Preserving geometric structure (and coherent structures) under discretization

Jason Frank

Mathematical Institute
Utrecht University

Transport in Unsteady Flows
16-20 Jan 2017 - Banff

Outline

- Motivation
- Hamiltonian structure
- Mean field statistics
- Time integration considerations
- Parameterization of unresolved scales

Geometric structure

- Conservation laws = invariant manifolds, important for physics and statistics:
    - Explicit (divergence-form): mass, momentum
    - Implicit (derived: kinetic energy, enstrophy, PV advection)
- Structural properties of phase space (important for tracer transport and ensemble spread):
    - Reversibility
    - (Ensemble) volume
- Hamiltonian/Poisson structure

Why conserve?

- Physically or mathematically pleasing
- Stability
- Correct transformation of energy from one form to another (Lorenz 60), response to forcing/diss.
- Coherent structures
- Statistics

Energy and Numerical Weather Prediction

By EDWARD N. LORENZ, Massachusetts Institute of Technology[1],
Cambridge, Mass., U.S.A.

(Manuscript received May 27, 1960)

Abstract

Since the study of energy transformations and the numerical integration of simplifiied equations are sometimes used as alternative approaches to the same physical problem, it is often desirable that the simplified equations conserve total energy under reversible adiabatic processes. Preferably, the equations should also conserve the sum of kinetic energy and available potential energy, and they should describe the tendency for static stability to increase as kinetic energy is released.

It is found that if the equation of balance is used as a filtering approximation, all the terms in

Why conserve?

- Physically or mathematically pleasing
- Stability
- Correct transformation of energy from one form to another (Lorenz 60), response to forcing/diss.
- Coherent structures
- Statistics

Coherent structures

- Many coherent structures are described by relative equilibria: extremal value of one conserved quantity constrained by a fixed value of another
    - KdV Soliton (min energy | fixed momentum)
    - Point vortex dipole (min energy | fixed angular momentum)
    - Taylor vortices (min. energy| fixed enstrophy)
    - Leith vortices (extrem. energy | fixed enstrophy & circulation)
    - Kirchhoff patches (extrem. energy & enstrophy | fixed circulation)
- Robust with respect to discretization, but shape and persistence depends on conservation

Why conserve?

- Physically or mathematically pleasing
- Stability
- Correct transformation of energy from one form to another (Lorenz 60), response to forcing/diss.
- Coherent structures
- Statistics

Hamiltonian structure

All *properly derived* inviscid fluid models possess Hamiltonian (Poisson) structure

$$\omega_t = \{\omega, \mathcal{H}\} \qquad \mathcal{H} = -\frac{1}{2}\iint \omega \cdot \psi \, dx \, dy$$

$$\{\mathcal{F}, \mathcal{G}\} = \iint \frac{\delta \mathcal{F}}{\delta \omega} \cdot J\left(\omega, \frac{\delta \mathcal{G}}{\delta \omega}\right) \, dx \, dy$$

$$J(a, b) = a_x b_y - a_y b_x$$

The Poisson bracket $\{\mathcal{F}, \mathcal{G}\}$:

- is skew-symmetric, encoding *energy conservation*
- satisfies the Jacobi identity, encoding *symplectic structure* and *phase volume conservation*
- is degenerate, encoding an *infinite class of (potential) vorticity conservation laws*

The Hamiltonian itself may admit additional symmetries.

Hamiltonian structure

All *properly derived* inviscid fluid models possess Hamiltonian (Poisson) structure

$$\omega_t = \{\omega, \mathcal{H}\} \qquad \mathcal{H} = -\frac{1}{2}\iint \omega \cdot \psi \, dx\, dy$$

$$\{\mathcal{F}, \mathcal{G}\} = \iint \frac{\delta \mathcal{F}}{\delta \omega} \cdot J\left(\omega, \frac{\delta \mathcal{G}}{\delta \omega}\right) \, dx\, dy$$

$$J(a, b) = a_x b_y - a_y b_x$$

Casimirs: for any functional of the vorticity $\mathcal{C}_\varphi[\omega] = \iint \varphi(\omega)\, dx\, dy$

$$\frac{d}{dt}\mathcal{C} = \{\mathcal{C}, \mathcal{H}\} = 0$$

⇒ Infinite class of conserved quantities

Enstrophy: $\mathcal{Z} = \dfrac{1}{2}\iint \omega^2 \, dx\, dy$

Hamiltonian structure

- What is the proper discrete analog PDE to ODE?
    - A finite dimensional Poisson bracket that converges to the continuum bracket? With a finite number of Casimir’s?
    - The Jacobi identity is difficult to satisfy, complex symmetries among derivatives of the discretization. One known example (Zeitlin 1991)
    - Particle-based methods (regularized point vortices).
    - Focus on quadratic and linear invariants, reversibility and phase volume: Arakawa (1966), Salmon (1989, 2004, 2005) (requires only matrix anti-symmetry considerations)

Statistics: mean field and fluctuations

- Quasigeostrophic PV with topographic forcing:

$$q(x,t) = \nabla \times u(x,t) + h(x)$$

$$q_t + \nabla^{\perp}\psi \cdot \nabla q = 0, \qquad \Delta\psi = q - h$$

- Problem parameters from Majda & Abramov (2003)

$$L = 2\pi, \quad M = 22, \quad h(x,y) = 0.2\cos x + 0.4\cos 2x, \quad E_M = 7, \quad Z_M = 20$$

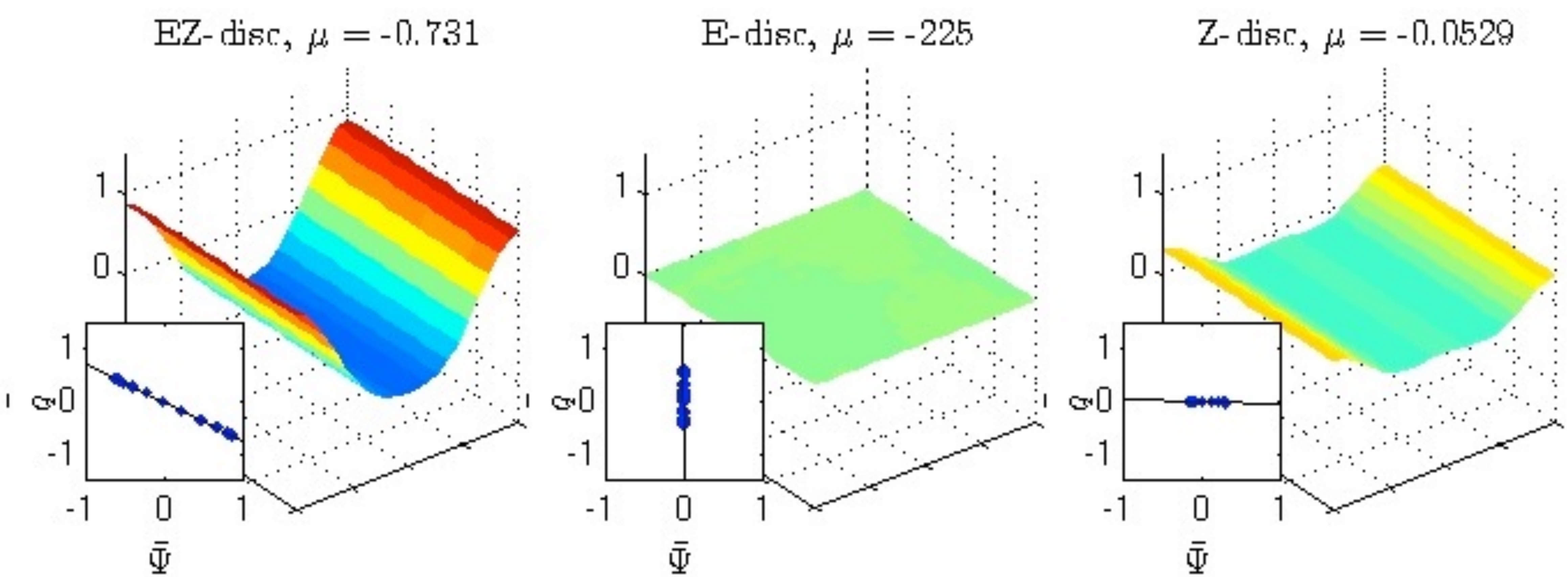
- Compare at the converged time averages of PV and stream function

$$\bar{q}_T = \frac{1}{N_T}\sum_n q^n, \quad \bar{\psi}_T = \frac{1}{N_T}\sum_n \psi^n,$$

- Three discretizations due to Arakawa (1966)

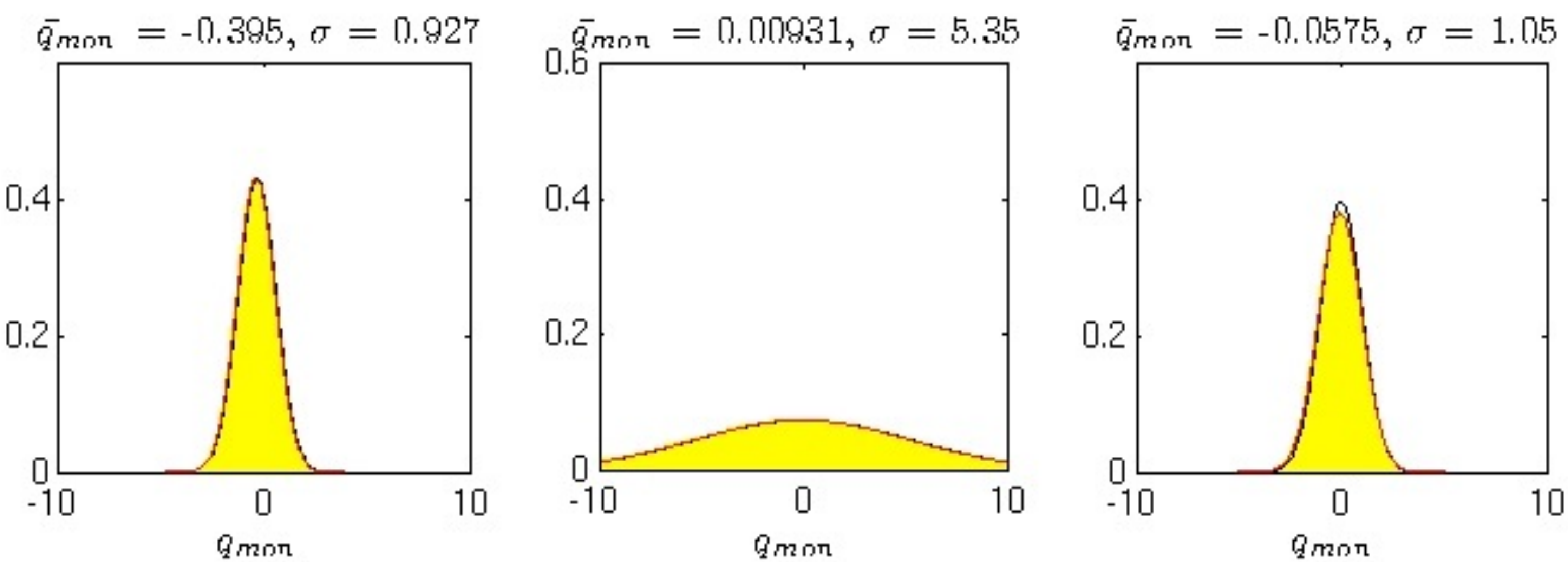
Mean states, $T_{av} = 10^6$

- Statistical predictions for E = 7, Z = 20
  - (EZ) $\langle q \rangle = \mu \langle \psi \rangle, \quad \mu = -0.730$
  - (E) $\langle \psi \rangle = 0$
  - (Z) $\langle q \rangle = 0 \Rightarrow \langle \psi \rangle = -\Delta^{-1} h$



Point statistics for vorticity fluctuations about the mean

- Statistical predictions for E=7, Z=20, (Gaussian with:)
  - (EZ) $\langle q_{\text{mon}} \rangle = -0.341, \quad \sigma_{q'} = 0.970$
  - (E) $\langle q_{\text{mon}} \rangle = -0.0740, \quad \sigma_{q'} = 5.36$
  - (Z) $\langle q_{\text{mon}} \rangle = 0, \quad \sigma_{q'} = 1.01$



Sine-bracket Poisson integrator

- Abramov & Majda (2003) used Zeitlin's (1991) Poisson truncation of the ideal fluid, which preserves N+1 integrals on an NxN grid, to study the statistical relevance of the higher moments of vorticity
- A nonzero third moment C_3 is statistically relevant
- Experimental setup suggests that higher moments could be irrelevant

$$\langle q \rangle = g(\langle \psi \rangle), \quad \forall x$$

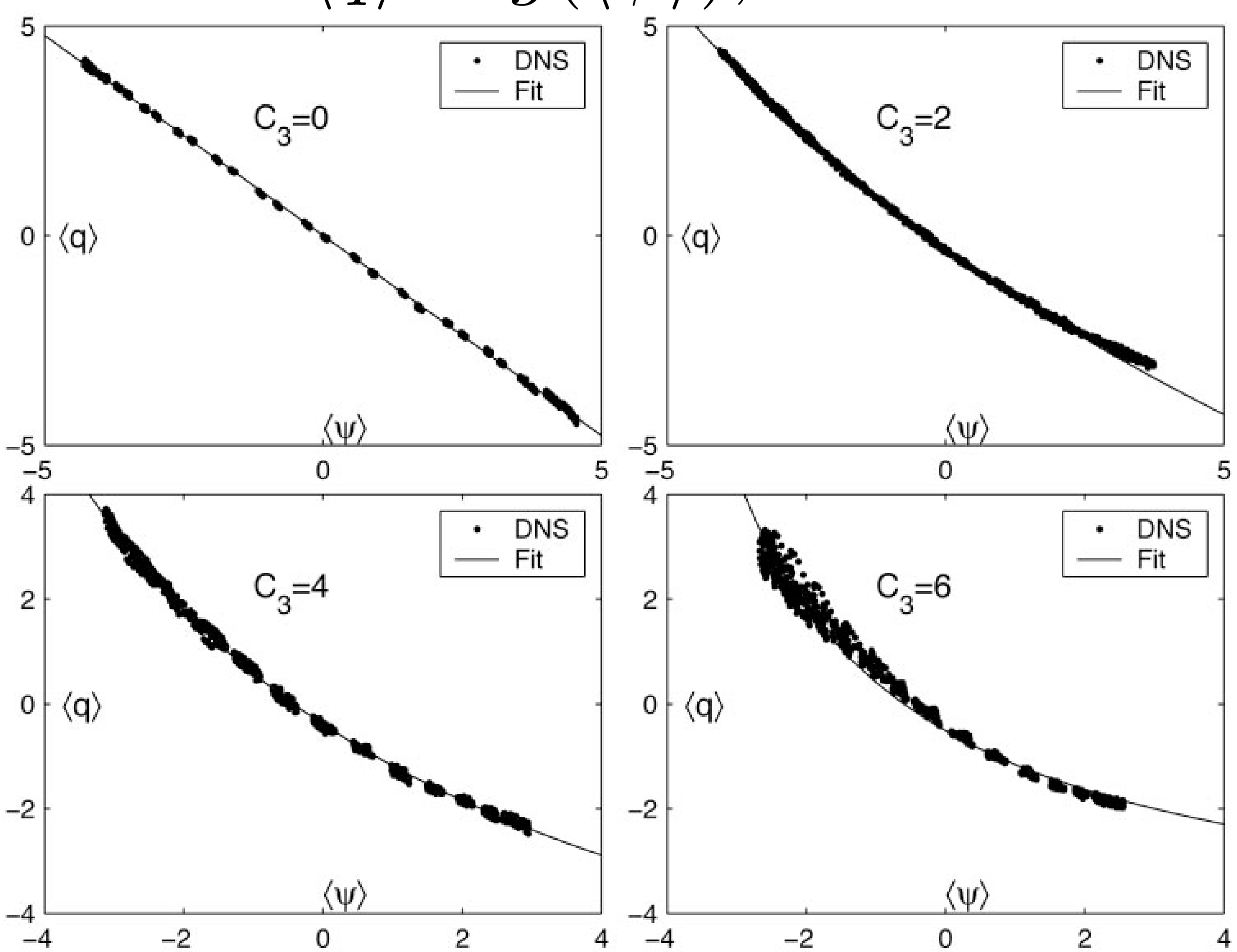


Fig. 3. The scatter plots $\bar{q}$ vs. $\bar{\psi}$ for the 23 × 23 sine-bracket truncation, layered topography, $\hat{C}_3 = 0, 2, 4, 6$.

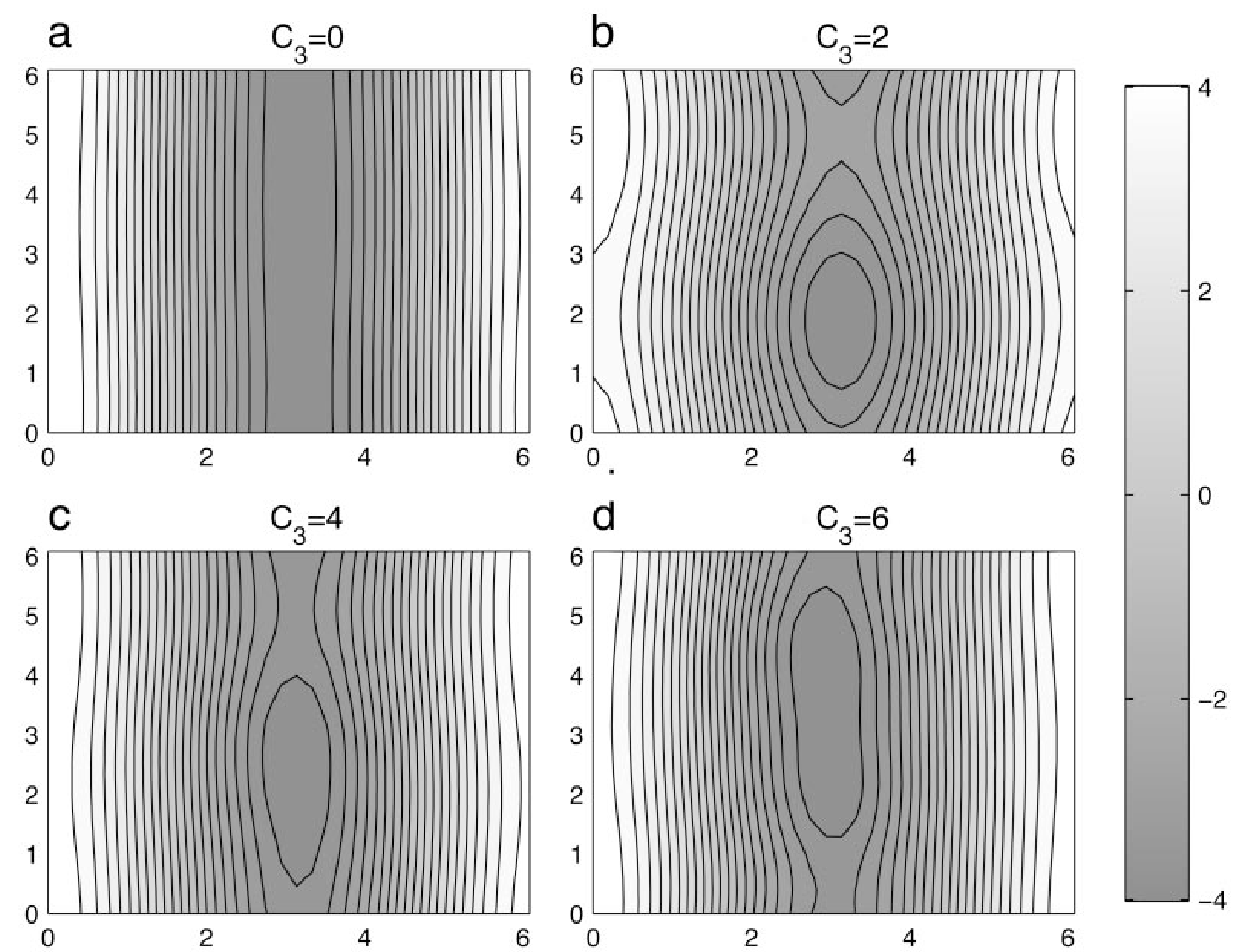


Fig. 4. The contour plots of the mean stream function, 23 × 23 sine-bracket truncation, layered topography, $\hat{C}_3 = 0, 2, 4, 6$.

Time integration

- Symplectic integrators are the preferred choice for Hamiltonian systems. They preserved volume and an approximate energy. But:
  - They are only symplectic if the discretization is Hamiltonian (or Poisson)
  - A symplectic method is only symplectic with respect to a specific Poisson bracket.
  - For Poisson systems, this means mostly only splitting methods will suffice
- The implicit midpoint rule is remarkable because it is

$$\frac{q^{n+1} - q^n}{\Delta t} = f\left(\frac{q^{n+1} + q^n}{2}\right)$$

  preserves any quadratic invariants (present in the discretization), e.g. kinetic energy and enstrophy.
- Kahan's method is related to midpoint, reversible, seems to conserve E and Z approximately, but is linearly implicit for quadratic vector fields.

Maximum entropy closure (Verkley et al. 2016)

- Verkley, Kalverla & Severijns (2016) propose a promising closure basd on maximum entropy theory.
- (Spectral) discretization decomposed in resolved and unresolved vorticity and stream function

$$\frac{\partial \zeta^{\mathcal{R}}}{\partial t} + P^{\mathcal{R}} J(\psi^{\mathcal{R}} + \langle \psi^{\mathcal{U}} \rangle, \zeta^{\mathcal{R}} + \langle \zeta^{\mathcal{U}} \rangle) \\ = \nu \nabla^2 \zeta^{\mathcal{R}} + \mu (F^{\mathcal{R}} - \zeta^{\mathcal{R}}).$$

- The unresolved modes are taken to be the ensemble means in (but for stochastic parameterization could be draw from) a probability density chosen to maximize entropy subject to constraints on the energy and enstrophy tendency

$$\langle \mathrm{d}E^{\mathcal{U}}/\mathrm{d}t \rangle = 0 \text{ and } \langle \mathrm{d}Z^{\mathcal{U}}/\mathrm{d}t \rangle = 0$$

- Mean can be explicitly computed in terms of resolved scale, no tuning parameters!

Maximum entropy closure (Verkley et al. 2016)

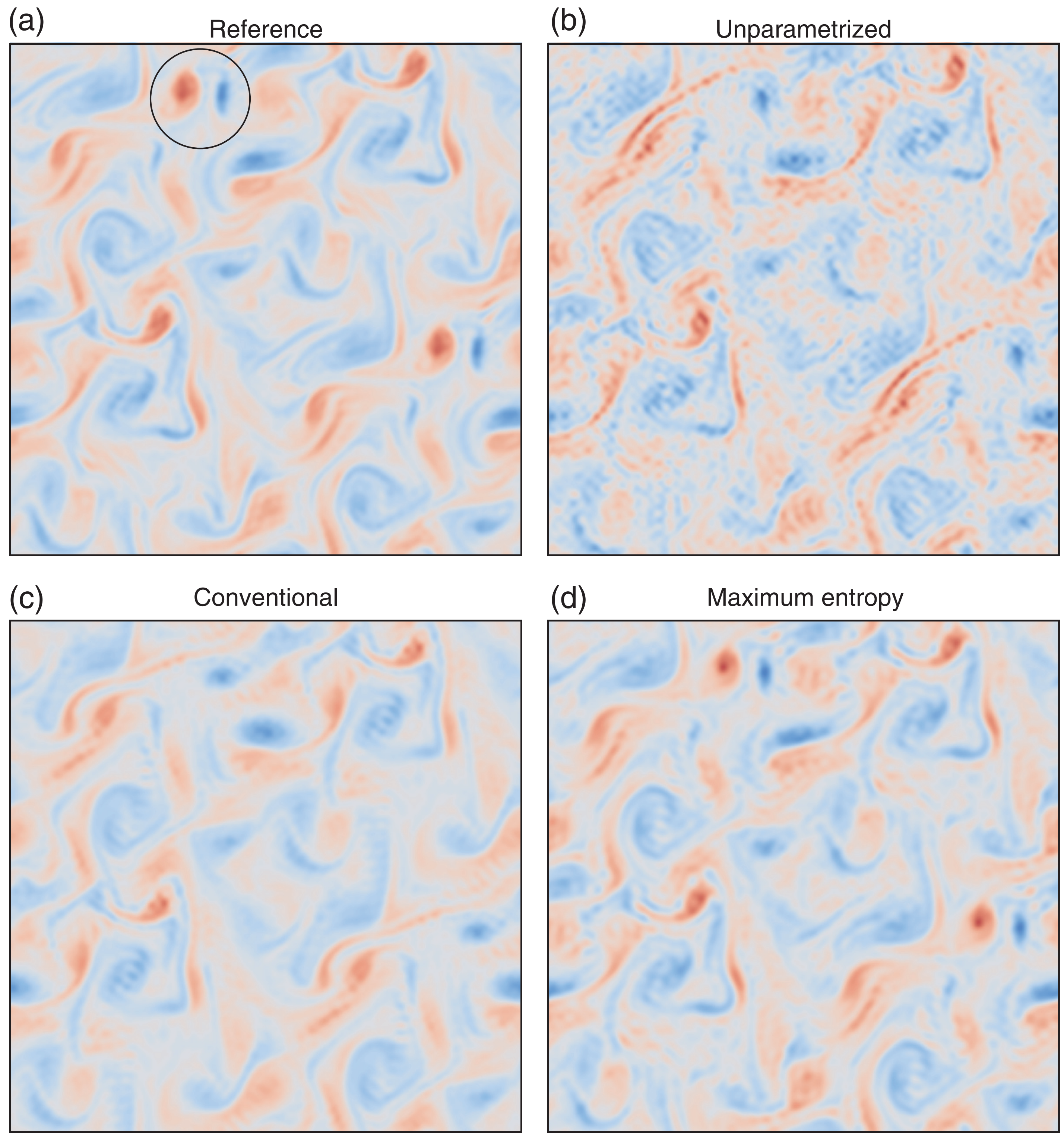


Figure 4. Vorticity fields from four model simulations at day 30 of the integration, starting from initial field 3, i.e. from the reference run after 600 days. A *T*42 truncation has been used to plot the vorticity fields, including the reference, on a 256 × 256 grid from 0−2π in both directions. (a) Reference run, (b) unparametrized run, (c) conventional run and (d) maximum entropy run. The circle in the upper left panel highlights a dipole structure that is only reproduced in the maximum entropy run.

Maximum entropy closure (Verkley et al. 2016)

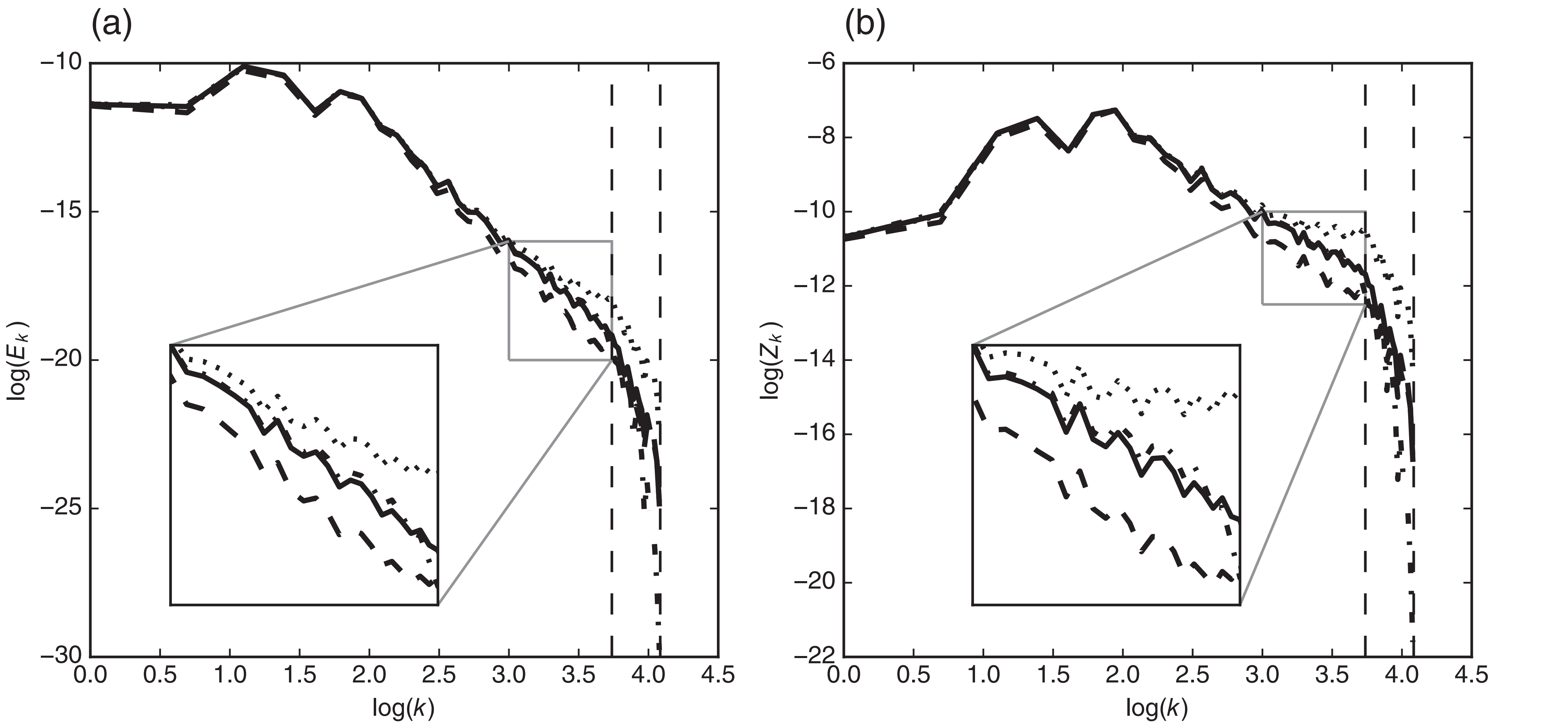


Figure 7. Energy and enstrophy spectra of the flow field as simulated with the reference model (solid lines), the unparametrized model (dotted lines), the conventional model (dashed lines) and the maximum entropy model (dash–dotted lines). All spectra are based on long 5000 day integrations, starting from initial state 3 in Figure 3, the spectra being averages over the data ten days apart. The insets show the differences between the spectra close to the truncation limit. Panel (a) refers to the energy, panel (b) to the enstrophy.

Perspectives

- Conservative discretizations ensure a correct transformation between different forms of energy.
- They should play a role in the formation and propagation of coherent structures.
- They clearly play an important role in statistics

- The Eternal question: is there an approach that allows us to derive Poisson discretizations of inviscid fluids in 3D, with physical boundary conditions, local methods, unstructured meshes?
- What is the role of volume preservation and reversibility in ensembles and tracer advection?
- How to construct parameterizations of unresolved motion that are minimally intrusive for resolved coherent structures?