Hamiltonian finite-dimensional models of baroclinic instability

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Abstract

A hierarchy of N-dimensional systems is constructed starting from the standard continuous two-layer quasi-geostrophic model of the geophysical fluid dynamics. These models ("truncations") preserve the Hamiltonian structure of the parent model and tend to it in the limit $N \to \infty$. The construction is based on the known correspondence $SU(N) \to SDiff(T^2)$ when $N \to \infty$ between the finite-dimensional group of unitary unimodular $N \times N$ matrices and the group of symplectic diffeomorphisms of the torus and the fact that the above-mentioned continuous model has an intrinsic geometric structure related to $SDiff(T^2)$ in the case of periodic boundary conditions. A fast symplectic solver for these truncations is proposed and used to study the baroclinic instability. © 1997 Published by Elsevier Science B.V.

1. Introduction

The baroclinic instability is one of the most fundamental features of rotating stratified fluids with vertical velocity shear, and hence is of primary importance in geophysical fluid dynamics (GFD). A proper account of the effects of this instability is one of the major challenges in the studies of weather and climate predictability and in observational data assimilation. However, the complexity of the description of this phenomenon in terms of the basic ("primitive") equations necessitates the use of intermediate models, like the simplest two-layer geostrophic model of the motions of large horizontal scale [1]. The model consists of two linearly coupled layers of fluid with different but constant densities and is governed by two parameters – Burger numbers for the two layers. In the absence

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of dissipation (the most important dissipative process at this scale is Ekman friction [1] which is small and spectrally uniform, i.e. relatively easy to deal with), the Euler equations of motion have Hamiltonian (symplectic) structure and, in addition, possess two infinite families of integrals of motion corresponding to the advection of individual potential vorticities of the layers (see, e.g., Ref. [2]).

In what follows we present a hierarchy of finite-dimensional models which preserve the original Hamiltonian structure of the two-layer continuous model and, at the same time, exhibit baroclinic instability. Our motivation in looking for such models is twofold.

First, from the point of view of numerical analysis of the PDEs governing the continuous model (i) a spatial discretization is needed which results in a system of ODEs and (ii) a temporal discretization of the ODEs is to be applied resulting in a discrete mapping

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in time, an integrator. The traditional spatial and temporal discretization strategies destroy the Hamiltonian structure of the original Euler equations of motion and, particularly for spatial discretizations, there is no general way to avoid this problem. (We believe that, at least in the physical literature, this was first pointed out in Ref. [3]; see also Refs. [4,5].) Increasing the spatial resolution cannot definitely cure this loss of basic geometric structure [6]. As to the relevance of such structure for real-world GFD, which is in general forced and dissipative, we must stress that a variety of stimulating results has been recently achieved by the application of Hamiltonian mechanics (see, e.g., Refs. [7–10] and references therein) and interest in related methods in GFD is growing rapidly.

Second, the use of low-order dynamical systems is a traditional tool of analysis in GFD both from the point of view of conceptual understanding of the basic processes (for a recent instructive example see Ref. [8]) and that of testing the standard procedures of data assimilation and forecast (see, e.g., Ref. [11]).

The first example of a structure-preserving spatial truncation, the sine-bracket approach to the 2D Euler equations, was proposed in Refs. [12,4]. It was shown in Ref. [13] that there exists an efficient explicit Lie–Poisson integrator for this finite-dimensional system. Below, it will be shown that a modified version of this discretization scheme can be applied to the two-layer quasi-geostrophic equations. Moreover, the baroclinic instability arises in the finite-mode system even at the lowest-order truncation.

2. The continuous system

The simplest physical system which retains baroclinic features consists of two linearly coupled layers with different but constant densities. As a further simplification the velocity and the pressure are related by geostrophic balance, i.e., the stream function is defined by the pressure and the velocity potential is zero. A detailed discussion and the derivation of the model equations for this system can be found in Ref. [1].

The system of governing PDEs defines an infinite-dimensional Hamiltonian system [2],

\[
\begin{align*}
q^{(1)}(x, y, t) & = \partial(q^{(1)}, \psi^{(1)}), \\
q^{(2)}(x, y, t) & = \partial(q^{(2)}, \psi^{(2)}),
\end{align*}
\]

where \( \partial(f, g) = (\partial f/\partial x) \partial g/\partial y - (\partial f/\partial y) \partial g/\partial x \). With periodic boundary conditions the equivalent Hamiltonian system of ODEs is written in terms of the Fourier modes

\[
\begin{align*}
\dot{q}^{(1)}_m & = \sum_n (m \times n) q^{(1)}_{m+n} \beta^{(11)}_n q^{(1)}_{-n} + \beta^{(12)}_n q^{(2)}_{-n}, \\
\dot{q}^{(2)}_m & = \sum_n (m \times n) q^{(2)}_{m+n} \beta^{(21)}_n q^{(1)}_{-n} + \beta^{(22)}_n q^{(2)}_{-n},
\end{align*}
\]

where \( m \times n = m_1 n_2 - m_2 n_1 \). The Fourier transform of the \( i \)th layer potential vorticity associated with the two-dimensional wavenumber \( n \) is denoted by \( q^{(i)}_n \), where the superscript \( 1 \) (2) refers to the the upper (lower) layer variables and parameters. The potential vorticities and the stream functions \( \psi^{(1)} \) are related by

\[
\dot{\psi}^{(i)} = -D^{(i)} \left[ \nabla^2 \psi^{(i)} + (-1)^i F^{(i)} (\psi^{(1)} - \psi^{(2)}) \right]
\]

so that their Fourier coefficients are related by

\[
(\psi^{(1)}_n, \psi^{(2)}_n)^T = B_n (q^{(1)}_n, q^{(2)}_n)^T \equiv B_n q_n,
\]

where

\[
B_n = \begin{pmatrix}
\beta^{(11)}_n & \beta^{(12)}_n \\
\beta^{(21)}_n & \beta^{(22)}_n
\end{pmatrix}
\]

and

\[
C_n = \left\{ \left( F^{(1)} D^{(2)} \right) \left( (n^2 + F^{(1)}) (n^2 + F^{(2)}) \right)^{-1} \right\}^{-1}
\]

and we write \( n^2 \) for \( |n|^2 \). The Burger numbers \( F^{(1)} \) and \( F^{(2)} \) are defined as \( F^{(i)} = (\rho^{(i)} + \rho^{(1)}) f^2 L^2 / (g \rho^{(i)} - \rho^{(1)} D^{(i)}) \) and satisfy the constraint \( F^{(1)} D^{(1)} = F^{(2)} D^{(2)} \), where \( f \) is the Coriolis parameter, \( L \) is the characteristic horizontal scale, \( \rho^{(i)} \) is the density, and \( D^{(i)} \) is the thickness of the \( i \)th layer in the absence of motion. The total (dimensionless) thickness is \( D^{(1)} + D^{(2)} = 1 \). Note that our potential vorticities \( q \) are related to Pedlosky’s \( II \) [1] by \( q^{(i)} = -D^{(i)} II^{(i)} \). This scaling is chosen to make \( B_n \) symmetric, which is necessary for \( II \) to be a Lie–Poisson system.
The total energy of the system is

$$H = K^{(1)} + K^{(2)} + AP = \frac{1}{2} \sum_n q_n^T B_n q_{-n},$$  \hspace{1cm} (5)

where

$$K^{(i)} = \frac{1}{2} \sum_n \langle \mathbf{D}^{(i)} | \mathbf{\psi}_n^{(i)} \rangle^2 \quad (i = 1, 2)$$  \hspace{1cm} (6)

is the kinetic energy (KE) of the $i$th layer and

$$AP = (\mathbf{F}^{(1)} \cdot \mathbf{D}^{(1)}) \sum_n \lvert \mathbf{\psi}_n^{(1)} - \mathbf{\psi}_n^{(2)} \rvert^2$$  \hspace{1cm} (7)

is the available potential energy (APE).

Now, the crucial observation is that this continuous two-layer system may be rewritten as “generalized Euler equations” [12,14] of the form

$$\dot{\mathbf{\omega}}_i = a^{ml} c_m^k \omega_k \omega_l,$$  \hspace{1cm} (8)

where $\mathbf{\omega}_i$ are coordinates on the dual of a Lie algebra, $a^{ml}$ is a metric and summation over the repeated indices is understood. The dynamical variables in (2) correspond to coordinates on the dual of the Lie algebra of the direct product of area-preserving diffeomorphisms of the torus $\text{SDiff}(T^2) \times \text{SDiff}(T^2)$ while the structure constants of each diffeomorphisms’ group are given by

$$c_{jm}^{(i)} = \delta(k - j - m)(j \times m) \quad (i = 1, 2).$$  \hspace{1cm} (9)

The coupling between layers is due to a nontrivial metric (which is symmetric in both $(k,l)$ and $(i,j)$).

$$a^{(ij)kl} = \delta(k + l) \beta^{(ij)} \quad (i, j = 1, 2).$$  \hspace{1cm} (10)

With these definitions, (2) takes the form (8) and define a Lie–Poisson system with Hamiltonian (5), and Casimir invariants

$$Q_i^{(i)M} = \sum_{I^M} q_i^{(i)} \ldots q_{I^M}^{(i)} \quad (i = 1, 2),$$  \hspace{1cm} (11)

$$I^M = \{ (i_1, \ldots, i_M) | \sum_{j=1}^M i_j = 0 \}.$$  \hspace{1cm} (12)

3. The finite-mode system

There are two differences between the two-dimensional vorticity equation considered in Refs. [4,12] and the two-layer system presented here: (i) the choice of the metric, and (ii) the direct product group structure. Neither is an obstacle to applying essentially the same truncation strategy to get a finite-dimensional Lie–Poisson system. The dynamical variables of the truncated system will be coordinates on the dual of the Lie algebra of $\text{SU}(N) \times \text{SU}(N)$, where the odd number $N$ will determine the resolution of the numerical model. The finite-mode system built with the help of the structure constants of the su$(N)$ algebra is

$$\dot{q}_m^{(1)} = \sum_{n \in I} (1/\varepsilon) \sin(\varepsilon m \times n) q_{m+n}^{(1)} (\beta_n^{(1)} q_{-n}^{(1)}$$

$$+ \beta_n^{(2)} q_{-n}^{(2)}),$$

$$\dot{q}_m^{(2)} = \sum_{n \in I} (1/\varepsilon) \sin(\varepsilon m \times n) q_{m+n}^{(2)} (\beta_n^{(2)} q_{-n}^{(1)}$$

$$+ \beta_n^{(2)} q_{-n}^{(2)}),$$  \hspace{1cm} (13)

where $\varepsilon = 2\pi/N$, the index set is defined by

$$I = \{i \in \mathbb{Z}^2 | -T \leq i_1, i_2 \leq T, i \neq 0, T = \frac{1}{2}(N - 1) \},$$  \hspace{1cm} (14)

and the sum of indices are taken modulo $N$. Thus, the preservation of structure was achieved at the price of introducing aliasing interactions (which, in a well-resolved simulation, would not be significant) and altering the interaction coefficients with respect to the original infinite-mode system written in the Fourier-space. This latter error is formally $O(N^{-2})$, but the interactions of the higher modes are not accurately represented. The Hamiltonian is defined by the truncated form of (5), while the analogy with the one-layer system gives immediately that the Casimirs are

$$Q_s^{(1)M} = \sum_{I^M} q_i^{(i)} \ldots q_{I^M}^{(i)} \cos(2A(i_1, \ldots, i_M))$$

$$\quad (i = 1, 2),$$  \hspace{1cm} (15)

$$I^M = \{ (i_1, \ldots, i_M) | \sum_{j=1}^M i_j = 0 \text{ mod } N \},$$  \hspace{1cm} (16)

where $M \leq 2T$ and $A(i_1, \ldots, i_M)$ denotes the area spanned by the index vectors:

$$A(i_1, \ldots, i_M) = \frac{1}{2} [i_2 \times i_1 + i_3 \times (i_1 + i_2)$$

$$+ \ldots + i_M \times (i_1 + \ldots + i_{M-1})].$$  \hspace{1cm} (17)
Thus, for any odd $N$ we get a finite-mode system of dimension $2(N^2 - 1)$ preserving the symplectic structure of the parent continuous system and having $2(N - 1)$ conserved quantities. In the limit $N \to \infty$ both equations and integrals of motion tend towards the parent ones.

4. Stationary solutions and linear stability analysis

Traditional stability analyses for (1) focus on the fixed point solutions associated with two different but constant velocities of the layers [1]. These solutions are, obviously, forbidden in the doubly periodic case, and we therefore start from the simplest sinusoidal zonal wind profile (a so-called Kolmogorov flow, much studied in the one-layer case, cf. Ref. [15] and references therein). We note that a solution of a Lie–Poisson system is a fixed point if and only if the gradient of the Hamiltonian is equal to the gradient of some linear combination of Casimirs on this solution. Setting for simplicity the stream function to zero at the upper layer, we see that stream functions which are zero at all but one selected wavenumber in the lower layer define steady states. A solution of this type is

\[
\text{Re} q_n^{(1)} = -D^{(1)} F^{1} \quad \text{if} \quad n = (0, 1),
\]

\[
= 0 \quad \text{otherwise}
\]

\[
\text{Re} q_n^{(2)} = D^{(2)} (F^{(2)} + 1) \quad \text{if} \quad n = (0, 1),
\]

\[
= 0 \quad \text{otherwise}
\]

(18)

or equivalently

\[
q_n^{(1)}(x, y) = -D^{(1)} F^{1} \cos y,
\]

\[
q_n^{(2)}(x, y) = D^{(2)} (F^{(2)} + 1) \cos y,
\]

(19)

which corresponds to

\[
\psi_n^{(1)}(x, y) = 0, \quad \psi_n^{(2)}(x, y) = \cos y.
\]

(20)

This initial field is a steady-state solution both of the original system and of the truncated one, independently of the resolution. The detailed analysis of the linear stability problem for the full system (1) is out of the scope of the present paper. We note, however, that, unlike the barotropic one-layer case, the formal stability analysis of (1) along the lines of Refs. [2,15] does not give any definite conclusions. We now consider the linear stability analysis of its finite-dimensional counterpart.

The equations linearized around (20) for (2) and (13) decouple into two independent systems of real and imaginary variables. The Jacobian matrix for the real part at the lowest-order truncation $T_1$ ($N = 3$) is

\[
\begin{pmatrix}
0 & -a & a & 0 & -b & b \\
c & 0 & -a & d & 0 & -c \\
-c & a & 0 & -d & b & 0 \\
o & e & -e & 0 & -f & f \\
-c & 0 & e & -d & 0 & -f \\
c & -e & 0 & d & f & 0
\end{pmatrix}
\]

where

\[
a = r F_1 \beta^{(11)}_1, \quad b = r F_1 \beta^{(12)}_1, \quad c = r F_1 \beta^{(11)}_0, \\
d = r F_1 \beta^{(12)}_0, \quad e = r (F_2 + 1) \beta^{(21)}_1, \\
f = r (1 - (F_2 + 1) \beta^{(22)}_1),
\]

(21)

and $r = \sqrt{3}/4$. The order of variables in the linearized state vector is $q_{00}^{(1)}, q_{11}^{(1)}, q_{11}^{(-1)}, q_{02}^{(2)}, q_{12}^{(2)}, q_{12}^{(-2)}$. The $q_{00}^{(i)}$ ($i = 1, 2$) do not appear in the linearized system because all the coefficients are zero for these variables due to the Liouville theorem on conservation of phase-space volume. The characteristic polynomial is

\[
\lambda^2 (\lambda^4 + B \lambda^2 + C) = 0,
\]

(22)

where $B$ and $C$ are functions of $a, b, c, d, e, f$. The eigenvalues are of the form

\[
\lambda_{1,2} = 0, \quad \lambda_{3,4,5,6} = \pm \alpha \pm i \beta.
\]

(23)

Because of the Hamiltonian character of the model, the spectrum has the desirable property of having two zero eigenvalues corresponding to the two Casimirs, with the other four having the correct symmetry. The steady state is stable if and only if all the following conditions hold: (i) $C > 0$; (ii) $B > 0$; and (iii) $B^2 - 4C > 0$. Conditions (i) and (ii) are always satisfied independently of the particular positive values of the Burger numbers. The key condition is (iii). The critical values of $F^{(1)}$ and $F^{(2)}$ are shown in Fig. 1. If the Burger numbers go to zero the system decouples into two one-layer systems, for which the initial conditions define stable fixed point solutions. The eigenproblem for the linearized imaginary variables has the
same physical solution as for the real part, since the only differences are in the imaginary part of the eigenvectors. This means that there are two unstable directions in the phase space, the same combination of cosine and sine functions as the initial perturbation will grow with the same amplification factor.

5. Numerical integration

By analogy with the one-layer system, (13) can be solved by an explicit Lie–Poisson integrator [13]. Such a method preserves all the Casimir invariants and is symplectic on their level set, promoting good long-time behavior of the numerical solution. The key point is that the terms associated with the coupling of the layers are linear and, therefore, have no effect on the commutation rules between the variables. To be brief we only summarize the algorithm for prime $N$; the extension of the one-layer algorithm to nonprime $N$ of [6] can be easily applied to the two-layer equations as well. The algorithm splits the Hamiltonian into a sum of terms, each of which can be solved explicitly using a fast Fourier transform. In this way one time step takes time $O(N^3 \log N)$, rather than the $O(N^4)$ needed just to evaluate the right hand side of (2). Let

$$K = \{(0,1)\} \cup \{(1,m) : 0 \leq m < N\},$$

$$a_n^{(1)} = -\frac{\sin(enj \times k)}{\varepsilon} (\beta_{nk}^{(1)} q_{nk}^{(1)} + \beta_{nk}^{(2)} q_{nk}^{(2)}),$$

$$a_n^{(2)} = -\frac{\sin(enj \times k)}{\varepsilon} (\beta_{nk}^{(2)} q_{nk}^{(1)} + \beta_{nk}^{(1)} q_{nk}^{(2)}),$$

and $F$ be the discrete Fourier transform

$$F_{jk} = \frac{1}{N} e^{-2\pi i jk/N}.$$  

We may summarize the algorithm as follows: (i) for $k \in K$ do, (ii) for $j = 1, \ldots, N$th translation of $k$ do, (iii) with $z_m^{(1)} = q_{j-mk}^{(1)}$ set $\tilde{z}^{(1)} = F^{-1} e^{\Delta t A_1} F z^{(1)}$, $A_1 = \text{diag}(Fa^{(1)})$; with $z_m^{(2)} = q_{j+mk}^{(2)}$ set $\tilde{z}^{(2)} = F^{-1} e^{\Delta t A_2} F z^{(2)}$, $A_2 = \text{diag}(Fa^{(2)})$, (iv) copy $\tilde{z}^{(1)}$ into $q_{-(j+mk)}^{(1)}$ and $\tilde{z}^{(2)}$ into $q_{-(j+mk)}^{(2)}$, (v) end do, (vi) end do.

The above algorithm is a first-order explicit Lie–Poisson integrator, say $q \mapsto S(t)q$; in practice we use the second-order scheme $q \mapsto S(t/2)S^{-1}(-t/2)q$, which is still explicit. Numerical experiments with the second order integrator were carried out in order to test the numerical algorithm and study the nonlinear stage of the instability predicted by the linear analysis. A small random noise was added to the steady state (20) at the initial time. The bound for the relative error of energy is $10^{-6}$ at a time step $\Delta t = 10^{-2}$, while the errors in the Casimirs grow by the average computer roundoff (about $5 \times 10^{-15}$). The parameters were chosen as $F^{(1)} = F^{(2)} = 1$ and $D^{(1)} = D^{(2)} = \frac{1}{2}$ at resolution T1, hence the APE = $K^{(2)}$ and $K^{(1)} = 0$ for the unstable basic state. Experiments confirmed that baroclinic instabilities with the above predicted features occur for any random initial perturbation. Fig. 2 shows the results of experiments with the same parameters but at resolution T2 ($N = 5$). The qualitative behavior of the T1 and the T2 results is similar, though the transfer of APE to KE is more efficient in the T2 system and the nonlinear saturation arises later. The minimum in the APE appears shortly after the nonlinear saturation and it is about 5 and 18 percent of the total energy for T2 and T1, respectively. Most of the APE is converted to upper layer KE, but there is a weaker, simultaneous increase in the bottom layer KE as well. This feature seems to be independent of the resolution. After the nonlinear saturation the flow is dominated by a chaotic exchange of energy between the layers.
6. Concluding remarks

The aim of the present paper was to demonstrate that a hierarchy of models preserving the Lie–Poisson structure of the original continuous two-layer quasigeostrophic model both in space and time exists and the phenomenon of baroclinic instability already arises at the lowest-order truncation. The finite-mode truncations obtained may serve as a neat model of baroclinic instability suitable for testing data assimilation and forecast algorithms. The symplectic solver developed in Ref. [5] allows fast numerical integration of these truncations, even for large numbers of modes, without destroying the underlying geometric structure.

The whole approach is based on the notion of symmetry underlying the motion of the incompressible fluid in the two-dimensional domain. This symmetry with respect to area preserving changes of variables (symplectic diffeomorphisms) corresponds, physically, to the relabelling of fluid particles. It provides the Lie–Poisson structure of the Euler equations of motion and, at the same time, the existence of the Casimir invariants [15]. Fortunately, the Lie algebra of the symplectic diffeomorphisms of the torus (corresponding to the doubly periodic boundary conditions in the domain of the flow) may be thought of as a large $N$ limit of the Lie algebra of the group of $N \times N$ unitary unimodular matrices [16] which allows the construction of structure-preserving truncations of the 2D ideal hydrodynamics [4,12] and their generalization presented here. The second known example of this kind, also discovered in Ref. [16], is the Lie algebra of symplectic diffeomorphisms of the sphere which is also a limit of the $su(N)$ algebras and, thus, creates the possibility of applying our approach to another kind of boundary condition. Due to the technical difficulties in the calculation of explicit expressions for the structure constants of the corresponding infinite-dimensional Lie algebras (for a discussion of this point see, e.g., Ref. [14]) it is unknown at the present time whether a similar construction may be carried out for other types of boundary conditions, i.e. for two-dimensional manifolds other than the torus and the sphere.

Another open problem is related to the correspondence (in the functional analysis sense) between solutions of the parent system and those of the truncated one. Remember that the latter is obtained by identi-
fying the Fourier modes of the former modulo $N$ and simultaneously changing the interaction coefficients, which represents a very special aliasing procedure introducing nonlocal interactions in the real space.

Finally, let us mention that there exists an alternative approach to the problem of structure-preserving truncations in fluid dynamics based on discretization of the action principle for the system in question [17]. While it has the advantage of conceptual transparency, this approach requires a Lagrangian rather than Eulerian description of the fluid dynamical problem. Finding a variational principle for a given set of PDEs may be a problem by itself and for the system (1) the corresponding variational principle is presently unknown. Of course, this system originates from the full hydrodynamical set of equations admitting a Lagrangian description and, hence, a variational formulation; however due to a very special character of the quasi-geostrophic approximation used to derive (1), finding a corresponding variational principle is a non-trivial task. The solution of this problem will be presented elsewhere [18]. Let us add that the Eulerian Lie–Poisson structure is not preserved by discretization of the Lagrangian variational principle due to the fact that the particle relabelling symmetry is destroyed by the spatial discretization and that, inevitably, the Lagrangian approach increases the number of dynamically active variables in the problem as compared to the Eulerian one.

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