Statistical mechanics and numerical modelling of geophysical fluid dynamics
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Citation for published version (APA):
Dubinkina, S. B. (2010). Statistical mechanics and numerical modelling of geophysical fluid dynamics

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Chapter 2

Statistical mechanics of Arakawa’s discretizations

2.1 Introduction

In applications such as weather and climate predictions, long numerical simulations are run for dynamical systems that are known to be chaotic, and for which it is consequently impossible to simulate a particular solution with any accuracy in the usual sense of numerical analysis. Instead, the goal of such simulations is to obtain a data set suitable for computing statistical averages or otherwise to sample the probability distribution associated with the continuous problem.

Different numerical discretizations have very different discrete dynamics, however. Recent work on geometric integration [35, 45, 79, 84] relies on backward error analysis, in which the numerical solution generated by a given method is viewed as the exact solution of a perturbed problem. The properties of different discrete dynamics become more pronounced when the numerical map is iterated over a very large number of time steps. Therefore it is important to establish the influence that a particular choice of method has on the statistical results obtained from simulations. Ideally, one would like to determine criteria which a method should satisfy to yield meaningful statistics, and to understand statistical accuracy in terms of discretization parameters.

To that end, in this chapter we consider three related discretizations for an ideal fluid in vorticity-stream function form, originally proposed by Arakawa [2]. The three discretizations conserve discrete approximations of energy, enstrophy, or both. We analyze the three methods through appropriate (trivial) modifications of the statistical mechanics theory of quasigeostrophic flow over topography—based on the original work of Kraichnan [40], Salmon et al. [76] and Carnevale & Frederiksen [11], and recently expounded in Majda & Wang [48]. The resulting theories predict entirely different statistical behavior for the three methods. Numerical experiments with conservative and projected time integrators agree with the statistical predictions, confirming that the conservation properties of a discretization define the backdrop, or climatic mean, against which the dynamics takes place.

It should be mentioned at the outset that the energy-enstrophy statistical
theory is a model and is known to be incomplete. In [1], Abramov & Majda show that nonzero values of the third moment of potential vorticity can cause significant deviation from the statistical predictions. In Section 2.6 we use the numerical setup of [1] to facilitate comparison with their results. We wish to stress, however, that the focus of this thesis is not the statistical mechanics of ideal fluids per se, but rather the application of statistical mechanics as a tool for the numerical analysis of discretizations.

The chapter is organized as follows. In Section 2.2 we briefly recall the quasigeostrophic potential vorticity equation and its conservation properties. Section 2.3 we review Arakawa’s discretizations, their conservation properties, and prove that all of these define divergence-free vector fields. In Section 2.4, the equilibrium statistical mechanical theories are developed for the three discretizations. Most of this section is simply a summary of material in Chapters 7 and 8 of [48] for the energy-enstrophy theory. Once established, it is a simple matter to extend the results to the cases in which only one of these quantities is conserved, and we do this in Section 2.4.4. Time integration aspects are discussed in Section 2.5. The numerical experiments confirming the statistical predictions are presented in Section 2.6.

2.2 The quasigeostrophic model

This section addresses the statistical mechanics of conservative discretizations of the quasigeostrophic potential vorticity model (QG) on a doubly periodic domain, \( \Omega = \{ x = (x, y) \ | \ x, y \in [0, 2\pi) \} \). The QG equation [67, 74] is

\[
\begin{align*}
q_t &= \mathcal{J}(q, \psi), \quad \text{(2.1a)} \\
\Delta \psi &= q - h, \quad \text{(2.1b)}
\end{align*}
\]

where the potential vorticity (PV) \( q(x, t) \), the stream function \( \psi(x, t) \), and the orography \( h(x) \) are scalar fields, periodic in \( x \) and \( y \) with period \( 2\pi \). The Laplace operator is denoted by \( \Delta \), and the operator \( \mathcal{J} \) is defined by

\[
\mathcal{J}(q, \psi) = q_x \psi_y - q_y \psi_x. \quad \text{(2.2)}
\]

The QG equation is a Hamiltonian PDE [57] having Poisson bracket

\[
\{ \mathcal{F}, \mathcal{G} \} = \int_{\mathcal{D}} q \mathcal{J} \left( \frac{\delta \mathcal{F}}{\delta q}, \frac{\delta \mathcal{G}}{\delta q} \right) dx. \quad \text{(2.3)}
\]

and Hamiltonian functional

\[
\mathcal{E}[q] = -\frac{1}{2} \int_{\mathcal{D}} \psi \cdot (q - h) dx. \quad \text{(2.4)}
\]

The Poisson bracket is degenerate with Casimir invariants the generalized enstrophies \( \mathcal{C}[f] = \int_{\mathcal{D}} f(q) dx \) for arbitrary function \( f \), see Section 1.1. Of particular interest are the PV moments \( \mathcal{C}_r = \int_{\mathcal{D}} q^r dx, \ r = 1, 2, \ldots \). The most
important of these are the total circulation
\[ C \equiv C_1[q] = \int_D q \, dx. \tag{2.5} \]
and the second moment of vorticity, i.e. the enstrophy
\[ Z \equiv \frac{1}{2} C_2[q] = \frac{1}{2} \int_D q^2 \, dx. \tag{2.6} \]

2.3 Spatial semi-discretization

We first consider the discretization of (2.1) in space only. The resulting system of ordinary differential equations will be referred to as the semi-discretization, and we will primarily be concerned with its analysis and statistical mechanics.

When discretizing Hamiltonian PDEs, it is advisable to consider the discretizations of the Poisson bracket and the Hamiltonian separately. As noted in [51], if a discrete Poisson bracket can be constructed to maintain skew-symmetry and satisfy the Jacobi identity, then any quadrature for the Hamiltonian will yield a semi-discretization that is a Hamiltonian ODE, and consequently will conserve energy and (possibly some subclass of) Casimirs. From the point of view of statistical mechanics, it is also natural to consider the discretizations of the bracket and the Hamiltonian separately. The bracket ensures the conservation of energy and enstrophy and preservation of volume, which are necessary ingredients for the existence of a statistical theory at all. But only the conserved quantities themselves enter into the probability distribution. Thus the predictions of the theory depend only on the discretization of these conserved quantities. The discretization of the Hamiltonian (2.4) amounts to a choice for the discrete Laplacian in (2.1b) and will be treated latter. The bracket will be discretized with (generalized) Arakawa schemes in Section 2.3.1.

For Eulerian fluid models, the only known discretization with Poisson structure is the sine-bracket truncation of Zeitlin [88], which is limited to 2D, incompressible flows on periodic geometry, see Section 1.2. This truncation conserves \( M \) polynomial enstrophies on an \( M \times M \) grid. Its statistics are investigated in [1]. For more general fluid problems, no Poisson discretizations are available. In lieu of a semi-discretization with Poisson structure, one may attempt to construct discretizations which conserve desired first integrals and are volume preserving. The flow of energy is important for statistics, and the spatial discretization determines the local flow. In numerical weather prediction, energy conserving discretizations were advocated by Lorenz in 1960 [46]. Motivated by Lorenz’s work, Arakawa [2] constructed discretizations that conserved energy, enstrophy or both. As we will see, these discretizations are also all volume preserving.

We discretize (2.1) on a uniform \( M \times M \) grid. Let \( \Delta x = \Delta y = 2\pi/M \) and consider a grid function \( q(t) \in \mathbb{R}^{M \times M} \), with components \( q_{i,j}(t) \approx q(i\Delta x, j\Delta y, t) \), \( i, j = 0, \ldots, M-1 \), where periodicity is realized by identifying the indices \( M \).
and 0. We think of $q$ as a vector in an $M^2$-dimensional phase space; that is, we identify $\mathbb{R}^{M^2}$ and $\mathbb{R}^{M \times M}$, and use vector notation, e.g., $\Psi^T q$ for the vector inner product of two such vectors.

### Spectral solution of the stream function

The linear elliptic PDE (2.1b) is solved using the Fourier spectral method. Let the Fourier transform of $q \in \mathbb{R}^{M \times M}$ be defined by

$$\hat{q} = \mathcal{F}q \iff \hat{q}_{k,\ell} = \frac{1}{M^2} \sum_{i,j=0}^{M-1} q_{i,j} e^{-i(k+i+j\ell)}, \quad k, \ell = -M/2 + 1, \ldots, M/2.$$  

(2.7)

The inverse transform is $\mathcal{F}^{-1} = \mathcal{F}^*$, and Parseval’s identity reads

$$\sum_{i,j} q_{i,j}^2 = \sum_{k,\ell} |\hat{q}_{k,\ell}|^2.$$

Equation (2.1b) is solved exactly in Fourier-space. Denote the discrete Laplace operator by $\Delta_M$:

$$\Delta_M \psi = q - h \iff -(k^2 + \ell^2) \hat{\psi}_{k,\ell} = \hat{q}_{k,\ell} - \hat{h}_{k,\ell}, \quad k, \ell = -M/2 + 1, \ldots, M/2.$$  

(2.8)

This relation is solved for stream function field $\psi$ with mean zero. The inverse Laplacian restricted to the hyperplane $\hat{\psi}_{0,0} = 0$ is denoted by $\Delta_{M}^{-1}$, i.e.

$$\psi = \Delta_{M}^{-1} (q - h) \iff \hat{\psi}_{k,\ell} = \begin{cases} 0, & k = \ell = 0, \\ -(\hat{q}_{k,\ell} - \hat{h}_{k,\ell})/(k^2 + \ell^2), & \text{otherwise}. \end{cases}$$

### 2.3.1 Arakawa’s discretizations

Arakawa [2] constructed finite difference discretizations of (2.2) that preserve discrete versions of energy (2.4), enstrophy (2.6), or both. We consider generalizations to Arakawa’s discretizations with the Nambu bracket approach of [75].

Let $D_x$ and $D_y$ denote discretization matrices that (i) are skew symmetric: $D_x^T = -D_x$, $D_y^T = -D_y$, and (ii) approximate the first derivative in $x$ and $y$, respectively:

$$(D_x q)_{i,j} \approx q_x (i \Delta x, j \Delta y), \quad (D_y q)_{i,j} \approx q_y (i \Delta x, j \Delta y).$$

Arakawa’s classical discretizations [2] use the central differences

$$(D_x q)_{i,j} = \frac{q_{i+1,j} - q_{i-1,j}}{2 \Delta x}, \quad (D_y q)_{i,j} = \frac{q_{i,j+1} - q_{i,j-1}}{2 \Delta y},$$  

(2.9)

and these will also be used in our numerical experiments. However, we wish to stress that the statistical predictions in Section 2.4 remain unchanged for a different choice of (skew-symmetric) $D_x$ and $D_y$. 

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2.3. Spatial semi-discretization

Denote the element-wise product of two vectors by \((u \ast v)_{i,j} = u_{i,j}v_{i,j}\). The scalar product
\[
(u^T v) = \sum_{i,j} u_{i,j}v_{i,j}
\]
is fully symmetric with respect to the vectors \(u, v\) and \(w\).

Arakawa’s discretizations can be viewed as discrete approximations to the equivalent formulations of (2.2)
\[
\mathcal{J}(q, \psi) = q_x\psi_y - q_y\psi_x, \\
\mathcal{J}(q, \psi) = \partial_x(q\psi_y) - \partial_y(q\psi_x), \\
\mathcal{J}(q, \psi) = \partial_y(q_x \psi) - \partial_x(q_y \psi),
\]
and are given by
\[
J_0(q, \psi) = (D_x q) \ast (D_y \psi) - (D_y q) \ast (D_x \psi), \\
J_E(q, \psi) = D_x(q \ast D_y \psi) - D_y(q \ast D_x \psi), \\
J_Z(q, \psi) = D_y(\psi \ast D_x q) - D_x(\psi \ast D_y q),
\]
and the average of these
\[
J_{EZ}(q, \psi) = \frac{1}{3} [J_0(q, \psi) + J_E(q, \psi) + J_Z(q, \psi)].
\]
That is, the semi-discretizations are defined by (2.8) and
\[
\frac{d}{dt} q = J(q, \psi)
\]
for \(J\) taken to be one of (2.11)–(2.14).

The Arakawa schemes are interesting for us, because they are all based on the standard central difference operators applied in various ‘conservation forms’ and hence, for short simulations with smooth solutions, there is often little noticeable difference between different discretizations. One might therefore expect that they yield similar statistics. On the contrary, the long-term statistics differ greatly.

The conservation properties of these three discretizations were established for the case of second order differences (2.9) in [2]. The case (2.14) has been generalized using the Nambu bracket formalism [59, 60, 75]. Define the associated bracket (the gradients are with respect to \(q\))
\[
\{F, G, H\}_0 = -\nabla F^T J_0(\nabla G, \nabla H), \\
\{F, G, H\}_E = -\nabla F^T J_E(\nabla G, \nabla H), \\
\{F, G, H\}_Z = -\nabla F^T J_Z(\nabla G, \nabla H), \\
\{F, G, H\}_{EZ} = \frac{1}{3} [\{F, G, H\}_0 + \{F, G, H\}_E + \{F, G, H\}_Z]
\]
for arbitrary differentiable $F(q), G(q), H(q) : \mathbb{R}^{M^2} \rightarrow \mathbb{R}$.

The derivative $dF/dt$ of any function $F(q)$ along a solution $q(t)$ to the discrete equations (2.15) is given by the associated bracket of $F$ with $Z_M$ and $E_M:
\[
\frac{dF}{dt} = \{F, Z_M, E_M\}.
\]
(2.20)

where $E_M$ and $Z_M$ are discrete approximations to the energy
\[
E_M(q) = -\frac{1}{2} \psi^T(q - h) \Delta x \Delta y = \frac{1}{2} \sum_{k,\ell} (k^2 + \ell^2)|\hat{\psi}_{k,\ell}|^2 \Delta x \Delta y
\]
(2.21)

and enstrophy
\[
Z_M(q) = \frac{1}{2} q^T q \Delta x \Delta y = \frac{1}{2} \sum_{k,\ell} |\hat{q}_{k,\ell}|^2 \Delta x \Delta y.
\]
(2.22)

This fact can be used to prove the conservation properties of the various discretizations.

The proofs rely on the antisymmetry of (2.16) with respect to its last two arguments,
\[
\{F, G, H\}_0 = -\{F, H, G\}_0,
\]
as well as the identities
\[
\{F, G, H\}_E = \{G, H, F\}_0, \quad \{F, G, H\}_Z = \{H, F, G\}_0,
\]
all of which follow from the skew-symmetry of $D_x$ and $D_y$ and the symmetry of (2.10).

Taking $F \equiv E_M$ in (2.20), it follows that for $J_E,$
\[
\frac{dE_M}{dt} = \{E_M, Z_M, E_M\}_E = \{Z_M, E_M, E_M\}_0 = 0.
\]

Similarly, taking $F \equiv Z_M$ in (2.20), it follows that for $J_Z,$
\[
\frac{dZ_M}{dt} = \{Z_M, Z_M, E_M\}_Z = \{E_M, Z_M, Z_M\}_0 = 0.
\]

The bracket (2.19) is fully antisymmetric in all three arguments (hence it is a proper Nambu bracket), and therefore conserves both $E_M$ and $Z_M$. Finally, taking $F = C_M = \sum_{i,j} q_{i,j} \Delta x \Delta y$, one can show that all of the discretizations (2.16)-(2.19) conserve total circulation.

In reference to their conservation properties, we will refer to the discretizations (2.11)-(2.14) as the 0, $E$, $Z$ and $EZ$ discretizations, respectively.

One can check that a solution of the form $q = \mu \psi$, $\mu$ a scalar, is an exact steady state for the 0 and EZ discretizations. Such a solution is not, in general, a steady state solution for the $E$ and $Z$ discretizations. However, the limit cases \{$\psi \equiv 0, q = h$\} and \{$q \equiv 0, \psi = -\Delta^{-1}_h h$\} obviously are steady states to these discretizations.
2.3.2 Volume preservation

In addition to conservation, a second important ingredient for statistical mechanics is the preservation, by the flow map, of the phase space volume element. In this section we demonstrate that each of the discretizations from Section 2.3.1 is volume preserving. Let us define the matrix $D(a) = \text{diag}(a)$ to be the diagonal matrix whose diagonal elements are the components of the vector $a$ (i.e. $D(a)_{ij} = a_i \delta_{ij}$).

Recall that for an ODE

$$y' = f(y)$$

the divergence of the vector field $f$ satisfies

$$\text{div} \ f = \text{tr}(f'),$$

where $f'$ denotes the Jacobian matrix of $f$. In particular, for a matrix $A$, $\text{div} Af(y) = \text{tr}(Af')$. Furthermore, for

$$y' = f(y) = g(y) * h(y)$$

it holds that

$$f' = D(g)h' + D(h)g'.$$

In the following calculations we make ready use of the commutative and transpose properties of the trace $\text{tr}(AB) = \text{tr}(BA) = \text{tr}(B^T A^T)$. We also need the following properties of our discretization matrices. The difference operators $D_x$ and $D_y$ are given by symmetric finite difference stencils, are skew-symmetric and commute $D_x D_y - D_y D_x = 0$. The discrete inverse Laplacian matrix $\Delta_M^{-1}$ is symmetric and represents a (global) central finite difference stencil. In this case, the matrices $D_x \Delta_M^{-1}$ and $D_y \Delta_M^{-1}$ have zeros on the diagonal.

Let us write the discretizations (2.11)-(2.13) as functions of $q$ only

$$J_0(q) = (D_x q) * (D_y \Delta_M^{-1} q) - (D_y q) * (D_x \Delta_M^{-1} q),$$

(2.23)

$$J_E(q) = D_x (q * D_y \Delta_M^{-1} q) - D_y (q * D_x \Delta_M^{-1} q),$$

(2.24)

$$J_Z(q) = D_y ((D_x q) * \Delta_M^{-1} q) - D_x ((D_y q) * \Delta_M^{-1} q).$$

(2.25)

Proposition 2.1. The vector fields defined by (2.23)-(2.25) and their average $J_{EZ} = (J_0 + J_E + J_Z)/3$ are divergence free.

**Proof.** We calculate, for (2.23),

$$\text{div} \ J_0(q) = \text{tr} \ (D(D_y \Delta_M^{-1} q)D_x) + \text{tr} \ (D(D_x q)D_y \Delta_M^{-1})$$

$$- \text{tr} \ (D(D_x \Delta_M^{-1} q)D_y) - \text{tr} \ (D(D_y q)D_x \Delta_M^{-1}) = 0,$$

(2.26)

since each term is the trace of the product of a diagonal matrix and a matrix with zero diagonal.
Chapter 2. Statistical mechanics of Arakawa’s discretizations

2.4 Energy-enstrophy statistical theory

The equilibrium statistical mechanical theory for 2D ideal fluids was developed by Kraichnan [40], Salmon et al. [76], and Carnevale & Frederiksen [11]. It is based on a finite truncation of the spectral decomposition of the equations of motion. Statistical predictions are obtained for the truncated system, and these are extended to the infinite dimensional limit, see Section 1.3.3.

Here we would like to adapt the analysis to the semi-discretizations outlined in the previous section. For the discretization $EZ$, which conserves both energy and enstrophy, the analysis is identical to the spectral case developed by Carnevale & Frederiksen [11]. Consequently, most of the material in Sections 2.4.1, 2.4.2 and 2.4.3 is simply summarized from Chapters 7 and 8 of Majda & Wang [48]. In Section 2.4.4 we modify the statistical predictions of the energy-enstrophy theory to the cases of only one quantity conserved.

As previously noted, semi-discretization of (2.1) using the bracket (2.14) yields a system of $M^2$ ordinary differential equations having the Liouville property and two first integrals that approximate the energy (2.21) and enstrophy (2.22). Due to the Liouville property, one can speak of transport of probability density functions by this semi-discrete flow, and consider equilibrium solutions to Liouville’s equation. Any normalized function of the two first integrals is an equilibrium distribution.

\[ \text{div } J_E(q) = \text{tr} (D_x [D(q)D_y \Delta^{-1}_M + D(D_q \Delta^{-1}_M q)]) \\
- \text{tr} (D_y [D(q)D_x \Delta^{-1}_M + D(D_q \Delta^{-1}_M q)]) \\
= \text{tr}(D(q)(D_y \Delta^{-1}_M D_x - D_x \Delta^{-1}_M D_y)) \\
+ \text{tr}(D_x D_y \Delta^{-1}_M q) - D_y D_y \Delta^{-1}_M q) = 0. \]

The term in bracket in the last expression is identically zero by symmetry considerations.

Similarly, for (2.25) we have

\[ \text{div } J_Z(q) = \text{tr} (D_y [D(\Delta^{-1}_M q)D_x + D(D_q \Delta^{-1}_M)]) \\
- \text{tr} (D_x [D(\Delta^{-1}_M q)D_y + D(D_q \Delta^{-1}_M)]) \\
= \text{tr}(D(\Delta^{-1}_M q)(D_x D_y - D_y D_x)) \\
+ \text{tr}(D(D_q \Delta^{-1}_M q) - D_y D_y \Delta^{-1}_M q) = 0. \]

Finally, discretization $EZ$ is divergence-free because it is a linear combination of divergence-free vector fields. □

\[ 1 \text{All discretizations also conserve the discrete total circulation } C_M = \sum_{i,j} q_{i,j} \Delta x \Delta y. \text{ Since } C_M \text{ is a linear first integral, any standard integrator will conserve it exactly in time. A nonzero value of } C_M \text{ will give a constant displacement in (2.32). For a periodic domain one may assume that } C_M = 0 \text{ so that its effects can be ignored. We do so in the numerical experiments.} \]
2.4. Energy-enstrophy statistical theory

We note in advance that that a solution of the semidiscrete equations (2.15) is constrained to the intersection of hypersurfaces defined by the relevant first integrals of the the discretization. The probability distributions obtained from the maximum entropy theory have nonzero probability everywhere in phase space, and as such, are a very crude approximation to the statistics of a single trajectory. Nonetheless, we will see that the maximum entropy theory accurately predicts the differences in long term averages observed for the discretizations (2.12)-(2.14). More on this will be said in Section 2.5.

2.4.1 Mean field predictions

The equilibrium distribution of least bias maximizes entropy under the constraints imposed by conservation of energy and enstrophy. Let \( \mathbf{y} \) parameterize the \( M^2 \) dimensional phase space; that is, each \( \mathbf{y} \in \mathbb{R}^{M \times M} \) corresponds to a particular realization of the grid function (or discrete field) \( q \). Consider the class of probability distribution \( \rho : \mathbb{R}^{M \times M} \rightarrow \mathbb{R} \) on phase space, satisfying

\[
\rho(\mathbf{y}) \geq 0, \quad \int_{\mathbb{R}^{M \times M}} \rho(\mathbf{y}) \, d\mathbf{y} = 1. \tag{2.27}
\]

The least biased distribution \( \rho^* \) maximizes the entropy functional

\[
S[\rho] = -\int_{\mathbb{R}^{M \times M}} \rho(\mathbf{y}) \ln \rho(\mathbf{y}) \, d\mathbf{y} \tag{2.28}
\]

under constraints on the ensemble averages of energy:

\[
\int_{\mathbb{R}^{M \times M}} E_M(\mathbf{y}) \rho(\mathbf{y}) \, d\mathbf{y} - E_M^* = 0, \tag{2.29}
\]

and enstrophy:

\[
\int_{\mathbb{R}^{M \times M}} Z_M(\mathbf{y}) \rho(\mathbf{y}) \, d\mathbf{y} - Z_M^* = 0, \tag{2.30}
\]

where \( E_M^* \) and \( Z_M^* \) are prescribed values. Additionally, there is the constraint implied by (2.27). Using the method of Lagrange multipliers, the maximizer is the Gibbs-like distribution (i.e. \( \rho^* = \mathcal{G} \))

\[
\mathcal{G}(\mathbf{y}) = N^{-1} \exp \left\{ -\alpha (Z_M(\mathbf{y}) + \mu E_M(\mathbf{y})) \right\}, \tag{2.31}
\]

where \( N, \alpha \), and \( \mu \) are chosen to ensure (2.27), (2.29) and (2.30).

The expected value of a function \( F(\mathbf{y}) \) is the ensemble average of \( F \) with the measure \( \mathcal{G} \), denoted

\[
\langle F \rangle = \int_{\mathbb{R}^{M \times M}} F(\mathbf{y}) \mathcal{G}(\mathbf{y}) \, d\mathbf{y}.
\]

The mean state is obtained from the observation

\[
\left\langle \frac{\partial Z_M}{\partial \mathbf{y}} + \mu \frac{\partial E_M}{\partial \mathbf{y}} \right\rangle = \int_{\mathbb{R}^{M \times M}} \left( \frac{\partial Z_M}{\partial \mathbf{y}} + \mu \frac{\partial E_M}{\partial \mathbf{y}} \right) N^{-1} e^{-\alpha (Z_M(\mathbf{y}) + \mu E_M(\mathbf{y}))} \, d\mathbf{y}
\]

\[
= -\alpha^{-1} \int_{\mathbb{R}^{M \times M}} \frac{\partial}{\partial \mathbf{y}} \mathcal{G}(\mathbf{y}) \, d\mathbf{y} = 0,
\]
assuming $G$ decays sufficiently fast at infinity. Since $\nabla_q E_M = -\psi$ and $\nabla_q Z_M = q$, the mean field relation
\begin{equation}
\langle q \rangle = \mu(\psi) \tag{2.32}
\end{equation}
follows. In other words, the ensemble averages of potential vorticity and stream function are linearly related. Combining (2.32) with the second relation of (2.1) yields a modified Helmholtz problem for the mean stream function given $\mu_r$:
\begin{equation}
(\mu - \Delta_m)\langle \psi \rangle = h. \tag{2.33}
\end{equation}

### 2.4.2 PV fluctuation predictions

In this section we adapt the point statistics of Majda & Wang [48] to yield predictions in terms of potential vorticity. The mean state (2.32) is a nonlinearly stable equilibrium [11]. Solutions to (2.1) may be decomposed into mean and fluctuation parts
\[ q = \langle q \rangle + q', \quad \psi = \langle \psi \rangle + \psi', \quad \langle q \rangle = \mu(\psi). \]
The fluctuation quantities satisfy
\begin{equation}
q_i' = J(q', \psi') + J(q', \psi) + J(q', \psi'), \quad \Delta_m \psi' = q'. \tag{2.34}
\end{equation}
This differential equation has the first integral
\begin{equation}
I_M(q') = Z'_M + \mu E'_M, \quad Z'_M = \frac{1}{2}(q')^T q' \Delta x \Delta y, \quad E'_M = -\frac{1}{2} (\psi')^T q' \Delta x \Delta y. \tag{2.35}
\end{equation}
One can also set up a statistical mechanics for the fluctuation equations and obtain predictions. To do so, let
\begin{equation}
\hat{p}_{k,\ell} = \left(1 + \frac{\mu}{k^2 + \ell^2}\right)^{1/2} \hat{q}_{k,\ell}'. \tag{2.36}
\end{equation}
Then the Fourier transform of (2.35) gives
\begin{equation}
I_M = \frac{1}{2} \sum_{k,\ell} \left(1 + \frac{\mu}{k^2 + \ell^2}\right) |q_{k,\ell}'|^2 \Delta x \Delta y = \frac{1}{2} \sum_{k,\ell} |\hat{p}_{k,\ell}'|^2 \Delta x \Delta y = \frac{1}{2} \sum_{i,j} \hat{p}_{i,j}^2 \Delta x \Delta y. \tag{2.37}
\end{equation}
The maximum entropy condition for this first integral yields the Gibbs distribution $\mathcal{G}(p) = N^{-1} \exp \left(-\beta I_M(p)\right)$, which is the product of identical Gaussian distributions with mean zero and standard deviation
\[ \eta_p = \sqrt{\frac{2 \langle I_M \rangle}{M^2 \Delta x \Delta y}} = \sqrt{\frac{\langle I_M \rangle}{2\pi^2}}. \]
The energy is equipartitioned.
Let us also assume that the $p_{i,j}$ are independent. Let $P = \mathbf{a}^T \mathbf{p}$ denote a linear combination of the $p_{i,j}$. Since these are identically distributed, $P$ is Gaussian with variation

$$\eta(P)^2 = \mathbf{a}^T \mathbf{a} \eta_p^2 = |\mathbf{a}|^2 \eta_p^2.$$  

From (2.36) we have

$$\mathbf{q}' = \mathcal{F}^{-1} \text{diag} \left( \left( 1 + \frac{\mu}{k^2 + \ell^2} \right)^{-1/2} \right) \mathcal{F} \mathbf{p} = A \mathbf{p},$$

where $A$ is real and symmetric. It follows that the $q'_{i,j}$ at each grid point $i, j$ are identically normally distributed with mean zero and variance

$$\eta_q^2 = |\mathbf{a}|^2 \eta_p^2 = |\mathbf{a}|^2 \langle I_M \rangle / 2\pi^2,$$

where for $\mathbf{a}$ we can take any row of $A$.

### 2.4.3 Approximation of $\mu$ and $\alpha$

The ensemble averages of energy and enstrophy can be split into a mean part and a fluctuation part [11, 48]:

$$\langle E_M \rangle = E_M(\langle \mathbf{q} \rangle) + E'_M, \quad \langle Z_M \rangle = Z_M(\langle \mathbf{q} \rangle) + Z'_M,$$

where, using (2.33),

$$E_M(\langle \mathbf{q} \rangle) = -\frac{1}{2} \langle \psi \rangle^T (\langle \mathbf{q} \rangle - \mathbf{h}) \Delta x \Delta y = \frac{1}{2} \sum_{k,\ell=-M/2+1}^{M/2} (k^2 + \ell^2) |\hat{h}_{k,\ell}|^2 (\mu + k^2 + \ell^2)^2 \Delta x \Delta y,$$

(2.40a)

$$E'_M = \frac{1}{2\alpha} \sum_{k,\ell=-M/2+1}^{M/2} \frac{1}{\mu + k^2 + \ell^2},$$

(2.40b)

and

$$Z_M(\langle \mathbf{q} \rangle) = \frac{1}{2} \langle \psi \rangle^T (\mathbf{q}) \Delta x \Delta y = \frac{1}{2} \sum_{k,\ell=-M/2+1}^{M/2} \frac{\mu^2 |\hat{h}_{k,\ell}|^2}{(\mu + k^2 + \ell^2)^2} \Delta x \Delta y,$$

(2.41a)

$$Z'_M = \frac{1}{2\alpha} \sum_{k,\ell=-M/2+1}^{M/2} \frac{k^2 + \ell^2}{\mu + k^2 + \ell^2}.$$  

(2.41b)

Given guesses for $\mu$ and $\alpha$, it is straightforward to compute $\langle E_M \rangle$ and $\langle Z_M \rangle$ by solving (2.40) and (2.41) and then substituting into (2.39). To estimate $\mu$ and $\alpha$, we proceed iteratively to implicitly solve (2.29) and (2.30) under that assumptions $E''_M \approx E_0$ and $Z''_M \approx Z_0$. 
2.4.4 Alternative statistical theories

In this section we derive alternative statistical models for the cases where either energy or enstrophy, but not both, is conserved numerically.

**Energy-based statistical mechanics**

For a semi-discretization that only preserves the energy $E_M$, the least biased distribution (2.31) becomes

$$G_E(y) = N^{-1} \exp \left[ -\lambda E_M(y) \right].$$

The mean field prediction (2.32) gives

$$\langle \psi \rangle \equiv 0, \quad \langle q \rangle = \mathbf{h}. \quad (2.42)$$

The fluctuation dynamics (2.34) becomes

$$\dot{q}_i = J_E(h + q', \psi'), \quad \psi' = \Delta_M^{-1} q',$$

which preserves the pseudo-energy

$$I_M = -\frac{1}{2} (\psi')^T q' \Delta x \Delta y = E'_M \approx E_0.$$

We define

$$\hat{p}_{k,\ell} = \frac{\hat{q}'_{k,\ell}}{(k^2 + \ell^2)^{1/2}}.$$

The fluctuation Gibbs distribution is again Gaussian with $\eta_p = (\langle I_M \rangle/2\pi^2)^{1/2}$. The standard deviation $\eta_q$ of the fluctuation vorticity is given by (2.38) with $A = (-\Delta_M)^{1/2}$.

**Enstrophy-based statistical mechanics**

For a semi-discretization that only preserves the enstrophy $Z_M$, the least biased distribution (2.31) becomes

$$G_E(y) = N^{-1} \exp \left[ -\lambda Z_M(y) \right].$$

The mean field prediction (2.32) gives

$$\langle q \rangle \equiv 0, \quad \langle \psi \rangle = -\Delta_M^{-1} \mathbf{h}. \quad (2.43)$$

The fluctuation dynamics (2.34) becomes

$$\dot{q}' = J_Z(q', \langle \psi \rangle + \psi'), \quad \psi' = \Delta_M^{-1} q',$$

and the pseudo-energy is just the enstrophy, i.e.

$$I_M = \frac{1}{2} (q')^T q' \Delta x \Delta y = Z'_M \approx Z_0.$$

The fluctuation Gibbs distribution is Gaussian with $\hat{p}_{k,\ell} = \hat{q}'_{k,\ell}$ and

$$\eta_q = \sqrt{\frac{\langle I_M \rangle}{2\pi^2}}.$$
2.5 Time integration

To test the statistical predictions of the previous section with computations, the semi-discretizations of Section 2.3 must be supplemented with a time stepping scheme. One would prefer to have a scheme that conserves the invariants \( E_M \) and \( Z_M \) in time whenever these are first integrals of the spatial discretization. Additionally, one would like to have a scheme that preserves volume. There is much literature on the preservation of first integrals under discretization; see [35] for an overview. Much less is known about preserving volume.

Time discretizations

Since both invariants \( E_M \) and \( Z_M \) of the discretizations are quadratic functions of \( q \), they are automatically conserved if the equations are integrated with a Gauss-Legendre Runge-Kutta method [35]. The simplest such method is the implicit midpoint rule

\[
\frac{q^{n+1} - q^n}{\Delta t} = J \left( \frac{q^{n+1} + q^n}{2}, \frac{\psi^{n+1} + \psi^n}{2} \right).
\]

The discretization is also symmetric, and in the case of zero topography \( h(x) \equiv 0 \), preserves the time reversal symmetry \( t \mapsto -t, \ q \mapsto -q \) of (2.1). Although it is symplectic for Hamiltonian systems with constant structure operators, the midpoint rule is not volume preserving in general. Indeed, it does not preserve volume exactly for our discretizations. However, numerical experiments indicate that volume is approximately conserved on long intervals, even for a relatively large step size.

The implicit midpoint rule requires the solution of a nonlinear system of dimension \( M^2 \) at every time step. As a more efficient alternative, we can take any explicit Runge-Kutta method and project the solution onto the integral manifolds as desired. Let the Runge-Kutta method be represented by a map \( q^{n+1} = \Phi_{\Delta t}(q^n) \) and compute a predicted step

\[
q^* = \Phi_{\Delta t}(q^n).
\]

Then project \( q^* \) onto the desired constraint manifolds by solving

\[
q^{n+1} = q^* + g'(q^*)^T \lambda,
\]

\[
g(q^{n+1}) = 0
\]

for \( \lambda \), where \( g(q) : \mathbb{R}^{M \times M} \rightarrow \mathbb{R}^r \), \( r \) the number of first integrals, and \( \lambda \in \mathbb{R}^r \) is a vector of Lagrange multipliers. For example, we can take \( (r = 3) \)

\[
g(q) = \begin{pmatrix}
E_M(q) - E_0 \\
Z_M(q) - Z_0 \\
C_M(q) - 0
\end{pmatrix},
\]
where the last constraint ensures that there is no drift in total vorticity. At each
time step, projection requires solving a small nonlinear problem of dimension 
$r$. Projected Runge-Kutta methods will not preserve volume in general.

## Time averages

Our interest is in the statistics applied to numerical data obtained from sim-
ulations over long times. To apply the theory from the previous sections, we
additionally have to assume that the semi-discrete dynamics are ergodic. De-
ote the time average of a quantity $F(q(t))$ by

$$
\overline{F}_T = \frac{1}{T} \int_{t_0}^{t_0+T} F(q(t)) \, dt.
$$

Then the assumption of ergodicity implies that the long time average converges
to the ensemble average:

$$
\overline{F} = \lim_{T \to \infty} \overline{F}_T = \langle F \rangle.
$$

On the other hand, suppose one chooses discrete initial conditions to have
a prescribed energy and enstrophy consistent with the continuum problem, i.e.

$$
E_M(q(0)) = E_0, \quad Z_M(q(0)) = Z_0.
$$

Then it is clear that since $E_M(q(t)) = E_M(q(0))$ and $Z_M(q(t)) = Z_M(q(0))$ are
conserved, the dynamics only samples at most a codimension two subspace of
$\mathbb{R}^{M \times M}$, so one may ask to what extent the averages will converge. Indeed, one
has inequality

$$
\overline{E}_M = \langle E_M \rangle \neq E_0, \quad \overline{Z}_M = \langle Z_M \rangle \neq Z_0,
$$

in general. By analogy with molecular dynamics, the Gibbs distribution (2.31)
determines expectations in the canonical ensemble, whereas a constant energy-
enstrophy simulation determines expectations in the microcanonical ensemble
(assuming ergodicity). It is only in the ‘thermodynamic limit’ $M \to \infty$ that
these averages coincide, giving equality in the above relations.

### 2.6 Numerical experiments

For the numerical experiments we use the test problem of [1]. The grid resolution
is $M = 22$. The orography is a function of $x$ only, specifically

$$
h(x, y) = 0.2 \cos x + 0.4 \cos 2x.
$$

(As a result the predicted mean fields $\overline{q}$ and $\overline{\psi}$ should be functions of $x$ only.)
The integrations were carried out using a step size of $\Delta t = 0.1$. 

2.6. Numerical experiments

For initial conditions we take a uniformly random field, \( q = (q_{i,j}), i,j = 1, \ldots, M \) and project this onto the constraints
\[
E_M(q) = \mathcal{E}_0, \quad Z_M(q) = \mathcal{Z}_0, \quad C_M(q) = 0.
\]
The same initial condition is used for all simulations. The discrete energy and enstrophy were taken to be \( \mathcal{E}_0 = 7 \) and \( \mathcal{Z}_0 = 20 \).

With these values prescribed, the statistical predictions of Section 2.4 can be computed for the three discretizations (2.12), (2.13), and (2.14). The Lagrange multiplier \( \mu \) is computed using the procedure described at the end of Section 2.4.3. Fluctuation statistics apply to the time series of PV at an arbitrarily chosen monitor point on the grid \( q_{\text{mon}} = q_{3,12} \).

For the energy-enstrophy theory we obtain the mean state (2.32) and estimates
\[
E_Z: \quad \mu = -0.730, \quad \langle q_{\text{mon}} \rangle = -0.341, \quad \eta_q = 0.970. \tag{2.44}
\]
For the energy theory of Section 2.4.4 we obtain the mean state (2.42) and estimates
\[
E: \quad \langle \psi \rangle = 0, \quad \langle q_{\text{mon}} \rangle = 0.0740, \quad \eta_q = 5.36. \tag{2.45}
\]
For the enstrophy theory of Section 2.4.4 we obtain the mean state (2.43) and estimates
\[
Z: \quad \mu = 0, \quad \langle q_{\text{mon}} \rangle = 0, \quad \eta_q = 1.01. \tag{2.46}
\]

The discretization (2.11), which conserves neither energy nor enstrophy, was found to be exponentially unstable under time discretization by the implicit midpoint rule, and no experiments with that discretization will be reported here.

Results using implicit midpoint

We first present results obtained using the implicit midpoint discretization in time. The nonlinear relations were solved using fixed point iteration to a tolerance of \( 10^{-13} \), which was the smallest tolerance that gave convergence at each step size for all discretizations. The solutions were averaged over the interval \( 10^3 \leq t \leq T \), for \( T = 10^4, 10^5 \) and \( 10^6 \). Averages were computed from time \( t = 1000 \) to allow the initially uniformly random initial condition to de-correlate, and this time is consistent with that used in [1] for a spectral discretization.

Given the average fields \( \overline{q} \) and \( \overline{\psi} \), the best linear fit to (2.32) yields an estimate of the Lagrange multiplier \( \overline{\mu} \), i.e.
\[
\overline{\mu} = \frac{\overline{\psi}^{-1} \overline{q}}{\overline{\psi} \overline{\psi}}.
\]

\(^2\)Experiments with smooth initial conditions typically show no noticeable difference, however.
The relative change in energy and enstrophy for each discretization is plotted in Figure 2.1 on the interval $[0, 10^5]$. The relative change is defined as

$$\Delta E_M^n = \frac{E_M^n - E_0}{E_0}, \quad \Delta Z_M^n = \frac{Z_M^n - Z_0}{Z_0}.$$  

For the $EZ$ discretization, both quantities are conserved up to the tolerance of the fixed point iteration, which leads to a small drift of magnitude $3 \times 10^{-11}$ (relative) over this interval. For the $E$ discretization, energy is conserved to the tolerance of the fixed point iteration, but enstrophy makes a rapid jump to a mean state roughly 30 times its initial value and subsequently undergoes bounded fluctuations with amplitude about $10 \times Z_0$. In contrast, for the $Z$ discretization, enstrophy is similarly conserved, but energy drifts gradually with a negative trend, to about 25% of its initial value.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig21.png}
\caption{Relative change in energy and enstrophy with $EZ$ (left), $E$ (middle) and $Z$ (right) discretizations.}
\end{figure}

**Long-time mean fields**

The time-averaged stream function $\overline{\psi}$ obtained by averaging over the interval $[10^3, 10^4]$ is shown in Figure 2.2 for the three $EZ$, $E$ and $Z$ discretizations. Also shown is a scatter plot of the locus $(\overline{\psi}_{i,j}, \overline{T}_{i,j})$ and a linear best fit to this data for the respective discretizations.

For the $EZ$ discretization, the mean stream function is similar to that predicted by the energy-enstrophy statistical theory (2.32), with $\overline{\psi} = -0.734$. For the $E$ discretization, the mean stream function satisfies $\overline{\psi} \approx 0$, consistent with (2.42), and the linear regression is inaccurate. For the $Z$ discretization, we observe a similar mean state with $\overline{\psi} = -0.715$ on this averaging interval, which is inconsistent with prediction (2.46).

In Figures 2.3 and 2.4 we examine more closely the mean fields for the $EZ$ and $Z$ discretizations, for longer averaging times of $T = 10^5$ and $T = 10^6$. For the energy-enstrophy discretization (2.14) in Figure 2.3, the mean field appears to converge to an equilibrium state with $\overline{\psi} \approx -0.732$. The tendency in Figure 2.4 is toward a mean field with zero vorticity, consistent with (2.43).
However the relaxation time is much longer than for the other discretizations. For $T = 10^6$, the mean flow has $\bar{\psi} = -0.0529$. Note that the relation $\bar{\psi} = \bar{\psi} \bar{\psi}$ approximates the data well for all averaging times, however. Below in this section, we show that the convergence of the $Z$ discretization is in agreement with the $EZ$ predictions on short time intervals, so that we can think of the system staying near statistical equilibrium with slowly drifting energy.

**PV fluctuation statistics**

In Figure 2.5, the time series for potential vorticity $\eta_{\text{mon}}$ at an arbitrarily chosen grid point $(3, 12)$ is analyzed. As discussed in Section 2.4.2, the statistical theory for fluctuations predicts that the PV should be distributed normally about the mean field according to (2.44)–(2.46). For the longest simulation time of $T = 10^6$, the $EZ$ discretization exhibits Gaussian fluctuations with mean $\bar{\eta}_{\text{mon}} = -0.395$ and standard deviation $\eta = 0.927$; the $E$ discretization with mean $\bar{\eta}_{\text{mon}} = -0.0093$ and standard deviation $\eta = 5.35$; and the $Z$ discretization with mean $\bar{\eta}_{\text{mon}} = -0.0575$ and standard deviation $\eta = 1.05$. These observations are approximately in agreement with (2.44)–(2.46).

We mention that the value $\bar{\psi} = -0.732$, to which the $EZ$ discretization seems to relax, corresponds to a mean energy value of $\langle E_M \rangle = 7.07$. For this value of mean energy, the prediction of Section 2.4.2 gives $\eta = 0.928$, which is much closer to the value observed in Figure 2.5. This indicates that for implicit midpoint, the mean energy is somewhat perturbed from the microcanonical energy $E_0$.

**Time-dependent energy-enstrophy model**

In Figure 2.6, the convergence of $\bar{\psi}$ is plotted as a function of averaging interval $T$ for both the $Z$ and $EZ$ discretizations. The $EZ$ dynamics relaxes very rapidly to give $\bar{\psi} \approx -0.73$, whereas the $Z$ dynamics converges rather slowly towards $\bar{\psi} = 0$.

Given the relatively fast relaxation of the energy-enstrophy conserving discretization to statistical equilibrium (2.32) and the slow drift of energy in Figure 2.1 for the enstrophy conserving discretization (2.13), a natural model for the approach to equilibrium would be to consider a state $\bar{\psi}_T = \bar{\mu}_T \bar{\psi}_T$ with $\bar{\mu}_T$ corresponding to the instantaneous energy $E_M(T)$. To test this idea, we define

$$\bar{\psi}_T = \frac{1}{N_T} \sum_{n=N_0}^{N_T+N_0} \psi^n, \quad \bar{\eta}_T = \frac{1}{N_T} \sum_{n=N_0}^{N_T+N_0} \eta^n,$$

where $T = N_T \cdot \Delta t$, and

$$\bar{\mu}_T = \frac{(\bar{\psi}_T)T \bar{\psi}_T}{(\bar{\psi}_T)T}.$$

The energy of the associated equilibrium state is denoted $E_M(\bar{\mu}_T)$ and is determined from the relations in Section 2.4.3. This energy is plotted in Figure 2.7.
Chapter 2. Statistical mechanics of Arakawa’s discretizations

Figure 2.2: Mean fields with averaging time $10^4$, EZ (left), E (middle), and Z (right). The insets show the best linear fit to the relation $\psi_{i,j} = \theta q_{i,j}$ at all grid points.

Figure 2.3: Mean fields for EZ discretization with averaging times $10^4$ (left), $10^5$ (middle), and $10^6$ (right). The insets show the best linear fit to the relation $\psi_{i,j} = \theta q_{i,j}$ at all grid points.

Figure 2.4: Mean fields for discretization $J_Z$ with averaging times $10^4$ (left), $10^5$ (middle), and $10^6$ (right). The insets show the best linear fit to the relation $\psi_{i,j} = \theta q_{i,j}$ at all grid points.
2.6. Numerical experiments

Figure 2.5: Fluctuation statistics for the potential vorticity about the predicted mean. Solid line is a Gaussian fit to the numerical observation. Dash line is the predicted distribution. Discretizations $EZ$, $E$, and $Z$ in left, middle and right columns. Integration intervals of $10^4$, $10^5$ and $10^6$ in top, middle and bottom rows.

next to the actual discrete energy function, for increasing averaging intervals $T = 10$, $T = 100$ and $T = 1000$. The agreement supports this model. That is, the $Z$ dynamics relaxes on a fast time scale to the statistical equilibrium predicted by energy-enstrophy theory for the instantaneous energy, while the energy drifts on a slow time scale towards the equilibrium state predicted by the enstrophy theory.

Results using projected Heun’s method

Besides preserving quadratic first integrals exactly, the implicit midpoint rule is symmetric. It is unclear what effect, if any, this may have on statistics. Furthermore, the implicit midpoint rule is fully implicit and therefore not a very practical choice for integrating a nonstiff system such as (2.1). For these reasons we repeat the experiments of the previous section using the second order, explicit Runge-Kutta method due to Heun [36], coupled with projection onto the discrete energy and/or enstrophy manifolds. It should be noted that
Figure 2.6: Convergence of parameter $\bar{\mu}_T$ as a function of the averaging interval $T$ for the $EZ$ and $Z$ discretizations.

Heun’s method is linearly unstable with respect to a center equilibrium, and it is only due to projection that we can carry out long integrations with this method.

Figure 2.8 compares the convergence of the parameter $\bar{\mu}_T$ as a function of $T$ for the implicit midpoint and projected Heun integrators for the $EZ$ and $Z$ discretizations. In both cases, it appears that the projected method approaches equilibrium faster than implicit midpoint.

Figures 2.9, 2.10 and 2.11 are analogous to Figures 2.2, 2.3 and 2.4 for implicit midpoint. Again we note that the projected method converges more rapidly and more accurately to the mean states (2.44)–(2.46).

The fluctuation statistics for the projection method are illustrated in Figure 2.12. Here, too, we see that the projection method is very close to the statistically predicted value for mean and standard deviation of PV fluctuations in (2.44)–(2.46). However, it is important to note that since a measure of predictability is the deviation from the statistical equilibrium, a numerical method that approaches equilibrium excessively fast is undesirable from a prediction perspective.

Discrete volume preservation

Although the spatial discretizations were shown to be volume preserving, neither the implicit midpoint rule nor the projected Heun integrator preserves volume for the discrete map. To get an impression of the degree of volume contraction, we computed the determinant of the Jacobian of the discrete flow maps, e.g.

$$c^n = \det \left( \frac{dq^{n+1}}{dq^n} \right)$$
2.7 Conclusions

![Energy drift with Z discretization comparison](image)

Figure 2.7: Energy drift with $Z$ discretization, compared to the energy associated with the best linear fit $\mu_T$ with averaging intervals $T = 10$, $T = 100$ and $T = 1000$.

in each time step. The cumulative volume ratio was defined to be

$$V^n = \prod_{m=0}^{n} c^m.$$

This volume ratio is plotted as a function of time in Figure 2.13 for the implicit midpoint and projected Heun methods. In both cases, a grid of size $M = 12$ was and step size $\Delta t = 0.1$ were used. The $EZ$ discretization (2.14) was employed, with in the second case, projection onto the energy and enstrophy manifolds.

Remarkably, the implicit midpoint rule conserves volume to within $3 \times 10^{-3}$ over the entire interval, exhibiting only a small positive drift.

For the projected method, volume is greatly contracted—to $10^{-4}$ at time $t = 10$ (100 time steps).

2.7 Conclusions

We have constructed statistical mechanical theories for three conservative discretizations of the quasigeostrophic model due to Arakawa [2], based on conser-
Figure 2.8: Convergence of $\pi_T$ as a function of averaging interval $T$ for EZ (left) and Z (right) discretizations, comparing the projected Heun's method and implicit midpoint.

vation of energy, enstrophy, or both. Numerical experiments indicate that the statistical theories can give insight into the long time behavior of the discretizations, making this approach a useful tool for numerical analysis.

Time integration of the semi-discretization was done with the symmetric implicit midpoint method—which automatically conserves any quadratic first integrals of the semi-discrete system—and with a projected Runge-Kutta method. Long time averages with the implicit midpoint discretization relax to the predicted equilibrium at a slower rate than for the projected method, suggesting that implicit midpoint has higher potential for prediction. The implicit midpoint rule was also found to approximately conserve volume for long time intervals. This is in stark contrast to the projection method, for which phase space volume is rapidly contracted.

The three statistical theories predict dramatically different behavior, and this is confirmed by the numerical experiments. In other words, the three discretizations exhibit dramatically different behavior in simulations over long intervals. The statistical equilibrium states define a backdrop on which the discrete dynamics occurs, and that backdrop depends on the conservation properties of the spatial discretization. Assuming the energy-enstrophy theory to be correct, it is thus essential for any code to preserve both quantities (under semi-discretization) if statistical consistency is desired. The results of this work make a strong argument for the use of conservative discretizations in weather and climate simulations.

On the other hand, it has been shown by Abramov & Majda [1] that the energy-enstrophy theory is incomplete. In [1], the Poisson discretization of [88] is integrated using the Poisson splitting of McLachlan [50]. The semi-discretization preserves, in addition to the Hamiltonian, $M$ Casimirs corre-
2.7. Conclusions

Figure 2.9: Same as Figure 2.2, but using projected Heun’s method.

Figure 2.10: Same as Figure 2.3, but using projected Heun’s method.

Figure 2.11: Same as Figure 2.4, but using projected Heun’s method.
Figure 2.12: Same as Figure 2.5, but using projected Heun’s method.

Figure 2.13: Volume contraction ratio for implicit midpoint (left) and projected Heun (right) methods, EZ discretization (2.14), $M = 12, 10^4$ time steps.

Sponding to the first $M$ moments of potential vorticity (PV), and these are
preserved by the splitting (the energy is only preserved approximately, in the sense of backward error analysis [35]). Abramov & Majda give convincing evidence that nonzero values of the third moment of PV, when conserved by the discretization, can significantly skew the predictions of the standard theory of [11, 40, 48, 76]. In Chapter 3 we will consider statistical theories for the Hamiltonian particle-mesh method, which in addition to the energy preserves any function of PV on the particles.