla F_\theta)\cdot(\nabla\theta \times \boldsymbol{H_s}) - (\nabla\theta \times \nabla H_\theta)\cdot(\nabla\theta \times \boldsymbol{F_s})] \tag{4.13}$$

and

$$\{F, H\}_{\boldsymbol{ss}} = \iiint \mathrm{d}\boldsymbol{x}\,[\boldsymbol{\omega}\cdot(\nabla\times(\nabla\theta\times\boldsymbol{F_s}))\times(\nabla\times(\nabla\theta\times\boldsymbol{H_s})) + \nabla\theta\cdot(\nabla\times(\nabla\theta\times\boldsymbol{F_s}))\nabla\cdot(\boldsymbol{\omega}\times\boldsymbol{H_s}) - \nabla\theta\cdot(\nabla\times(\nabla\theta\times\boldsymbol{H_s}))\nabla\cdot(\boldsymbol{\omega}\times\boldsymbol{F_s})]. \tag{4.14}$$

As in previous sections, we focus on the moments

$$Z_n = \frac{1}{2+n}\iiint \mathrm{d}\boldsymbol{x}\, q^{2+n}. \tag{4.15}$$

Once again, potential enstrophy corresponds to $n = 0$. Since Z_n depends only on q, it follows that $\{F, Z_n\}_{\boldsymbol{ss}} = \{F, Z_n\}_{\theta s} = 0$ for arbitrary F. Thus (4.13) and (4.14) are analogous to (3.8); arbitrary discretizations of (4.13) and (4.14) conserve arbitrary discrete H and

$$Z_n = \frac{1}{2+n}\sum_{ij} q_{ij}^{2+n}. \tag{4.16}$$

To maintain the properties $\{F, Z_n\}_{qq} = \{F, Z_n\}_{qs} = 0$ for arbitrary F, we express (4.11) and (4.12) as Nambu brackets. We find that

$$\{F, H\}_{qq} = \{F, H, Z_n\}_{qqq} \equiv -\iiint \mathrm{d}\boldsymbol{x}\frac{\theta}{(1+n)q^n}(\nabla F_q \times \nabla H_q)\cdot\nabla(Z_n)_q \tag{4.17}$$

and

$$\{F, H\}_{qs} = \{F, H, Z_n\}_{qqs} \equiv \iiint \mathrm{d}\boldsymbol{x}[(\nabla q \times \nabla F_q)\cdot(\nabla\theta\times\boldsymbol{H_s}) - (\nabla q \times \nabla H_q)\cdot(\nabla\theta\times\boldsymbol{F_s})]\frac{(Z_n)_q}{q^{1+n}} + \mathrm{cyc}(F, H, Z_n). \tag{4.18}$$

Discretizations that maintain the antisymmetry properties of (4.17) and (4.18) automatically conserve discrete analogues of H and Z_n. Both (4.17) and (4.18) contain apparent singularities at $q = 0$. However, these apparent singularities are very mild and are easily handled by the methods in sections 2 and 3.

Besides Z_n, we may wish to conserve an additional Casimir of the form

$$R = \iiint \mathrm{d}\boldsymbol{x}\, W(\theta). \tag{4.19}$$

Since $R_s = R_q = 0$, R is also a Casimir of (4.17), (4.18) and (4.14). R is a Casimir of (4.13) because $\nabla\theta \times \nabla R_\theta = 0$. Noting that

$$\{F, H\}_{\theta s} = \{F, H, R\}_{\theta\theta s} \equiv \iiint \mathrm{d}\boldsymbol{x}[(\nabla\theta\times\nabla F_\theta)\cdot(\nabla\theta\times\boldsymbol{H_s}) - (\nabla\theta\times\nabla H_\theta)\cdot(\nabla\theta\times\boldsymbol{F_s})]\frac{R_\theta}{W'(\theta)} + \mathrm{cyc}(F, H, R) \tag{4.20}$$

we pose the primitive-equation dynamics in the form

$$\frac{\mathrm{d}F}{\mathrm{d}t} = \{F, H, Z_n\}_{qqq} + \{F, H, Z_n\}_{qqs} + \{F, H, R\}_{\theta\theta s} + \{F, H\}_{ss}, \tag{4.21}$$

where the three triple brackets are defined by (4.17)–(4.19), and the double bracket may be written as a triple bracket in an infinite number of ways, because neither Z_n nor R depends on $\boldsymbol{s}$. By maintaining the antisymmetry properties of all the brackets in (4.21)—a very easy task—we construct numerical models of the primitive equations that automatically conserve Z_n and R. The rhs of (4.21) is *not*, strictly speaking, a Nambu bracket, because it involves the two *distinct* triplets (F, H, Z_n) and (F, H, R). In important work, Nevir (1998) gives many more examples of such 'generalized' Nambu brackets.

5. Discussion

Although no general proof has been found, the foregoing examples strongly suggest that any Hamiltonian system with Casimirs can be written in a Nambu-bracket form in which an arbitrary Casimir plays the role of the 'second Hamiltonian', and, moreover, that the Nambu bracket is not unique. Many more examples could be given. For instance, a Nambu bracket for general (compressible) homentropic flow—the most general case for which helicity is conserved—is given by

$$\{F, H, \Omega\} = \iiint \mathrm{d}\boldsymbol{x}[\rho^{-1}(F_{\boldsymbol{v}} \times H_{\boldsymbol{v}}) \cdot \Omega_{\boldsymbol{v}} - (\boldsymbol{\alpha} \cdot \boldsymbol{\omega})^{-1}(F_\rho \nabla \cdot H_{\boldsymbol{v}} - H_\rho \nabla \cdot F_{\boldsymbol{v}})\boldsymbol{\alpha} \cdot \boldsymbol{\Omega}_{\boldsymbol{v}} + \mathrm{cyc}(F, H, \Omega)], \tag{5.1}$$

where

$$H = \frac{1}{2} \iiint \mathrm{d}\boldsymbol{x}\, \rho \boldsymbol{v} \cdot \boldsymbol{v} \tag{5.2}$$

is the energy, Ω is the helicity (1.17) and $\boldsymbol{\alpha}$ is an arbitrary vector. Natural choices are $\boldsymbol{\alpha} = \boldsymbol{\omega}$ and $\boldsymbol{\alpha} = \boldsymbol{v}$.

The manifest antisymmetry of Nambu brackets makes it easy, in principle, to construct numerical algorithms that exactly conserve discrete analogues of the energy and Casimir; one need only preserve the antisymmetry property of the exact bracket. In practice, apparent singularities like those encountered in sections 2 and 3 may pose a significant challenge, but here again the examples offer encouragement. Although I have not yet found a singularity-free, discrete analogue of (3.29), the discrete Poisson brackets discovered by AL and S04 suggest that one exists, whereas the alternative formulations (3.16) and (3.17) show that it is also unnecessary.

Poisson brackets obey the Jacobi identity

$$\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0 \tag{5.3}$$

for any three functionals A, B, C, so it is natural to ask whether Nambu brackets obey an identity analogous to (5.3). Takhtajan (1994) proposes a generalized Jacobi identity which implies that arbitrary contractions of the Nambu bracket obey (5.3). However, the contraction of (1.9) with H yields

$$\{F, Z\} = \iint \mathrm{d}\boldsymbol{x}\, \psi J(F_\zeta, Z_\zeta), \tag{5.4}$$

which does not obey (5.3), as was apparently first realized by Benjamin (1984). Thus, to insist on the generalized Jacobi property for Nambu brackets would be to disallow our prototypical example. In any case, our applications require only that the Nambu bracket be antisymmetric.

All the explicit examples given in this paper have only second-order accuracy in the grid-spacing, but the state of the art probably requires algorithms that are at least fourth-order accurate. However, the results of sections 2 and 3 may be easily extended to fourth-order accuracy. The critical factor allowing this extension is that the discrete Casimirs (2.7) and (3.15) do not involve finite differences. The same cannot be said of (3.28), and in fact no completely fourth-order-accurate counterpart to (3.26) is known.

Throughout this paper, we have assumed, to great computational advantage, that the boundary conditions are periodic. This condition must certainly be relaxed. However, all of our discrete brackets correspond to *local* operations. This guarantees that the discrete dynamical equations for energy and the conserved Casimir involve the divergence of a flux. From this we may infer the form of the fluxes, and the boundary conditions must be such that these discrete fluxes vanish. That is, the boundaries must not be artificial sources of energy or potential enstrophy. Except for this, the boundary conditions are as arbitrary as the Hamiltonian itself.

Is it ever possible to conserve *two* Casimirs by generalizing (1.7) to the form

$$\frac{\mathrm{d}F}{\mathrm{d}t} = \{F, H, Z, X\}, \tag{5.5}$$

in which X is the additional Casimir? If so, then X is itself a Casimir of (1.7). The *single* Casimir of (2.3) is

$$X = \iint \mathrm{d}\boldsymbol{x}\, \zeta^{1+n/3} \propto Z_{n/3-1}. \tag{5.6}$$

This suggests that the dynamics (1.2) and (1.3) can be written in the form

$$\frac{\mathrm{d}F}{\mathrm{d}t} = \{F, H, Z_n, Z_{n/3-1}\}_n, \tag{5.7}$$

but (except for the easy case $n = 0$) no such quadruple bracket has been found.

The extensive literature on Nambu brackets is unconcerned with numerical applications. However, McLachlan (2003) advocates an antisymmetric-tensor approach to deriving conservative numerical algorithms. He notes that any system of coupled ordinary differential equations,

$$\frac{\mathrm{d}u_i}{\mathrm{d}t} = f_i(u) \tag{5.8}$$

in the dynamical variables $\{u_1(t), u_2(t), \ldots, u_n(t)\}$ that conserves the quantities $\{H_1(u), H_2(u), \ldots, H_m(u)\}$ can be written in the form

$$\frac{\mathrm{d}u_{i_0}}{\mathrm{d}t} = \sum_{i_1,\ldots,i_m} J_{i_0,\ldots,i_m} \frac{\partial H_1}{\partial u_{i_1}} \cdots \frac{\partial H_m}{\partial u_{i_m}} \equiv \{u_{i_0}, H_1, H_2, \ldots, H_m\}, \tag{5.9}$$

where the tensor $J(u)$ is antisymmetric in all of its indices. The system (5.9) corresponds to numerical algorithms in which all the spatial derivatives (but, again, not the time derivative) have been replaced by discrete approximations. Thus, any numerical algorithm—obtained by any method whatsoever—that conserves the m H_i, must take the form (5.9). The strategy of seeking a completely antisymmetric bracket of the form (5.9) is, therefore, a general starting point for obtaining conservative numerical algorithms. In this view, the challenge is to find the antisymmetric J that makes (5.9) a sufficiently accurate approximation to the set of partial differential equations governing the fluid. Although he gives no completely satisfactory general method, McLachlan shows how group theoretic ideas aid the search for J, and he recovers Arakawa's Jacobian as one of many interesting examples.

In this paper we proceed from somewhat the opposite direction. Like McLachlan, we use antisymmetry to construct conservative numerical algorithms, but rather than beginning at (5.9), we first seek Nambu-bracket formulations of the *partial* differential equations governing the fluid. However, we also fail to find a general, cookbook method for deriving exact Nambu brackets and their discrete, singularity-free counterparts. In fact, virtually all our results have been obtained by various tricks and guesses that would be pointless to elaborate. The deduction of (3.29) was particularly painful.

Bialynicki-Birula and Morrison (1991)—hereafter BM—offer a general method of constructing a Nambu bracket corresponding to a Hamiltonian system of ordinary differential equations in which the Poisson bracket takes the form of a Lie–Poisson bracket. Since virtually all the equations of fluid mechanics may be written in Lie–Poisson form—see Shepherd (1990)—and may be posed as an infinite system of ordinary differential equations by (e.g.) changing the variables to the Fourier coefficients of the fields, the BM method appears to apply. However, in every example that I have tried, the method leads to divergent integrals. For shallow-water dynamics this is not surprising, since the BM method predicts a Casimir that is quadratic in the dependent variables, and no such Casimir exists. But for the dynamics (1.2) and (1.3) the BM method fails even to capture the Nambu bracket (1.9) in which the Casimir (1.8) *is* quadratic. We evidently require a still more general method.

Acknowledgments

This work was supported by National Science Foundation Grant OCE-0100868. I thank P J Dellar, G I Ierley, P J Morrison and T G Shepherd for helpful conversations. I am especially grateful to P Nevir for sending me a copy of his Habilitationsschrift.

References

Arakawa A 1966 *J. Comput. Phys.* **1** 119
Arakawa A and Lamb V R 1981 *Mon. Wea. Rev.* **109** 18
Batchelor G K 1970 *An Introduction to Fluid Dynamics* (Cambridge: Cambridge University Press)
Benjamin T B 1984 *IMA J. Appl. Math.* **32** 3
Bialynicki-Birula I and Morrison P J 1991 *Phys. Lett.* A **158** 453
Guha P 2004 *J. Nonlinear Math. Phys.* **11** 223
Hsu Y J G and Arakawa A 1990 *Mon. Wea. Rev.* **118** 1933
McLachlan R I 2003 *IMA J. Numer. Anal.* **23** 645
Nambu Y 1973 *Phys. Rev.* D **7** 2405
Nevir P and Blender R 1993 *J. Phys. A: Math. Gen.* **26** L1189
Nevir P 1998 Die Nambu-Felddarstellungen der Hydro-Thermodynamik und ihre Bedeutung fur die dynamische Meteorologie *Habilitationsschrift* Freie Universitat Berlin
Sadourny R 1975 *J. Atmos. Sci.* **32** 680
Salmon R 1998 *Lectures on Geophysical Fluid Dynamics* (Oxford: Oxford University Press)
Salmon R 2004 *J. Atmos. Sci.* **61** 2016
Salmon R and Talley L D 1989 *J. Comput. Phys.* **83** 247
Shepherd T G 1990 *Adv. Geophys.* **32** 287
Takhtajan L 1994 *Commun. Math. Phys.* **160** 295