

DIRECT STATISTICAL SIMULATION OF CHAOS AND TURBULENCE

by

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Chapter 1

Introduction and Overview

1.1 Planetary Turbulence

In his book, Richard Feynman described turbulence as a “central problem which we ought to solve some day, and we have not.” [1]. Half a century later the problem of turbulence remains largely unsolved. A large part of the difficulty in understanding turbulent flows arises from the nonlinearity which couples all length scales of the flow. These length scales can span many orders of magnitude from the microscopic up to planetary scales, giving rise to complex phenomena with no closed-form expressions. This chaotic state of fluid flow has an extreme sensitivity to initial conditions where small perturbations grow spontaneously.

Our solar system offers a rich selection of planetary turbulence, some instances of which are illustrated in Fig. 1.1.1. For example, the Jovian atmosphere exhibits banded zonal structures (Fig. 1.1.1a) and large coherent vortices (Fig. 1.1.1b). The most well-known instance of this is the Great Red Spot which is a large atmospheric storm that has been observed for centuries and continues to rage [2]. Such a red spot is also found in Saturn’s atmosphere (Fig. 1.1.1c). Although smaller than Jupiter’s, it bears similar features [3]. The other gas giant, Neptune, also has a similar feature

in its atmosphere (Fig. 1.1.1d). Known as the Great Dark Spot, it has a shorter lifespan - a few years instead of a few centuries - but it reemerges every few years [4]. Like the Great Red Spot, the Great Dark Spot is also an anticyclonic storm.

While these gas giants are orders of magnitude times larger than the Earth and exhibit more violent dynamics, similar structures also exist in the Earth's atmosphere in the form of jet streams and storms, though diminished in comparison to Jupiter's. For example, the Earth's troposphere contains two polar and two subtropical jets, one in each hemisphere. These jets, which travel in an easterly direction, can reach speeds of over 160 km/hr and are a driving force for the weather. Fig. 1.1.2a shows a visualization of the polar jet stream in the Northern hemisphere. Unlike Jupiter, the jet streams on Earth tend to meander, often to such an extent that a portion can get cut off from the main jet stream, causing anomalous weather over the region until it dissipates. This mechanism is illustrated in Fig. 1.1.2b. Understanding such coherent structures is not only an interesting problem in turbulence but also of practical benefit for developing more accurate short-term weather predictions and long-term climate predictions. This is of particular relevance in today's context of climate change as scientists seek to gain a more precise understanding of the extent of anthropogenic changes to global circulation patterns and ways of mitigating these effects.

The relatively large ratio between the horizontal to vertical scales in these planetary systems renders them amenable to a two dimensional approximation. In this thesis the governing equations of two dimensional turbulence will be shown to produce many of the features found in planetary turbulence such as the banded zonal structures (jets) and large coherent vortices (cyclones), features that will be understood using statistical techniques. I will begin by justifying the quasi-two-dimensionality of planetary turbulence in the next section.

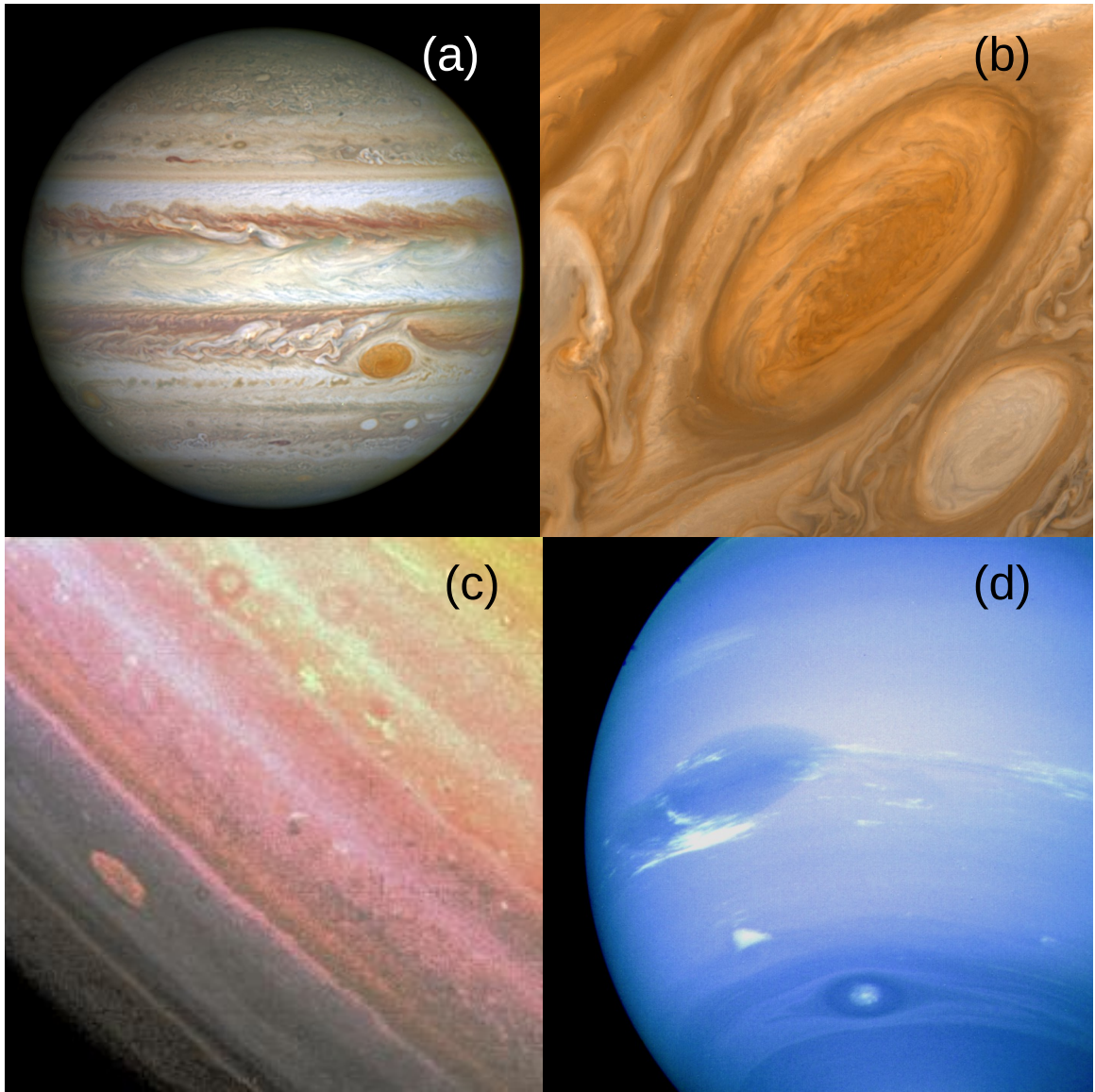


Figure 1.1.1: Planetary turbulence in our solar system. (a) An image taken by NASA's Hubble's wide-field camera showing Jupiter's zonal bands and vortices. (b) Close-up of the Great Red Spot. (c) A false-color image taken by NASA's Voyager 1's narrow-angle camera showing Saturn's redspot which is similar to but smaller than Jupiter's. (d) Reconstruction of two images taken by NASA's Voyager 2's narrow-angle camera. The Great Dark spot, seen to the top left of the image, is an anticyclonic storm similar to Jupiter's Great Red Spot. (Credit: JPL/University of Arizona/NASA's Goddard Space Flight Center).

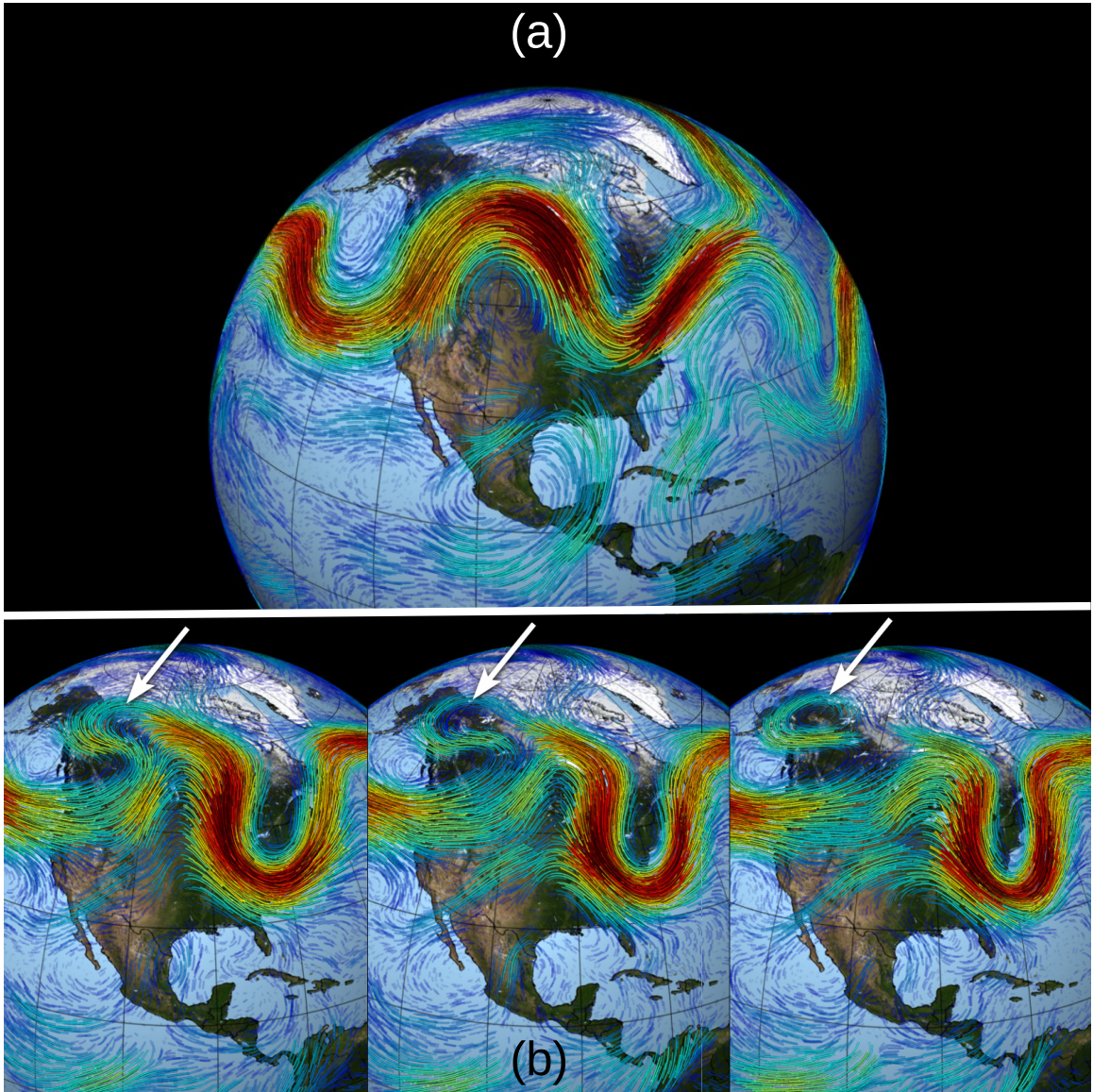


Figure 1.1.2: (a) A visualization of the polar jet stream in the Northern hemisphere using weather observations by NASA's MERRA dataset. (b) Snapshots showing a mechanism by which a portion of warm air from the jet stream can get cut off, resulting in a period of unusual weather in the region (indicated by the arrow). (Credit: NASA's Goddard Space Flight Center.)

1.2 Incompressibility and Quasi-two-dimensionality

Conservation of mass requires that the fluid flow satisfy the mass continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0, \quad (1.2.1)$$

where $\vec{u}(\vec{r}, t)$ is the velocity field and $\rho(\vec{r}, t)$ is the density of the fluid. This can be reexpressed using the material derivative as:

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \vec{u} = 0, \quad (1.2.2)$$

where the material derivative is defined as:

$$\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + \vec{u} \cdot \nabla, \quad (1.2.3)$$

and describes the rate of change of a fluid parcel in time as it is advected along its trajectory. Following a fluid parcel, it is clear that the material derivative of the density must vanish in order for the fluid to be incompressible. Therefore incompressibility requires that the velocity field be solenoidal (divergence-free):

$$\nabla \cdot \vec{u} = 0. \quad (1.2.4)$$

This statement of incompressibility motivates a two dimensional approximation for planetary turbulence because by scale analysis,

$$\left[\frac{U_x}{L_x} \right] \sim \left[\frac{U_y}{L_y} \right] \sim \left[\frac{U_z}{L_z} \right], \quad (1.2.5)$$

where U_i is the fluid velocity in the i direction and L_i is the length scale in the i direction. When the ratio of vertical length scale to horizontal length scale is small,

scale analysis of the continuity equation requires that flow in the vertical dimension be negligible compared to flow in the horizontal direction. This condition is met in the case of planetary systems where the vertical length scale of the atmosphere is on the scale of kilometers while the horizontal length scale is thousands of times larger.

1.3 Single Layer Barotropic Vorticity Equation

Having made a case for the validity of a quasi-two-dimensional approximation for planetary atmospheres, I will proceed to deriving the equation governing two dimensional turbulence. The fundamental equation of hydrostatics states that:

$$f_{app} - \frac{1}{\rho} \nabla p = 0, \quad (1.3.1)$$

where p is the pressure of the fluid and f_{app} is the applied force per unit mass on the fluid. In the systems studied in this thesis, the applied force is the acceleration due to gravity $\vec{g}$. If instead the fluid is in motion then this expression continues to be satisfied by a parcel of fluid moving along its trajectory so that:

$$\frac{D\vec{u}}{Dt} = \vec{g} - \frac{1}{\rho} \nabla p. \quad (1.3.2)$$

This is Newton's second law for an ideal fluid. Together with the incompressibility constraint, they constitute the incompressible Euler equations of nonviscous hydrodynamics. In a rotating frame and in the presence of viscous forces, the equation is appended with two more terms - a Coriolis force term and a viscous dissipation term - leading to the incompressible three dimensional Navier-Stokes equation in a rotating frame:

$$\frac{D\vec{u}}{Dt} + 2\vec{\Omega} \times \vec{u} = \vec{g} - \frac{1}{\rho} \nabla p + \nu \nabla^2 \vec{u}, \quad (1.3.3)$$

where ν is the kinematic viscosity and $\vec{\Omega}$ is the angular velocity vector of the system.

At this stage the vorticity can be defined as the curl of the velocity:

$$\vec{\omega} = \nabla \times \vec{u}. \quad (1.3.4)$$

An equation of motion governing the vorticity of the fluid can then be derived by taking the curl of the Navier-Stokes equation:

$$\frac{\partial \vec{\omega}}{\partial t} + \vec{u} \cdot \nabla (\vec{\omega} + 2\vec{\Omega}) = \vec{\omega} \cdot \nabla \vec{u} - \frac{\nabla p \times \nabla \rho}{\rho^2} + \nu \nabla^2 \vec{\omega}. \quad (1.3.5)$$

This is the general vorticity equation in three dimensions. In general, the density of a fluid can be a function of both pressure and temperature. However, the systems studied in this thesis will assume constant temperature along each constant pressure surface so that the density of the fluid depends only on its pressure. Therefore surfaces of constant density are parallel to surfaces of constant pressure:

$$\nabla \rho = B \nabla p, \quad (1.3.6)$$

where the constant coefficient B is known as the barotropy parameter. Since fluid motion does not vary with height under this approximation, the system effectively has only a single layer. This is known as the barotropic model of the atmosphere. A less simplified model is the baroclinic model which can accommodate two or more coupled layers. In this thesis I will consider only the barotropic model as it can offer insight into the nature of two dimensional turbulence whilst paying a relatively smaller computational cost.

Since the cross product of a vector with itself vanishes, so too does the second term on the RHS of Eq. 1.3.5. Furthermore, the scale analysis of the continuity equation presented in the previous section shows that the velocity field has a negligible component normal to the surface. Therefore the first term, known as the vortex

stretching term, vanishes too. This leads to the vorticity equation for two dimensional turbulence:

$$\frac{\partial \omega}{\partial t} + \vec{u} \cdot \nabla \omega = \nu \nabla^2 \omega, \quad (1.3.7)$$

where ω is the scalar vorticity defined by $\vec{\omega} = \omega \hat{n}$ and $\hat{n}$ is the normal unit vector to the surface. The rotation of the system has been temporarily neglected but will be reintroduced later. Thus vorticity obeys an advection-diffusion type equation where viscosity acts as a diffusive term.

The absence of this vortex stretching term in the governing equation for vorticity has significant implications. In the three dimensional case, it provides a mechanism for energy to be transmitted from the macroscopic scales down to the Kolmogorov scale, at which stage viscous forces between molecules dissipate the energy. This is known as the energy cascade process. However, this enhanced dissipation is absent in the two dimensional case where there exists dynamically conserved quantities such as energy and Casimirs (see Eq. 1.3.13) which result in an *inverse* cascade process causing energy to instead be transported upwards from the small scales up to the macroscopic length scales of the system, growing the size of the structures accordingly. This accounts for much of the qualitatively different behavior between two dimensional turbulence and its three dimensional counterpart as I will show in this thesis.

Under the assumption that the flow is divergence-free, the two dimensional vorticity equation can be further simplified using a streamfunction ψ defined such that:

$$\vec{u} = \nabla \times \psi \hat{z} \quad (1.3.8)$$

The scalar vorticity is then related to the streamfunction by a Laplacian operation,

$$\omega = \nabla^2 \psi, \quad (1.3.9)$$

so that the advective term can be reexpressed as:

$$\begin{aligned}\vec{u} \cdot \nabla \omega &= \hat{n} \cdot (\nabla \psi \times \nabla \omega) \\ &= J[\psi, \omega],\end{aligned}\tag{1.3.10}$$

where J is the Jacobian. See Appendix D.1 for details. Since this thesis studies barotropic models in the context of planetary turbulence, problems will be solved on the surface of a sphere where the Jacobian takes the form:

$$J[A, B] = \frac{1}{\sin \theta} \left(\frac{\partial A}{\partial \theta} \frac{\partial B}{\partial \phi} - \frac{\partial A}{\partial \phi} \frac{\partial B}{\partial \theta} \right).\tag{1.3.11}$$

Since the Coriolis force resulting from the rotating reference frame was absorbed into the vorticity term in Eq. 1.3.5, it is useful to explicitly define an absolute and relative vorticity, q and ζ such that $q = \zeta + f$ where $f = 2\Omega \cos \theta$ is the planetary vorticity. Eq 1.3.7 can then be written in terms of a scalar equation, known as the single-layer barotropic vorticity equation:

$$\frac{\partial q}{\partial t} = J[q, \psi] + \nu \nabla^2 q,\tag{1.3.12}$$

where $\zeta = \nabla^2 \psi$. In the absence of viscous dissipation this equation reduces to the two dimensional Euler equation which is a statement about the conservation of absolute vorticity under advection. A corollary of this statement is that an infinite hierarchy of Casimirs must also be conserved, defined as:

$$\Gamma_n \equiv \int q^n d^2 \vec{r}.\tag{1.3.13}$$

See Appendix D.1 for details of the proof. The conservations of these quantities accounts for the inverse cascade described above, allowing the flow to spontaneously

self-organize into coherent structures such as jets and vortices as in Fig. 1.1.1 and 1.1.2. This thesis will attempt to gain insight into these coherent structures by applying statistical methods to the prognostic and diagnostic equations of the vorticity.

1.4 Chaos & The Lorenz Attractor

An even simpler idealized model for atmospheric convection is the Lorenz system, a three dimensional chaotic system and a hallmark of chaos theory. As with the coherent structures found in turbulent flow such as banded zonal structures and vortices, chaotic systems too exhibit persistent structures. For example, the Lorenz attractor has double lobes visible on the macroscopic scale and delicate rings on a finer scale. And like turbulent systems, chaotic systems too pose a unique challenge to scientists. With no closed-form analytic solution, computational simulations are a major tool for learning about them. It is unsurprising that their discovery - or rather, formal classification - occurred shortly after the advent of the modern computer [5]. Since then, they have been observed in a vastly diverse set of unconnected systems, ranging from electric circuits [6], chemical reactions [7], population dynamics [8] and stock markets [9]. In a chaotic system, two points in phase space initialized infinitesimally close to each other will diverge in exponential time. This inherent sensitivity to initial conditions means that even with perfect knowledge of the governing laws, the imperfections in the knowledge of the state of a system will quickly grow until predictability is lost. Therefore chaotic systems serve as a good challenge for testing new numerical and statistical techniques.

The Lorenz-63 attractor was motivated by Rayleigh-Bénard convection, a type of convection where a uniform layer of fluid between two horizontal plates is heated from beneath. Such a system has a steady-state solution in which the temperature gradient is constant. However, this solution is unstable and a small perturbation

results in convection of the fluid. Applying a severe Galerkin approximation to the equations of motion (EOMs) of the system with stress-free boundary conditions gives the EOMs of the Lorenz attractor [10]. In addition to this deterministic system, in this thesis I will study an extension with additive stochastic forcing [11–15] which is Gaussian white noise δ -correlated in time. Such additive white noise can model uncertainties in observations or else fast or unresolved physical processes that are not explicitly described.

$$\begin{aligned}\dot{x} &= \sigma(y - x) + \eta_1(t) \\ \dot{y} &= x(\rho - z) - y + \eta_2(t) \\ \dot{z} &= xy - \beta z + \eta_3(t).\end{aligned}\tag{1.4.1}$$

In this context x is proportional to convective intensity, y to the difference in temperature between ascending and descending currents, and z to the vertical temperature profile’s deviation from linearity. Parameters β , ρ , and σ are a geometric factor, the Rayleigh number, and the Prandtl number respectively.

For $\beta = 1.0$, $\sigma = 3.0$, and $\rho = 5$, the system behaves like a damped oscillator. Increasing ρ to 15 does not qualitatively change this behavior. However, a further increase of ρ to 26.5 results in a system with very different behavior. x , y and z lose their periodicity and motion becomes irregular, with two attractors emerging on either side of the $x - z$ plane, as shown in Fig. 1.4.1. An analysis of this object’s Hausdorff dimension in this chaotic regime yields a value of around 2.06 [16]. This fractional dimension of the Lorenz attractor has led to it being termed a “strange attractor”.

This thesis studies this strange attractor for two different sets of parameters. The conventional (classic) set of parameters for which the Lorenz system enters the chaotic regime is $\beta = 1.0$, $\rho = 26.5$, and $\sigma = 3.0$. In addition, the case where the

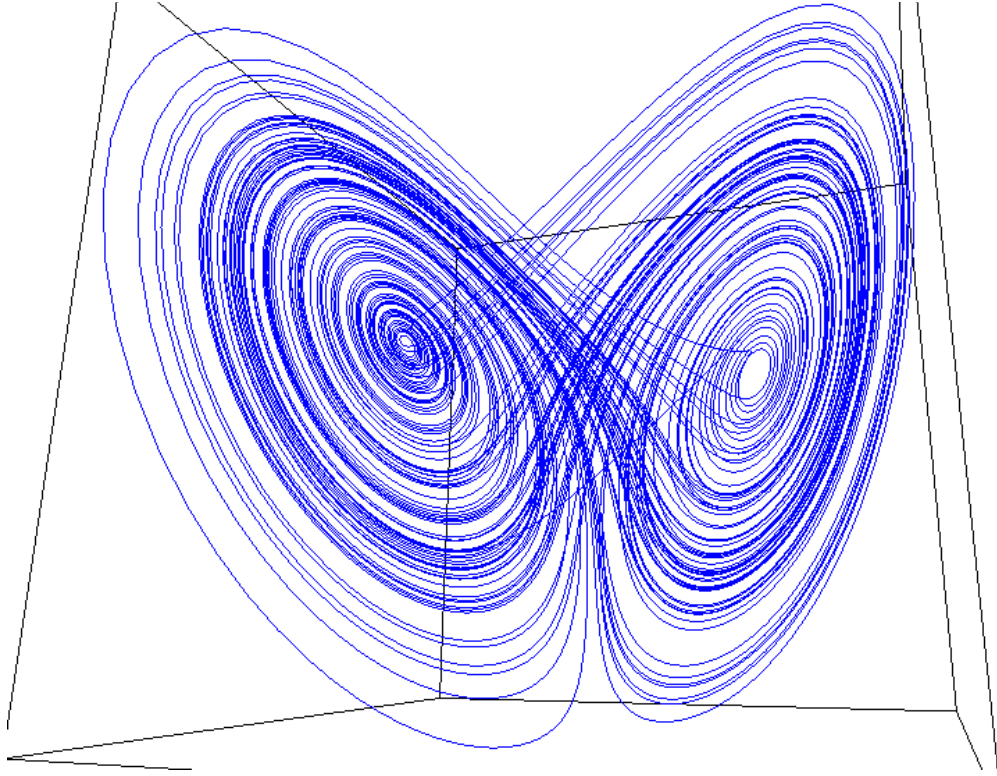


Figure 1.4.1: Direct numerical simulation of the deterministic Lorenz-63 attractor in the x, y, z phase space using the classic parameters for the chaotic regime.

geometric factor is changed to $\beta = 0.16$ will also be studied as this modification enhances layering in its probability distribution. Each attractor has a slow time scale corresponding to transitions between the wings, and a fast time scale for orbits about each wing. The fast time-scale is $\tau = \mathcal{O}(1)$. This thesis will introduce techniques to directly solve for the statistics of this strange attractor.

1.5 Direct Statistical Simulation

Statistical descriptions are well-suited for both chaotic systems as well as turbulent systems of large-scale planetary flows which exhibit coherent structures with relatively slow time-scales. Physical and numerical experiments each offer unique benefits and

drawbacks for studying the statistics of such structures. Laboratory experiments have the advantage that they can be run for long times without the introduction of errors associated with the finite resolution of flows. However the relatively small size of flow chambers means that they cannot achieve the high Reynolds flows observed in the atmosphere. In addition, extracting the data from the observations of flow visualizations presents another difficulty because techniques such as particle image velocimetry and particle tracking velocimetry introduce a source of imprecision.

Another method of studying the statistics of such flows which offers more precise data extraction is Direct Numerical Simulation (DNS) where the fields are evolved forward in time according to the EOMs of the system. Statistics are then formed by performing a long temporal average on the data. Since DNS is not limited by physical design constraints, it can allow for more precise modeling of the system of interest. However accumulating statistics via DNS can be inefficient because convergence to a statistically steady-state is slow, especially in systems with rare but large deviations as are often found in turbulent flows. Another drawback of DNS is that it is difficult to extract the physics from the computed numbers. As Edward Lorenz remarked [17]: “More than any other theoretical procedure, numerical integration is also subject to the criticism that it yields little insight into the problem. The computed numbers are not only processed like data but they look like data, and a study of them may be no more enlightening than a study of real meteorological observations. An alternative procedure which does not suffer this disadvantage consists of deriving a new system of equations whose unknowns are the statistics themselves.” Accordingly, in this thesis I propose a shift in ethos from Direct Numerical Simulation to one of Direct Statistical Simulation (DSS), where the statistics are solved for directly.

Many well-established theories can be considered instances of DSS. For example numerical solutions of the Fokker-Planck equation directly solve for the probability distribution of a system, from which information about both low-order and high-order

statistics can be extracted. I will demonstrate this in Chapter 2 on the Lorenz attractor. However the Fokker-Planck equation scales with the number of degrees of freedom of the system and so the associated computational expense of simulations restricts its use to relatively low-dimensional systems of between one to four dimensions [18–22]. By contrast the highly turbulent behavior of geophysical fluid flows makes for extremely high dimensional systems where each mode contributes a new degree of freedom. For example, typical Reynolds numbers associated with large-scale planetary flows can exceed 10^{10} . Therefore for turbulent systems I will seek a different type of DSS. One option, Large Deviation Theory [23], solves for the probabilities of extreme or rare events. However these events contribute little to the statistics of turbulent flows because they get washed out over a temporal or ensemble average. Other methods such as those developed by Kolmogorov [24, 25] offer a description of the statistical properties of turbulent flows but assume isotropy and homogeneity. Since geophysical flows exhibit features such as coherent vortices and zonal banding (as seen in Fig. 1.1.1c&d), any statistical method that can appropriately treat such systems needs to respect the asymmetries of these large scale planetary flows.

One such scheme of DSS that satisfies these requirements involves perturbatively expanding in the equal-time cumulants of the flow. Since low-order statistics tend to be spatially smoother than the corresponding dynamical fields (or instantaneous flow), this method can capture the macroscopic features of turbulent flows using fewer degrees of freedom. An added benefit of such a cumulant expansion scheme is that the small-scale modes are integrated out, leaving only large-scale modes containing information about the coherent structures of interest. These modes are associated with the low-order statistics of the system and might be described by a fixed point or slow manifold, allowing for quicker convergence to a statistically steady state.

The aim of this thesis is to investigate both types of DSS - the Fokker-Planck technique and the cumulant expansion scheme - in the context of the two idealized

models of planetary atmospheres discussed in this chapter: barotropic models and the Lorenz attractor. Since the former is an instance of a turbulent system with many degrees of freedom while the latter is an instance of a chaotic system with minimal degrees of freedom, these two models combined offer a rich testbed for the theoretical and computational aspects of DSS.

1.6 Outline of Thesis

Chapter 2 introduces a Fokker-Planck equation and applies it to an Ornstein-Uhlenbeck process to directly solve for the statistics. It is then extended to a two dimensional version of the system where its two variables are coupled. An analytic solution is presented using an eigenvalue approach. This method is then applied to the highly chaotic stochastically-forced Lorenz-63 attractor and the results compared against Monte-Carlo simulations.

Chapter 3 introduces another type of DSS to directly access the quasi-steady-state statistics of a system with quadratic nonlinearity, this time using the Cumulant Expansion technique. Section 3.2 considers a third-order closure of this expansion, known as CE3, where cumulants are defined by an ensemble average. The technique is then applied to the stochastically-forced Lorenz attractor, as well as the unforced (deterministic) attractor. The calculated cumulants according to this method are again compared against Monte Carlo simulation which are used as a reference. Section 3.3 then considers a second-order closure, known as CE2, and applies it to two barotropic models. Traditionally CE2 has used a zonal average. However this form of CE2 neglects crucial eddy-eddy scattering processes required to accurately describe turbulent flows. Therefore a variant of CE2 using an ensemble average is used to capture the nonlinear processes inherent to turbulent flow. The validity of both schemes are discussed. In Section 3.3.3 this new scheme is tested on a deterministic barotropic

jet and a stochastically-forced barotropic jet, compared against traditional CE2 and DNS which is used as a reference.

Since the dimensionality of the system increases under an ensemble CE2 scheme, Chapter 4 examines a dimensional reduction scheme involving a Proper Orthogonal Decomposition of the eigenvectors of the system. Its theory is developed and then applied to the two types of CE2 as well as DNS, for both types of barotropics jets considered in the previous chapter. A substantial basis reduction with associated computational gains are observed.

Continuing on with the theme of numerical efficiency, a semi-implicit numerical integration scheme is presented in Chapter 5. This semi-implicit scheme is known as TR-BDF2 as it combines the trapezoidal rule (TR) with a backward differentiation formula (BDF2). TR-BDF2 is shown to offer a combination of the precision of a fourth-order Runge-Kutta (RK4) scheme, and the stability of the semi-implicit Euler (BDF1) scheme. The equations for TR-BDF2 are derived in Section 5.2 and then tested on the stochastically-forced barotropic jet, compared against both RK4 and BDF1 for clock speed, time step size and accuracy. Significant speed ups, as measured by both clock speed and mean time steps, are observed.

Chapter 6 will discuss the insights, limitations and future directions of this work.

Chapter 2

Fokker-Planck method

2.1 Introduction

The persistence of microscopic and macroscopic structures in chaotic systems (described in the previous chapter) despite the inherent unpredictability of individual trajectories hints at the utility of a statistical approach to chaos. Although the individual trajectories are chaotic, they often have a well-defined statistically steady state. One option for forming these statistics is by performing an ensemble over many different initializations, evolving each separately. But if the basin of attraction is ergodic, as is often true for chaotic systems [26], the ensemble average can be replaced by a long time average instead. This makes DNS well-suited for gaining statistical inferences about the chaotic system. But DNS has a drawback. Rare but large deviations in the individual trajectories may occur due to the chaotic nature of the dynamics, which increases the time required for a DNS run to converge to the true statistics of the dynamics. Therefore an alternative option is to solve for the statistics directly. This Direct Statistical Simulation (DSS) [27], introduced in Section 1.5, can offer a more efficient approach for accessing the statistical quantities such as the probability distribution function (PDF) or invariant measure. Such a DSS can be performed us-

ing the Fokker-Planck equation (FPE) [28] which is a statement of the conservation of local probability. Since the FPE is an EOM for the statistics (in particular, the PDF) derived from the EOM for the dynamics, it integrates out the rare and large deviations, thus converging at a steady-state solution quicker. In addition, statistical variables are often smoother in time than the underlying dynamical variables, which makes it computationally attractive. However the numerical solution of the FPE is subject to the well-known “curse of dimensionality”. Several different types of numerical solutions have been explored using finite differences [22]. However this method is often subject to numerical instabilities, prompting an exploration of other numerical approaches such as finite elements [18, 20] and path integrals [21].

In this chapter, I will present a numerically stable finite difference method that directly solves for the zero or null mode of a discretized FPE operator on a lattice. I will begin by illustrating in Section 2.2 the Fokker-Planck equation on a canonical Ornstein-Uhlenbeck process, which is a simple one-dimensional model for the motion of a Brownian particle under a restorative force. In Section 2.3 this approach will be extended to the Lorenz-63 system [10], a hallmark of chaos theory and nonlinear dynamics. Following previous works [11–15], a small amount of additive white noise is introduced to the strange attractor to wash out fractal structure below the lattice scale in order to ensure resolvability. Section 2.3.1 gives an outline of the numerical methods used to find the steady-state statistics of the Lorenz system via the FPE method as well as the traditional method of accumulating statistics by DNS, against which these DSS solutions are compared. Section 2.4 studies the scaling of the spectral gap of the linear FPE operator as the stochastic forcing is varied. Section 2.5 considers two extensions to the method: A self-adjoint construction of the linear operator, and the replacement of diffusion with hyperdiffusion. Each of these could be potentially advantageous in certain situations. Some brief conclusions are presented in Section 2.6.

2.2 Ornstein-Uhlenbeck Process

The FPE describes the conservation of total probability in phase space. Consider a trajectory governed by the EOM:

$$\frac{d\vec{x}}{dt} = \vec{V}(\vec{x}) + \vec{\eta}(t), \quad (2.2.1)$$

where $\vec{\eta}(t)$ is additive stochastic forcing. The FPE for this system is:

$$\frac{\partial P(\vec{x}, t)}{\partial t} = -\hat{L}_{FPE}P(\vec{x}, t), \quad (2.2.2)$$

where we will call $\hat{L}_{FPE}$ the (linear) FPE operator. The negative sign ensures that it is a semipositive-definite operator which will be useful later on. For noise with an unspecified structure, the FPE operator has an infinite number of terms by Pawula's theorem [28]. But in the special case where $\vec{\eta}$ is Gaussian white noise with zero mean and covariance given by

$$\langle \eta_i(t) \eta_j(t') \rangle = 2\Gamma \delta_{ij} \delta(t - t'), \quad (2.2.3)$$

with angular brackets $\langle \dots \rangle$ indicating a short time-average, only a finite number of terms appear in the FPE operator [29]:

$$\hat{L}_{FPE}P = \vec{\nabla} \cdot (\vec{V}P) - \Gamma \nabla^2 P. \quad (2.2.4)$$

Since the Gaussian white noise in the EOM of the dynamics appears as a diffusion term in the EOM of the PDF, stochastic forcing can be thought of as a low-pass filter for the statistics of the system. In other words, it smears out the PDF through diffusion in phase space.

The eigenvectors and eigenvalues of the FPE operator are wholly responsible for

the behavior of the PDF of the system. To see this, Eq. 2.2.2 can be solved using a propagator:

$$P(t) = e^{-\hat{L}_{FPE}t}P(0). \quad (2.2.5)$$

The initial-value PDF can be expanded in terms of the eigenvectors of the FPE operator:

$$P(0) = \sum_k \alpha_k \vec{v}_k, \quad (2.2.6)$$

which allows for the propagator to be written in terms of its eigenvalues:

$$P(t) = \sum_k e^{-\lambda_k t} \alpha_k \vec{v}_k. \quad (2.2.7)$$

Since eigenvectors with negative eigenvalues would cause the PDF to diverge, such eigenvectors cannot exist for systems with known steady-state PDFs. This means that the FPE operator must be positive definite. In addition it is readily seen as $t \rightarrow \infty$ that the contribution to the PDF of those eigenvectors with positive eigenvalues must exponentially go to zero. In fact, the steady-state PDF of the system is given by only the zero-mode eigenvector of the FPE operator (with the appropriate normalization factor) because in the large time limit:

$$\lim_{t \rightarrow \infty} P(t) = \alpha_0 \vec{v}_0. \quad (2.2.8)$$

Therefore rather than solving for the statistics of the dynamical system by integrating the PDF forward in time according to the FPE, a more novel approach is to solve for the eigenvalues and eigenvectors of the FPE operator. This converts a time-evolution problem into a linear algebra problem and is the main topic of this chapter.

I will first illustrate these ideas on a simple one-dimensional Ornstein-Uhlenbeck process which has an analytic solution. The system models a stochastically-forced

particle subject to a restorative force toward the origin. Its trajectory is governed by

$$\dot{x} = -ax + \eta(t), \quad (2.2.9)$$

where a sets the relaxation timescale of the system. The corresponding FPE is

$$\frac{\partial P(x, t)}{\partial t} = \frac{\partial}{\partial x} [axP(x, t)] + \Gamma \frac{\partial^2 P(x, t)}{\partial x^2}. \quad (2.2.10)$$

To find the steady-state solution, the LHS is set to zero to yield

$$\frac{\partial}{\partial x} [axP(x, t)] = -\Gamma \frac{\partial^2 P(x, t)}{\partial x^2}, \quad (2.2.11)$$

with a solution that is readily found analytically to be a Gaussian:

$$P(x) = \sqrt{\frac{a}{2\pi\Gamma}} e^{-ax^2/2\Gamma}. \quad (2.2.12)$$

Here the normalization constant has been chosen such that the PDF integrates to unity over the entire lattice domain.

But I present an alternative approach that solves for the eigenvalues and eigenvectors of the FPE operator instead of explicitly time-evolving the PDF. This too can be done analytically for this system. The calculations are presented in Appendix A.1. The eigenvalues and eigenvectors are given by:

$$P_n(x) = c_1 \exp\left(-\frac{\alpha x^2}{2\Gamma}\right) H_n\left(\sqrt{\frac{\alpha}{2\Gamma}}x\right) \quad (2.2.13)$$

$$E_n = \alpha n. \quad (2.2.14)$$

where n is a non-negative integer, c_1 is the appropriate normalization constant and $H_n(x)$ are the (physicists') Hermite polynomials. Setting $n = 0$ for the zero-mode

recovers Eq. 2.2.12, showing consistency between the two different approaches. In addition, the energy gap between the eigenvalues is set solely by a . Although the stochastic forcing has affected the eigenvectors of the FPE operator, it has not affected the eigenvalues in this system. This is not generally true, as will be seen in Section 2.4. In the case of strange attractors, stochastic forcing needs to be introduced to ensure resolvability of the fine, and often fractal, structures by preventing them from dropping below the resolution of the grid. As the fractal structure of a strange attractor cannot be resolved on a lattice, it is necessary to smoothen out the structure at the lattice length scale. The details of this are discussed in the next section.

2.3 Lorenz Attractor

As discussed in Section 2.2, the FPE is an attractive alternative to estimating equal-time statistics by DNS accumulation. The method of calculating the zero-mode of the FPE operator can be applied to the stochastically-forced Lorenz attractor, described in Chapter 1. Using the EOMs of the Lorenz system, the linear FPE operator can be constructed as,

$$\hat{L}_{FPE}P = \vec{\nabla} \cdot [(\sigma(y - x), x(\rho - z) - y, xy - \beta z)P] - \Gamma \nabla^2 P. \quad (2.3.1)$$

As before, the steady-state PDF of the FPE is the zero or null mode of $\hat{L}_{FPE}$. But unlike with the Ornstein-Uhlenbeck example, the zero-mode cannot be solved analytically. Computational methods do exist, however. By discretizing the operator on a lattice, the problem of finding the steady-state PDF can be converted to a sparse linear algebra problem.

2.3.1 Numerical Solution

A standard center-difference scheme is employed to discretize the derivatives that appear in Eq. 2.3.1:

$$\begin{aligned}\frac{df_i}{dx} &\approx \frac{f_{i+1} - f_{i-1}}{2\Delta x} \\ \frac{d^2f_i}{dx^2} &\approx \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2} .\end{aligned}\tag{2.3.2}$$

Dirichlet boundary conditions are applied such that the edges are fixed at zero. The PDF of the unforced Lorenz attractor has compact support but once stochastic forcing is included the PDF becomes non-zero but exponentially small throughout phase space. The zero-mode of $\hat{L}_{FPE}$ is found numerically using a preconditioned Jacobi-Davidson QR-style (JDQR) algorithm [30,31] which computes the partial Schur decomposition of a matrix with error tolerance set to 10^{-5} . The results do not change appreciably for tighter tolerances. The code is included in Appendix E.2. Although the JDQR algorithm is well-suited for sparse matrices, requiring only the action of a matrix multiplying a vector, the preconditioner selected was not sparse. A sparse preconditioner would enable a substantial increase in resolution and so finding such a preconditioner would be an interesting avenue of research. The Jacobi correction equation is preconditioned as in Section 3.2 of Ref. [31] and solved using the generalized minimal residual (GMRES) method. The finest resolution achieved is 160^3 with 500 GB of memory on a 64-bit version of Matlab. The

The mode with maximal wavenumber must go from zero to a maximum over one lattice spacing, below which it cannot have structure, and so this suggests the following Ansatz:

$$P(x, y, z, t) = e^{-t/\tau_d} \sin\left(\frac{\pi}{2\Delta x}x\right) \sin\left(\frac{\pi}{2\Delta y}y\right) \sin\left(\frac{\pi}{2\Delta z}z\right). \tag{2.3.3}$$

Inserting this mode into the diffusion equation yields the following dispersion relation:

$$\tau_d^{-1} = \frac{\pi^2 \Gamma}{4} [(\Delta x)^{-2} + (\Delta y)^{-2} + (\Delta z)^{-2}]. \quad (2.3.4)$$

This connects how modes at the maximal wavenumber decay diffusively due to stochastic forcing with a decay timescale τ_d . Equating this time scale to the timescale of fast dynamics τ provides an estimate of the effective resolution of the discretized FPE as a function of stochastic forcing.

Fig. 2.3.1 shows a scatter plot of the smallest 1000 eigenvalues of the FPE operator of the Lorenz attractor with classic parameters, calculated by the procedure outlined. As the eigenvalue magnitude increases, so too does the density of the eigenvalue distribution as shown on the scatter plot. Since each of the points on the scatter plot is associated with an eigenvector, the eigenvector associated with the eigenvalue at the origin is shown in Fig. 2.3.2, which corresponds to the steady-state PDF of the system.

The accuracy of these numerical results from the FPE method can be compared against DNS as a benchmark. The EOMs in Eq. 1.4.1 are integrated forward in time with the fourth-order accurate Runge-Kutta algorithm with fixed time step $\delta t = 0.01$. Stochastic forcing, drawn from a zero-mean normal distribution, is updated at intervals of $\Delta t = 0.1$ and interpolated at intermediate times δt . Since the natural time scale of the system, τ , is of order unity, to ensure a good separation of time scales, I chose the values $\Delta t = 0.1$ and $\delta t = 0.01$ so that $\tau \gg \Delta t \gg \delta t$ (as outlined in [32]).

Statistics via DNS are accumulated up to a final time $T = 2 \times 10^7$. The PDF is estimated from the histogram that results from binning the trajectory into cubic boxes. The PDF is projected onto a plane by integrating over the direction perpendicular to

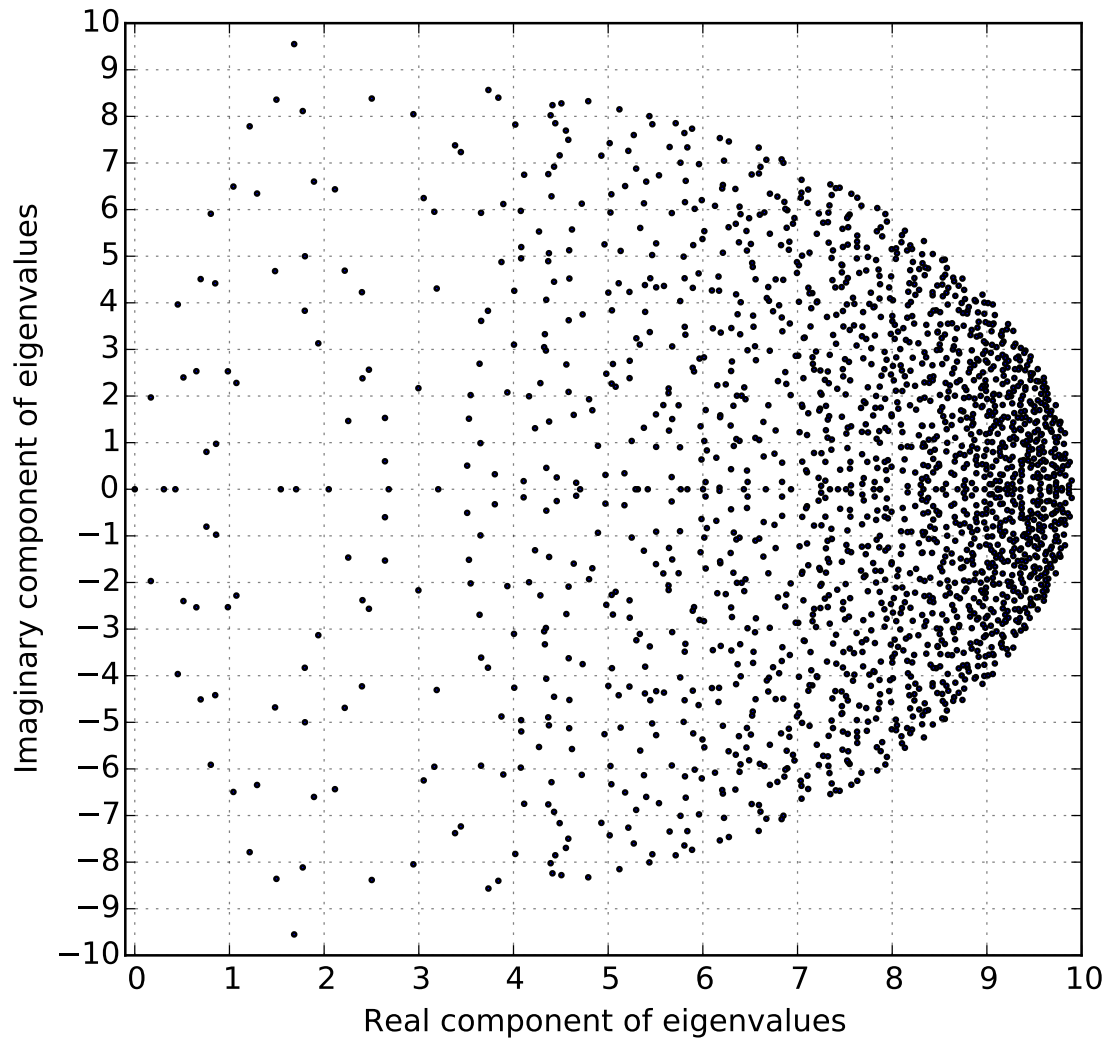


Figure 2.3.1: The smallest 1000 eigenvalues (by magnitude) of the FPE operator for the Lorenz attractor with classic parameters and $\Gamma = 0.2$. The eigenvector associated with the zero eigenvalue at the origin is the steady-state PDF.

the plane; for instance:

$$P(x, y) = \int_{-\infty}^{\infty} P(x, y, z) dz . \quad (2.3.5)$$

Fig. 2.3.2 shows that even small stochastic forcing smoothes out the fine structure of the strange attractor (in agreement with Ref. [?]) and in particular the ring-like steps in the PDF disappear.

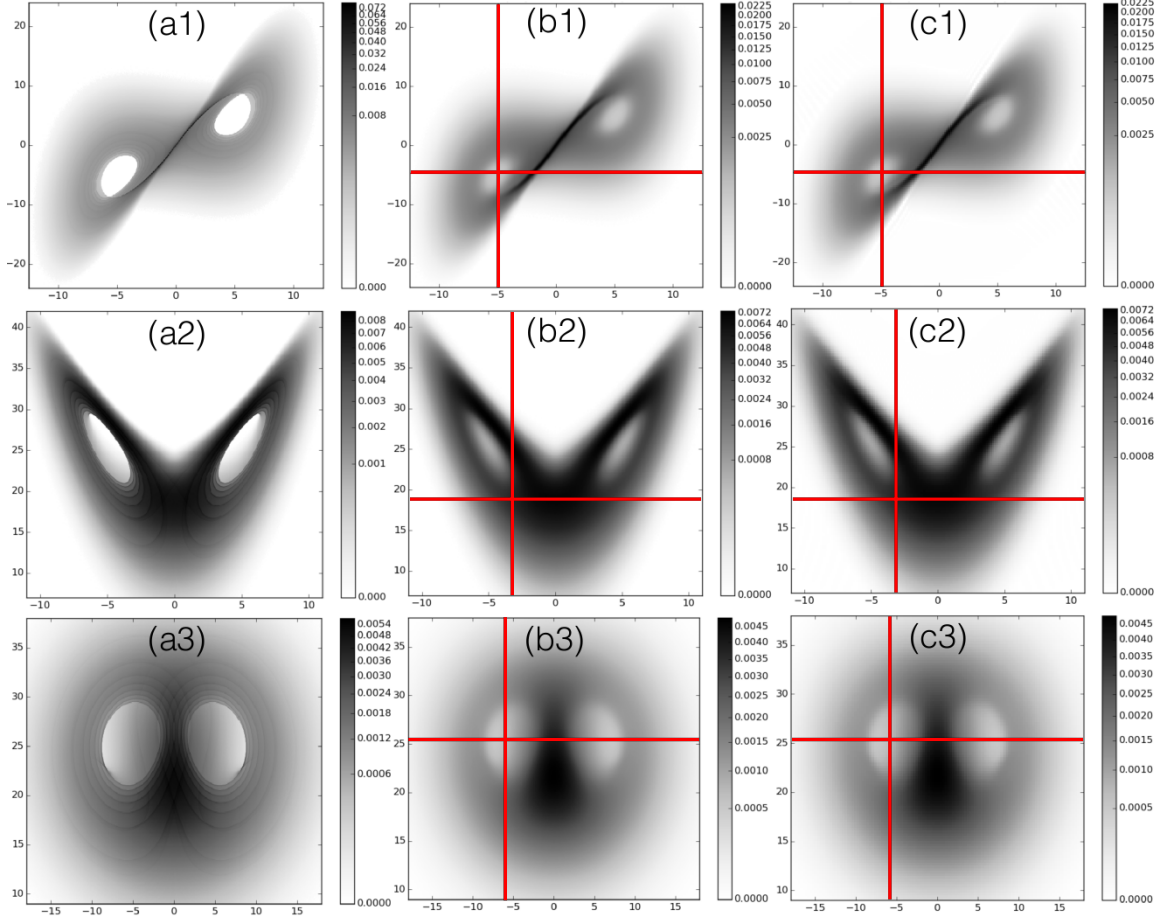


Figure 2.3.2: (a) PDF of the unforced Lorenz system (binned on a 637^3 grid) accumulated by DNS. Classic Lorenz parameters are used (see Sec. 1.4). (b) Same, but for the stochastically forced ($\Gamma = 0.2$) (438^3 grid). Note that the fine rings visible in the unforced system are washed out by the noise. (c) PDF of the stochastically forced attractor ($\Gamma = 0.2$) as obtained from the zero-mode of $\hat{L}_{FPE}$ on a 160^3 grid and for $x \in [-12.5, 12.5]$, $y \in [-24, 24]$ and $z \in [1, 45]$. The JDQR algorithm is employed. Rows (1), (2) and (3) correspond to the $x-y$, $x-z$ and $y-z$ projections of the PDF respectively. Good agreement between (b) DNS and (c) FPE is evident. Red lines correspond to the cross-sections shown in Fig. 2.3.3.

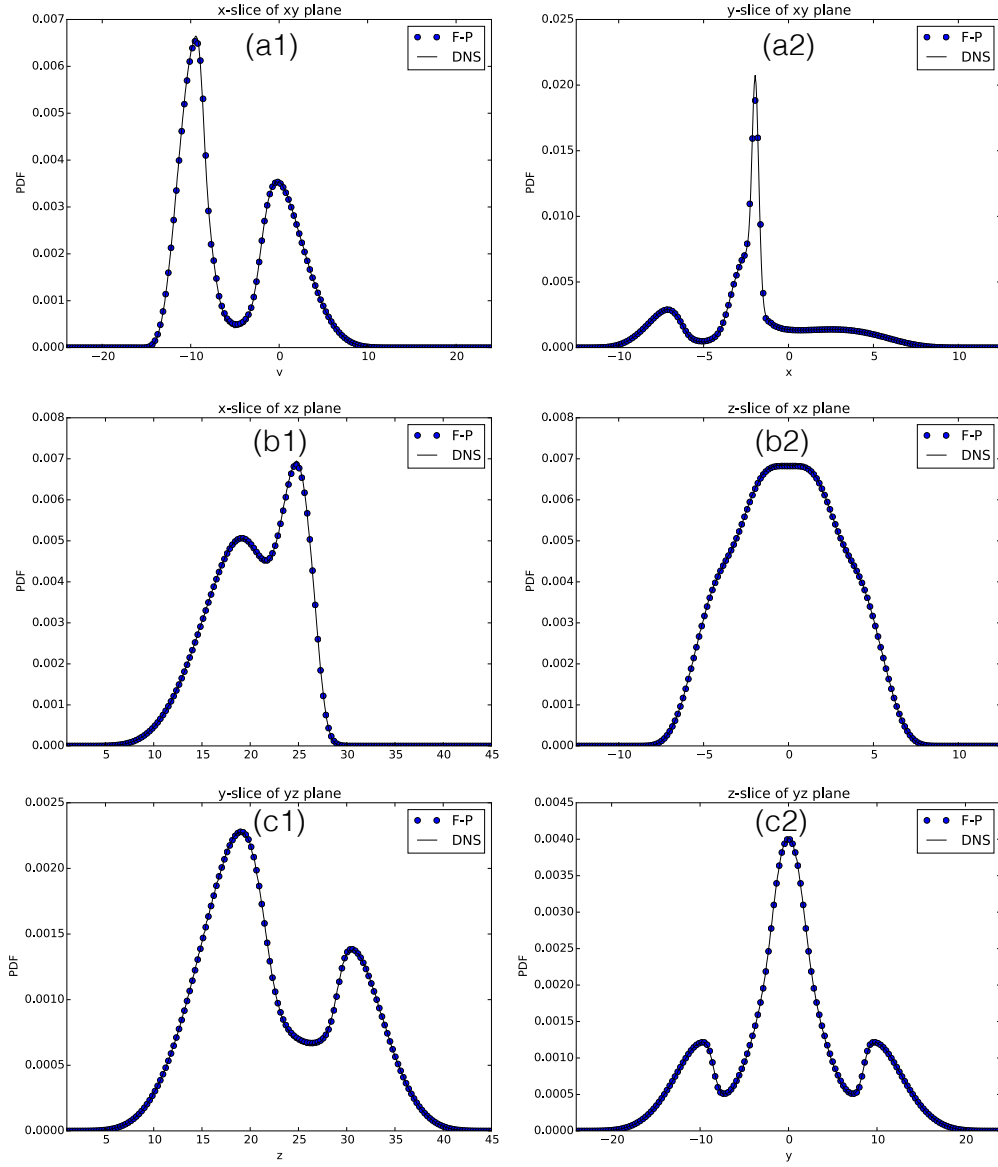


Figure 2.3.3: Slices along the (a) $x - y$, (b) $x - z$ and (c) $y - z$ cross-sections of the planar projections of the PDF with classic Lorenz parameters. Columns (1) and (2) correspond to the vertical and horizontal red lines shown in Fig. 2.3.2 respectively. The DNS and FPE methods agree quantitatively.

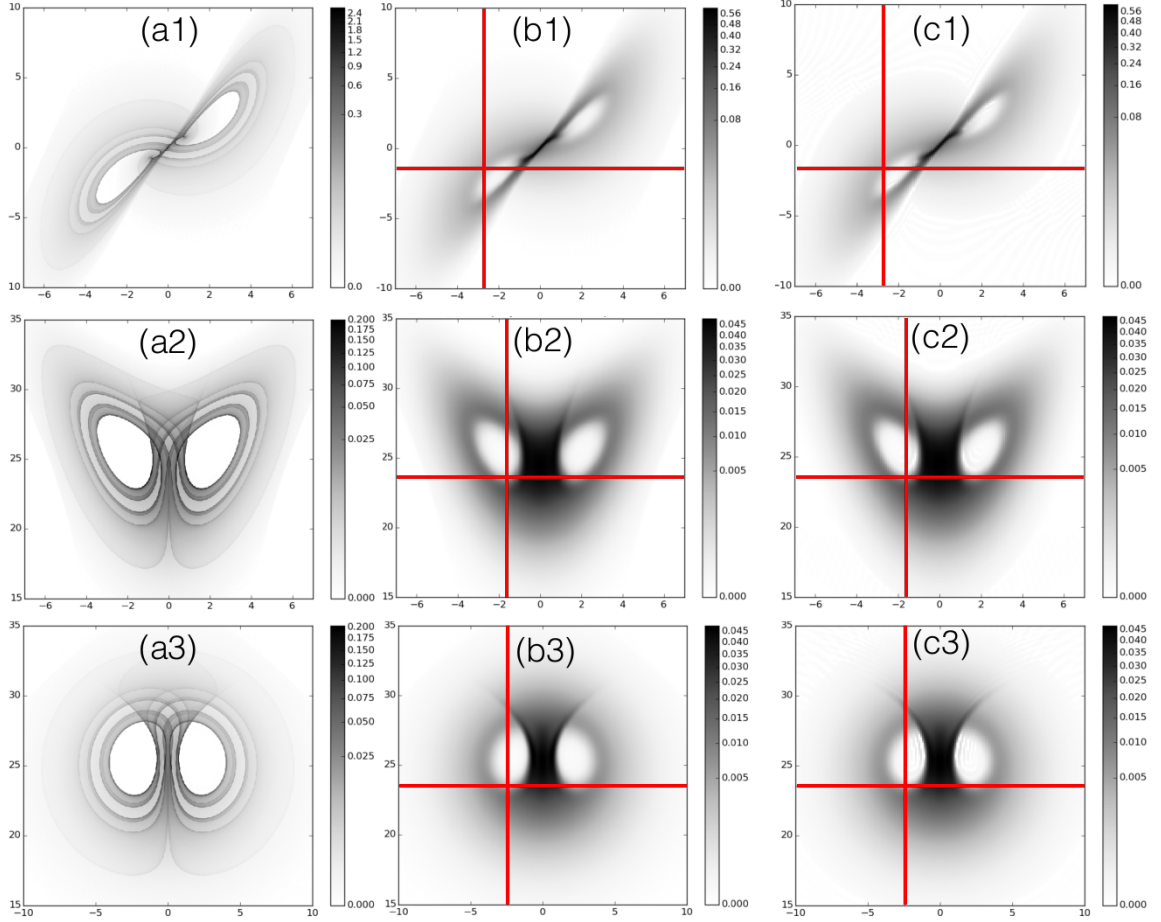


Figure 2.3.4: (a) PDF of the unforced Lorenz system (binned on a 637^3 grid) accumulated by DNS. Modified parameters are used (see Sec. 1.4). (b) Same, but for the stochastically forced ($\Gamma = 0.02$) (438^3 grid). Note that the fine rings visible in the unforced system are washed out by the noise. (c) PDF of the stochastically forced attractor ($\Gamma = 0.02$) as obtained from the zero-mode of $\hat{L}_{FPE}$ on a 160^3 grid and for $x \in [-7, 7]$, $y \in [-10, 10]$ and $z \in [15, 35]$. Rows (1), (2) and (3) correspond to the $x-y$, $x-z$ and $y-z$ projections of the PDF respectively. Good agreement between (b) DNS and (c) FPE is evident. Red lines correspond to the cross-sections shown in Fig. 2.3.5.

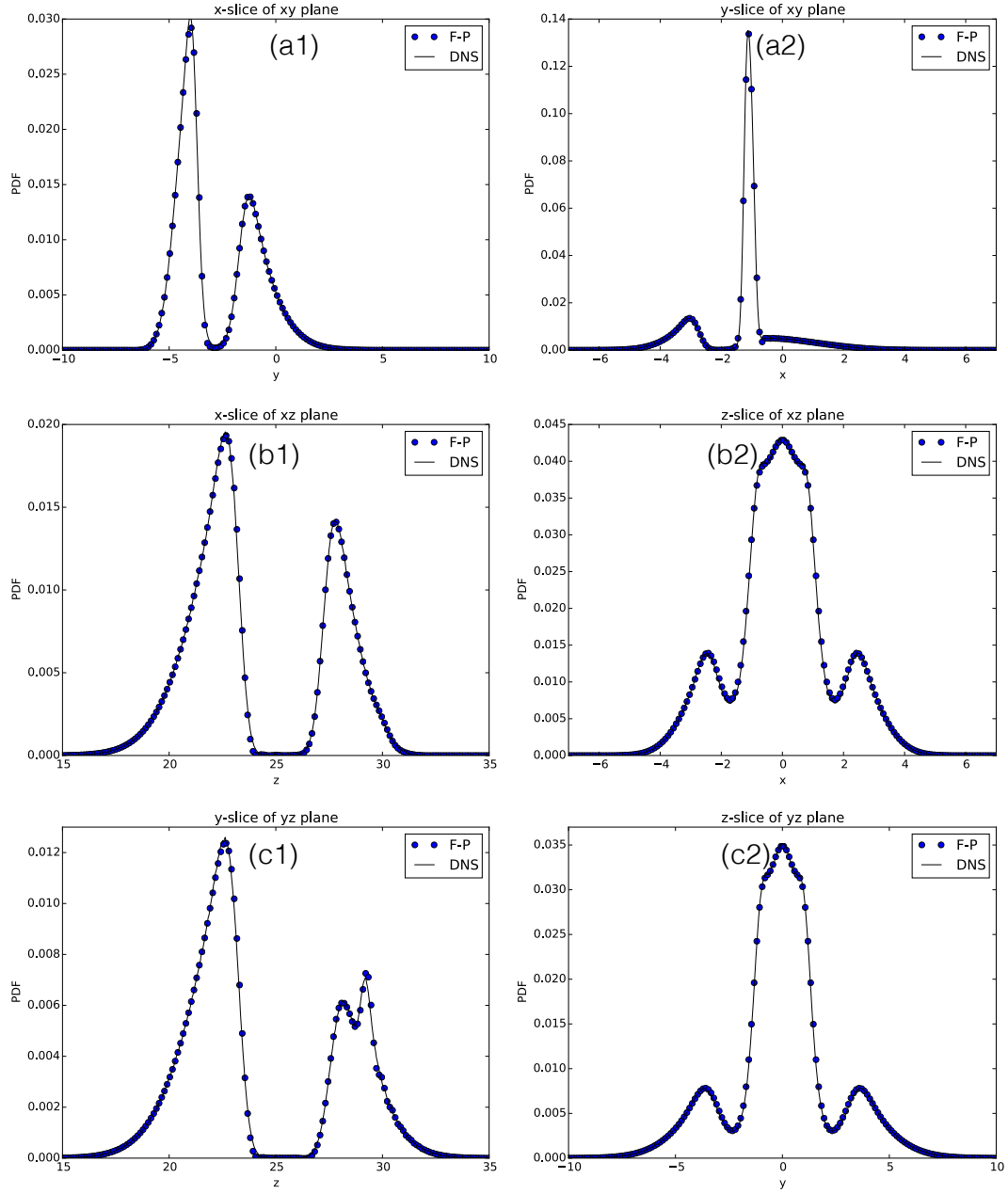


Figure 2.3.5: Slices along the (a) $x - y$, (b) $x - z$ and (c) $y - z$ cross-sections of the planar projections of the PDF with modified Lorenz parameters. Columns (1) and (2) correspond to the vertical and horizontal red lines shown in Fig. 2.3.2 respectively. The DNS and FPE method agree quantitatively.

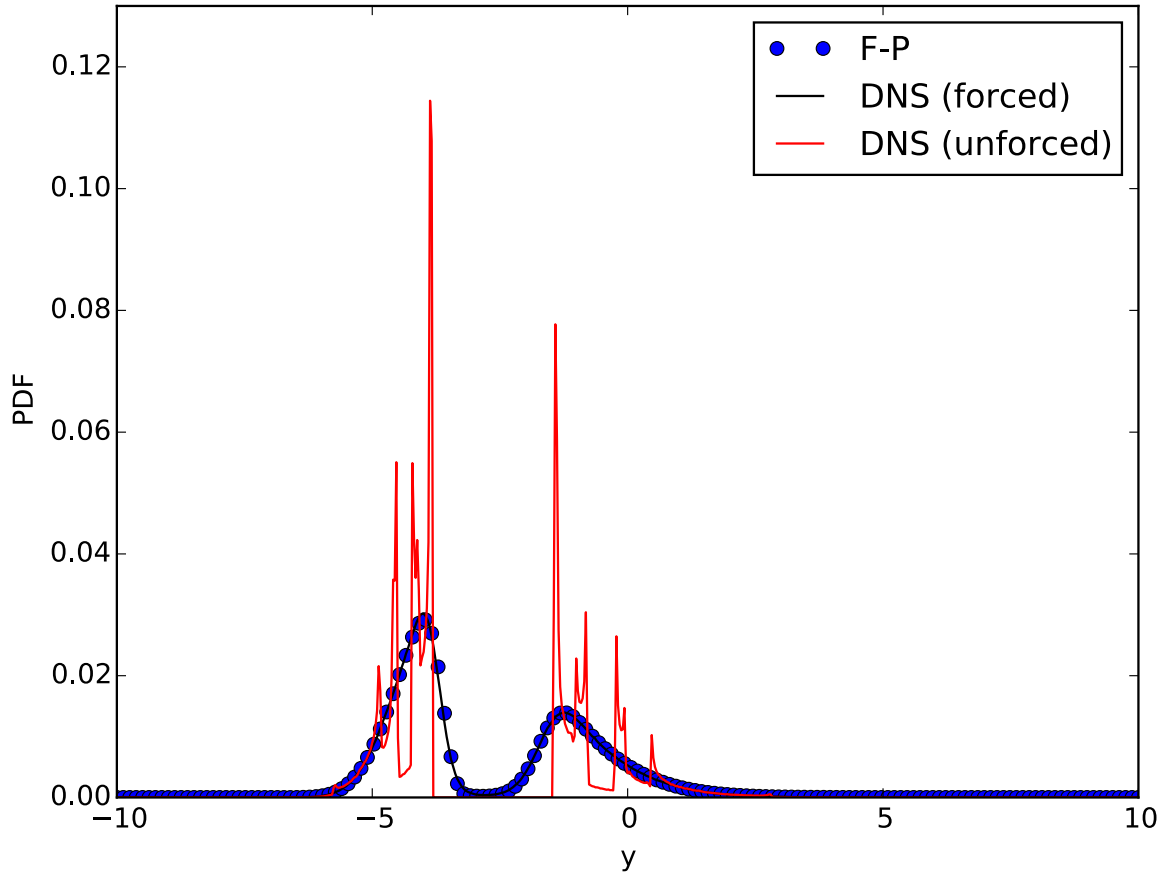


Figure 2.3.6: Cross-section through the $x - y$ planar projection of the PDF where $x = -2.77$ for unforced DNS, stochastically forced DNS, and stochastically forced FPE (with $\Gamma = 0.02$). Modified parameters are used. Sharp peaks in probability in the unforced Lorenz system (corresponding to the steps) are eliminated by the stochastic forcing.

Fig. 2.3.2, 2.3.3, 2.3.4, and 2.3.5 show good quantitative agreement between PDFs accumulated by DNS and those obtained from the zero mode of the FPE. Fine structure evident in the $x-z$ and $y-z$ projections of the PDF for the Lorenz attractor with modified parameters, Fig. 2.3.4, is reproduced by the FPE. The modified parameters also demonstrate the sensitivity of the fractal structure to stochastic forcing. Even forcing as small as $\Gamma = 0.02$ washes out the ring-like steps in the PDF. Fig. 2.3.6 offers a visualization of the dissipation of fine structure with forcing.

2.4 Spectral Gap

The imaginary component of the eigenvalues of the linear FPE operator sets the quasi-frequency of the dynamical system (see Section 1.4 for the slow and fast time scales). Additionally the real component of the eigenvalues sets the relaxation timescale of the system. This is most easily seen by separating the eigenvalues in Eq. 2.2.7 into real and imaginary parts, $\lambda_k^{(R)}$ and $\lambda_k^{(I)}$ respectively, so that the PDF as a function of time is given by:

$$P(t) = \sum_k e^{-\lambda_k^{(R)} t} \alpha_k \vec{v}_k + \sum_k e^{-i\lambda_k^{(I)} t} \alpha_k \vec{v}_k. \quad (2.4.1)$$

Since stochastic forcing smears out a corresponding amount of fine structure in the steady-state PDF of the Lorenz attractor resulting in a faster convergence time for an arbitrary initial PDF, it introduces a Γ -dependence to these real eigenvalues. This is numerically demonstrated in Fig. 2.4.1 where stochastic forcing increases the values of the real components of the eigenvalues of the FPE operator, in turn shortening the decay timescale. By contrast, this Γ -dependence is absent in systems that lack fine structure. This is readily illustrated with a non-chaotic two dimensional Ornstein-Uhlenbeck process modified so that motion in the x and y directions is coupled via

circular motion:

$$\begin{aligned}\dot{x} &= y - \alpha x + \eta_1(t) \\ \dot{y} &= -x - \alpha y + \eta_2(t).\end{aligned}\tag{2.4.2}$$

The eigenvalues of the FPE operator of this system are:

$$\lambda_{n,m} = \alpha n \pm im,\tag{2.4.3}$$

where m, n are non-negative integers of the same parity and $m \leq n$. The derivation of the eigenvalues of Eq. 2.4.3 and their associated eigenvectors, is presented in Appendix A.2. Note that since this system lacks fine structure, its eigenvalues are independent of stochastic forcing, presenting a crucial distinction between the two systems. In addition the presence of both real and imaginary parts in the eigenvalues reflects the presence of two different types of processes: Mean macroscopic behavior that decays toward a fixed point, and the individual orbits behaving quasi-periodically. For this system each has only one time scale. For the Lorenz attractor each has multiple time scales.

The energy gap between the zero-mode and the smallest real component of the excited eigenmodes is of particular importance as it corresponds to the slowest relaxation rate in the statistics towards the statistical steady state. This is trivially equal to α for the modified Ornstein-Uhlenbeck system. For the Lorenz attractor, a linear extrapolation to the unforced ($\Gamma = 0$) regime yields $Re(\lambda_{k=1}^{(\Gamma=0)}) = 0.0802$ which corresponds to a timescale of $\simeq 12$.

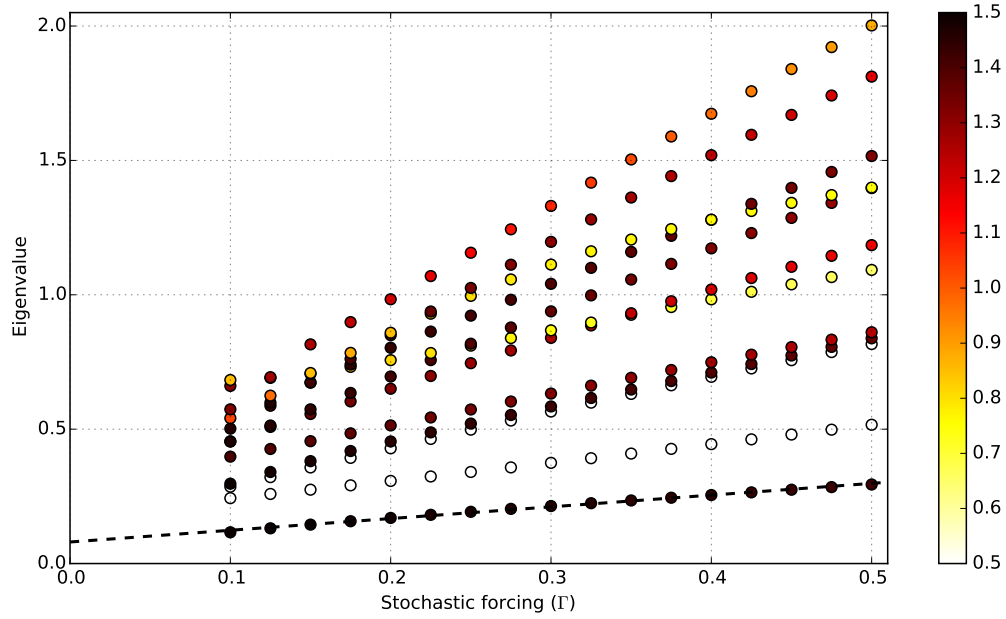


Figure 2.4.1: Real component of the first 12 excited eigenvalues of the linear FPE operator of the Lorenz system (on an 80^3 lattice grid) as a function of stochastic forcing (Γ). Modified parameters are used (see Sec. 1.4) with $x \in [-12.5, 12.5]$, $y \in [-17.5, 17.5]$ and $z \in [7.5, 42.5]$. The phase of the eigenvalue is represented by the color of the points where white filling corresponds to zero phase. Second and third excited eigenvalues are purely real.

2.5 Extensions

The FPE operator can be modified in two potentially advantageous ways. The first is a self-adjoint construction of the linear operator, and the second is the substitution of diffusion with hyperdiffusion.

2.5.1 Self-Adjoint Linear FPE Operators

Self-adjoint versions of the linear FPE operator may be advantageous as the eigenvectors form a complete basis. One way to construct such an operator is to double the size of the linear space and introduce

$$\hat{H}_2 = \begin{pmatrix} 0 & \hat{L} \\ \hat{L}^\dagger & 0 \end{pmatrix} \quad (2.5.1)$$

that by construction obeys $\hat{H}_2^\dagger = \hat{H}_2$. $\hat{H}_2$ is no longer positive-definite; instead its eigenvalue spectrum is symmetric about 0. Finding the zero mode therefore requires a numerical algorithm that can target the middle of the spectrum. Alternatively the operator

$$\hat{H}_1 \equiv \hat{L}^\dagger \hat{L} \quad (2.5.2)$$

is self-adjoint, positive-definite, and has the same ground state as $\hat{L}$. To see this define $|V\rangle \equiv \hat{L}|\Psi_0\rangle$ where $|\Psi_0\rangle$ is the zero mode eigenvector of $\hat{H}_1$. Then $\langle\Psi_0|\hat{L}^\dagger\hat{L}|\Psi_0\rangle = \langle V|V\rangle = 0$ which implies that $|V\rangle$ must have zero norm, $|V\rangle = |0\rangle$, and $|\Psi_0\rangle$ is the ground state of $\hat{L}$.

Since $\hat{H}_1$ is a Hermitian operator and its ground state might possibly be accessed adiabatically [33,34], it is of interest to investigate its numerical solution. A drawback of $\hat{H}_1$ is that the eigenvalues are clustered more tightly around 0 than those of $\hat{L}$, slowing convergence. Fig. 2.5.1(a) shows the projection of the PDF onto the $x - z$ plane, found by calculating the ground state of $\hat{H}_1$ by the Davidson algorithm [35,36].

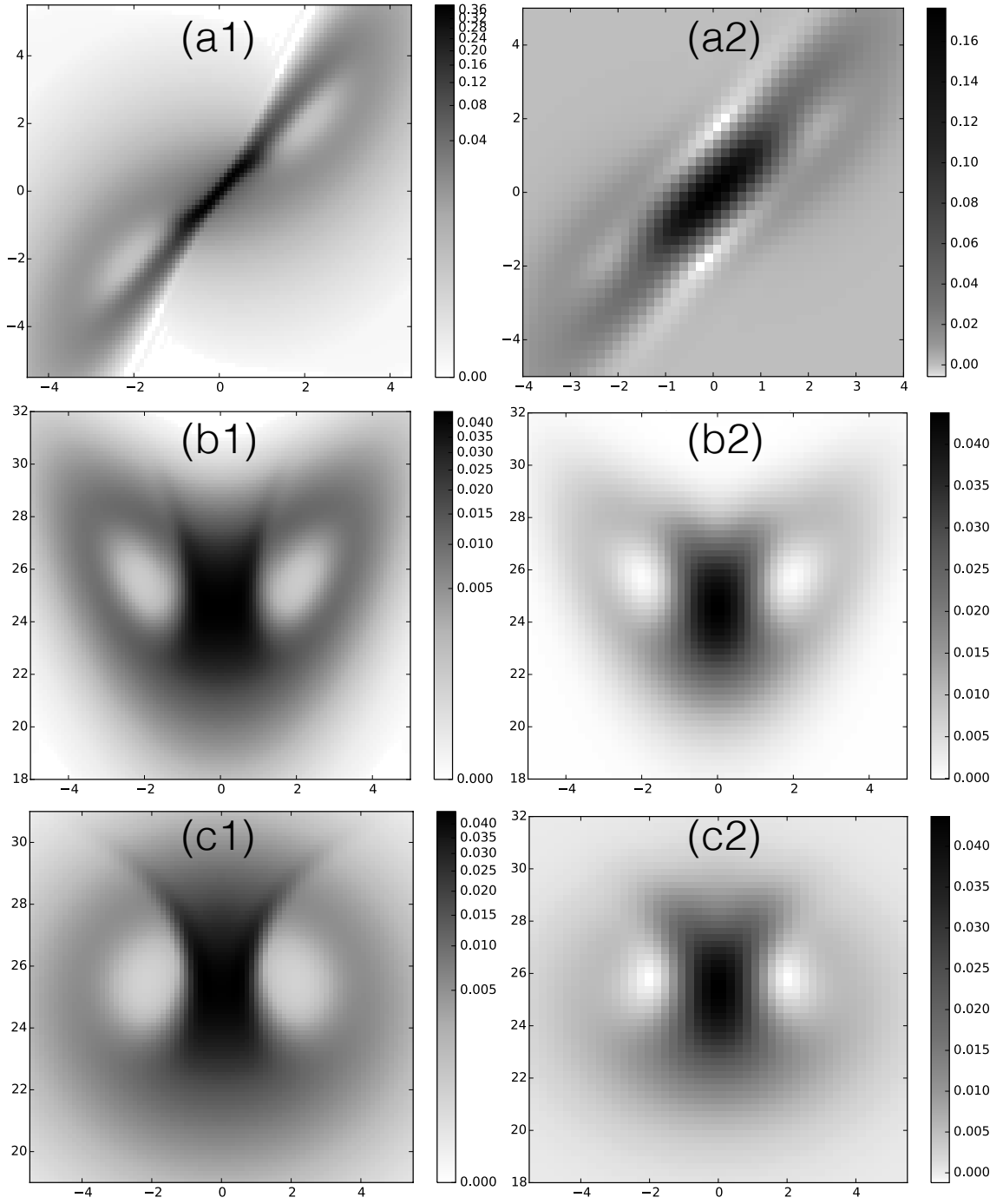


Figure 2.5.1: (a) $x - y$, (b) $x - z$ and (c) $y - z$ planar projections of the PDF with modified Lorenz parameters. Column 1 is the ground state of the self-adjoint operator $\hat{H}_1$ with diffusion coefficient of $\Gamma = 0.05$ on a 150^3 lattice. The lattice extends over $x \in [-7, 7]$, $y \in [-10, 10]$ and $z \in [15, 35]$. Column 2 is the Lorenz attractor PDF with a hyperdiffusion coefficient of $\Gamma_2 = 0.2$ on a 80^3 lattice. The lattice is $x \in [-7, 7]$, $y \in [-9.5, 9.5]$ and $z \in [15, 35]$.

2.5.2 Hyperdiffusion

Another interesting variant to investigate is to replace diffusion in Eq. 2.3.1 with hyperdiffusion:

$$-\Gamma \nabla^2 \rightarrow \Gamma_2 \nabla^4 \quad (2.5.3)$$

where the values of the PDF, as well as its first and second derivatives, are fixed at zero at the boundaries. Γ_2 now scales inversely with the quartic rather than the square of the lattice spacing Δx . As hyperdiffusion is more scale selective than ordinary diffusion, it acts to smooth out structure at the lattice scale while leaving larger structures intact. However, unlike ordinary diffusion that has its origin in stochastic forcing, hyperdiffusion violates realizability leading to negative probability densities. For example Section 4.3 of Ref. [28] discusses Pawula's theorem which shows that the FP equation with diffusion replaced by hyperdiffusion is guaranteed to have negative probabilities. And indeed even the 1D Orstein-Uhlenbeck system with diffusion replaced with hyperdiffusion has a steady-state PDF that drops below zero toward the edges. In addition, hyperdiffusion reduces the sparseness of the discretized linear FPE operator, slowing computation. Nevertheless computations are possible on smaller lattices and Fig. 2.5.1(b) shows the PDF computed with hyperdiffusion in place of diffusion. The negative values of the PDF are visible.

2.6 Summary

Finding the zero-mode of the FPE operator is an accurate and fast alternative to DNS for directly accessing the equal time statistics of the Lorenz-63 attractor. This technique is obviously general and can be extended to other nonlinear dynamical systems. An attractive feature of this technique is that the FPE operator can be expressed in a sparse form. The steady-state PDF, as computed by a matrix diagonalization of this operator, quantitatively matches with the PDF as computed by DNS. However,

although a sparse matrix diagonalizer was used, the pre-conditioner used was dense. It would be interesting to look for an appropriate sparse matrix diagonalizer, as this would allow for a drastic increase in resolution and a further decrease in the artificially introduced stochastic forcing.

The dependence of the real component of the eigenvalues of the Lorenz attractor on stochastic forcing allows for a linear extrapolation down to the deterministic case. This value, corresponding to a timescale of 12, represents the relaxation time scale of the system. But it is still unclear whether important information regarding the dynamics of the system is contained in the other excited eigenvalues of the operator. Another open question is why the density of the eigenvalue distribution in complex space increases as the magnitude of the eigenvalue increases.

Variants of the Fokker-Planck equation also have interesting properties. The replacement of diffusion with hyperdiffusion allows for the elimination of stochastic forcing altogether. Although this breaks realizability (by Pawula's theorem) and the PDF develops negative probabilities, this might still be useful in cases where only an approximate distribution is required. For example, if the negative values remain small and away from the regions of interest, hyperdiffusion can be a valuable tool. Other variants of the FPE operator, such as a self-adjoint form, break either positive-definiteness or clusters the eigenvalues more tightly around zero. But by gaining Hermiticity, the operator becomes amenable to solution by simulated/quantum annealing and adiabatic quantum computation. It would be interesting to check whether the theoretical computational gains of using a quantum algorithm could offset the added drawbacks of a slower convergence time due to a more clustered eigenvalue distribution around zero.

Chapter 3

Ensemble Cumulant Expansions

3.1 Introduction

The utility of Direct Statistical Simulation (DSS) for understanding chaotic systems was demonstrated in the previous chapter. An instance of DSS, involving the Fokker-Planck approach, was used to directly solve for the statistics of the Lorenz attractor. However because numerical solution of the FPE for dynamical systems of high dimensions is increasingly difficult, it is of interest to explore alternative forms of DSS. Here I use an expansion in low-order equal-time cumulants to find the statistics of the Lorenz attractor. Whereas the FPE approach grows exponentially with the dimensionality of the system, this cumulant expansion technique grows only polynomially with the size of the system (but exponentially with the truncation level) and so is more suitable for high-dimensional dynamical systems. This technique will be applied to the two main types of systems considered in this thesis: the Lorenz attractor and the idealized barotropic models, both introduced in Chapter 1. In both the cases, the low-order statistics will be seen to be well reproduced at second and third order truncation for the chaotic and turbulent systems respectively.

This chapter is organized as follows. Section 3.2 introduces the cumulant expan-

sion to directly access the steady-state statistics of a system with quadratic nonlinearity. The expansion is closed at second-order (CE2, CE2.5) and third-order (CE3) and the validity of these closures are discussed. CE3 is applied to the Lorenz system and its comparison to DNS is discussed. Section 3.3 then applies CE2 on two idealized barotropic models. Although this has been already been done using a zonal average [37, 38], it neglects crucial eddy-eddy scattering processes required to accurately describe turbulent flows. Therefore I instead use an ensemble average to capture these processes inherent to turbulent flow. The formalism of these two different flavors of CE2 is expounded in Sections 3.3.1 and 3.3.2. In Section 3.3.3 this scheme using an ensemble average is tested against traditional (zonal) CE2 and fully nonlinear DNS on the two different barotropic models: A deterministic barotropic jet relaxed toward an unstable profile in Section 3.3.3.1, and a stochastically-forced barotropic jet in Section 3.3.3.2. Some conclusions are presented in Section 3.4.

3.2 Lorenz Attractor

An equal-time expansion in the low order cumulants has been applied to the Orszag-McLaughlin attractor [39], as well as a number of high-dimensional problems in fluids using spatial averaging [27, 37, 38, 40–44]. However sometimes ensemble averages are employed instead [45, 46], as will be done here.

In addition to deriving the EOMs of the equal-time cumulants via the Hopf functional formalism [25, 40], they can also be derived directly from the EOMs of the dynamical system. Consider a general system with at most quadratic nonlinearities:

$$\dot{q}_i = F_i + L_{ij}q_j + Q_{ijk}q_jq_k + \eta_i. \quad (3.2.1)$$

Performing a Reynolds decomposition, $q_i = \overline{q}_i + q'_i$, its mean and fluctuating part

are required to satisfy the Reynolds rules of averaging:

$$\begin{aligned}\overline{\overline{q_i}} &= \overline{q_i} \\ \overline{q'_i} &= 0 \\ \overline{\overline{q_i} q_j} &= \overline{q_i} \overline{q_j}.\end{aligned}\tag{3.2.2}$$

Here the mean has been defined as an ensemble average over a large number of initial conditions:

$$\overline{q_i(t)} = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=0}^{N-1} q_i^{(n)}(t).\tag{3.2.3}$$

The mean of q_i is given by the first cumulant, c_i , and the second and third central-moments give the second and third cumulants respectively. However, the fourth cumulant is not a central moment:

$$\begin{aligned}c_i &\equiv \overline{q_i} \\ c_{ij} &\equiv \overline{q'_i q'_j} \\ c_{ijk} &\equiv \overline{q'_i q'_j q'_k} \\ c_{ijkl} &\equiv \overline{q'_i q'_j q'_k q'_l} - c_{ij} c_{kl} - c_{ik} c_{jl} - c_{il} c_{jk}.\end{aligned}\tag{3.2.4}$$

By these definitions only the second cumulant of a Gaussian distribution is nonzero. These cumulants can be solved for directly. Since the ensemble averaging operator commutes with the time derivative operator, an EOM for the first cumulant can be derived in terms of the first and second cumulants:

$$\begin{aligned}\frac{dc_i}{dt} &= \overline{\frac{dq_i}{dt}} \\ &= L_{im} \overline{q_m} + Q_{imn} \overline{q_m q_n} \\ &= L_{im} c_m + Q_{imn} (c_m c_n + c_{mn}).\end{aligned}\tag{3.2.5}$$

Similarly, the EOMs for the seconds cumulants contain the first, second and third cumulants:

$$\begin{aligned}
\frac{dc_{ij}}{dt} &= 2 \left\{ \overline{\frac{dq'_i}{dt} q'_j} \right\} \\
&= 2 \left\{ \overline{\left(\frac{dq_i}{dt} - \frac{d\bar{q}_i}{dt} \right) q'_j} \right\} \\
&= 2 \left\{ \overline{\frac{dq_i}{dt} q'_j} \right\} \\
&= 2 \left\{ \overline{L_{im} q_m q'_j + Q_{imn} q_m q_n q'_j} \right\} \\
&= \left\{ 2L_{im} c_{mj} + Q_{imn} (4c_m c_{nj} + 2c_{mnj}) \right\}, \tag{3.2.6}
\end{aligned}$$

where the symmetrization operator $\{\}$ performs an average over all permutations of the free indices. For example, in the case of a 2-index variable such as the second cumulant it is defined as $\{c_{ij}\} = \frac{1}{2}(c_{ij} + c_{ji})$ and similarly for higher cumulants.

The EOMs for the n -th cumulants contain the $(n+1)$ -th cumulants, forming an infinite hierarchy of cumulants resulting in the well-known closure problem. Since computing a higher cumulant requires an increase in the degrees of freedom of the system by an amount equal to the dimensionality of the system, a closure should be performed as soon as possible. Performing the closure at third order by setting $c_{ijk} = 0$ (known as CE2) is an adequate approximation for the dynamics of some systems but not the Lorenz attractor because neglecting the nonlocal cubic & higher correlations (eddy-eddy scattering) disallows for the inverse-cascade processes inherent to the attractor that gives rise to the fractal fine structure. Since the cumulants do not converge to a steady-state, closure is instead performed at fourth order by setting

$c_{ijkl} = 0$ along with all higher cumulants (known as CE3) as follows:

$$\begin{aligned}
\frac{dc_{ijk}}{dt} &= 3 \left\{ \overline{\frac{dq'_i}{dt} q'_j q'_k} \right\} \\
&= 3 \left\{ \overline{\left(\frac{dq_i}{dt} - \frac{d\bar{q}_i}{dt} \right) q'_j q'_k} \right\} \\
&= 3 \left\{ \overline{\frac{dq_i}{dt} q'_j q'_k} - \frac{dc_i}{dt} \overline{q'_j q'_k} \right\} \\
&= 3 \left\{ L_{im} c_{mjk} + Q_{imn} (2c_m c_{njk} - c_{mn} c_{jk} + \overline{q'_m q'_n q'_j q'_k}) \right\}, \quad (3.2.7)
\end{aligned}$$

where the symmetrization operator is defined for a 3-index variable as:

$$\{x_{abc}\} = \frac{1}{6} (x_{abc} + x_{bca} + x_{cab} + x_{acb} + x_{bac} + x_{cba}), \quad (3.2.8)$$

and the fourth central-moment $\overline{q'_m q'_n q'_j q'_k}$ can be expressed in terms of second and fourth cumulants as:

$$\begin{aligned}
\overline{q'_m q'_n q'_j q'_k} &= c_{mn} c_{jk} + c_{mj} c_{nk} + c_{mk} c_{jn} + c_{mnjk} \\
&\simeq c_{mn} c_{jk} + c_{mj} c_{nk} + c_{mk} c_{jn}. \quad (\text{CE3}) \quad (3.2.9)
\end{aligned}$$

Hence the EOMs for the third cumulants are:

$$\frac{dc_{ijk}}{dt} = \left\{ 3L_{im} c_{mjk} + 6Q_{imn} (c_m c_{njk} + c_{mj} c_{nk}) - \frac{c_{ijk}}{\tau_d} \right\}. \quad (3.2.10)$$

An eddy-damping parameter, τ_d , has been introduced to model the truncated higher-order cumulants [47]. This is necessary to ensure realizability because unlike even-ordered cumulants which are guaranteed to be non-negative [48, 49], the third cumulant (and hence CE3) has no such guarantee. The eddy damping timescale is required to be sufficiently smaller than the timescale of the system to ensure realizability. However excessively reducing τ_d has the effect of suppressing the third cumulant, causing

the behavior of the system to be similar to its behavior under the CE2 approximation; indeed CE2 is recovered in the limit $\tau_d \rightarrow 0$.

In addition to CE2, another way to achieve closure at the level of the second cumulant is by assuming that the third cumulant varies fast enough to remain close to equilibrium. This can be modeled by setting the time derivative of the third cumulant to zero in Eq. 3.2.10. A further simplification by neglecting the next two terms yields an approximation for the third cumulant in terms of the second:

$$c_{ijk} = 6\tau_d \{Q_{imn}c_{mj}c_{nk}\}. \quad (3.2.11)$$

This then provides closure for the EOM of the second cumulant. This approximation has been termed CE2.5 as it shares a mix of properties of both CE2 and CE3. For example, like CE2 it closes at the level of the second cumulant and has also been shown to be a conservative truncation scheme up to quadratic quantities [37]. But unlike CE2 and like CE3, it retains the nonlinear eddy-eddy scattering. In addition, numerical experiments suggest that it is a realizable truncation scheme for the Lorenz attractor (Saxena & Marston, unpublished). While its realizability status for a general quadratically nonlinear system remains an open question, one way forward might be to establish its connection (and possible equivalency) to another realizable scheme such as EDQNM [50]. In this thesis, CE2.5 is explored only in the context of testing a semi-implicit integration scheme (Chapter 5).

Since the timescale of the Lorenz system is $T \simeq 1$, the eddy damping timescale must be set accordingly. Tables 1 & 2 compare the low-ordered cumulants via DNS with DSS for the unforced and forced ($\Gamma = 0.02$) systems respectively where two different sets of eddy damping timescales are used. The cumulants associated with the larger timescale, $\tau_d = 0.5$, agree more closely with the DNS results than those cumulants associated with the shorter timescale, $\tau_d = 0.1$.

Irrespective of the eddy damping timescale, the first cumulants $\bar{x}$ and $\bar{y}$ are analytically zero because the EOMs for the Lorenz system remain unchanged under the transformation $\{x, y, z\} \rightarrow \{-x, -y, z\}$ and thus $P(x, y, z) = P(-x, -y, z)$. This symmetry is captured by the CE3 method but not by DNS, where $\bar{x}$ and $\bar{y}$ are as large as 10^{-4} despite a run time of $T = 2 * 10^7$. This is in comparison to the DSS run time of only $T = 100$. Thus although the DSS values for the cumulants are only approximate due to the truncation, the cumulants converged to their steady-state five orders of magnitude faster than DNS. This is shown in Table 3.1 which compares DNS and CE3 via the first and second cumulants of the unforced Lorenz attractor for two different choices of the time scale τ_d . The good qualitative agreement at both $\tau_d = 0.1$ and $\tau_d = 0.5$ demonstrates an insensitivity to the precise choice of the time scale. The same results are presented in Table 3.2 but for the stochastically forced attractor. Despite having a large effect on the fine structure of the PDF, the small stochastic forcing only changes the covariances slightly.

Table 3.1: Comparison of the low-order statistically steady state cumulants of the unforced Lorenz attractor ($\Gamma = 0$) as accumulated by DNS and as calculated with CE3. Modified Lorenz parameters are used (see Section 1.4). Entries such as $\mathcal{O}(10^{-4})$ indicate that these mean values are tending to zero as time-averaging of DNS extends over increasing intervals of time.

Cumulant	DNS	CE3 ($\tau_d = 0.1$)	CE3 ($\tau_d = 0.5$)
$\bar{x}$	$\mathcal{O}(10^{-4})$	0	0
$\bar{y}$	$\mathcal{O}(10^{-4})$	0	0
$\bar{z}$	24.796	25.188	25.000
$\overline{x'x'}$	3.966	4.030	4.000

$\overline{x'y'}$	3.966	4.030	4.000
$\overline{x'z'}$	$\mathcal{O}(10^{-5})$	0	0
$\overline{y'y'}$	5.395	4.392	4.908
$\overline{y'z'}$	$\mathcal{O}(10^{-5})$	0	0
$\overline{z'z'}$	8.513	5.592	6.825

Table 3.2: As in Table 3.1 but with added stochastic forcing ($\Gamma = 0.02$).

Cumulant	DNS	CE3 ($\tau_d = 0.1$)	CE3 ($\tau_d = 0.5$)
$\bar{x}$	$\mathcal{O}(10^{-5})$	0	0
$\bar{y}$	$\mathcal{O}(10^{-5})$	0	0
$\bar{z}$	24.834	25.192	25.004
$\overline{x'x'}$	3.977	4.034	4.004
$\overline{x'y'}$	3.971	4.031	4.001
$\overline{x'z'}$	$\mathcal{O}(10^{-5})$	0	0
$\overline{y'y'}$	5.350	4.396	4.912
$\overline{y'z'}$	$\mathcal{O}(10^{-4})$	0	0
$\overline{z'z'}$	8.150	5.610	6.829

3.3 Idealized Barotropic Model

Beyond chaotic systems such as the Lorenz attractor, an ensemble-averaged cumulant expansion can also be used in problems of geophysical turbulence. To develop this, I will consider a rotating barotropic model where relative vorticity is convected by a

bilinear Jacobian operator,

$$J[A, B] = \hat{r} \cdot (\nabla A \times \nabla B), \quad (3.3.1)$$

and damped by a frictional term with coefficient κ as well as a hyperviscosity term with coefficient ν_3 which models subgrid physics by soaking up enstrophy which cascades down to the grid scales,

$$L[A] \equiv - [\kappa - \nu_3 (\nabla^2 + 2) \nabla^4] A. \quad (3.3.2)$$

The governing EOM of the system is thus:

$$\dot{\zeta} = J[\zeta + f, \psi] + L[\zeta], \quad (3.3.3)$$

where ψ is the stream function, $\nabla^2 \psi = \zeta$ is the relative vorticity and $f = 2\Omega \cos(\theta)$ is the Coriolis parameter.

As in 3.2, the starting point for a cumulant expansion is a Reynolds decomposition into the relative vorticity into the sum of a hitherto unspecified average vorticity $\bar{\zeta}$ and a fluctuation about that average ζ' ,

$$\zeta(\theta, \phi) = \bar{\zeta}(\theta, \phi) + \zeta'(\theta, \phi). \quad (3.3.4)$$

Unlike in the previous section where the nature of the averaging operation was assumed to be an ensemble average, for now I will leave it as an as-yet undefined type of average and later discuss specific varieties in Sections 3.3.1 & 3.3.2. This general

averaging operation will satisfy the following Reynolds averaging rules:

$$\begin{aligned}
\overline{\zeta'(\theta, \phi)} &= 0 \\
\overline{\overline{\zeta(\theta, \phi)}} &= \overline{\zeta(\theta, \phi)} \\
\overline{\overline{\zeta\zeta}} &= \overline{\zeta} \overline{\zeta}.
\end{aligned} \tag{3.3.5}$$

This average relative vorticity is defined as the first cumulant whereas the second and third cumulants are defined as the centered moments of the fluctuations, which on the surface of a sphere are most naturally defined in terms of a co-latitude θ and azimuth angle ϕ :

$$\begin{aligned}
c(\theta_1, \phi_1) &\equiv \overline{\zeta(\theta_1, \phi_1)} \\
c(\theta_1, \phi_1; \theta_2, \phi_2) &\equiv \overline{\zeta'(\theta_1, \phi_1) \zeta'(\theta_2, \phi_2)} \\
c(\theta_1, \phi_1; \theta_2, \phi_2; \theta_3, \phi_3) &\equiv \overline{\zeta'(\theta_1, \phi_1) \zeta'(\theta_2, \phi_2) \zeta'(\theta_3, \phi_3)}.
\end{aligned} \tag{3.3.6}$$

It is useful to define as auxiliary cumulants the correlations of relative vorticity and the stream function,

$$\begin{aligned}
p(\theta_1, \phi_1) &\equiv \overline{\psi(\theta_1, \phi_1)} \\
p(\theta_1, \phi_1; \theta_2, \phi_2) &\equiv \overline{\zeta'(\theta_1, \phi_1) \psi'(\theta_2, \phi_2)} \\
p(\theta_1, \phi_1; \theta_2, \phi_2; \theta_3, \phi_3) &\equiv \overline{\zeta'(\theta_1, \phi_1) \zeta'(\theta_2, \phi_2) \psi'(\theta_3, \phi_3)}.
\end{aligned} \tag{3.3.7}$$

This allows for the re-expression of $\overline{\xi(\theta_1, \phi_1) \psi(\theta_2, \phi_2)}$ in terms of the cumulants and auxiliary cumulants:

$$\begin{aligned}
\overline{\xi(\theta_1, \phi_1) \psi(\theta_2, \phi_2)} &= \overline{\xi'(\theta_1, \phi_1) \psi'(\theta_2, \phi_2)} + \overline{\xi(\theta_1, \phi_1)} \overline{\psi(\theta_2, \phi_2)} \\
&= p(\theta_1, \phi_1; \theta_2, \phi_2) + c(\theta_1, \phi_1) p(\theta_2, \phi_2),
\end{aligned} \tag{3.3.8}$$

The equation of motion (EOM) of the first cumulant can then be derived by averaging over Eq. 3.3.3:

$$\frac{\partial}{\partial t} c(\vec{r}) = \overline{J[\zeta(\vec{r}) + f(\vec{r}), \psi(\vec{r})]} + L[\zeta(\vec{r})], \quad (3.3.9)$$

where $\vec{r} = (\theta, \phi)$. The averaging operation commutes with the time derivative operator and linear operator but does not commute with the quadratic operator. To evaluate the average of this quadratic operator, $\overline{J[A, \psi]}$ may be rewritten as:

$$\begin{aligned} \overline{J[A(\vec{r}_1), \psi(\vec{r}_1)]} &= \overline{\int \hat{n} \cdot (\nabla_1 A(\vec{r}_1) \times \nabla_1 \psi(\vec{r}_2) \delta(\vec{r}_1 - \vec{r}_2)) d^2 r_2} \\ &= \overline{\int \hat{n} \cdot (\nabla_1 A(\vec{r}_1) \psi(\vec{r}_2) \times \nabla_1 \delta(\vec{r}_1 - \vec{r}_2)) d^2 r_2} \\ &= \int J_1[\overline{A(\vec{r}_1) \psi(\vec{r}_2)}, \delta(\vec{r}_1 - \vec{r}_2)] d^2 r_2, \end{aligned} \quad (3.3.10)$$

where the subscript of the Jacobian is understood to denote the variable being differentiated. Therefore using Eq. 3.3.8 & 3.3.10, the EOM for the first cumulant becomes:

$$\begin{aligned} \frac{\partial}{\partial t} c(\vec{r}_1) &= \overline{J_1[\zeta(\vec{r}_1), \psi(\vec{r}_1)]} + J_1[f(\vec{r}_1), p(\vec{r}_1)] + L_1[c(\vec{r}_1)] \\ &= \int J_1[p(\vec{r}_1, \vec{r}_2) + c(\vec{r}_1) p(\vec{r}_2), \delta(\vec{r}_1 - \vec{r}_2)] d^2 r_2 \\ &\quad + J_1[\zeta(\vec{r}_1), p(\vec{r}_1)] + L_1[c(\vec{r}_1)] \\ &= \int J_1[p(\vec{r}_1, \vec{r}_2), \delta(\vec{r}_1 - \vec{r}_2)] d^2 r_2 \\ &\quad + J_1[c(\vec{r}_1) + f(\vec{r}_1), p(\vec{r}_1)] + L_1[c(\vec{r}_1)]. \end{aligned} \quad (3.3.11)$$

Since the equation of motion of the first cumulant involves both the first and second cumulant, the well-known closure problem results as a direct consequence of the non-commutivity of the averaging operator with the quadratic operator. This was also seen in Section 3.2. Therefore the equation of motion for the second cumulant

involves the first, second and third cumulant:

$$\begin{aligned}
\frac{\partial}{\partial t} c(\vec{r}_1, \vec{r}_2) &= 2 \left\{ \overline{\zeta'(\vec{r}_2) \frac{\partial}{\partial t} \zeta'(\vec{r}_1)} \right\} \\
&= 2 \left\{ \overline{\zeta'(\vec{r}_2) \frac{\partial}{\partial t} \zeta(\vec{r}_1)} \right\} \\
&= 2 \left\{ \overline{\zeta'(\vec{r}_2) J_1 [\zeta(\vec{r}_1) + f(\vec{r}_1), \psi(\vec{r}_1)]} + \overline{\zeta'(\vec{r}_2) L_1 [\zeta(\vec{r}_1)]} \right\} \\
&= 2 \left\{ \overline{\zeta'(\vec{r}_2) J_1 [c(\vec{r}_1) + f(\vec{r}_1), \psi(\vec{r}_1)]} + \overline{\zeta'(\vec{r}_2) J_1 [\zeta'(\vec{r}_1), \psi(\vec{r}_1)]} + \overline{\zeta'(\vec{r}_2) L_1 [\zeta'(\vec{r}_1)]} \right\} \\
&= 2 \left\{ \overline{J_1 [c(\vec{r}_1) + f(\vec{r}_1), \zeta'(\vec{r}_2) \psi(\vec{r}_1)]} + \overline{J_1 [\zeta'(\vec{r}_1) \zeta'(\vec{r}_2), \psi(\vec{r}_1)]} + L_1 [c(\vec{r}_1, \vec{r}_2)] \right\} \\
&= 2 \left\{ L_1 [c(\vec{r}_1, \vec{r}_2)] + J_1 [c(\vec{r}_1) + f(\vec{r}_1), \overline{\zeta'(\vec{r}_2) \psi(\vec{r}_1)}] \right\} \\
&\quad + 2 \left\{ \int J_1 [\overline{\zeta'(\vec{r}_1) \zeta'(\vec{r}_2) \psi(\vec{r}_3)}, \delta(\vec{r}_1 - \vec{r}_3)] d^2 r_3 \right\} \\
&= 2 \left\{ J_1 [c(\vec{r}_1) + f(\vec{r}_1), p(\vec{r}_2, \vec{r}_1)] + \int J_1 [\overline{\zeta'(\vec{r}_1) \zeta'(\vec{r}_2) \psi(\vec{r}_3)}, \delta(\vec{r}_1 - \vec{r}_2)] d^2 r_3 \right\} \\
&\quad + 2 \{ L_1 [c(\vec{r}_1, \vec{r}_2)] \}, \tag{3.3.12}
\end{aligned}$$

where the symmetrization operator $\{\dots\}$ performs an average over all interchanges of the field points. For example, in the case of a 2-point variable such as the second cumulant it is defined as before as $\{c(\vec{r}_1, \vec{r}_2)\} = \frac{1}{2} [c(\vec{r}_1, \vec{r}_2) + c(\vec{r}_2, \vec{r}_1)]$ and similarly for higher cumulants. This closure problem means that the EOMs for the n -th cumulants contain the $(n+1)$ -th cumulants, forming an infinite hierarchy where the degrees of freedom increase by an amount equal to the dimensionality of the system. A closure should be performed as soon as possible; one such option is CE2 where the third cumulant is decoupled from Eq. 3.3.12:

$$\begin{aligned}
\overline{\zeta'(\vec{r}_1) \zeta'(\vec{r}_2) \psi(\vec{r}_3)} &= p(\vec{r}_1, \vec{r}_2, \vec{r}_3) + c(\vec{r}_1, \vec{r}_2) p(\vec{r}_3) \\
&\simeq c(\vec{r}_1, \vec{r}_2) p(\vec{r}_3) \quad (\text{CE2}), \tag{3.3.13}
\end{aligned}$$

giving the (closed) EOM for the second cumulant:

$$\begin{aligned} \frac{\partial}{\partial t} c(\vec{r}_1, \vec{r}_2) = & 2 \{ J_1 [c(\vec{r}_1) + f(\vec{r}_1), p(\vec{r}_2, \vec{r}_1)] \} \\ & + 2 \{ J_1 [c(\vec{r}_1, \vec{r}_2), p(\vec{r}_1)] + L_1 [c(\vec{r}_1, \vec{r}_2)] \} \end{aligned} \quad (3.3.14)$$

Although this decoupling assumes Gaussianity, even for non-Gaussian statistics this can be a good approximation. When the system is stochastically forced with additive Gaussian white noise, $\eta(\vec{r}, t)$, the EOM for the second cumulant is appended with $\Gamma(\vec{r}_1, \vec{r}_2)$, the magnitude of the auto-correlation function of the white noise over a short time average $[\dots]$:

$$\frac{\partial}{\partial t} c(\vec{r}_1, \vec{r}_2) = \dots + 2\Gamma(\vec{r}_1, \vec{r}_2), \quad (3.3.15)$$

The EOM for the second cumulant, Eq. 3.3.14, thus becomes

$$[\eta(\vec{r}_1, t_1) \eta(\vec{r}_2, t_2)] = 2\Gamma(\vec{r}_1, \vec{r}_2) \delta(t_1 - t_2). \quad (3.3.16)$$

It is natural to expand in the basis of spherical harmonics because of the zonal symmetry of barotropic models on a rotating sphere:

$$\zeta(\theta, \phi, t) \simeq \sum_{l=0}^L \sum_{m=-\min\{l, M\}}^{\min\{l, M\}} \zeta_{lm}(t) Y_{lm}(\theta, \phi), \quad (3.3.17)$$

where the approximation results from introducing L and M as cutoffs for the spherical and zonal wavenumbers respectively. The EOM of the field in spectral space is then

given by:

$$\begin{aligned}\dot{\zeta}_{lm} &= A_l \delta_{m,0} + \sum_{l_1} B_{l;l_1 m} \zeta_{l_1 m} + \eta_{lm}(t) \\ &+ \sum_{l_1 l_2 m_1 m_2} Q_{l;l_1 m_1; l_2 m_2} \zeta_{l_1 m_1} \zeta_{l_2 m_2}.\end{aligned}\quad (3.3.18)$$

Here the coefficients A_l , $B_{l;l_1 m}$ and $Q_{l;l_1 m_1; l_2 m_2}$ are the amplitudes of the constant, linear and quadratic interactions governing the time evolution of the vorticity. $Q_{l;l_1 m_1; l_2 m_2}$ is the amplitude for the scattering of two waves which can be calculated using the associated Legendre functions P_l^m :

$$\begin{aligned}Q_{lm;l_1 m_1; l_2 m_2} &\equiv 2\pi i \int_0^\pi P_l^m(\cos \theta) [m_1 P_{l_1}^{m_1}(\cos \theta) \frac{\partial}{\partial \theta} P_{l_2}^{m_2}(\cos \theta) \\ &+ m_2 P_{l_2}^{m_2}(\cos \theta) \frac{\partial}{\partial \theta} P_{l_1}^{m_1}(\cos \theta)] d\theta.\end{aligned}\quad (3.3.19)$$

where $m = m_1 + m_2$. The EOMs for the cumulants in spectral space can then be found in a similar manner as for real space and is presented in Appendix B.2. This has been implemented in the ‘‘GCM’’ app ¹, a freely available application which simulates and visualizes statistics computed via real space DNS, spectral DNS and spectral DSS.

3.3.1 Zonal Average

CE2 has different flavors which are dictated by the nature of the averaging operation, $\overline{\cdots}$, which has been hitherto unspecified. Different choices exist such as temporal averages, spatial averages and ensemble averages. For systems with inherent zonal symmetry such as geophysical fluid models on rotating spheres, a zonal average is often the simplest, defined as:

$$\langle q(\theta, \phi) \rangle \equiv \frac{1}{2\pi} \int_0^{2\pi} q(\theta, \phi) d\phi. \quad (3.3.20)$$

¹Available on the Apple Mac App Store at <http://appstore.com/mac/gcm>

Since the average is a zonal average, the fluctuations q' represent eddies and the allowed triadic interactions represent wave-wave interactions. Therefore zonal CE2 (zCE2) allows for the interaction between a mean flow and an eddy to produce an eddy, and allows for the interaction between two eddies to produce a mean flow. However, it disallows for the interaction between two eddies to produce another eddy. Thus the eddy-eddy scattering process is neglected and so zCE2 is formally equivalent to the quasi-linear approximation [51, 52], a quadratically conservative truncation scheme. Since the neglect of the eddy-eddy scattering process is equivalent to deactivating the quadratic operator for certain pairs of wavenumbers, zCE2 remains physically realizable.

A virtue of using a zonal average is that it yields a dimensional reduction of the first and second cumulants in the zonal direction. The first cumulant depends only on the co-latitude,

$$c(\vec{r}_1) = c(\theta_1), \quad (3.3.21)$$

and the second cumulant depends only on the two co-latitudes of either points and the difference in longitudes,

$$c(\vec{r}_1, \vec{r}_2) = c(\theta_1, \theta_2, \phi_2 - \phi_1). \quad (3.3.22)$$

Since $c(\vec{r}_1)$, $p(\vec{r}_1)$ and $f(\vec{r}_1)$ have no zonal dependence,

$$J_1[c(\vec{r}_1) + f(\vec{r}_1), p(\vec{r}_1)] = 0, \quad (3.3.23)$$

and so the EOM for the first cumulant in this scheme reduces to:

$$\frac{\partial}{\partial t} c(\theta_1) = \int J_1[p(\vec{r}_1, \vec{r}_2), \delta(\vec{r}_1 - \vec{r}_2)] d^2 r_2 + L_1[c(\theta_1)]. \quad (3.3.24)$$

3.3.2 Ensemble Average

In systems where the eddy-eddy scattering processes dominate such as in turbulent flow, zCE2 can give an inaccurate reproduction of the statistics. An alternative version of the cumulant expansion that does not neglect these processes can be formulated instead using an ensemble average. The averaging operator $\overline{\cdot}$ will be used here onwards to denote specifically an ensemble average. In such a case, the triadic interactions allowed and disallowed in ensemble CE2 (eCE2) are identical to those in zCE2. But under this formulation, the average of the field represents coherent flow [46, 53, 54] instead of zonal mean flow and the fluctuations about this average represent incoherent flow instead of eddies. Therefore eCE2 allows for the interaction between coherent flow and incoherent flow to produce incoherent flow, the interaction between incoherent flows to form coherent flow, but neglects the interactions of incoherent flows to form yet more incoherent flow. Thus eCE2 does not necessarily neglect the eddy-eddy scattering process and can give rise to dynamics that zCE2 is unable to capture. An added benefit of this definition is that non-zonal structures are not *a priori* treated as incoherent and so can be captured in the first cumulant. While the derivations of CE2 presented here are performed in real space, Appendix B.2 and B.1 presents two alternative derivations of eCE2 (one in spectral space and the other in a generalized basis respectively).

Since an average over an ensemble of realizations converges to a time-average in ergodic systems, eCE- n as $n \rightarrow \infty$ is expected to flow to a single fixed point in systems that have a statistically-steady state. For $n = 2$ (that is, a second order truncation) the system might still flow to a quasi-steady-state which would approximate the steady-state statistics accumulated by DNS. Indeed it is shown in Section 3.3.3 that in two different barotropic models the first ensemble cumulant captures the steady-state coherent flow of the corresponding DNS simulations.

Like zCE2, eCE2 is also a conservative truncation scheme up to quadratic quanti-

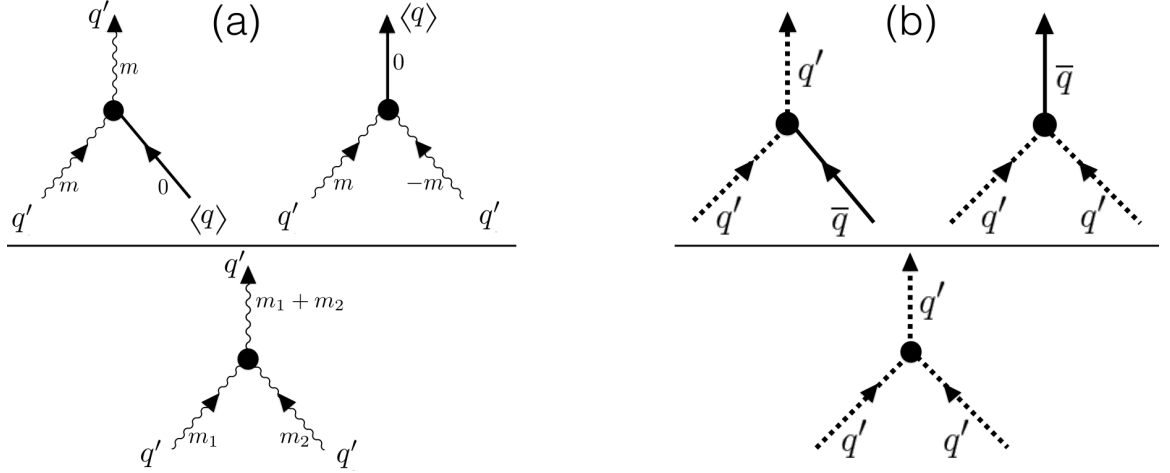


Figure 3.3.1: The allowed (top) and disallowed (bottom) triadic interactions in (a) zonal CE2 and (b) ensemble CE2. Wavy lines denote eddies with zonal wavenumber m whereas dashed lines denote the amplitude of the incoherent parts of the flow.

ties. Proofs are presented in Appendix D.1. But unlike zCE2, eCE2 is not guaranteed to be numerically stable and so this must be explicitly enforced by projecting out, as required, the non-physical modes of the second moment which can be identified by their negative eigenvalues (see Section 3.3.3.1). Alternatively, systems with a stochastic component are already likely to be realizable under eCE2 because even a small amount of stochastic forcing can wash out high-order ensemble-averaged cumulants, thus lessening the approximation introduced by the decoupling of the third cumulant (see Section 3.3.3.2).

Given a zonally symmetric initialization of the cumulants, however, eCE2 is guaranteed to be numerically stable because it reduces to zCE2. Indeed zCE2 can be considered a special case of eCE2 and such an example will be shown in the next section. The proof of zCE2's recovery from eCE2 is presented in Appendix B.3. Converting from ensemble-averaged zonal cumulants to zonally-averaged ensemble cumulants can have certain subtleties. These are expounded in Appendix C.2 and the conversions are stated explicitly.

3.3.3 Applications

This section implements eCE2 on two highly idealized barotropic models of planetary atmospheres on a unit sphere rotating at an angular velocity Ω . A spherical domain is selected since it can give rise to behavior not observed in β -plane turbulence [55]. Accordingly the equations are solved in the basis of spherical harmonics. The eCE2 simulations are compared with zCE2 and statistics gathered by DNS, which is used as a reference. Identical resolution and parameters are used for a fair comparison of the three methods.

3.3.3.1 Deterministic Jet

To illustrate the advantages of eCE2 over zCE2 for turbulent flows, I present a deterministic barotropic jet relaxed toward an unstable profile q_{jet} . The equation for the evolution of the flow is given by:

$$\frac{\partial q}{\partial t} = \frac{q_{jet} - q}{\tau} + J[q, \psi], \quad (3.3.25)$$

where q_{jet} is:

$$q_{jet} = f(\phi) - A \tanh\left(\frac{\phi}{\Delta\phi}\right). \quad (3.3.26)$$

Here J represents the Jacobian and q is the absolute vorticity which is the sum of the relative vorticity ξ and the Coriolis parameter f :

$$\begin{aligned} q &= \xi + f \\ \xi &= \nabla^2 \psi \\ f(\phi) &= 2\Omega \sin \phi \\ J[A, B] &= \hat{n} \cdot \left(\vec{\nabla} A \times \vec{\nabla} B \right). \end{aligned} \quad (3.3.27)$$

The latitude is given by ϕ , the stream-function by ψ and the angular rotation rate by Ω . The relaxation time τ determines the strength of the coupling to the fixed jet and so varies the flow from weakly nonlinear to strongly nonlinear, providing a good toy model for testing eCE2. This forcing and dissipation can be seen as a model for radiative forcing and Rayleigh drag. For short relaxation times where the flow is dominated by critical-layer waves, eddies are suppressed by the strong coupling to the fixed jet [38]. Since non-zonal coherent structure is absent, an ensemble average converges to a zonal average and so eCE2 reduces to zCE2 and differs from DNS, as demonstrated in Fig. 3.3.2 which shows the power spectra and second vorticity cumulants at a relaxation timescale of $\tau = 2$. This collapse of eCE2 to zCE2 in the absence of non-zonal structure is consistent with the proof presented in Appendix B.3.

The qualitative differences between DNS and eCE2/zCE2 can be explained by the neglect of the eddy-eddy scattering process which blocks the pathways for transporting power up to higher zonal wavenumber modes. However at longer relaxation times ($\tau = 20$) the flow enters the turbulent regime and non-zonal coherent structures form so that an ensemble average captures statistics that a zonal average is unable to capture. Fig. 3.3.3 shows that whereas zCE2 still has power only in the $m = 0$ and $m = 3$ modes, the power spectrum of eCE2 now matches that of DNS, mode for mode. It also shows that the second cumulant of the vorticity field as computed by fully nonlinear DNS is subject to the approximate symmetry $c_2(\theta_1, \theta_2, \Delta\phi)$. This can be seen from the EOM of the second cumulant. However, this symmetry is only approximate because coupling to the third cumulant breaks the symmetry. In the case of zCE2 where the third cumulant is decoupled from the evolution equation of the second cumulant, this symmetry becomes exact. An attractive feature of eCE2 is that it breaks this artificial symmetry by including the eddy-eddy interactions which spatially transports eddy enstrophy and thus agrees closely with fully nonlinear DNS.

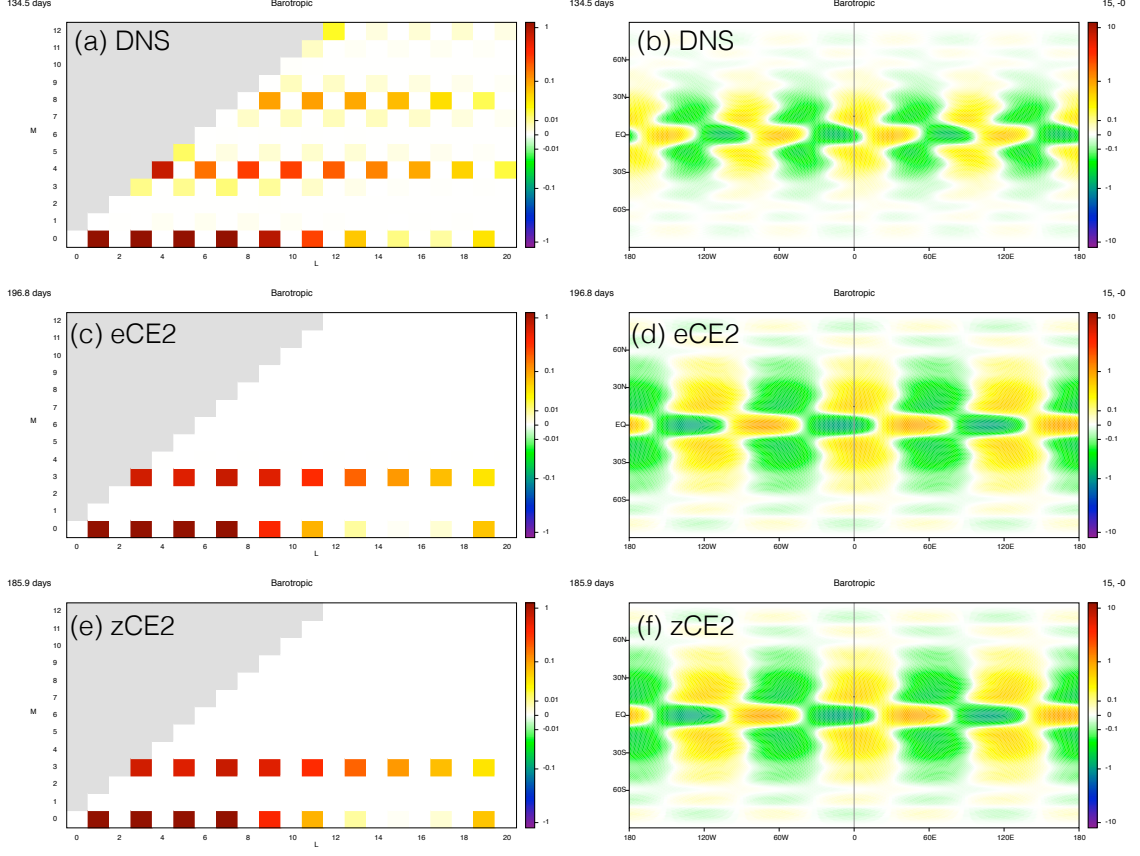


Figure 3.3.2: Power spectra (left) and second cumulant of relative vorticity field (right) at steady-state for $\tau = 2$. (a, b) DNS. (c, d) eCE2. (e, f) zCE2. The reference point for cross-correlations (black dot) is positioned along the central meridian at a latitude of 15°N . Spectral simulations truncated at $0 \leq l \leq L$ for $L = 20$ and $|m| \leq \min(l, M)$ for $M = 12$. The relative lack of non-zonal structure causes eCE2 to reduce to zCE2, as expected from Appendix B.3.

For this same reason, at low latitudes zCE2 is unable to capture the transition from the turbulent mixing layer in the middle of the jet to the non-mixing layer further from the equator whereas the mean absolute vorticity of eCE2 quantitatively agrees with DNS, as shown in Fig. 3.3.4. The remarkable agreement between eCE2 and DNS in this regime suggests that turbulence washes out the third and higher ensemble-averaged cumulants, thus lessening the approximation introduced by the eCE2 truncation. In fact, eCE2 performs even better than DNS for this turbulent regime as shown in Fig. 3.3.5 which shows snapshots of the cylindrical projections of the absolute vorticity evolved up to time $T = 1000$ days. Whereas a time-average is

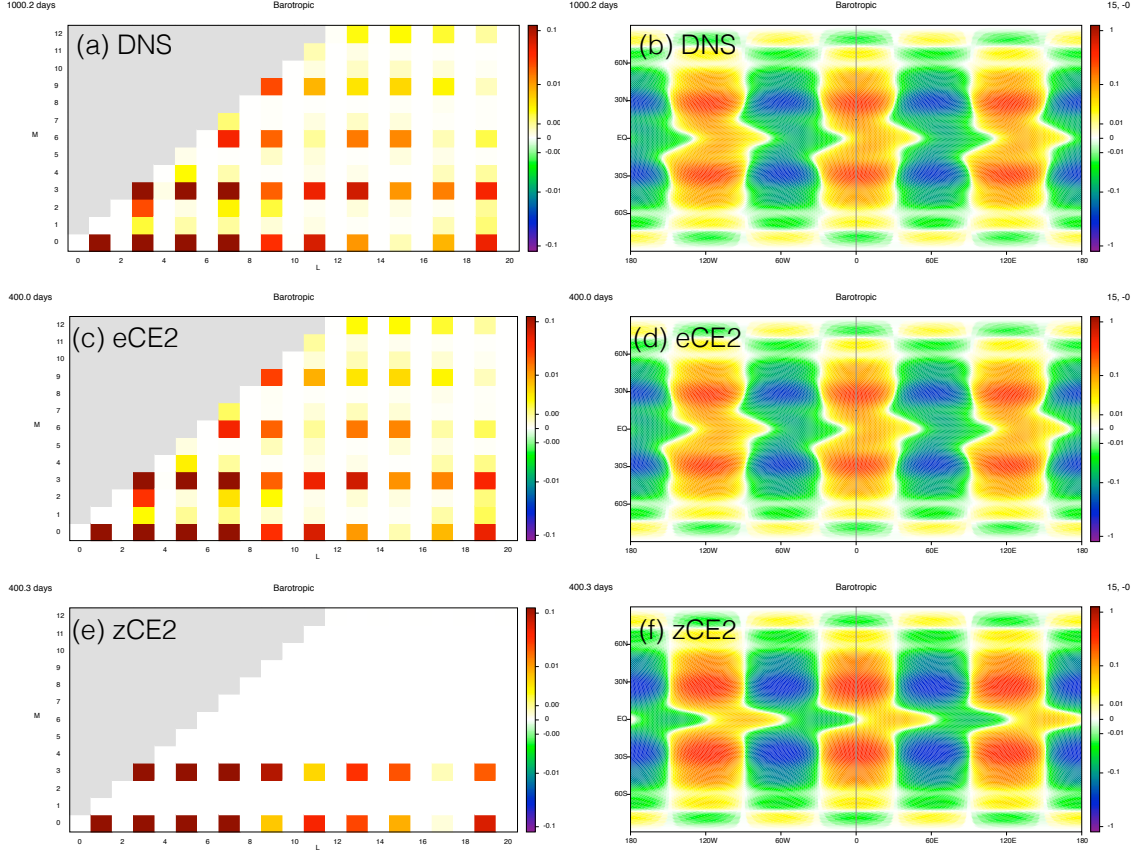


Figure 3.3.3: Power spectra (left) and second cumulant of relative vorticity field (right) at steady-state for $\tau = 20$. (a, b) DNS. (c, d) eCE2. (e, f) zCE2. The reference point for cross-correlations (black dot) is positioned along the central meridian at a latitude of 18°N . Spectral simulations truncated at $0 \leq l \leq L$ for $L = 20$ and $|m| \leq \min(l, M)$ for $M = 12$. eCE2 is in excellent agreement with DNS and breaks the artificial symmetry exhibited by zCE2.

required over the last 700 days to integrate out the incoherent structures of DNS, eCE2 directly solves for the time-averaged absolute vorticity without explicitly needing a time-average.

Since eCE2 is guaranteed to be convergent (see Section 3.3.2), physical realizability can be enforced by performing a Schmidt decomposition and zeroing out any eigenvectors of the second moment with negative eigenvalues. For the results presented here, the projection is carried out approximately every 1000 time steps, but more frequent projections do not effect the statistics.

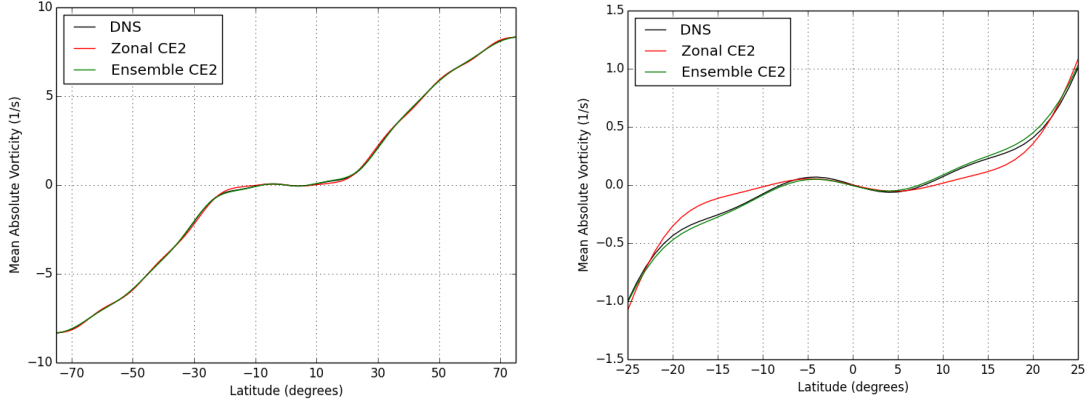


Figure 3.3.4: (a) Mean absolute vorticity as a function of latitude for $\tau = 20$ for DNS, eCE2 and zCE2. (b) Magnification of lower latitudes. Parameters as in Fig. 3.3.3.

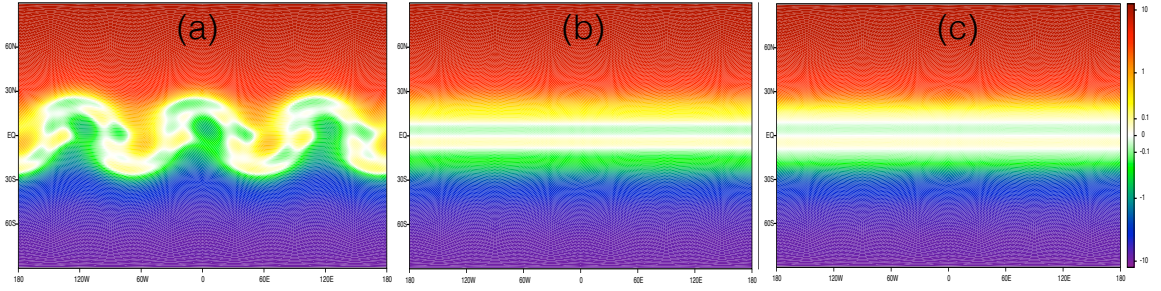


Figure 3.3.5: Snapshots of cylindrical projections at $T = 1000$ of the absolute vorticity for $\tau = 20$ as computed by (a) DNS, (b) DNS time-averaged for 300 days, (c) eCE2. Parameters as in Fig. 3.3.3. eCE2 has integrated out the incoherent structure present in the dynamics and is in good agreement with the time-averaged absolute vorticity field.

3.3.3.2 Stochastic Jet

Another barotropic model that illustrates the advantages of eCE2 for turbulent flows is the stochastically-forced jet,

$$\frac{\partial \xi}{\partial t} = J[\xi + f, \psi] - [\kappa - \nu_3 (\nabla^2 + 2) \nabla^4] \xi + \eta(t). \quad (3.3.28)$$

The relative vorticity of the flow evolves under the action of a Jacobian term, J , and a linear term which contains the linear friction term, κ , as well as a bi-cubic hyper-viscosity term, ν_3 , which soaks up enstrophy that cascades down to the Kolmogorov

scale. Stochastic forcing, $\eta(t)$, is additive Gaussian white noise satisfying Eq. 3.3.16. This Gaussian forcing is even more effective than deterministic turbulence (see Section 3.3.3.1) at washing out the high-order ensemble-averaged cumulants. This lessens the approximation introduced by the eCE2 truncation for stochastically-forced problems, ensuring the scheme remains numerically stable and obviating the projections of negative eigenmodes.

I study this model for the parameters $\nu_3 = 1.0$, $\kappa = 0.02$ with the autocorrelation of the stochastic forcing equal to $\Gamma = 0.1$, as in [37]. Spectral simulations are performed at a resolution of $0 \leq l \leq L$ for $L = 30$ and $|m| \leq \min(l, M)$ for $M = 20$. Fig. 3.3.6 compares the Hovmöller timelines (that is, the evolution of the zonal mean zonal velocity of the jet at each latitude) and the second vorticity cumulants (that is, the two-point correlation functions) simulated using all three methods. A prograde equatorial jet forms in all three methods. However, zCE2 is subject to persistent non-physical oscillations for which a time-average is required to smoothen out (commencing at $t = 300$ days). By contrast eCE2 does not exhibit these fast oscillations and better matches the DNS statistics. Similarly the correlations are manifestly non-local in DNS. However zCE2 exaggerates these correlations because the neglect of the non-linear interactions results in wave-dominated behavior. By contrast eCE2 is a closer match to DNS since it retains these interactions.

Another quantity to probe the effectiveness of eCE2 is the zonal mean velocity of the jet as a function of latitude as in Fig. 3.3.7. Since zCE2 neglects the eddy-eddy scattering processes, it has no efficient mechanism for the transport of eddy angular momentum from the equator toward the poles. Therefore it underestimates the mean zonal velocity at high latitudes, compared to DNS. By contrast, eCE2 better matches DNS because an ensemble average does not project out non-zonal features such as eddies.

In addition, the first cumulant computed via eCE2 approximates the time average

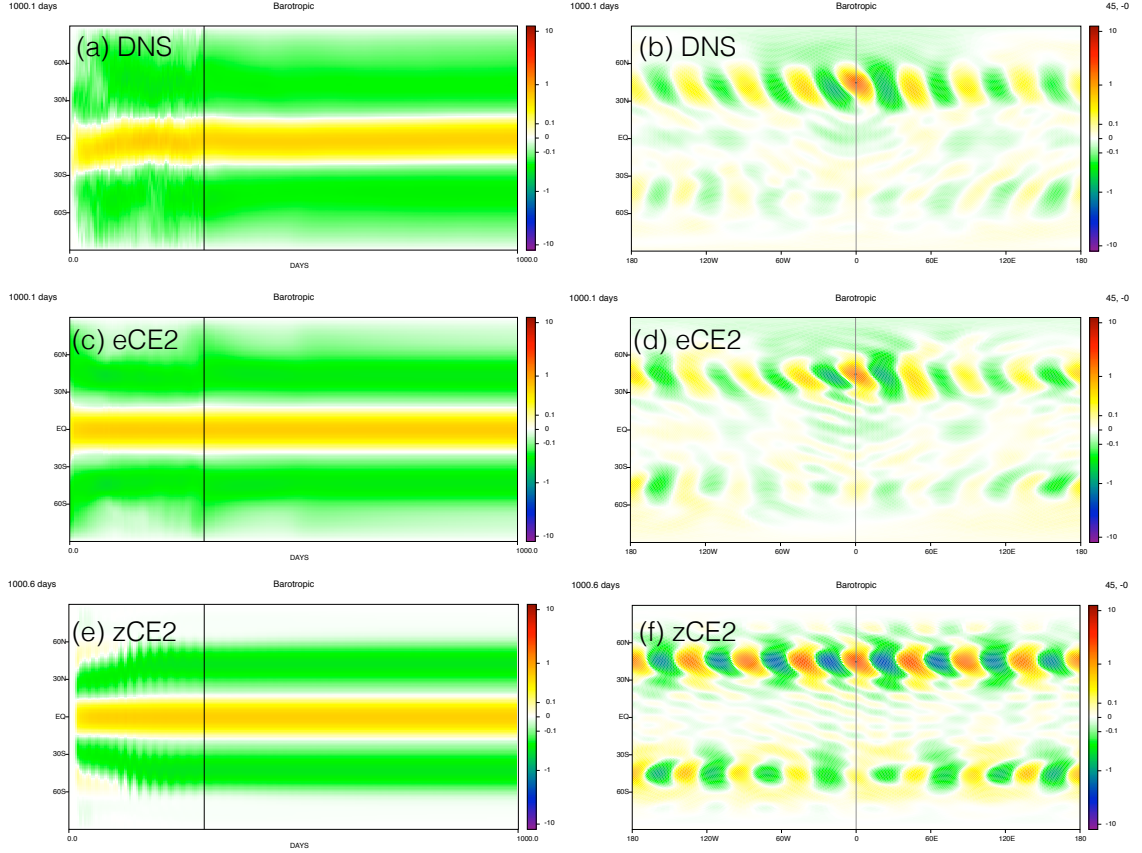


Figure 3.3.6: Hovmöller timelines of the zonal mean zonal velocity (left) and second cumulant of relative vorticity field (right) at $\Gamma = 0.1$ for (a, b) DNS. (c, d) eCE2. (e, f) zCE2 with North-South symmetry imposed. The black line at 300 days denotes the start of time-averaging. The reference point for cross-correlations (black dot) is positioned along the central meridian at a latitude of 45°N . Spectral simulations with truncation $0 \leq l \leq L$ for $L = 30$ and $|m| \leq \min(l, M)$ for $M = 20$. Equatorial symmetrization was imposed for zCE2 and DNS. zCE2 exhibits exaggerated coherent waves whereas eCE2 better reproduces the DNS statistics.

of the relative vorticity field computed via DNS as seen in Fig. 3.3.8, demonstrating that eCE2 accesses the coherent zonal bands directly without the need for long time averages to wash out the small scale and fast eddies seen in DNS which contribute little to the statistics.

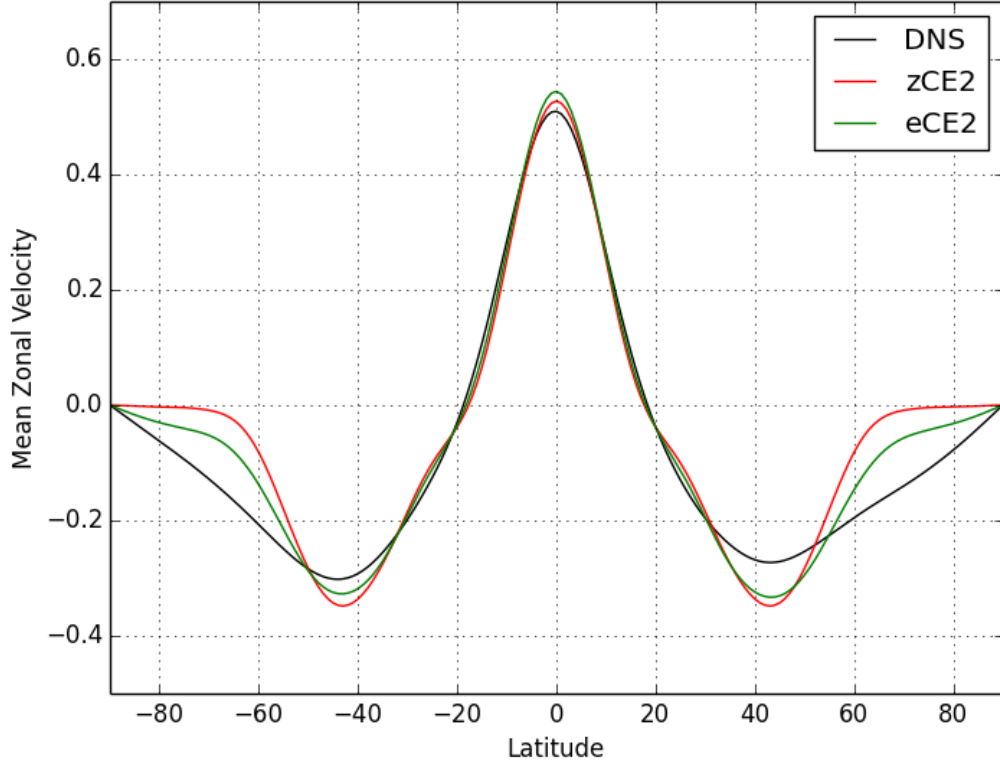


Figure 3.3.7: Comparison of the zonal mean velocity as a function of latitude for DNS, eCE2 and zCE2. eCE2 matches DNS better than zCE2 because it retains the eddy-eddy scattering process which transports eddy enstrophy poleward. Parameters as in Fig. 3.3.6.

3.4 Summary

Cumulant expansions offer a powerful form of Direct Statistical Simulation (DSS) for calculating the low-order statistics of chaotic and turbulent systems. In this chapter I showed that an expansion in equal-time cumulants is able to reproduce the low-order statistics of both the deterministic and stochastic forms of these systems, despite their highly nonlinear nature. This was first demonstrated on the deterministic and stochastically forced Lorenz attractor, where a CE3 approximation was used. It was found to respect the reflection symmetries of the system and qualitatively agree well with DNS. The efficiency of this technique in comparison to DNS, as measured by

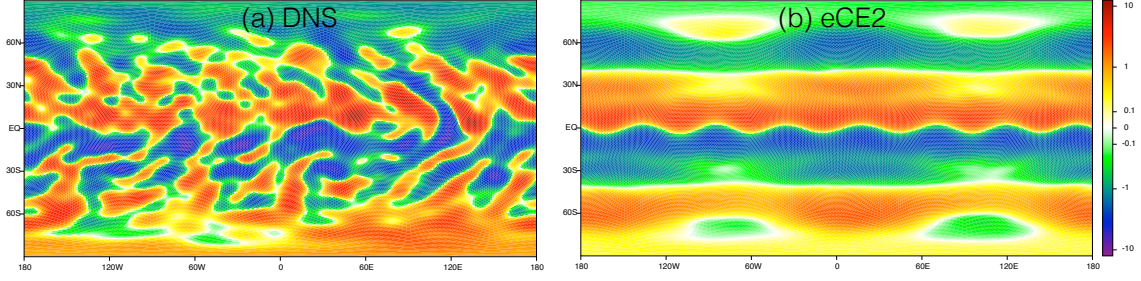


Figure 3.3.8: Cylindrical projections at $T = 1000$ days of (a) the relative vorticity field computed via DNS and (b) its ensemble average of the relative vorticity field computed via eCE2. Parameters as in Fig. 3.3.6. eCE2 has integrated out most of the incoherent structure present in DNS but still retains some wave-like behavior.

wall-clock time, is an attractive feature.

I then demonstrated the utility of a cumulant expansion technique on two idealized barotropic models, this time using a CE2 approximation. CE2 is usually performed using a zonal average. But this has the drawback of neglecting the eddy-eddy scattering processes which are important for the latitudinal transport of enstrophy in turbulent flows. Therefore I used an ensemble average in place of a zonal average and tested this on a stochastically-forced barotropic jet and a deterministic barotropic jet relaxed toward an unstable profile. This method better reproduced statistics accumulated via direct numerical simulation compared to zonal CE2.

Ensemble CE2 is slower than zonal CE2 because the second ensemble-averaged cumulant has a higher dimensionality than the second zonally-averaged cumulant. But unlike a zonal average which fails to capture the eddy-eddy scattering processes, I have shown that ensemble average closely matches the statistics accumulated by a temporal average of DNS. This agreement, which is exceptionally good for the deterministic barotropic jet, hints that turbulence washes out the third and higher ensemble-averaged cumulants and so diminishes the error associated with the ensemble CE2 truncation, allowing it to directly access the statistics of turbulent flows. In the next chapter, I will present a way to overcome this higher dimensionality associated with an ensemble average using an unsupervised machine learning technique.

Chapter 4

Dimensional Reduction

4.1 Introduction

In addition to spherical harmonics, it is sometimes advantageous to work in other bases too. By rotating into the basis formed by the eigenvectors of the second zonally-averaged moment and discarding the less important eigenvectors, a dimensional reduction can be achieved. Such a Proper Orthogonal Decomposition (POD) [56, 57], known in other fields as Principal Component Analysis (PCA), is especially useful for systems with many degrees of freedom that are slow to simulate, such as the ensemble CE2 technique where the use of the ensemble-averaged cumulant retains a larger dimensionality than the zonally-averaged cumulant. This computational intractability at high resolutions calls for a dimensional reduction scheme.

In this chapter I investigate a reduced basis method based on a POD of the eigenvectors of the second moment. Since knowledge about the second cumulant is a key ingredient for performing a POD, a cumulant expansion is a better candidate than DNS because it solves for the cumulants directly. In addition its eigenvalue spectrum decays more quickly than that of DNS, allowing for a more severe truncation in the reduced basis. Accordingly I implement a POD on both zonal CE2 (zCE2)

and ensemble CE2 (eCE2). For completeness, I also implement a POD on DNS to compare its behavior.

This chapter is organized as follows. Since an ensemble average retains a larger dimension compared to a zonal average, Section 4.2 develops an explicit dimensional reduction scheme using the POD described above. In Section 4.3, this scheme is implemented in DNS, zCE2 and eCE2 and tested on the two different idealized barotropic models introduced in the previous chapter: A deterministic barotropic jet relaxed toward an unstable profile in Section 4.3.1, and a stochastically-forced barotropic jet in Section 4.3.2. This reduced order model is shown to offer substantial computational gains with little loss to accuracy. Some conclusions are presented in Section 4.4.

4.2 Proper Orthogonal Decomposition

To perform a POD, a new basis should be constructed which includes information about both the first and the second cumulant. Therefore instead of using only the second cumulant, I will form the basis using the second zonally-averaged moment, defined as:

$$\begin{aligned} m(\vec{r}_1, \vec{r}_2) &= \langle q(\vec{r}_1) q(\vec{r}_2) \rangle \\ &= c(\vec{r}_1, \vec{r}_2) + c(\vec{r}_1) c(\vec{r}_2) \end{aligned} \quad (4.2.1)$$

Since the average is zonal, an order reduction occurs which is most evidently seen in spectral space:

$$m_{ll'm} \equiv c_{ll'm} + c_l c_{l'} \delta_{m,0}, \quad (4.2.2)$$

where c_l and $c_{ll'm}$ are the first and second zonally-averaged cumulants respectively. (Note that under a time-average, the first cumulants become entangled and so the $m = 0$ component of the second moment does not decompose into their product). The

dimensional reduction can then be performed via POD by the following prescription:

1. Since $m_{ll'm}$ is zonally-averaged, and therefore diagonal in m , it is more convenient to treat the second zonally-averaged moment as a collection of M different matrices of dimension $\mathcal{O}(L)$:

$$m_{ll'm} \rightarrow m_{ll'}^{(m)}, \quad (4.2.3)$$

so that instead of performing an eigendecomposition on a single matrix of dimension $\mathcal{O}(LM)$, the eigendecomposition can more efficiently be performed on M matrices of dimension $\mathcal{O}(L)$:

$$m_{ll'}^{(m)} = \sum_{ij} U_{li}^{(m)} \lambda_{ij}^{(m)} \left[U_{l'j}^{(m)} \right]^{-1}, \quad (4.2.4)$$

where λ_{ij} forms a diagonal matrix containing the eigenvalues of $m_{ll'm}$ which are real and non-negative [48], and $U_{li}^{(m)}$ is a collection of M unitary matrices with rows containing the eigenvectors of $m_{ll'm}$. Since $m_{ll'm}$ is self-adjoint for fixed m (that is, $m_{ll'm} = m_{l'l m}^*$), these eigenvectors form an orthonormal basis. They can then be combined into a single $\mathcal{O}(LM)$ dimensional unitary rotation matrix $U_{lm;i}$. I will refer to this as the “change of basis” matrix.

2. Once the change of basis matrix has been constructed, the system can be rotated from the spectral basis into the new basis formed by the eigenvectors of $m_{ll'm}$ so that, for example, the eCE2 EOMs become:

$$\begin{aligned} \dot{c}_i &= F_i + \sum_n L_{in} c_n + \sum_{m,n} Q_{inp} (c_n c_{np} + c_{np}) \\ \dot{c}_{ij} &= 2 \left\{ \sum_m L_{im} c_{mj} + 2 \sum_{m,n} Q_{imn} c_m c_{nj} + \Gamma_{ij} \right\}, \end{aligned} \quad (4.2.5)$$

where the coefficients in the new basis are found using the change of basis

matrix:

$$\begin{aligned}
F_i &= \sum_l U_{lm=0;i}^* F_l \\
\Gamma_{ij} &= \sum_{lm} \sum_{l_1} U_{lm;i}^* \Gamma_{ll_1 m} U_{l_1 m;n} \\
L_{in} &= \sum_{lm} \sum_{l_1} U_{lm;i}^* L_{l;l_1 m} U_{l_1 m;n} \\
Q_{inp} &= \sum_{lm} \sum_{l_1, l_2, m_1, m_2}^{m=m_1+m_2} U_{lm;i}^* Q_{l;l_1 m_1; l_2 m_2} U_{m_1 l_1; n} U_{m_2 l_2; p}. \tag{4.2.6}
\end{aligned}$$

A derivation of these transformations is presented in Appendix C.1. The quadratic coefficient can be split up into $Q_{inp}^{(-)}$ and $Q_{inp}^{(+)}$ as before, satisfying the following symmetries (derived in Appendix C.3):

$$\begin{aligned}
Q_{inp}^{(+)} &= Q_{ipn}^{(+)} \\
Q_{inp}^{(-)} &= Q_{ipn}^{(-)*}. \tag{4.2.7}
\end{aligned}$$

3. The dimension of the system can now be reduced by setting some critical value λ_c such that all the eigenvalues below this value are discarded, along with their associated eigenvectors. Although this breaks conservation laws, it does not cause divergences in the driven/damped non-conservative systems studied here.

The second zonally-averaged moment required to construct the basis can be formed in a number of different ways. Since the zonally-averaged statistics of turbulent systems fluctuate in time, in this study a temporal average over these oscillations is performed in the full-dimensional system until a statistically steady state is reached, but other types of averages would be interesting to explore too. This temporal average is performed after an initial spin-up which ensures the system is in a state of fully developed turbulent flow. Section 4.3 shows that this procedure allows for significant dimensional reductions in DNS, eCE2 and zCE2 for two different barotropic models.

4.3 Tests

As in the previous chapter, two different idealized barotropic models (a deterministic jet and a stochastic jet) are used as a testbed for this new approach with the same parameters as before. I will compare DNS, eCE2 and zCE2 with their reduced-order counterparts using the POD scheme outlined. As before, a spherical domain is selected since it can give rise to unique behavior not permitted on a β -plane [55]. Identical resolution and parameters are used for an “apples to apples” comparison of the reduced systems against the full dimensional systems. To further ensure a fair comparison, the second zonally-averaged moments used to form the reduced basis, which are unique to each of these three methods, are identical across each level of truncation.

4.3.1 Deterministic Jet

As in the previous chapter, I consider the deterministic barotropic jet relaxed toward an unstable profile where $\tau = 20$ sets the relaxation time scale. For this choice of τ , the flow is in the turbulent regime and eCE2 agrees with DNS unlike zCE2. All three runs are evolved for 1000 days, with DNS time-averaged for the last 700 days.

Fig. 4.3.1 shows the first cumulants, or zonal mean absolute vorticities, at different levels of truncation. While POD offers a substantial dimensional reduction for DNS and eCE2 with slight loss of accuracy, zCE2 allows for the severest truncation where the retention of just 2 modes agrees quantitatively with the full (195 mode) simulation. This can also be seen from an inspection of the size of the eigenvalues of its second cumulant as shown in Fig. 4.3.2. The steep decay of the eigenvalues of zCE2 is unsurprising because the quasi-linear approximation, to which it is formally equivalent, excites fewer modes in comparison to eCE2 or full DNS. This is also evident from Fig. 3.3.3 of the previous chapter where the power remains confined to

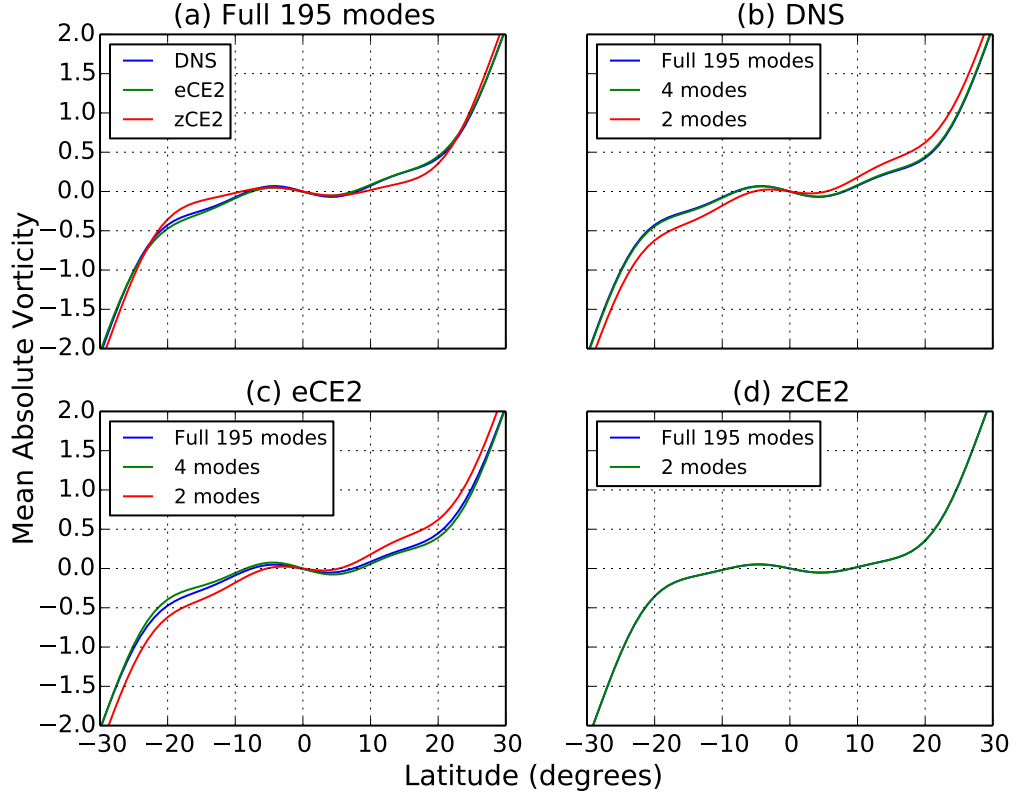


Figure 4.3.1: (a) The first cumulant, or zonal mean absolute vorticity, as a function of latitude for $\tau = 20$ for DNS, eCE2 and zCE2. (b)-(d) Comparison of the first cumulant of the untruncated system against different levels of truncation for DNS, eCE2 and zCE2 respectively. Each run is evolved until a statistically-steady state is reached, which occurs for all runs by $T=10,000$ days without time-averaging. Spectral simulations truncated at $0 \leq l \leq L$ for $L = 20$ and $|m| \leq \min(l, M)$ for $M = 12$.

relatively few modes, lending itself particular well to a dimensional reduction.

4.3.2 Stochastic Jet

This subsection continues testing the POD dimensional reduction scheme, this time on the stochastic jet. As before, statistics are time-averaged starting from $T = 300$ days and collected up to $T = 1,000$ days. For all three methods, prograde flow persists at the equator with retrograde flow elsewhere. Fig. 4.3.3 shows the zonal mean zonal velocities as a function of latitude at different levels of truncation for

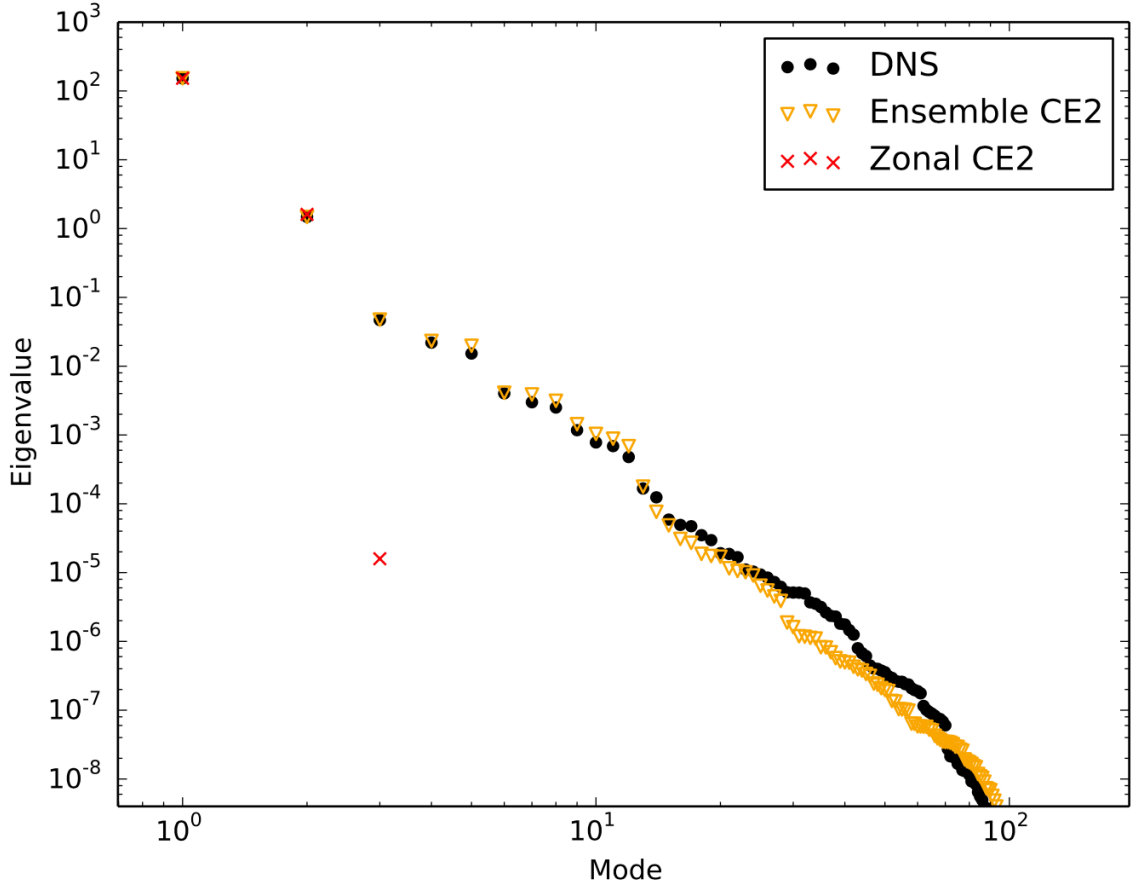


Figure 4.3.2: Eigenvalues of the second moment of the barotropic jet for $\tau = 20$ arranged in descending order for DNS, eCE2 and zCE2. Parameters as in Fig. 4.3.1. zCE2 permits the most severe truncation.

DNS, eCE2 and zCE2.

Once again zCE2 allows for a severer truncation compared to eCE2 and DNS, though all three methods benefit substantially from the dimensional reduction. This is also seen in Fig. 4.3.4 which compares the size of the eigenvalues of the second moments of DNS, eCE2 and zCE2. In the case of zCE2, retaining 13 eigenvectors of the second moment speeds up the problem by a factor of 10,000 compared to the full dimensional system with 441 modes. Although the reduced system requires more time to evolve to a statistically-steady state (by approximately a factor of 10), this is small relative to the speed-up. The convergence of the statistics as the number of retained modes increases is most clearly observed with an inspection of the second

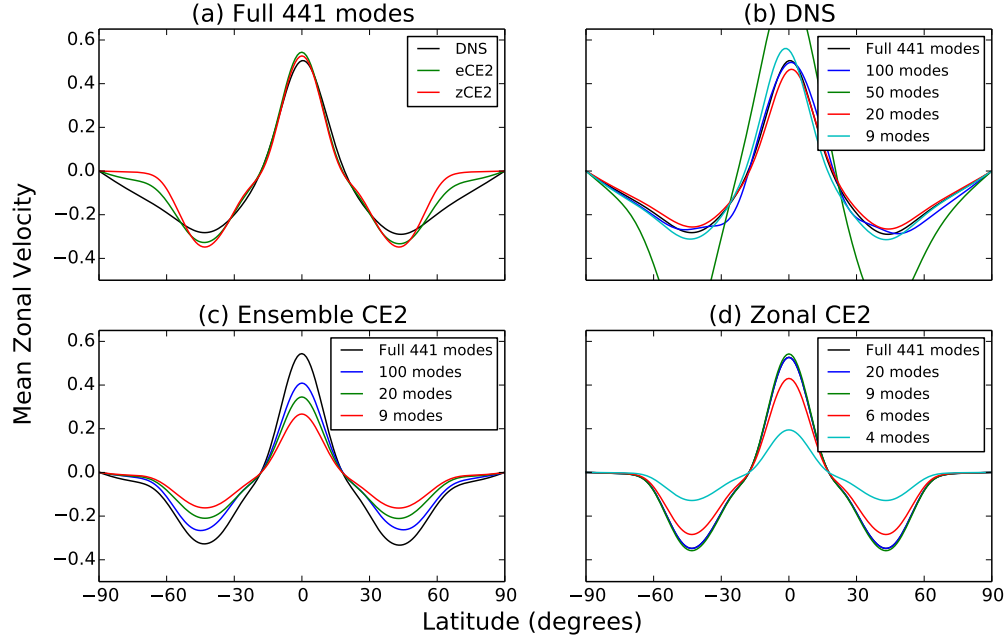


Figure 4.3.3: Comparison of the zonal mean velocity as a function of latitude for the stochastically-forced barotropic jet. Spectral simulations with truncation $0 \leq l \leq L$ for $L = 30$ and $|m| \leq \min(l, M)$ for $M = 20$. (a) DNS, eCE2 and zCE2 runs in an unreduced basis. eCE2 matches DNS better than zCE2 because it retains the eddy-eddy scattering process that transports eddy enstrophy poleward. (b)-(d) Comparison of the untruncated system against different levels of truncation for DNS, eCE2 and zCE2 respectively. Each run is evolved until a statistically-steady state is reached, which occurs for all runs by $T=10,000$ days with the last 1,000 days time-averaged.

zonal cumulants, as in Fig. 4.3.5 and 4.3.6 and 4.3.7 for DNS, eCE2 and zCE2 respectively.

In the basis of the second zonally-averaged moment, the number of operations required in zCE2 and eCE2 scale as $\mathcal{O}(N_{ret}^3)$ where N_{ret} is the number of retained eigenvectors and $\mathcal{O}(N_{ret}) = \mathcal{O}(LM)$. Therefore a dimensional reduction from $N_{ret} = 441$ to $N_{ret} = 13$ equates to a gross speed up of order 10^4 . This is numerically demonstrated for zCE2. Without any dimensional reduction ($N_{ret} = 441$) a Mac Mini 2.6GHz Intel Core i7 (with 16 GB of 1600MHz DDR3 memory) takes 26 hours to complete the simulation. By contrast, when a dimensional reduction ($N_{ret} = 13$) is performed, the same problem takes only 10 seconds on the same machine; a speed

up of order 10^4 as expected.

However in the basis of spherical harmonics, the number of operations required in zCE2 and eCE2 scale instead as $\mathcal{O}(L^3M)$ and $\mathcal{O}(L^3M^2)$. This is because the spectral basis can exploit zonal symmetries which remain concealed in a generalized basis. Therefore a fairer comparison would be between the wall-clock time for zCE2 in a transformed and truncated system (at $N_{ret} = 13$) against the wall-clock time in the *original spectral basis* (at $N_{ret} = 441$), which is 10 seconds and 284 seconds respectively - still a considerable speed-up.

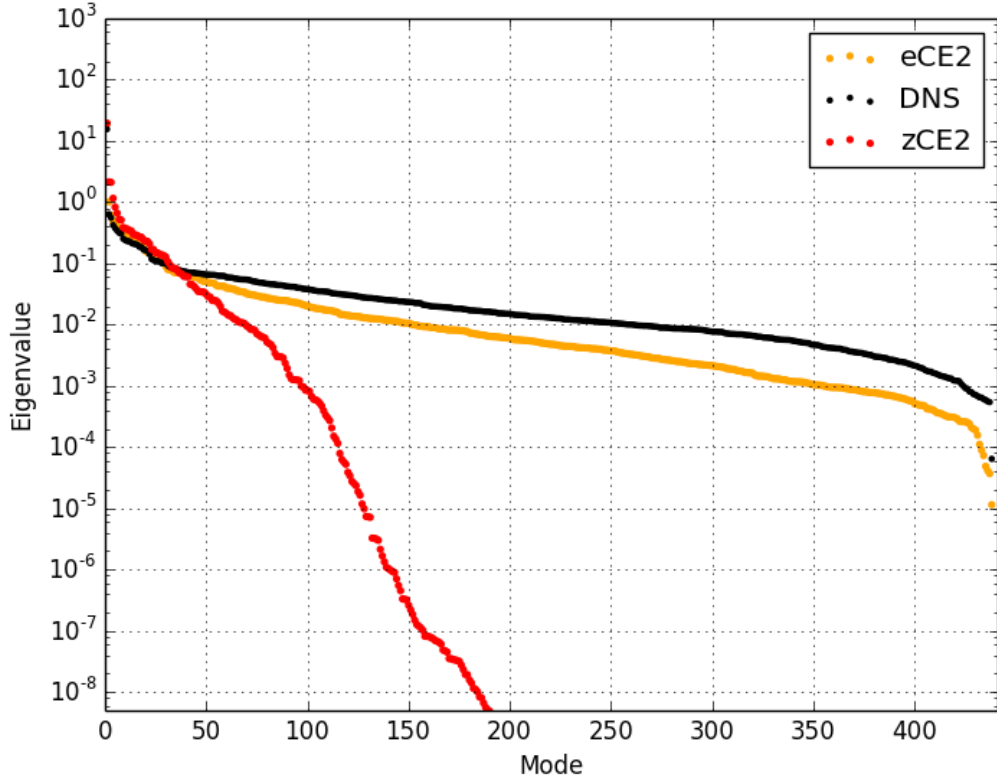


Figure 4.3.4: Eigenvalues arranged in descending order of the second moment of the stochastic jet for DNS, eCE2 and zCE2. Parameters as in Fig. 4.3.3. The curve decays exponentially, though less steep than for the deterministic jet.

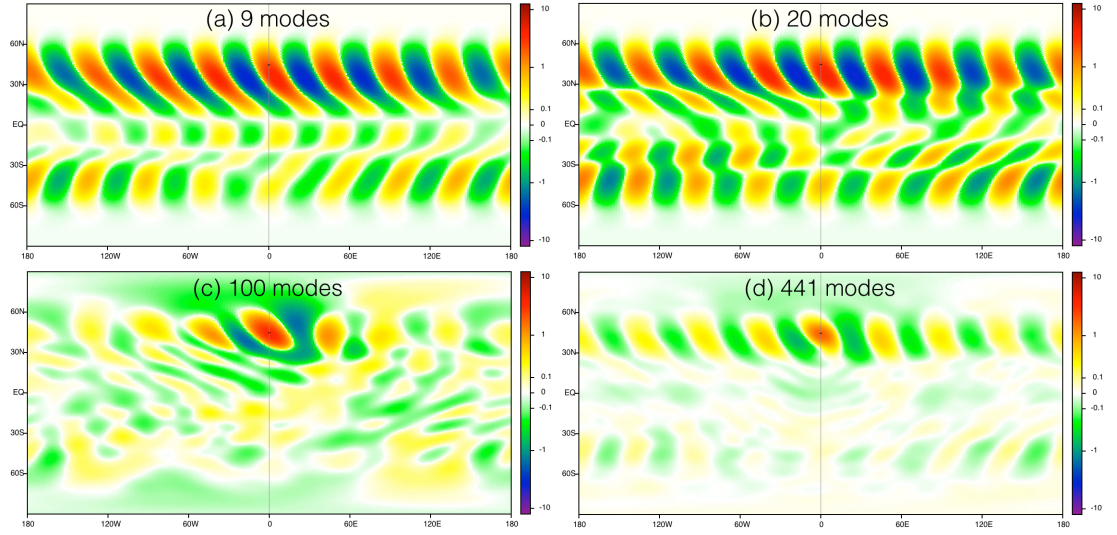


Figure 4.3.5: Comparison of the second vorticity cumulants of the stochastic jet at a statistically steady state via DNS for different truncation levels against the untruncated system (d). Parameters as in Fig. 4.3.3.

4.4 Discussion and conclusion

A Proper Orthogonal Decomposition (POD) can be used to reduce the dimension of a system by discarding modes that contribute little to the dynamics. Since most of the power is seen in relatively few modes, a substantial reduction can be performed leading to a speed up of orders of magnitude. This is especially true for zCE2 which permits the most severe truncations because relatively fewer modes get excited in the quasi-linear approximation, allowing more to be discarded. However because ensemble-averaged cumulants have a larger dimension than zonally-averaged cumulants, the POD truncation scheme finds its greatest utility in eCE2 which is the more computationally demanding of the two.

The severity with which a POD truncation can be made at a given accuracy depends on the specifics of the system. The presence of stochastic forcing diffuses power into adjacent modes, requiring a larger number of retained modes. By contrast, the power spectra of the deterministic jet is more localized and permits a more highly

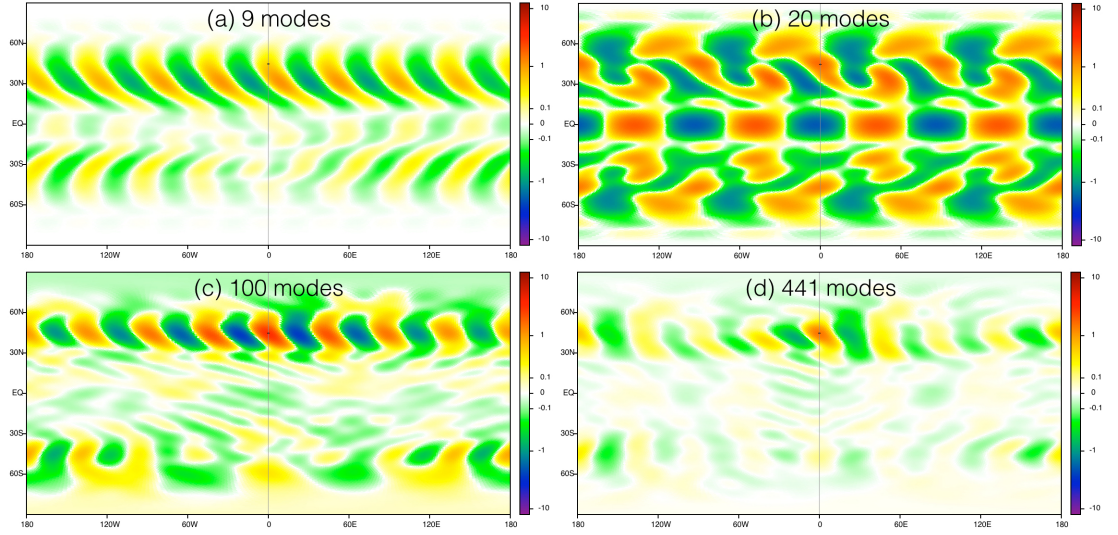


Figure 4.3.6: Comparison of the second vorticity cumulants of the stochastic jet at a statistically steady state via eCE2 for different truncation levels against the untruncated system (d). Parameters as in Fig. 4.3.3.

dimensionally-reduced system with little loss of accuracy. It would be interesting to extend the POD scheme to baroclinic models as in Ref [?, 44, 51, 58, 59] and possibly explore other types of averages with which to form the second moments for the reduced basis. An even more interesting extension, leading to yet greater time savings, would dynamically update the basis “on the fly” since most of the simulation time is spent gathering enough statistics in the full dimensional system to form the basis.

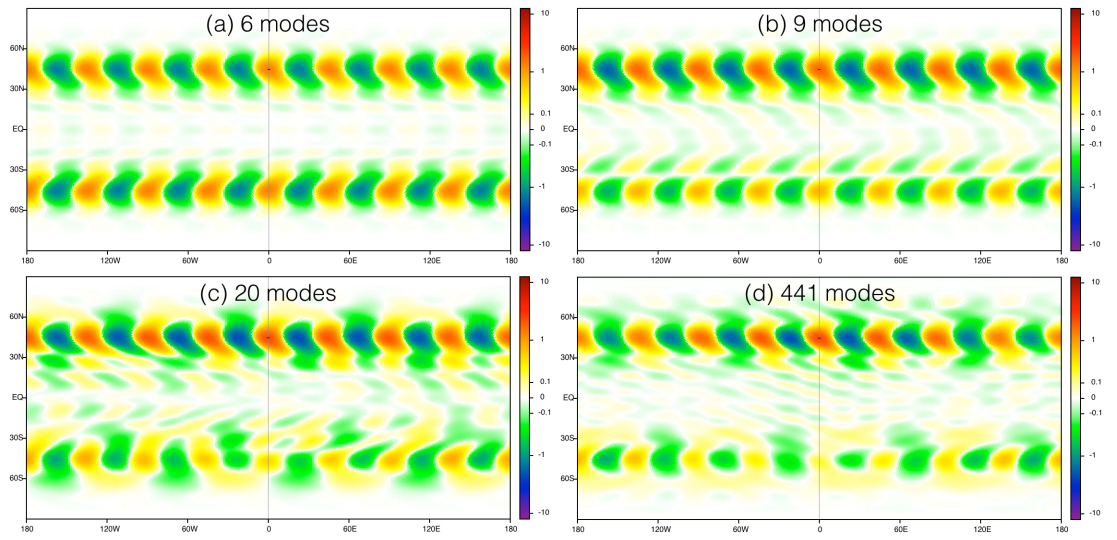


Figure 4.3.7: Comparison of the second vorticity cumulants of the stochastic jet at a statistically steady state via zCE2 for different truncation levels against the untruncated system (d). Parameters as in Fig. 4.3.3.

Chapter 5

TR-BDF2

5.1 Introduction

Given the need for numerical efficiency for turbulent flow problems where there exist many degrees of freedom, it is worthwhile to explore alternative integration schemes too. Numerical integrators of differential equations can be broadly classified as either explicit, implicit and semi-implicit schemes. Since the low-order statistics of a system tend to evolve slower in time than the dynamics, one of the potential applications of a semi-implicit integration scheme is in evolving the equations of the cumulants with the expectation that it will take much larger time steps than explicit schemes.

To illustrate the difference between explicit, implicit and semi-implicit integration schemes, it is instructive to consider a simple one-dimensional system governed by a differential equation of the form,

$$\frac{dx}{dt} = f(x, t). \quad (5.1.1)$$

Explicit integration schemes take the form,

$$x_{n+1} = x_n + \Delta t f(x_n, t_n), \quad (5.1.2)$$

where the derivative is being evaluated at the time-step n . Such a scheme is relatively straight forward to implement because knowledge about x_n and its EOM is sufficient to solve for x_{n+1} . However, maintaining numerical stability for stiff problems often requires extremely small time steps. By contrast, implicit schemes evaluate the derivative at a subsequent time step and take a form such as,

$$x_{n+1} = x_n + \Delta t f(x_{n+1}, t_{n+1}). \quad (5.1.3)$$

This type of implicit formula is known as a “backward differentiation formula”. This particular formula is the backward Euler formula or BDF1. In fact, there is an entire family of BDF formulae of increasing order. For example, BDF2 is given by:

$$x_{n+2} = \frac{4}{3}x_{n+1} - \frac{1}{3}x_n + \frac{2}{3}\Delta t f(x_{n+2}, t_{n+2}). \quad (5.1.4)$$

The virtue of implicit schemes is that they are better suited for stiff differential equations than explicit schemes, allowing for larger time steps and superior stability. However, solving BDF equations requires information about the derivative at a subsequent time step. This can be approximated by linearizing the derivative in time, which leads to a semi-implicit form:

$$\begin{aligned} x_{n+1} &= x_n + \Delta t f(x_n + \Delta x_n) \\ \rightarrow \Delta x_n &= \Delta t \left[f(x_n) + \frac{\partial f}{\partial x} \Big|_{x_n} \Delta x_n \right], \end{aligned} \quad (5.1.5)$$

where the temporal index for f has now been dropped under the assumption of a derivative term with no explicit time dependence (which is true for all the systems addressed in this thesis). Having performed a linear expansion on $f(x_n + \Delta x_n)$, the equation can now be solved for Δx_n .

Although BDF2 is more accurate than BDF1 (second order compare to first or-

der), it requires extra memory since information about both x_n and x_{n+1} needs to be stored in order to compute x_{n+2} . It was found by Bank et al. in [60] that combining BDF2 with the trapezoidal method (an explicit method) in alternating time steps can produce a solver with superior accuracy than BDF2, superior stability than the trapezoidal method, and without the memory drawback of having to store the intermediate solution [61]. This combination of the trapezoidal rule and BDF2 is known as TR-BDF2 and is also second-order accurate. Given its attractive features, TR-BDF2 was implemented by Tumolo and Bonaventura in [62] for numerical weather prediction. The algorithm enabled an increase in time step size of two orders of magnitude in comparison to explicit integration methods. In addition, an adaptive time stepper was used which reduced the computational cost of their simulation. This was tested on the shallow water and fully compressible Euler equations. Inspired by these results, I implement a semi-implicit form of the TR-BDF2 numerical integration scheme on the stochastically-forced barotropic jet with an adaptive time-stepper and then compare it against semi-implicit BDF1 (given by Eq. 5.1.5) and fully explicit RK4 as a benchmark.

Section 5.2 derives the TR-BDF2 algorithm in an implementation-ready form. This is tested on the stochastically-forced barotropic jet in Section 5.3 and its performance is benchmarked against both RK4 and BDF1 under a CE2 and CE2.5 approximation. In the case of the former, significant computational gains are observed. A summary is presented in Section 5.4.

5.2 Derivation

The TR-BDF2 equations are presented in Equation (9) of [62] as:

$$\begin{aligned}
\vec{k}_1 &= \vec{f}(\vec{u}_n, t_n) \\
\vec{k}_2 &= \vec{f}\left(\vec{u}_n + \gamma\Delta t\vec{k}_1 + \gamma\Delta t\vec{k}_2, t_n + \gamma\Delta t\right) \\
\vec{k}_3 &= \vec{f}\left(\vec{u}_n + \frac{1-\gamma}{2}\Delta t\vec{k}_1 + \frac{1-\gamma}{2}\Delta t\vec{k}_2 + \gamma\Delta t\vec{k}_3, t_{n+1}\right) \\
\vec{u}_{n+1} &= \vec{u}_n + \Delta t\left(\frac{1-\gamma}{2}\vec{k}_1 + \frac{1-\gamma}{2}\vec{k}_2 + \gamma\vec{k}_3\right),
\end{aligned} \tag{5.2.1}$$

where γ is an implicitness parameter. For example, the choice of $\gamma = 0$ reduces the equations to a forward Euler scheme:

$$\vec{u}_{n+1} = \vec{u}_n + \Delta t \vec{f}(\vec{u}_n), \tag{5.2.2}$$

whereas setting $\gamma = 1$ reduces the equations to a backward Euler scheme:

$$\vec{u}_{n+1} = \vec{u}_n + \Delta t \vec{f}(\vec{u}_{n+1}). \tag{5.2.3}$$

As outlined in [60], this parameter can be optimized for stability by equating the Jacobians of the two implicit steps, yielding $\gamma = 1 - 1/\sqrt{2}$.

Although the equations for TR-BDF2 above are technically correct, they can be further simplified. Since $\vec{f}$ is time-independent for the barotropic models being studied in here, the temporal index can be neglected. In addition, the following two quantities can be defined,

$$\begin{aligned}
\vec{k}^* &\equiv \frac{1}{2}(\vec{k}_1 + \vec{k}_2) \\
\Delta\vec{u}_n &\equiv \vec{u}_{n+1} - \vec{u}_n,
\end{aligned} \tag{5.2.4}$$

enabling the simplification of the TR-BDF2 equations to:

$$\begin{aligned}\vec{k}^* &= \frac{1}{2} \left[\vec{f}(\vec{u}_n) + \vec{f}(\vec{u}_n + 2\gamma\Delta t\vec{k}^*) \right] \\ \Delta\vec{u}_n &= \Delta t \left[\gamma\vec{f}(\vec{u}_n + \Delta\vec{u}_n) + (1-\gamma)\vec{k}^* \right].\end{aligned}\tag{5.2.5}$$

This form is tidier for implementation purposes as the two explicit steps have been eliminated - though the number of implicit steps (two) to be solved remains the same.

To produce a semi-implicit method out of this fully implicit method, the derivative term can be linearized in time as was done in the one-dimensional example. Taylor expanding yields:

$$\begin{aligned}\vec{k}^* &= \vec{f}(\vec{u}_n) + \gamma\Delta t J \left[\vec{f} \right] |_{\vec{u}_n} \vec{k}^* \\ \Delta\vec{u}_n &= \Delta t \left(\gamma\vec{f}(\vec{u}_n) + \gamma J \left[\vec{f} \right] |_{\vec{u}_n} \Delta\vec{u}_n + (1-\gamma)\vec{k}^* \right),\end{aligned}\tag{5.2.6}$$

where $J \left[\vec{f} \right] |_{\vec{u}_n}$ is the Jacobian matrix of $\vec{f}$ evaluated at $\vec{u}_n$. Collecting $\vec{k}^*$ and $\Delta\vec{u}_n$ above gives:

$$\begin{aligned}\left(I - \gamma\Delta t J \left[\vec{f} \right] |_{\vec{u}_n} \right) \vec{k}^* &= \vec{f}(\vec{u}_n) \\ \left(I - \gamma\Delta t J \left[\vec{f} \right] |_{\vec{u}_n} \right) \Delta\vec{u}_n &= \Delta t \left[\gamma\vec{f}(\vec{u}_n) + (1-\gamma)\vec{k}^* \right].\end{aligned}\tag{5.2.7}$$

These equations are now in the linear algebraic form $AX = B$ and can be solved, for example, using an iterative scheme such as a Krylov subspace method. The error vector is:

$$\vec{r}_0 = \Delta\vec{u}_n - \Delta t \left(\gamma\vec{f}(\vec{u}_k) + (1-\gamma)\vec{k}^* + \gamma J \left[\vec{f} \right] |_{\vec{u}_n} \Delta\vec{u}_n \right).\tag{5.2.8}$$

It might be tempting to go one step further and combine the two implicit steps into a single implicit step by eliminating $\vec{k}^*$. Acting the operator $\left(I - \gamma\Delta t J \left[\vec{f} \right] |_{\vec{u}_k} \right)$ on the

second step and then combining this with the first step gives:

$$\left(I - \gamma \Delta t J \left[\vec{f} \right] |_{\vec{u}_n} \right)^2 \Delta \vec{u}_n = \Delta t \left(I - \gamma^2 \Delta t J \left[\vec{f} \right] |_{\vec{u}_n} \right) \vec{f}(\vec{u}_n). \quad (5.2.9)$$

However this would be a mistake. Although the form has been simplified into a single analytically equivalent linear equation of the form $AX = B$, in practice the inversion of a matrix (using Krylov methods, as in Appendix E.3) introduces an error term, rendering this simplification numerical different from its two parent equations. Therefore I content myself with solving the two linear equations of Eq. 5.2.7 for each time step.

5.3 Benchmarks

As in the previous chapter, I will use the stochastically-forced barotropic jet in the turbulent regime as a testbed for the TR-BDF2 integration scheme, compared against RK4 and BDF1. Identical parameters and spectral resolutions are used as before but this time time-averaging is not performed, in order to observe and then compare the fast temporal oscillations produced via the three numerical schemes. The relevant portions of the GCM code are produced in Appendix E.3.

5.3.1 CE2

CE2 is performed using all three numerical integrators (RK4, BDF1 and TR-BDF2), implemented with a dynamically adaptive time stepper. By tracking the time steps of each scheme, their performances are benchmarked. In order to add an additional layer of difficulty for these solvers, North-South symmetry is no longer imposed which results in visible temporal oscillations. These oscillations are visible in Fig. 5.3.1 which shows the Hovmöller timelines of the relative vorticity and zonal mean zonal velocity of the stochastically-forced barotropic jet using each numerical integrator.

While both RK4 and TR-BDF2 are able to capture these oscillations, BDF1 is unable to reproduce them. This reflects its first-order accuracy in comparison to the second-order accuracy of the other two solvers.

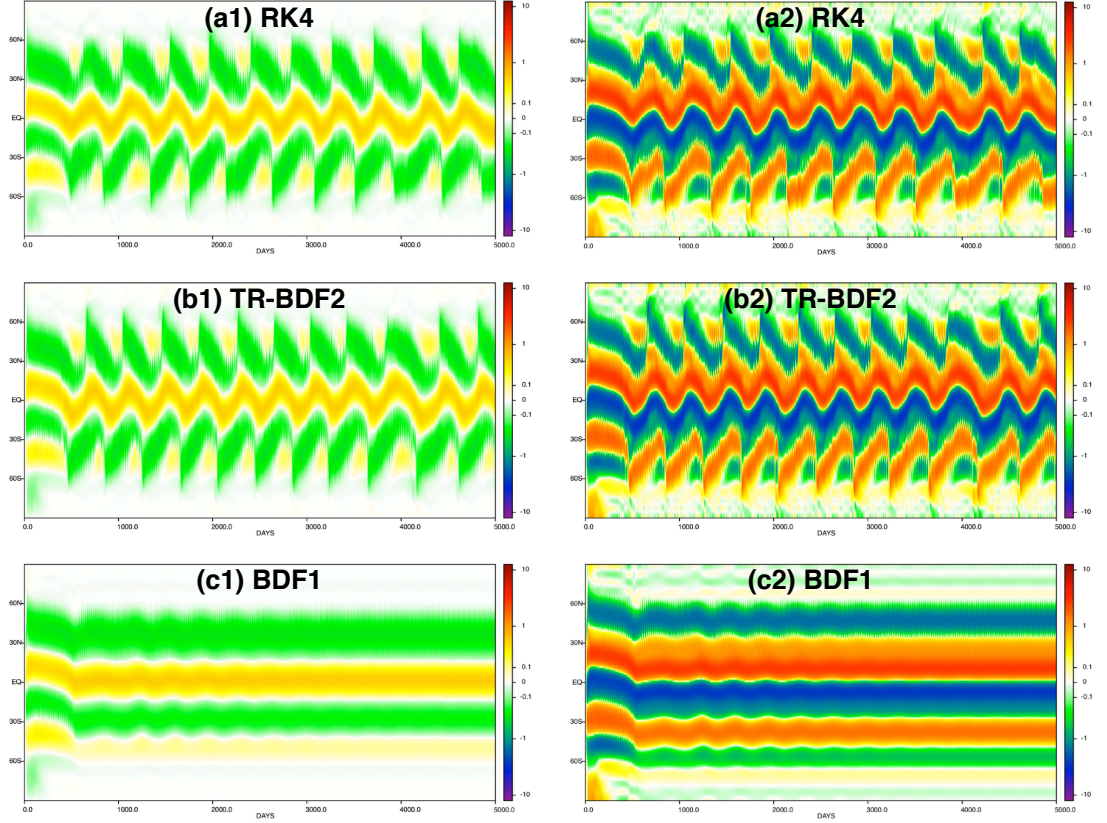


Figure 5.3.1: Hovmöller timelines of the (1) zonal mean zonal velocity and (2) relative vorticity of the stochastically-forced barotropic jet at $\Gamma = 0.1$ evolved via CE2 under (a) RK4, (b) TR-BDF2 and (c) BDF1. Spectral simulations with truncation $0 \leq l \leq L$ for $L = 30$ and $|m| \leq \min(l, M)$ for $M = 20$ and error tolerance set to 10^{-8} and Krylov subspace dimension of 12.

While both TR-BDF2 and RK4 are in agreement, the former is able to integrate the statistics of the jet considerably faster than the explicit scheme. Table 5.1 benchmarks the wall-clock times and mean time steps of each of the three numerical integrators. While BDF1 is the fastest of the three, it is also the most imprecise as already shown in Fig. 5.3.1. By contrast, although RK4 does not suffer from this deficiency since it is a second-order accurate scheme, it is the slowest of the three and

	RK4	BDF1	TR-BDF2
Arithmetic mean time step	0.036	0.171	0.224
Geometric mean time step	0.033	0.067	0.125
Wall-clock time (mins)	6780	1920	2280

Table 5.1: Benchmarks for RK4, BDF1 and TR-BDF2 with wall-clock times and mean time steps (arithmetic and geometric) of each. Simulation parameters as in Fig. 5.3.1.

takes the smallest time steps. This is expected because, as an explicit integration scheme, it requires a smaller time step in order to maintain stability. However, TR-BDF2 offers both speed and precision. It has the largest mean time step of the three methods whilst being a second-order accurate scheme. In addition, it is only slightly slower than BDF1 and 3x faster than RK4.

Thus the added computational work of solving the linear algebra problem in Eq. 5.2.7 for TR-BDF2 is offset by its larger time step. The distribution of the time steps for all three numerical integrators are visualized in Fig. 5.3.2. As expected, the size of RK4’s time step remains relatively constant. However, BDF1’s time step is mostly *smaller* than RK4’s time step because its lower precision causes its error vector to grow large for large time steps and so the adaptive time stepper responds by suppressing its magnitude. By contrast, TR-BDF2 has a more uniform distribution of time step magnitudes, ranging from the size of RK4’s time step up to 20x larger.

5.3.2 CE2.5

Beyond CE2, TR-BDF2 is also tested on the CE2.5 approximation (introduced in Section 3.2). In the case of high precision, TR-BDF2 gives extremely small time steps and becomes infeasible. However, this can be rectified by reducing the subspace dimension of the Krylov solver used to solved Eq. 5.2.7 from 12 to 10. In this case, Fig. 5.3.3 shows the Hovmöller timelines of the relative vorticity and zonal mean zonal velocity of the stochastically-forced barotropic jet using each of the three numerical

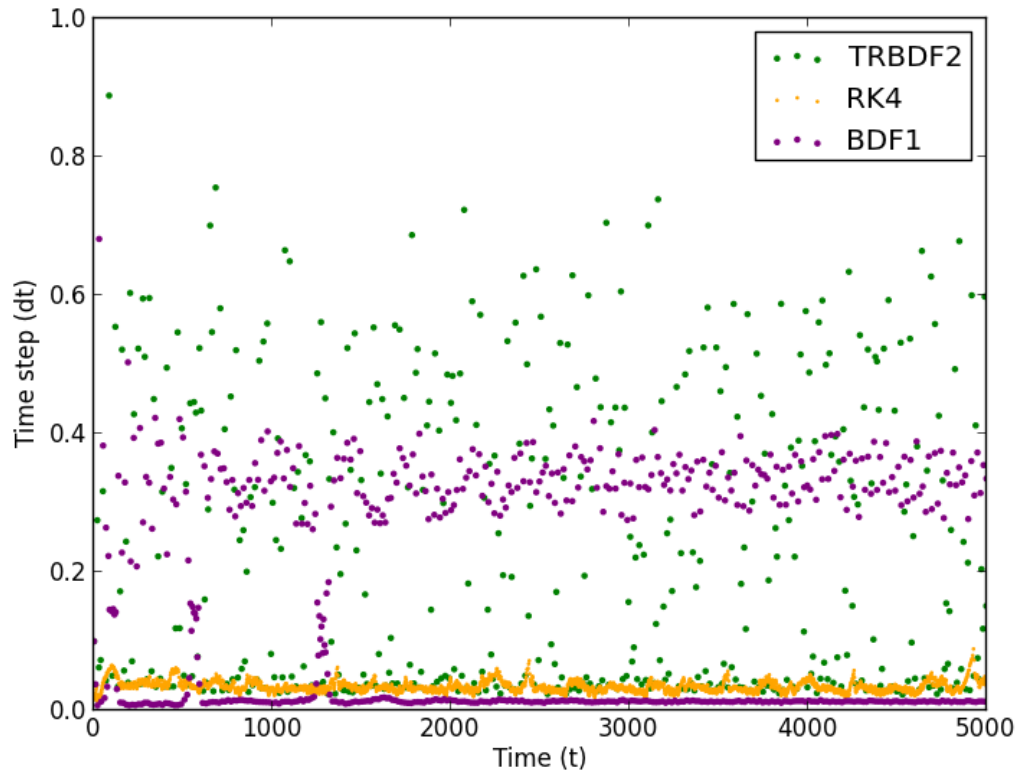


Figure 5.3.2: Time steps of the RK4, BDF1 and TR-BDF2 integration schemes as a function of time, sampled every 49 time steps. Simulation parameters as in Fig. 5.3.1.

integrators. For the case of a stochastically-forced barotropic jet evolved via CE2.5, the jet has less time dependence than in the previous example where CE2 was used and thus all three methods give indistinguishable results.

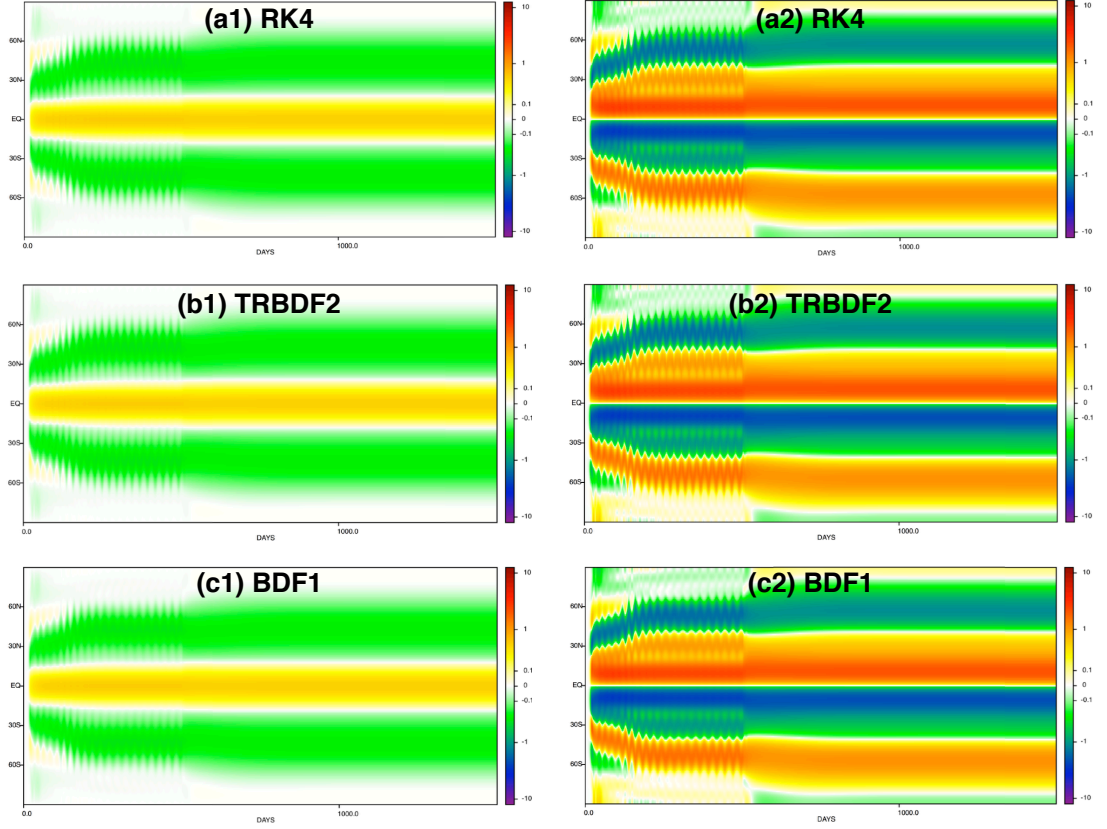


Figure 5.3.3: Hovmöller timelines of the (1) zonal mean zonal velocity and (2) relative vorticity of the stochastically-forced barotropic jet evolved via (a) RK4, (b) TR-BDF2 and (c) BDF1. CE2 was run up to $T = 500$ days and then CE2.5 for the remaining 1000 days. Simulation parameters as in Fig. 5.3.1 with error tolerance set to 10^{-10} and Krylov subspace dimension of 10.

However, there remains a noticeable difference in performance. TR-BDF2 performs comparably to RK4 in terms of wall-clock times and better in terms of the permitted time step size. Table 5.2 gives a quantitative comparison, where the averages have been performed only after $T = 500$ days which is when CE2.5 gets activated. While BDF1 takes larger time steps than RK4, the added computational expense associated with the semi-implicit method results in a longer run time. How-

	RK4	BDF1	TR-BDF2
Arithmetic mean time step	0.134	0.193	0.453
Geometric mean time step	0.083	0.161	0.341
Wall-clock time (mins)	1200	1605	1232

Table 5.2: Benchmarks for RK4, BDF1 and TR-BDF2 with wall-clock times and mean time steps (arithmetic and geometric) of each, averaged starting from $T = 500$ (i.e. only the CE2.5 section of the simulation). Simulation parameters as in Fig. 5.3.3.

ever, TR-BDF2’s significantly larger time steps as compared to RK4 are able to offset this added computational expense.

These larger time steps are illustrated in Fig. 5.3.4 which visualizes the distribution of the time steps for all three numerical integrators. The time steps of TR-BDF2 continuously increase up to ~ 1 day, at which point they plateau off and the variance of the distribution increases. However the accuracy of RK4 begins to degrade at a smaller time step (~ 0.5 days) due to a larger error vector and therefore the adaptive time stepper adjusting the time step to remain small for the majority of the rest of the simulation. Although a maximum time step of 0.5 days was set for RK4 in order to prevent numerical instabilities, it is still unable to prevent the oscillations in the time steps of RK4. By contrast, the time step of TR-BDF2 increases to 3x larger before the same effects became observable.

5.4 Summary

A semi-implicit TR-BDF2 integration scheme offers a faster and more precise alternative to the conventional explicit RK4 and semi-implicit BDF1 schemes in certain cases. In this chapter, I tested the performance of the scheme on a stochastically-forced barotropic jet.

In the case of CE2, where the first cumulant undergoes fast oscillations, BDF1 is unable to capture this behavior due to its first-order accuracy. However, TR-BDF2

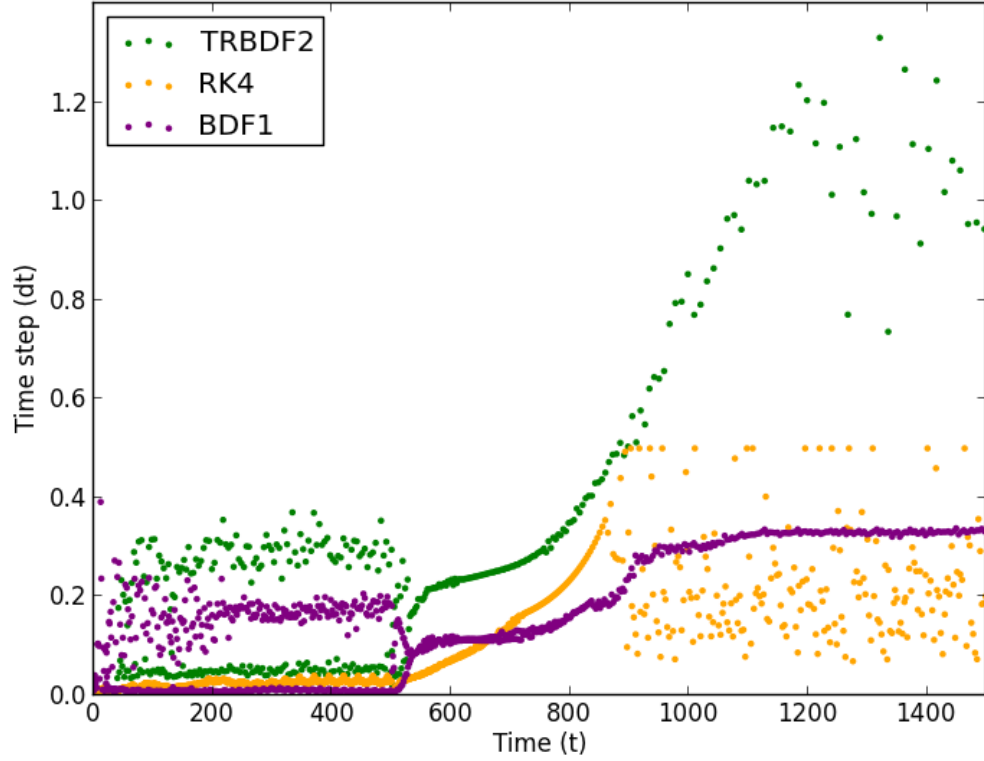


Figure 5.3.4: Time steps of the RK4, BDF1 and TR-BDF2 integration schemes as a function of time, sampled every 13 time steps. Simulation parameters as in Fig. 5.3.3.

and RK4 both reproduce the oscillations. Additionally, TR-BDF2 outperforms RK4 in both wall-clock times and mean time steps - by a drastic order of magnitude in the case of the latter.

For CE2.5, the difference in precision between the three methods is less pronounced because the cumulants have fewer fluctuations. However, TR-BDF2 still outperforms BDF1 by both wall-clock time and mean time steps. Although it also permits a larger mean time step than RK4, its wall-clock time is comparable. This is because (semi)implicit methods require the solution of a linear equation at each time step (usually via an iterative approach) which entails a larger computational expense than explicit time-stepping. It would be interesting to *a priori* select the more appropriate

solver for an arbitrary turbulent flow problem by performing an analytic comparison of TR-BDF2 and RK4 for a general quadratically nonlinear system.

Chapter 6

Concluding Remarks

Direct statistical simulation (DSS) is an attractive alternative to the accumulation of statistics by direct numerical simulation (DNS). This thesis explores a new technique for finding the equal-time statistics of dynamical systems by re-expressing a time-evolution problem of the Fokker-Planck equation (FPE) as a sparse linear algebra problem. This technique offers an elegant alternative to the traditional approach of DNS. While other studies have found that deterministic chaos and stochastic noise have similar effects on the low-order statistics of dynamical systems [13,63], this study finds a fundamental distinction between the two in the case of the Lorenz attractor where its deterministic dynamics produce high-order statistics that stochastic forcing erases, indicating competing effects.

For systems of one to four dimensions, this FPE technique is computationally tractable and, for low resolutions, even faster than DNS. One drawback is that it requires the introduction of small stochastic noise to ensure resolvability of the PDF on the lattice scale by washing out the fine, and often fractal, structure. Since this forcing can be made arbitrarily small for increasing resolution, an interesting direction of future work would be to employ a sparse preconditioner for the large nonsymmetric FPE operator studied here, allowing for even higher resolutions to be reached and,

for the case of the Lorenz attractor, revealing its fine fractal steps.

Another interesting extension of this work is the proposed self-adjoint representation of the FPE operator. This Hermiticity makes it equivalent to a Hamiltonian operator and allows for the FPE to be related to the Schrodinger equation by a Wick rotation. By gaining Hermiticity, the operator becomes amenable to solution by simulated/quantum annealing and adiabatic quantum computation. It would be interesting to check whether the theoretical computational gains of using a quantum algorithm could offset the added drawbacks of a slower convergence time due to a more clustered eigenvalue distribution around zero. If so and if the efforts of quantum computing come to fruition, it might be possible to solve for the steady-state statistics of entirely classical systems using entirely quantum mechanical algorithms and processes, offering a direct way to access the extremely high order steady-state statistics of deterministic chaotic systems.

Other variants of the Fokker-Planck equation also have interesting properties. Stochastic forcing can be entirely eliminated by replacing diffusion with hyperdiffusion. Although the PDF develops negative probabilities since Pawula's theorem shows that realizability gets violated, if the negative values remain small and away from the vicinities of interest then hyperdiffusion might still be a valuable tool for problems where an approximate distribution suffices.

An open question in this thesis is about the eigenvalue distribution of the FPE operator. The dependence of the real component of the eigenvalues of the Lorenz attractor on stochastic forcing allows for a linear extrapolation down to the deterministic case. This value is related to the relaxation time scale of the system. But it is still unclear whether important information regarding the dynamics of the system is contained in the other excited eigenvalues of the operator. For example, what (if any) is the significance of those eigenvalues that are purely real? Another open question is why density of the clustering of eigenvalues in complex space increases with distance

from the origin.

This thesis also investigated the steady-state statistics of the Lorenz attractor in the context of a perturbative expansion in the equal-time cumulants of the system. Its utility is highlighted by the order of magnitude speed ups compared to DNS and the FPE technique as measured by wall-clock time. Unlike the FPE technique which scales exponentially with system dimensionality, the cumulant expansion technique scales exponentially with truncation level instead, and so it is especially well-suited for higher dimensional systems where the former fails. Another attractive feature of this technique is that it explicitly respects the reflection symmetries of the system, unlike DNS where the statistics only slowly converge to the correct symmetries.

The inability of the CE2 approximation to adequately capture the statistics of the Lorenz attractor underscores the importance of its nonlocal cubic higher correlations. It provides evidence that this eddy-eddy scattering allows for the inverse-cascade processes inherent to the attractor which gives rise to the fractal fine structure. A CE3 approximation is able to capture these essential processes.

However CE2 does suffice for dynamical systems that are less nonlinear than the Lorenz attractor, such as the two idealized barotropic models explored in this thesis. An interesting type of CE2 that I investigate for these barotropic models is the use of an ensemble average in place of a zonal average. By retaining the eddy-eddy scattering processes that are important for the latitudinal transport of enstrophy in turbulent flows, it does a better job than zonal CE2 at reproducing the statistics accumulated via direct numerical simulation. In fact for some deterministic barotropic systems, the agreement between ensemble CE2 and temporally-averaged DNS is so remarkable that it suggests turbulence is almost entirely washing out the third and higher ensemble-averaged cumulants and thus essentially reducing temporally-averaged DNS to ensemble CE2 by ergodicity. If so then this hints at a fundamental distinction between deterministic barotropic turbulence and the Lorenz system where in the case

of the latter, chaos in fact *produces, not erases*, higher order statistics.

An open question is whether ensemble CE2 has an equivalent formalism under general conditions, in the same way that zonal CE2 is equivalent to the quasi-linear approximation. If such an equivalency exists then it might offer insight into its realizability conditions. Computational evidence presented in this thesis suggests that ensemble CE2 is realizable when sufficient stochastic noise is present to stabilize the scheme by washing out the higher order statistics. But in the case of the deterministic barotropic jet being relaxed toward a fixed profile, frequent projections of nonphysical eigenmodes are required to maintain positivity. Knowing *a priori* whether ensemble CE2 is suitable for an arbitrary problem by developing a rigorous set of requirements for its realizability condition will bolster its attractiveness as an alternative to zonal CE2.

However a drawback of ensemble CE2 is its sluggishness as it retains more modes than zonal CE2. Therefore I have also presented a prescription for a dimensional reduction using an unsupervised machine learning technique. The Proper Orthogonal Decomposition (POD) scheme developed in this thesis gives order of magnitude speeds up for certain barotropic systems. Unlike in the case of the stochastically-forced barotropic jet where power is forced into adjacent modes, the deterministic jet has most of the power in relatively fewer modes and so a substantial basis reduction can be performed. These savings are further pronounced when POD is coupled with a zonal CE2 truncation scheme, since relatively fewer modes get excited in the quasi-linear approximation, allowing more to be discarded. However the POD truncation scheme finds its greatest utility in eCE2 which is the most computationally demanding of the two. Its varying performance shows that its effectiveness depends on the specifics of the system, and must be considered on a case by case basis.

Since this thesis looked at barotropic models, an interesting future direction of research is to extend the POD scheme to baroclinic models as in Ref [?, 44, 51, 58, 59].

It would also be worthwhile to compare performance by forming the second moments of the reduced basis using other types of averages too. But perhaps the biggest savings in time could come from developing a way to dynamical update the basis “on the fly”. This would avoid having to first gather the statistics in the full dimensional system to form the basis, which at present is where the majority of the simulation time is spent.

Finally, there are other ways to achieve numerical speed ups too. One option is to change the integration scheme itself. While a fourth-order Runge-Kutta (RK4) scheme is the main workhorse used for the simulations performed in this thesis, I also investigated semi-implicit schemes since they tend to have superior stability than explicit schemes. One such scheme, BDF1, is unable to capture the fast oscillations of the first cumulant in the case of CE2 on a stochastically-forced barotropic jet due to its first-order accuracy. However, a second-order accurate TR-BDF2 scheme is able to reproduce the oscillations seen in RK4. Additionally, TR-BDF2 outperforms RK4 in both wall-clock times and mean time steps. It would be interesting to develop a heuristic to automatically infer the appropriateness of TR-BDF2 over traditional RK4 for an arbitrary turbulent flow problem.

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Appendix A

Ornstein-Uhlenbeck System

A.1 One Dimensional Ornstein-Uhlenbeck System

Consider a Fokker-Planck equation cast as the following eigenvalue problem:

$$EP = L_{FPE}P, \tag{A.1.1}$$

where in the case of the Ornstein-Uhlenbeck system, the FPE operator is defined as:

$$L_{FPE} = \frac{\partial}{\partial x} (-\alpha x P) - \Gamma \frac{\partial^2 P}{\partial x^2}. \tag{A.1.2}$$

Under the transformation,

$$y = \sqrt{\Gamma}x, \tag{A.1.3}$$

the eigenvalue equation simplifies to:

$$\begin{aligned}
EP &= -\frac{\partial^2 P}{\partial y^2} - \alpha \frac{\partial}{\partial y} (yP) \\
\rightarrow 0 &= \frac{\partial^2 P}{\partial y^2} + \alpha y \frac{\partial P}{\partial y} + (E + \alpha) P.
\end{aligned} \tag{A.1.4}$$

This ODE can now be solved by the Frobenius method using a series solution of the form:

$$P = y^k \sum_{n=0}^{\infty} a_n y^n, \tag{A.1.5}$$

where the first and second derivatives are given by:

$$\frac{\partial P}{\partial y} = \sum_{n=0}^{\infty} (n+k) a_n y^{n+k-1} \tag{A.1.6}$$

$$\frac{\partial^2 P}{\partial y^2} = \sum_{n=0}^{\infty} (n+k)(n+k-1) a_n y^{n+k-2}. \tag{A.1.7}$$

Plugging these into the eigenvalue equation gives:

$$\begin{aligned}
0 &= \sum_{n=0}^{\infty} (n+k)(n+k-1) a_n y^{n+k-2} \\
&\quad + \sum_{n=0}^{\infty} [E + \alpha(n+k+1)] a_n y^{n+k} \\
&= k(k-1) a_0 y^{k-2} + k(k+1) a_1 y^{k-1} \\
&\quad + \sum_{n=-2}^{\infty} (n+k+2)(n+k+1) a_{n+2} y^{n+k} \\
&\quad + \sum_{n=0}^{\infty} [E + \alpha(n+k+1)] a_n y^{n+k},
\end{aligned} \tag{A.1.8}$$

where in the last step the dummy index of the first term is redefined such that

$n \rightarrow n + 2$.

To find k , obtain the indicial equation by considering the equality for the coefficient of the lowest power polynomial:

$$0 = k(k-1)a_0y^{k-2}. \quad (\text{A.1.9})$$

Since a_0 is defined as the smallest non-zero coefficient of a_i , it must be that

$$\begin{aligned} 0 &= k(k-1) \\ \rightarrow k &= 0, 1. \end{aligned} \quad (\text{A.1.10})$$

Both choices of k should be checked. First let $k = 0$. Equating equal powers of y from Equation A.1.8 gives:

$$\begin{aligned} 0 &= \sum_{n=-2}^{\infty} (n+2)(n+1)a_{n+2}y^n \\ &\quad + \sum_{n=0}^{\infty} [E + \alpha(n+1)]a_ny^n \\ &= \sum_{n=0}^{\infty} (n+2)(n+1)a_{n+2}y^n \\ &\quad + \sum_{n=0}^{\infty} [E + \alpha(n+1)]a_ny^n. \end{aligned} \quad (\text{A.1.11})$$

Since this equality must hold for all powers of y , it must hold for all values of n :

$$0 = (n+1)(n+2)a_{n+2} + [E + \alpha(n+1)]a_n. \quad (\text{A.1.12})$$

The recursion relation for the coefficients is thus:

$$a_n = -a_{n-2} \frac{E + \alpha(n-1)}{n(n-1)}, n \geq 2. \quad (\text{A.1.13})$$

To find an analytic expression, first express the indices in consecutively ascending order by the substitution $n = 2m$ for even n and $n = 2m + 1$ for odd n , where $m \geq 1$:

$$\begin{aligned} a_{2m}^{(even)} &= -a_{2m-2} \frac{E + \alpha(2m-1)}{2m(2m-1)} \\ &= a_0 \prod_{j=1}^m \left[-\frac{E + \alpha(2j-1)}{2j(2j-1)} \right] \\ &= a_0 \frac{2^m (-\alpha)^m \Gamma\left(\frac{E}{2\alpha} + m + \frac{1}{2}\right)}{\Gamma(2m+1) \Gamma\left(\frac{E}{2\alpha} + \frac{1}{2}\right)} \end{aligned} \quad (\text{A.1.14})$$

$$\begin{aligned} a_{2m+1}^{(odd)} &= a_1 \prod_{j=1}^m \left[-\frac{E + 2\alpha j}{2j(2j+1)} \right] \\ &= a_1 \frac{2^m (-\alpha)^m \Gamma\left(\frac{E}{2\alpha} + m + 1\right)}{\Gamma(2m+2) \Gamma\left(\frac{E}{2\alpha} + 1\right)}. \end{aligned} \quad (\text{A.1.15})$$

Thus the $k = 0$ part of the solution is:

$$\begin{aligned} P &= \sum_{n=0}^{\infty} a_n y^n \\ &= \sum_{m=0}^{\infty} a_{2m} y^{2m} + \sum_{m=0}^{\infty} a_{2m+1} y^{2m+1} \\ &= \exp\left(-\frac{\alpha y^2}{2}\right) \left[c_1 H_{\frac{E}{\alpha}} \left(\sqrt{\frac{\alpha}{2}} y \right) + c_2 y L_{\frac{E}{2\alpha} - \frac{1}{2}}^{\frac{1}{2}} \left(\frac{\alpha y^2}{2} \right) \right] \\ &= (c_1 + c_2) \exp\left(-\frac{\alpha y^2}{2}\right) H_{\frac{E}{\alpha}} \left(\sqrt{\frac{\alpha}{2}} y \right), \end{aligned} \quad (\text{A.1.16})$$

since the weighted Laguerre polynomial reduces to the Hermite polynomial.

Now let $k = 1$. This time note that Equation A.1.8 implies that $a_1 = 0$ and thus the solution has only an even contribution. Equating equal powers of y from Equation

A.1.8 gives:

$$\begin{aligned}
0 &= \sum_{n=-2}^{\infty} (n+3)(n+2) a_{n+2} y^{n+1} \\
&\quad + \sum_{n=0}^{\infty} [E + \alpha(n+2)] a_n y^{n+1} \\
&\quad + \sum_{n=0}^{\infty} (n+3)(n+2) a_{n+2} y^{n+1} \\
&\quad + \sum_{n=0}^{\infty} [E + \alpha(n+2)] a_n y^{n+1}.
\end{aligned} \tag{A.1.17}$$

Since this equality must hold for all powers of y , it must hold for all values of n :

$$0 = (n+2)(n+3) a_{n+2} + [E + \alpha(n+2)] a_n \tag{A.1.18}$$

The recursion relation for the coefficients is thus:

$$a_n = -a_{n-2} \frac{E + \alpha n}{n(n+1)}, n \geq 2. \tag{A.1.19}$$

To find an analytic expression, first express the indices in consecutively ascending order by the substitution $n = 2m$ for even n , where $m \geq 1$:

$$\begin{aligned}
a_{2m} &= -a_{2m-2} \frac{E + 2\alpha m}{2m(2m+1)} \\
&= a_0 \prod_{j=1}^{\infty} \left[-\frac{E + 2\alpha j}{2j(2j+1)} \right] \\
&= a_0 \frac{2^m (-\alpha)^m \Gamma\left(\frac{E}{2\alpha} + m + 1\right)}{\Gamma(2m+2) \Gamma\left(\frac{E}{2\alpha} + 1\right)}.
\end{aligned} \tag{A.1.20}$$

Thus the $k = 1$ part of the solution is:

$$\begin{aligned}
P &= y \sum_{n=0}^{\infty} a_n y^n \\
&= \sum_{m=0}^{\infty} a_{2m} y^{2m+1}.
\end{aligned} \tag{A.1.21}$$

This has reduced to the same equation from the odd contribution of the $k = 0$ case and so it reduces to the same weighted Hermite polynomial.

Therefore the full solution to Equation A.1.2 is:

$$P(y) = c \exp\left(-\frac{\alpha y^2}{2}\right) H_{\frac{E}{\alpha}}\left(\sqrt{\frac{\alpha}{2}}y\right). \tag{A.1.22}$$

The eigenvalues and eigenvectors of the FPE operator are thus:

$$P_n(x) = c_1 \exp\left(-\frac{\alpha x^2}{2\Gamma}\right) H_n\left(\sqrt{\frac{\alpha}{2\Gamma}}x\right) \tag{A.1.23}$$

$$E_n = \alpha n, \tag{A.1.24}$$

where c_1 is the appropriate normalization constant and $n \geq 0$ to ensure boundedness of the integral.

A.2 Two Dimensional Ornstein-Uhlenbeck Modified System

Consider a two dimensional modified Ornstein-Uhlenbeck process where motion in the x and y directions is coupled via circular motion with coupling strength β :

$$\dot{x} = \beta y - \alpha x + \eta_1(t) \quad (\text{A.2.1})$$

$$\dot{y} = -\beta x - \alpha y + \eta_2(t). \quad (\text{A.2.2})$$

For this system, the FPE operator becomes:

$$\begin{aligned} L_{FPE}P = & -\Gamma \left(\frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} \right) - 2\alpha P \\ & - (\alpha x - \beta y) \frac{\partial P}{\partial x} - (\alpha y - \beta x) \frac{\partial P}{\partial y}. \end{aligned} \quad (\text{A.2.3})$$

My goal is to find the eigenvalue spectrum of this operator, as was done with the one-dimensional unmodified Ornstein-Uhlenbeck system. Due to the circular symmetry of the system, it is natural to transform from Cartesian to polar coordinates,

$$x = r \cos \theta \quad (\text{A.2.4})$$

$$y = r \sin \theta. \quad (\text{A.2.5})$$

The relevant derivatives of the PDF can be found by the chain rule:

$$\frac{\partial P}{\partial x} = \frac{\partial P}{\partial \theta} \frac{\partial \theta}{\partial x} + \frac{\partial P}{\partial r} \frac{\partial r}{\partial x} \quad (\text{A.2.6})$$

$$\frac{\partial P}{\partial y} = \frac{\partial P}{\partial \theta} \frac{\partial \theta}{\partial y} + \frac{\partial P}{\partial r} \frac{\partial r}{\partial y}, \quad (\text{A.2.7})$$

to yield:

$$\begin{aligned}
L_{FPE}P &= - (\alpha r \cos \theta - \beta r \sin \theta) \left(-\frac{\partial P}{\partial \theta} \frac{\sin \theta}{r} + \frac{\partial P}{\partial r} \cos \theta \right) \\
&\quad - (\alpha r \sin \theta + \beta r \cos \theta) \left(\frac{\partial P}{\partial \theta} \frac{\cos \theta}{r} + \frac{\partial P}{\partial r} \sin \theta \right) \\
&\quad - 2\alpha P - \Gamma \left(\frac{\partial^2 P}{\partial r^2} + \frac{1}{r} \frac{\partial P}{\partial r} + \frac{1}{r^2} \frac{\partial^2 P}{\partial \theta^2} \right) \tag{A.2.8}
\end{aligned}$$

$$\begin{aligned}
&= -\beta \frac{\partial P}{\partial \theta} - \alpha r \frac{\partial P}{\partial r} - 2\alpha P \\
&\quad - \Gamma \left(\frac{\partial^2 P}{\partial r^2} + \frac{1}{r} \frac{\partial P}{\partial r} + \frac{1}{r^2} \frac{\partial^2 P}{\partial \theta^2} \right). \tag{A.2.9}
\end{aligned}$$

The eigenvalue problem for this system,

$$EP = L_{FPE}P, \tag{A.2.10}$$

thus becomes:

$$\begin{aligned}
0 &= \beta \frac{\partial P}{\partial \theta} + \alpha r \frac{\partial P}{\partial r} + (2\alpha + E) P \\
&\quad + \Gamma \left(\frac{\partial^2 P}{\partial r^2} + \frac{1}{r} \frac{\partial P}{\partial r} + \frac{1}{r^2} \frac{\partial^2 P}{\partial \theta^2} \right). \tag{A.2.11}
\end{aligned}$$

To solve this, I first set $\beta = 0$. Since the system is now decoupled, the PDF is expected to have a separable form,

$$P(r, \theta) = R(r) \Theta(\theta), \tag{A.2.12}$$

leading to:

$$\begin{aligned}
0 &= \alpha \frac{r}{R} \frac{\partial R}{\partial r} + (2\alpha + E) \\
&\quad + \Gamma \left(\frac{1}{R} \frac{\partial^2 R}{\partial r^2} + \frac{1}{R} \frac{1}{r} \frac{\partial R}{\partial r} + \frac{1}{\Theta} \frac{1}{r^2} \frac{\partial^2 \Theta}{\partial \theta^2} \right)
\end{aligned} \tag{A.2.13}$$

$$\begin{aligned}
\rightarrow 0 &= \frac{\alpha r^3}{\Gamma R} \frac{\partial R}{\partial r} + \frac{2\alpha + E}{\Gamma} r^2 \\
&\quad + \left(\frac{r^2}{R} \frac{\partial^2 R}{\partial r^2} + \frac{r}{R} \frac{\partial R}{\partial r} + \frac{1}{\Theta} \frac{\partial^2 \Theta}{\partial \theta^2} \right).
\end{aligned} \tag{A.2.14}$$

Consistent with the separability of the solution, for R and Θ to be independent the last term must be constant:

$$-m^2 = \frac{1}{\Theta} \frac{\partial^2 \Theta}{\partial \theta^2} \tag{A.2.15}$$

$$\rightarrow -m^2 \Theta = \frac{\partial^2 \Theta}{\partial \theta^2}, \tag{A.2.16}$$

giving the general solution,

$$\Theta(\theta) = A \exp(mi\theta) + B \exp(-mi\theta). \tag{A.2.17}$$

Applying periodic boundary conditions to both $\Theta(\theta)$ and $\Theta'(\theta)$ yields:

$$\Theta(\theta) = A \exp(mi\theta), \tag{A.2.18}$$

where m is constrained to be an integer.

Next I turn to the radial equation:

$$\begin{aligned}
m^2 &= \frac{r^2}{R} \frac{\partial^2 R}{\partial r^2} + \frac{r}{R} \frac{\partial R}{\partial r} \\
&\quad + \frac{\alpha}{\Gamma} \frac{r^3}{R} \frac{\partial R}{\partial r} + \frac{2\alpha + E}{\Gamma} r^2
\end{aligned} \tag{A.2.19}$$

$$\begin{aligned}
\rightarrow 0 &= r^2 \frac{\partial^2 R}{\partial r^2} + \left(r + \frac{\alpha}{\Gamma} r^3 \right) \frac{\partial R}{\partial r} \\
&\quad + \left(\frac{2\alpha + E}{\Gamma} r^2 - m^2 \right) R.
\end{aligned} \tag{A.2.20}$$

This can be solved using confluent hypergeometric functions of the first kind, ${}_1F_1(a; b; x)$, as:

$$\begin{aligned}
R(r) &= c_1 r^{-m} {}_1F_1 \left[\frac{1}{2} \left(\frac{E}{\alpha} - m \right); 1 - m; \frac{-ar^2}{2\Gamma} \right] \\
&\quad + c_2 r^m {}_1F_1 \left[\frac{1}{2} \left(\frac{E}{\alpha} + m \right); 1 + m; \frac{-ar^2}{2\Gamma} \right].
\end{aligned} \tag{A.2.21}$$

Since ${}_1F_1(a; b; x)$ is undefined for $b \leq 0$, the radial solution can be re-expressed as:

$$R(r) = c r^{|m|} {}_1F_1 \left[\frac{1}{2} \left(\frac{E}{\alpha} + |m| \right); 1 + |m|; \frac{-ar^2}{2\Gamma} \right], \tag{A.2.22}$$

which can in turn be re-expressed as,

$$R(r) = c \exp \left(-\frac{ar^2}{2\Gamma} \right) r^{|m|} {}_1F_1 \left[\frac{1}{2} \left(\frac{E}{\alpha} + |m| \right); 1 + |m|; \frac{ar^2}{2\Gamma} \right]. \tag{A.2.23}$$

The solution can now be converted to generalized Laguerre polynomials:

$$R(r) = c \exp\left(-\frac{ar^2}{2\Gamma}\right) r^{|m|} L_n^{|m|}\left(\frac{ar^2}{2\Gamma}\right), \quad (\text{A.2.24})$$

where c is the appropriate normalization constant and the subscript n has been introduced as,

$$n = \frac{1}{2} \left(\frac{E}{\alpha} - |m| \right), \quad (\text{A.2.25})$$

and is constrained to be an integer. In addition, $R(r)$ is non-normalizable for $n < 0$. Under these constraints, the Laguerre polynomial has a finite number of terms. Therefore the full solution for Equation A.2.11 is:

$$P_{n,m}(r, \theta) = c \exp\left(-\frac{ar^2}{2\Gamma}\right) r^{|m|} L_n^{|m|}\left(\frac{ar^2}{2\Gamma}\right) \exp(im\theta), \quad (\text{A.2.26})$$

where eigenvalues given by

$$E_{n,m} = \alpha (2n + |m|), \quad (\text{A.2.27})$$

with $\{n, m\} \in \mathbb{Z}$ and $n \geq 0$.

Recall that the coupling factor, β , was set to zero at the start. Examining the neglected term, $\beta \frac{\partial P}{\partial \theta}$, reveals that the eigenfunction of Equation A.2.26 is also an eigenfunction of the neglected term with eigenvalue $i\beta m$. Thus the neglected term can now be re-introduced into the eigenproblem without affecting the validity of the calculated eigenfunction, by modifying the eigenvalues to:

$$E_{n,m} = \alpha (2n + |m|) + i\beta m. \quad (\text{A.2.28})$$

This expression can be further simplified with the substitution

$$l = 2n + |m|, \tag{A.2.29}$$

where manifestly $l \geq 0$ and is of the same parity as m . Equation A.2.28 then becomes:

$$E_{l,m} = \alpha l + i\beta m, \tag{A.2.30}$$

where now m is constrained such that $|m| = l - 2n \leq l$. Although m structurally relates to l similar to how the azimuthal quantum number relates to the magnetic quantum number, recall that unlike the quantum numbers, m determines not only the spherical component of the solution but also the radial component.

Appendix B

Ensemble CE2 Equations of Motion

B.1 Derivation in a Generalized Basis

Consider the EOMs for the field in a generalized basis, where the two quadratic terms are kept separate:

$$\frac{dq_i}{dt} = A_i + L_{im}q_m + Q_{imn}^{(+)}q_mq_n + Q_{imn}^{(-)}q_mq_n^*. \quad (\text{B.1.1})$$

The usual Reynolds decomposition can be performed, $q_i = \bar{q}_i + q'_i$ where $\bar{\bar{q}}_i = \bar{q}_i$ and $\bar{q}'_i = 0$. Here the mean has been defined as an ensemble average over initial conditions:

$$\overline{q_i(t)} = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=0}^{N-1} q_i^{(n)}(t) \quad (\text{B.1.2})$$

The first cumulant is defined as $c_i \equiv \bar{q}_i$. Then the EOM for the first cumulant is thus:

$$\frac{dc_i}{dt} = \overline{\frac{dq_i}{dt}} \quad (\text{B.1.3})$$

$$= A_i + L_{im}\bar{q}_m + Q_{imn}^{(+)}\bar{q}_m\bar{q}_n + Q_{imn}^{(-)}\overline{q_mq_n^*} \quad (\text{B.1.4})$$

$$= A_i + L_{im}c_m + Q_{imn}^{(+)}c_mc_n + Q_{imn}^{(-)}c_mc_n^* + Q_{imn}^{(+)}\overline{q'_mq'_n} + Q_{imn}^{(-)}\overline{q'_mq_n'^*} \quad (\text{B.1.5})$$

Here the Einstein summation convention is being used. Since there are two terms of second order which cannot be expressed in terms of the first cumulants, instead define two different types of second order cumulants as $c_{ij}^{(S)} = \overline{q'_i q'_j}$ and $c_{ij}^{(H)} = \overline{q'_i q_j'^*}$. Consequently, also define two different kinds of symmetrization operators for symmetric and self-adjoint variables:

$$\{a_{ij}\}_S = \frac{1}{2} (a_{ij} + a_{ji}) \quad (\text{B.1.6})$$

$$\{a_{ij}\}_H = \frac{1}{2} (a_{ij} + a_{ji}^*) . \quad (\text{B.1.7})$$

The EOMs for the two second cumulants then become:

$$\frac{dc_{ij}^{(S)}}{dt} = 2 \left\{ \overline{\frac{dq'_i}{dt} q'_j} \right\}_S \quad (\text{B.1.8})$$

$$= 2 \left\{ \overline{\frac{dq_i}{dt} q'_j} \right\}_S \quad (\text{B.1.9})$$

$$= 2 \left\{ A_i q'_j + L_{im} q_m q'_j + Q_{imn}^{(+)} q_m q_n q'_j + Q_{imn}^{(-)} q_m q_n^* q'_j \right\}_S \quad (\text{B.1.10})$$

$$= 2 \left\{ L_{im} c_{mj}^{(S)} + Q_{imn}^{(+)} \left(c_m c_{nj}^{(S)} + c_n c_{mj}^{(S)} \right) \right\}_S \quad (\text{B.1.11})$$

$$+ 2 \left\{ Q_{imn}^{(-)} \left(c_m c_{nj}^{(H)*} + c_n^* c_{mj}^{(S)} \right) \right\}_S \quad (\text{B.1.12})$$

$$\frac{dc_{ij}^{(H)}}{dt} = 2 \left\{ \overline{\frac{dq'_i}{dt} q_j'^*} \right\}_H \quad (\text{B.1.13})$$

$$= 2 \left\{ \overline{\frac{dq_i}{dt} q_j'^*} \right\}_H \quad (\text{B.1.14})$$

$$= 2 \left\{ L_{im} q_m q_j'^* + Q_{imn}^{(+)} q_m q_n q_j'^* + Q_{imn}^{(-)} q_m q_n^* q_j'^* \right\}_H \quad (\text{B.1.15})$$

$$= 2 \left\{ L_{im} c_{mj}^{(H)} + Q_{imn}^{(+)} \left(c_m c_{nj}^{(H)} + c_n c_{mj}^{(H)} \right) \right\}_H \quad (\text{B.1.16})$$

$$+ 2 \left\{ Q_{imn}^{(-)} \left(c_m c_{nj}^{(S)*} + c_n^* c_{mj}^{(H)} \right) \right\}_H . \quad (\text{B.1.17})$$

Thus the two EOMs for the second cumulants can be expressed as a single EOM

as follows:

$$\frac{dc_{ij}^{(S,H)}}{dt} = 2 \left\{ L_{im} c_{mj}^{(S,H)} + 2Q_{imn}^{(+)} c_m c_{nj}^{(S,H)} + Q_{imn}^{(-)} \left(c_m c_{nj}^{(H,S)*} + c_n^* c_{mj}^{(S,H)} \right) \right\}_{S,H}. \quad (\text{B.1.18})$$

Note that $Q_{ijk}^{(+)} = Q_{ikj}^{(+)}$ whereas $Q_{ijk}^{(-)} \neq Q_{ikj}^{(-)*}$ because $Q_{ijk}^{(\pm)}$ assumes that the field/cumulant produced by the eddy-eddy interaction of two fields/cumulants has an m -mode greater than zero.

B.2 Jacobian-free Derivation in Spectral Space

Consider the vorticity $q(\theta, \phi)$ in real space. Expanding in spherical harmonics gives:

$$q(\theta, \phi) = \sum_{lm} q_{lm} Y_l^m(\theta, \phi). \quad (\text{B.2.1})$$

The first and second cumulants are given by:

$$c_1(\theta, \phi) = \overline{q(\theta, \phi)} \quad (\text{B.2.2})$$

$$= \sum_{lm} c_{lm} Y_l^m(\theta, \phi) \quad (\text{B.2.3})$$

$$c_2(\theta_1, \phi_1, \theta_2, \phi_2) = \overline{q'(\theta_1, \phi_1) q'(\theta_2, \phi_2)} \quad (\text{B.2.4})$$

$$= \sum_{l_1 m_1} \sum_{l_2 m_2} c_{l_1 m_1; l_2 m_2} Y_{l_1}^{m_1}(\theta_1, \phi_1) Y_{l_2}^{m_2}(\theta_2, \phi_2), \quad (\text{B.2.5})$$

where the coefficients c_{lm} and $c_{l_1 m_1; l_2 m_2}$ are given by:

$$c_{lm} = \overline{q_{lm}} \quad (\text{B.2.6})$$

$$c_{l_1 m_1; l_2 m_2} = \overline{q'_{l_1 m_1} q'_{l_2 m_2}}. \quad (\text{B.2.7})$$

The ensemble CE2 EOMs for a system with at most quadratic nonlinearities in a generalized basis are:

$$\frac{dc_i}{dt} = \sum_m L_{im} c_m + \sum_{m,n} Q_{imn} (c_m c_n + c_{mn}) \quad (\text{B.2.8})$$

$$\frac{dc_{ij}}{dt} = 2 \sum_m L_{im} c_{mj} + 4 \sum_{m,n} Q_{imn} c_m c_{nj}. \quad (\text{B.2.9})$$

Thus in the basis of spherical harmonics they are expressed as:

$$\frac{dc_{lm}}{dt} = \sum_{l_1 m_1} L_{lm;l_1 m_1} c_{l_1 m_1} \quad (\text{B.2.10})$$

$$+ \sum_{l_1 m_1} \sum_{l_2 m_2} Q_{lm;l_1 m_1; l_2 m_2} (c_{l_1 m_1} c_{l_2 m_2} + c_{l_1 m_1; l_2 m_2}) \quad (\text{B.2.11})$$

$$\frac{dc_{lm;l' m'}}{dt} = 2 \sum_{l_1 m_1} L_{lm;l_1 m_1} c_{l_1 m_1; l' m'} \quad (\text{B.2.12})$$

$$+ 4 \sum_{l_1 m_1} \sum_{l_2 m_2} Q_{lm;l_1 m_1; l_2 m_2} c_{l_1 m_1} c_{l_2 m_2; l' m'} \quad (\text{B.2.13})$$

Here m_1 and m_2 can be either both positive, both negative, or one positive and the other negative. But if the constraint is imposed that $0 \leq m < M$ where $m = m_1 + m_2$ for the Q term, then each of the four cases allows for only the following possibilities.

Case 1 ($++$): $m_1 \geq 0, m_2 \geq 0$ and $m_1 + m_2 < M$

Case 2 ($+ -$): $m_1 > 0, m_2 < 0$ and $|m_2| \leq m_1$

Case 3 ($- +$): $m_2 > 0, m_1 < 0$ and $|m_1| \leq m_2$

Case 4 ($--$): No combinations

Since Q is symmetric about interchange of l_1, m_1 and l_2, m_2 , the second and third cases are usually the same but not always. The quadratic term of the EOM for c_{lm} can be split into the three possible cases as:

$$\begin{aligned}
& \sum_{l_1 m_1} \sum_{l_2 m_2} Q_{lm;l_1 m_1; l_2 m_2} (c_{l_1 m_1} c_{l_2 m_2} + \overline{q'_{l_1 m_1} q'_{l_2 m_2}}) \\
&= \sum_{l_1 l_2 m_1 m_2 \geq 0}^{m_1+m_2 < M} Q_{lm;l_1 m_1; l_2 m_2} (c_{l_1 m_1} c_{l_2 m_2} + \overline{q'_{l_1 m_1} q'_{l_2 m_2}}) \\
&+ \sum_{l_1 l_2 \geq 0, m_1 m_2 > 0}^{m_2 \leq m_1} Q_{lm;l_1 m_1; l_2 - m_2} (c_{l_1 m_1} c_{l_2 m_2}^* + \overline{q'_{l_1 m_1} q_{l_2 m_2}^*}) \\
&+ \sum_{l_1 l_2 \geq 0, m_1 m_2 > 0}^{m_1 \leq m_2} Q_{lm;l_2 m_2; l_1 - m_1} (c_{l_2 m_2} c_{l_1 m_1}^* + \overline{q'_{l_2 m_2} q_{l_1 m_1}^*}) \quad (B.2.14)
\end{aligned}$$

These terms can be combined to yield the following EOM for c_{lm} :

$$\begin{aligned}
\frac{dc_{lm}}{dt} &= \sum_{l_1 m_1} L_{lm;l_1 m_1} c_{l_1 m_1} + \sum_{l_1 l_2 m_1 m_2 \geq 0}^{m_1+m_2 < M} Q_{lm;l_1 m_1; l_2 m_2}^{(+)} (c_{l_1 m_1} c_{l_2 m_2} + c_{l_1 m_1; l_2 m_2}^{(S)}) \\
&+ \sum_{l_1 l_2 \geq 0, m_1 m_2 > 0}^{m_2 \leq m_1} 2Q_{lm;l_1 m_1; l_2 m_2}^{(-)} (c_{l_1 m_1} c_{l_2 m_2}^* + c_{l_1 m_1; l_2 m_2}^{(H)}). \quad (B.2.15)
\end{aligned}$$

Similarly the quadratic term in the EOM for $c_{lm;l'm'}^{(S)}$ has three possible cases:

$$\begin{aligned}
\sum_{l_1 m_1} \sum_{l_2 m_2} Q_{lm;l_1 m_1; l_2 m_2} c_{l_1 m_1} \overline{q'_{l_2 m_2} q'_{l' m'}} &= \sum_{l_1 l_2 m_1 m_2 \geq 0}^{m_1+m_2 < M} Q_{lm;l_1 m_1; l_2 m_2} c_{l_1 m_1} \overline{q'_{l_2 m_2} q'_{l' m'}} \\
&+ \sum_{l_1 l_2 \geq 0, m_1 m_2 > 0}^{m_2 \leq m_1} Q_{lm;l_1 m_1; l_2 - m_2} c_{l_1 m_1} \overline{q'_{l_2 m_2} q_{l' m'}^*} \\
&+ \sum_{l_1 l_2 \geq 0, m_1 m_2 > 0}^{m_1 \leq m_2} Q_{lm;l_2 m_2; l_1 - m_1} c_{l_2 m_2}^* \overline{q'_{l_2 m_2} q_{l' m'}^*}.
\end{aligned}$$

These can be combined to yield the EOM for $c_{lm;l'm'}^{(S)}$:

$$\begin{aligned}
\frac{dc_{lm;l'm'}^{(S)}}{dt} = & 2 \sum_{l_1 m_1} L_{lm;l_1 m_1} c_{l_1 m_1;l'm'}^{(S)} + 4 \sum_{l_1, l_2, m_1, m_2 \geq 0}^{m=m_1+m_2} Q_{lm;l_1 m_1; l_2 m_2}^{(+)} c_{l_1 m_1} c_{l_2 m_2;l'm'}^{(S)} \\
& + 4 \sum_{l_1 l_2 \geq 0, m_1 m_2 > 0}^{m_1 \leq m_2} Q_{lm;l_1 m_1; l_2 m_2}^{(-)} \left(c_{l_1 m_1} c_{l_2 m_2;l'm'}^{(H)*} + c_{l_2 m_2}^* c_{l_1 m_1;l'm'}^{(S)} \right).
\end{aligned}$$

Now consider the three possible cases for the quadratic term in the EOM for $c_{lm;l'm'}^{(H)}$:

$$\begin{aligned}
\sum_{l_1 m_1} \sum_{l_2 m_2} Q_{lm;l_1 m_1; l_2 m_2} c_{l_1 m_1} \overline{q'_{l_2 m_2} q'_{l'-m'}} = & \sum_{l_1 l_2 m_1 m_2 \geq 0}^{m_1+m_2 < M} Q_{lm;l_1 m_1; l_2 m_2} c_{l_1 m_1} \overline{q'_{l_2 m_2} q'^*_{l'm'}} \\
& + \sum_{l_1 l_2 \geq 0, m_1 m_2 > 0}^{m_2 \leq m_1} Q_{lm;l_1 m_1; l_2 -m_2} c_{l_1 m_1} \overline{q'^*_{l_2 m_2} q'^*_{l'm'}} \\
& + \sum_{l_1 l_2 \geq 0, m_1 m_2 > 0}^{m_1 \leq m_2} Q_{lm;l_2 m_2; l_1 -m_1} c_{l_1 m_1}^* \overline{q'_{l_2 m_2} q'^*_{l'm'}}.
\end{aligned}$$

These can similarly be combined to yield the EOM for $c_{lm;l'm'}^{(H)}$:

$$\begin{aligned}
\frac{dc_{lm;l'm'}^{(H)}}{dt} = & 2 \sum_{l_1 m_1} L_{lm;l_1 m_1} c_{l_1 m_1;l'm'}^{(H)} + 4 \sum_{l_1, l_2, m_1, m_2 \geq 0}^{m=m_1+m_2} Q_{lm;l_1 m_1; l_2 m_2}^{(+)} c_{l_1 m_1} c_{l_2 m_2;l'm'}^{(H)} \\
& + 4 \sum_{l_1 l_2 \geq 0, m_1 m_2 > 0}^{m_2 \leq m_1} Q_{lm;l_1 m_1; l_2 m_2}^{(-)} \left(c_{l_1 m_1} c_{l_2 m_2;l'm'}^{(S)*} + c_{l_2 m_2}^* c_{l_1 m_1;l'm'}^{(H)} \right).
\end{aligned}$$

Note that the EOMs for $c_{lm;l'm'}^{(H,S)}$ can be written in a combined form as:

$$\begin{aligned}
\frac{dc_{lm;l'm'}^{(S,H)}}{dt} = & 2 \sum_{l_1 m_1} L_{lm;l_1 m_1} c_{l_1 m_1;l'm'}^{(S,H)} + 4 \sum_{l_1, l_2, m_1, m_2 \geq 0}^{m=m_1+m_2} Q_{lm;l_1 m_1; l_2 m_2}^{(+)} c_{l_1 m_1} c_{l_2 m_2;l'm'}^{(S,H)} \\
& + 4 \sum_{l_1 l_2 \geq 0, m_1 m_2 > 0}^{m_1 \leq m_2} Q_{lm;l_1 m_1; l_2 m_2}^{(-)} \left(c_{l_1 m_1} c_{l_2 m_2;l'm'}^{(H,S)*} + c_{l_2 m_2}^* c_{l_1 m_1;l'm'}^{(S,H)} \right).
\end{aligned}$$

In the presence of stochastic forcing drawn from a Gaussian distribution which is δ -correlated in time (white noise) as follows:

$$\langle \eta_{lm}(t) \eta'_{l'm'}(t) \rangle = 2\Gamma \delta(t - t') \delta_{l,l'} \delta_{m,m'}, \quad (\text{B.2.16})$$

the EOM for $c_{lm;l'm'}^{(H)}$ is appended with:

$$\frac{d}{dt} c_{lm;l'm'}^{(H)} = \dots + 2\Gamma. \quad (\text{B.2.17})$$

Note that the EOM for $c_{lm;l'm'}^{(S)}$ remains unchanged by the addition of white noise because $\eta'_{lm} \eta'_{l'm'}$ contains a complex phase and therefore vanishes under an ensemble average.

B.3 From Ensemble CE2 to Zonal CE2

It has been shown that the EOMs for the first and second cumulants of ensemble CE2 are given by:

$$\frac{dc_i}{dt} = A_i + L_{im} c_m + Q_{imn}^{(+)} c_m c_n + Q_{imn}^{(-)} c_m c_n^* + Q_{imn}^{(+)} c_{mn}^{(S)} + Q_{imn}^{(-)} c_{mn}^{(H)} \quad (\text{B.3.1})$$

$$\frac{dc_{ij}^{(S,H)}}{dt} = 2 \left\{ L_{im} c_{mj}^{(S,H)} + 2Q_{imn}^{(+)} c_m c_{nj}^{(S,H)} + Q_{imn}^{(-)} \left(c_m c_{nj}^{(H,S)*} + c_n^* c_{mj}^{(S,H)} \right) \right\}_{S,H} \quad (\text{B.3.2})$$

Note that $Q_{ijk}^{(+)} = Q_{ikj}^{(+)}$ whereas $Q_{ijk}^{(-)} \neq Q_{ikj}^{(-)*}$ because $Q_{ijk}^{(\pm)}$ assume that the

field/cumulant produced by the eddy-eddy interaction of two fields/cumulants has an m -mode greater than zero.

Two further simplifications can be made under the assumption that c_i and c_{ij} have been zonally averaged.

Simplification 1: $\sum_m Q_{imn}^{(-)} \langle c_m \rangle = 0, \forall_{i,n}$ and $\sum_n Q_{imn}^{(-)} \langle c_n \rangle = 0, \forall_{i,m}$ because $Q_{imn}^{(-)}$ is only nonzero for when the m -modes of the fields/cumulants that it connects are greater than zero. If either the modes are zero, then it represents an *eddy* $\pm$ *mean* $\rightarrow$ *eddy* interaction which is already captured by $Q_{imn}^{(+)}$.

Simplification 2: $\sum_m Q_{imn}^{(+)} \langle c_m^{(S)} \rangle = 0, \forall_{i,n}$ because $\langle c_{mj}^{(S)} \rangle = \langle \overline{q_m q_j} \rangle - \langle c_m c_j \rangle = \overline{\langle q_m \rangle \langle q_j \rangle} - \langle c_m \rangle \langle c_j \rangle$ since q_i (and thus c_i) are constrained to have non-negative m -modes. Thus $\sum_m Q_{imn}^{(+)} c_{mj}^{(S)} = \overline{\sum_m Q_{imn}^{(+)} \langle q_m \rangle \langle q_j \rangle} - \sum_m Q_{imn}^{(+)} \langle c_m \rangle \langle c_j \rangle = 0, \forall_{i,n}$ since $Q_{l_1 l_2 m_1 m_2}^{(\pm)} = 0$ and thus *mean* $\pm$ *mean* $\rightarrow$ *mean* interactions are zero.

Therefore the EOMs for the cumulants reduce down to:

$$\frac{dc_i}{dt} = A_i + L_{im} c_m + Q_{imn}^{(-)} c_{mn}^{(H)} \quad (\text{B.3.3})$$

$$\frac{dc_{ij}^{(S)}}{dt} = 2 \left\{ L_{im} c_{mj}^{(S)} \right\}_S \quad (\text{B.3.4})$$

$$\frac{dc_{ij}^{(H)}}{dt} = 2 \left\{ \left(L_{im} + 2Q_{imn}^{(+)} c_n \right) c_{mj}^{(H)} \right\}_H. \quad (\text{B.3.5})$$

Note that the EOM for $c_{ij}^{(S)}$ is now decoupled and so can be ignored. Furthermore, the cumulants maintain their zonal symmetry under time evolution. These EOMs are equivalent to the EOMS for zCE2 and therefore eCE2 reduces to zCE2 under a zonal initialization of the cumulants.

Appendix C

Basis Conversions

C.1 Basis Transformation

Let $q_{ml} \equiv \langle Y_l^m | q \rangle$ and $q_i \equiv \langle i | q \rangle$ where $|Y_l^m\rangle$ forms the basis of spherical harmonics and $|i\rangle$ is the basis formed by the eigenvectors of the second moment.

A basis transformation connects the EOM of q_i with q_{lm} as follows:

$$\dot{q}_i = \langle i | \dot{q} \rangle \quad (\text{C.1.1})$$

$$= \sum_{lm} \langle i | Y_l^m \rangle \langle Y_l^m | \dot{q} \rangle \quad (\text{C.1.2})$$

$$= \sum_{lm} U_{i \rightarrow ml}^* \dot{q}_{lm}, \quad (\text{C.1.3})$$

where $U_{i \rightarrow ml} \equiv \langle Y_l^m | i \rangle$ and $U_{i \rightarrow ml}^* \equiv \langle i | Y_l^m \rangle$ are the basis rotation matrix elements.

In the case of a non-stochastic barotropic jet, the EOM of q_{lm} is given by:

$$\begin{aligned}
\dot{q}_{lm} = & A_l \delta_{m,0} + \sum_{l_1} B_{l;l_1 m} q_{l_1 m} + \eta_{lm}(t) \\
& + \sum_{l_1, l_2, m_1, m_2}^{m=m_1+m_2} C_{l;l_1 m_1; l_2 m_2}^{(+)} q_{l_1 m_1} q_{l_2 m_2} \\
& + \sum_{l_1, l_2, m_1, m_2}^{m=m_1-m_2} C_{l;l_1 m_1; l_2 m_2}^{(-)} q_{l_1 m_1} q_{l_2 m_2}^*.
\end{aligned} \tag{C.1.4}$$

Thus using the basis transformation, the EOM of q_i is given by:

$$\begin{aligned}
\dot{q}_i = & \sum_{lm} U_{i \rightarrow ml}^* \dot{q}_{lm} \\
= & \sum_{lm} U_{i \rightarrow ml}^* A_l \delta_{m,0} \\
& + \sum_{lm} \sum_{l_1} U_{i \rightarrow ml}^* B_{l;l_1 m} \langle Y_{l_1}^m | q \rangle \\
& + \sum_{lm} U_{i \rightarrow ml}^* \eta_{lm}(t) \\
& + \sum_{lm} \sum_{l_1, l_2, m_1, m_2}^{m=m_1+m_2} U_{i \rightarrow ml}^* C_{l;l_1 m_1; l_2 m_2}^{(+)} \langle Y_{l_1}^{m_1} | q \rangle \langle Y_{l_2}^{m_2} | q \rangle \\
& + \sum_{lm} \sum_{l_1, l_2, m_1, m_2}^{m=m_1-m_2} U_{i \rightarrow ml}^* C_{l;l_1 m_1; l_2 m_2}^{(-)} \langle Y_{l_1}^{m_1} | q \rangle \langle q | Y_{l_2}^{m_2} \rangle.
\end{aligned} \tag{C.1.5}$$

Now inserting complete states where appropriate, the EOM is given by:

$$\begin{aligned}
\dot{q}_i &= \sum_{lm} U_{i \rightarrow ml}^* A_l \delta_{m,0} \\
&+ \sum_n \sum_{lm} \sum_{l_1} U_{i \rightarrow ml}^* B_{l;l_1 m} U_{n \rightarrow ml_1} q_n \\
&+ \sum_{lm} U_{i \rightarrow ml}^* \eta_{lm}(t) \\
&+ \sum_p \sum_n \sum_{lm} \sum_{l_1, l_2, m_1, m_2}^{m=m_1+m_2} U_{i \rightarrow ml}^* C_{l;l_1 m_1; l_2 m_2}^{(+)} U_{n \rightarrow m_1 l_1} U_{p \rightarrow m_2 l_2} q_n q_p \\
&+ \sum_p \sum_n \sum_{lm} \sum_{l_1, l_2, m_1, m_2}^{m=m_1-m_2} U_{i \rightarrow ml}^* C_{l;l_1 m_1; l_2 m_2}^{(-)} U_{n \rightarrow m_1 l_1} U_{p \rightarrow m_2 l_2}^* q_n q_p^*. \quad (\text{C.1.6})
\end{aligned}$$

And therefore the EOM of q_i in the basis $|i\rangle$ is given by:

$$\dot{q}_i = A_i + \sum_n B_{in} q_n + \eta_i(t) + \sum_p \sum_n \left(C_{inp}^{(+)} q_n q_p + C_{inp}^{(-)} q_n q_p^* \right), \quad (\text{C.1.7})$$

where the coefficients are defined in the new basis as:

$$A_i = \sum_{lm} U_{i \rightarrow ml}^* A_l \delta_{m,0} = \sum_l U_{i \rightarrow m=0,l}^* A_l \quad (\text{C.1.8})$$

$$B_{in} = \sum_{lm} \sum_{l_1} U_{i \rightarrow ml}^* B_{l;l_1 m} U_{n \rightarrow ml_1} \quad (\text{C.1.9})$$

$$\eta_i(t) = \sum_{lm} U_{i \rightarrow ml}^* \eta_{lm}(t) \quad (\text{C.1.10})$$

$$C_{inp}^{(+)} = \sum_{lm} \sum_{l_1, l_2, m_1, m_2}^{m=m_1+m_2} U_{i \rightarrow ml}^* C_{l;l_1 m_1; l_2 m_2}^{(+)} U_{n \rightarrow m_1 l_1} U_{p \rightarrow m_2 l_2} \quad (\text{C.1.11})$$

$$C_{inp}^{(-)} = \sum_{lm} \sum_{l_1, l_2, m_1, m_2}^{m=m_1-m_2} U_{i \rightarrow ml}^* C_{l;l_1 m_1; l_2 m_2}^{(-)} U_{n \rightarrow m_1 l_1} U_{p \rightarrow m_2 l_2}^*. \quad (\text{C.1.12})$$

C.2 Cumulant and Basis Conversions

This section states (and derives) the relations for converting from ensemble averages to zonal averages and/or the basis of spherical harmonics to a generalized basis.

C.2.1 Definitions

Let $\langle \overline{\cdots} \rangle$ denote an ensemble average, $\langle \cdots \rangle$ denote a zonal average. Then define the following:

$$c_i \equiv \overline{q_i} \quad (\text{C.2.1})$$

$$c_{ij}^{(S)} \equiv \overline{q'_i q'_j} \quad (\text{C.2.2})$$

$$c_{ij}^{(H)} \equiv \overline{q'_i q_j^*} \quad (\text{C.2.3})$$

$$c_l \equiv q_{l,m=0} \quad (\text{C.2.4})$$

$$c_{l_1 l_2 m} \equiv q_{l_1 m} q_{l_2 m}^* - q_{l_1 m=0} q_{l_2 m=0} \delta_{m,0} \quad (\text{C.2.5})$$

C.2.2 Properties

Using the property of a zonal average:

$$\begin{aligned} \langle q_{lm} \rangle &= q_{l,m=0} \delta_{m,0} \\ &= c_l \delta_{m,0} \end{aligned} \quad (\text{C.2.6})$$

$$\begin{aligned} \langle q_{l_1 m_1} q_{l_2 m_2}^* \rangle &= q_{l_1 m_1} q_{l_2 m_2}^* \delta_{m_1, m_2} \\ \Rightarrow \langle q_{l_1 m} q_{l_2 m}^* \rangle &= q_{l_1 m} q_{l_2 m}^* \\ &= c_{l_1 l_2 m} + c_{l_1} c_{l_2} \delta_{m,0} \end{aligned} \quad (\text{C.2.7})$$

$$\begin{aligned} \langle q_{l_1 m_1} q_{l_2 m_2} \rangle &= q_{l_1 m_1=0} q_{l_2 m_2=0} \delta_{m_1,0} \delta_{m_2,0} \\ &= c_{l_1} c_{l_2} \delta_{m_1,0} \delta_{m_2,0} \end{aligned} \quad (\text{C.2.8})$$

$$\Rightarrow \langle q_{l_1 m} q_{l_2 m} \rangle = c_{l_1} c_{l_2} \delta_{m,0} \quad (\text{C.2.9})$$

C.2.3 Ensemble cumulants

$\Rightarrow$ Ensemble-averaged zonal cumulants

$$\begin{aligned}
 q_{lm} &\equiv \langle Y_l^m | q \rangle \\
 &= \sum_i \langle Y_l^m | i \rangle \langle i | q \rangle \\
 &= \sum_i \langle Y_l^m | i \rangle q_i
 \end{aligned} \tag{C.2.10}$$

$$\Rightarrow \langle \overline{q_{lm}} \rangle = \sum_i \langle Y_l^m | i \rangle \langle \overline{q_i} \rangle \tag{C.2.11}$$

$$\Rightarrow \overline{c_l} \delta_{m,0} = \sum_i \langle Y_l^m | i \rangle \langle c_i \rangle \tag{C.2.12}$$

$$m = 0 : \overline{c_l} = \sum_i \langle Y_l^{m=0} | i \rangle \langle c_i \rangle \tag{C.2.13}$$

And:

$$\begin{aligned}
 q_{l_1 m} q_{l_2 m}^* &\equiv \langle Y_{l_1}^m | q \rangle \langle q | Y_{l_2}^m \rangle \\
 &= \sum_i \sum_j \langle Y_{l_1}^m | i \rangle \langle i | q \rangle \langle q | j \rangle \langle j | Y_{l_2}^m \rangle \\
 &= \sum_i \sum_j \langle Y_{l_1}^m | i \rangle \langle j | Y_{l_2}^m \rangle q_i q_j^*
 \end{aligned} \tag{C.2.14}$$

$$\begin{aligned}
 q_{l_1 m} q_{l_2 m} &\equiv \langle Y_{l_1}^m | q \rangle \langle Y_{l_2}^m | q \rangle \\
 &= \sum_i \sum_j \langle Y_{l_1}^m | i \rangle \langle i | q \rangle \langle Y_{l_2}^m | j \rangle \langle j | q \rangle \\
 &= \sum_i \sum_j \langle Y_{l_1}^m | i \rangle \langle Y_{l_2}^m | j \rangle q_i q_j
 \end{aligned} \tag{C.2.15}$$

So from (10) & (13):

$$\begin{aligned}
c_{l_1 l_2 m} &= \langle q_{l_1 m} q_{l_2 m}^* \rangle - \langle q_{l_1 m} q_{l_2 m} \rangle \\
c_{l_1 l_2 m} &= \sum_i \langle Y_{l_1}^m | i \rangle \left[\sum_j \langle j | Y_{l_2}^m \rangle \langle q_i q_j^* \rangle - \langle Y_{l_2}^m | j \rangle \langle q_i q_j \rangle \right] \\
\Rightarrow \overline{c_{l_1 l_2 m}} &= \sum_i \langle Y_{l_1}^m | i \rangle \left[\sum_j \langle j | Y_{l_2}^m \rangle \langle \overline{q_i q_j^*} \rangle - \langle Y_{l_2}^m | j \rangle \langle \overline{q_i q_j} \rangle \right] \\
&= \sum_i \langle Y_{l_1}^m | i \rangle \left[\sum_j \langle j | Y_{l_2}^m \rangle \langle c_{ij}^{(H)} + c_i c_j^* \rangle \right] \\
&\quad - \sum_i \langle Y_{l_1}^m | i \rangle \left[\langle Y_{l_2}^m | j \rangle \langle c_{ij}^{(S)} + c_i c_j \rangle \right] \\
&= \sum_i \langle Y_{l_1}^m | i \rangle (c_i \alpha_i + \beta_j) \tag{C.2.16}
\end{aligned}$$

where:

$$\begin{aligned}
\alpha_i &= \sum_j (\langle j | Y_{l_2}^m \rangle \langle c_j^* \rangle - \langle Y_{l_2}^m | j \rangle \langle c_j \rangle) \\
\beta_i &= \sum_j (\langle j | Y_{l_2}^m \rangle \langle c_{ij}^{(H)} \rangle - \langle Y_{l_2}^m | j \rangle \langle c_{ij}^{(S)} \rangle)
\end{aligned}$$

But in the case of non-zonally averaged cumulants, we need a different representation to express $\overline{c_{l_1 l_2 m}}$. In this case recognize that:

$$\begin{aligned}
c_{l_1 l_2 m} &= \langle q_{l_1 m} q_{l_2 m}^* \rangle - \langle q_{l_1 m} q_{l_2 m} \rangle \\
&= q_{l_1 m} q_{l_2 m}^*, \quad m \geq 1 \tag{C.2.17}
\end{aligned}$$

$$\begin{aligned}
\Rightarrow \overline{c_{l_1 l_2 m}} &= \overline{q_{l_1 m} q_{l_2 m}^*}, \quad m \geq 1 \\
&= \sum_i \sum_j \langle Y_{l_1}^m | i \rangle \langle j | Y_{l_2}^m \rangle \overline{q_i q_j^*}, \quad m \geq 1 \\
&= \sum_i \sum_j \langle Y_{l_1}^m | i \rangle \langle j | Y_{l_2}^m \rangle (c_i c_j^* + c_{ij}^{(H)}), \quad m \geq 1 \tag{C.2.18}
\end{aligned}$$

C.2.4 Ensemble-averaged zonal cumulants

$\Rightarrow$ Zonally-averaged ensemble cumulants

$$\begin{aligned}
q_i &\equiv \langle i|q \rangle \\
&= \sum_{lm} \langle i|Y_l^m \rangle \langle Y_l^m|q \rangle \\
&= \sum_{lm} \langle i|Y_l^m \rangle q_{lm} \\
\Rightarrow \langle \overline{q_i} \rangle &= \sum_{lm} \langle i|Y_l^m \rangle \langle \overline{q_{lm}} \rangle \\
\Rightarrow \langle c_i \rangle &= \sum_{lm} \langle i|Y_l^m \rangle \overline{c_l} \delta_{m,0} \\
&= \sum_l \langle i|Y_l^{m=0} \rangle \overline{c_l}
\end{aligned} \tag{C.2.19}$$

And:

$$\begin{aligned}
q_i q_j^* &\equiv \langle i|q \rangle \langle q|j \rangle \\
&= \sum_{l_1 m_1} \sum_{l_2 m_2} \langle i|Y_{l_1}^{m_1} \rangle \langle Y_{l_1}^{m_1}|q \rangle \langle q|Y_{l_2}^{m_2} \rangle \langle Y_{l_2}^{m_2}|j \rangle \\
&= \sum_{l_1 m_1} \sum_{l_2 m_2} \langle i|Y_{l_1}^{m_1} \rangle \langle Y_{l_2}^{m_2}|j \rangle q_{l_1 m_1} q_{l_2 m_2}^* \\
\Rightarrow \langle \overline{q_i q_j^*} \rangle &= \sum_{l_1 m_1} \sum_{l_2 m_2} \langle i|Y_{l_1}^{m_1} \rangle \langle Y_{l_2}^{m_2}|j \rangle \langle \overline{q_{l_1 m_1} q_{l_2 m_2}^*} \rangle \\
\Rightarrow \langle c_{ij}^{(H)} \rangle &= \sum_{l_1 m_1} \sum_{l_2 m_2} \langle i|Y_{l_1}^{m_1} \rangle \langle Y_{l_2}^{m_2}|j \rangle \overline{q_{l_1 m_1} q_{l_2 m_2}^*} \delta_{m_1, m_2} \\
&= \sum_{l_1 l_2 m} \langle i|Y_{l_1}^m \rangle \langle Y_{l_2}^m|j \rangle \overline{c_{l_1 l_2 m} + c_{l_1} c_{l_2} \delta_{m,0}}
\end{aligned} \tag{C.2.20}$$

And:

$$\begin{aligned}
q_i q_j &\equiv \langle i|q \rangle \langle j|q \rangle \\
&= \sum_{l_1 m_1} \sum_{l_2 m_2} \langle i|Y_{l_1}^{m_1} \rangle \langle Y_{l_1}^{m_1}|q \rangle \langle j|Y_{l_2}^{m_2} \rangle \langle Y_{l_2}^{m_2}|q \rangle \\
&= \sum_{l_1 m_1} \sum_{l_2 m_2} \langle i|Y_{l_1}^{m_1} \rangle \langle j|Y_{l_2}^{m_2} \rangle q_{l_1 m_1} q_{l_2 m_2} \\
\Rightarrow \langle \overline{q_i q_j} \rangle &= \sum_{l_1 m_1} \sum_{l_2 m_2} \langle i|Y_{l_1}^{m_1} \rangle \langle j|Y_{l_2}^{m_2} \rangle \langle \overline{q_{l_1 m_1} q_{l_2 m_2}} \rangle \\
\Rightarrow \langle c_{ij}^{(S)} \rangle &= \sum_{l_1 m_1} \sum_{l_2 m_2} \langle i|Y_{l_1}^{m_1} \rangle \langle j|Y_{l_2}^{m_2} \rangle \overline{c_{l_1} c_{l_2}} \delta_{m_1,0} \delta_{m_2,0} \\
&= \sum_{l_1 l_2} \langle i|Y_{l_1}^{m=0} \rangle \langle j|Y_{l_2}^{m=0} \rangle \overline{c_{l_1} c_{l_2}} \tag{C.2.21}
\end{aligned}$$

C.3 Symmetries of the quadratic coefficients

It has already been shown that the EOM of the vorticity q_i in the basis $|i\rangle$ is given by:

$$\dot{q}_i = A_i + \sum_n B_{in} q_n + \sum_p \sum_n \left(C_{inp}^{(+)} q_n q_p + C_{inp}^{(-)} q_n q_p^* \right), \tag{C.3.1}$$

where the coefficients are defined in the new basis as:

$$A_i = \sum_{lm} U_{i \rightarrow ml}^* A_l \delta_{m,0} = \sum_l U_{i \rightarrow m=0,l}^* A_l \tag{C.3.2}$$

$$B_{in} = \sum_{lm} \sum_{l_1} U_{i \rightarrow ml}^* B_{l;l_1 m} U_{n \rightarrow m l_1} \tag{C.3.3}$$

$$C_{inp}^{(+)} = \sum_{lm} \sum_{l_1, l_2, m_1, m_2}^{m=m_1+m_2} U_{i \rightarrow ml}^* C_{l;l_1 m_1; l_2 m_2}^{(+)} U_{n \rightarrow m_1 l_1} U_{p \rightarrow m_2 l_2} \tag{C.3.4}$$

$$C_{inp}^{(-)} = \sum_{lm} \sum_{l_1, l_2, m_1, m_2}^{m=m_1-m_2} U_{i \rightarrow ml}^* C_{l;l_1 m_1; l_2 m_2}^{(-)} U_{n \rightarrow m_1 l_1} U_{p \rightarrow m_2 l_2}^*. \tag{C.3.5}$$

The symmetry of $C_{inp}^{(+)}$, in particular that $C_{ipn}^{(+)} = C_{inp}^{(+)}$, can be easily shown by interchanging $n \rightleftharpoons p$ above and then redefining the dummy indices.

Now let's consider the symmetry of $C_{inp}^{(-)}$, in particular whether $C_{ipn}^{(-)*} = C_{inp}^{(-)}$.

Using Eq. C.3.5:

$$\begin{aligned}
C_{ipn}^{(-)*} &= \sum_{lm} \sum_{l_1, l_2, m_1, m_2}^{m=m_1-m_2} U_{i \rightarrow ml} C_{l; l_1 m_1; l_2 m_2}^{(-)*} U_{p \rightarrow m_1 l_1}^* U_{n \rightarrow m_2 l_2} \\
&= \sum_{lm} \sum_{l_1, l_2, m_1, m_2}^{m=m_1-m_2} U_{i \rightarrow -ml} C_{l; l_2 m_2; l_1 m_1}^{(-)*} U_{p \rightarrow m_2 l_2}^* U_{n \rightarrow m_1 l_1}, \quad (C.3.6)
\end{aligned}$$

where $\{m_1, l_1\}$ and $\{m_2, l_2\}$ have been interchanged since they are dummy variables.

However in doing so, m becomes $-m$ since $m = m_1 - m_2$.

Since $C_{l; l_2 m_2; l_1 m_1}^{(-)*} = C_{l; l_1 m_1; l_2 m_2}^{(-)}$, Eq. C.3.5 and Eq. C.3.6 can be compared to reveal that $C_{ipn}^{(-)*} = C_{inp}^{(-)}$ if and only if $U_{i \rightarrow m, l}^* = U_{i \rightarrow -m, l}$. To prove this, use the symmetry of the spherical harmonics, $Y_l^{-m}(\theta, \phi) = Y_l^m(\theta, \phi)^*$ and therefore $\langle \theta, \phi | Y_l^{-m} \rangle = \langle Y_l^m | \theta, \phi \rangle$. Thus using the definition of the basis rotation matrix elements:

$$\begin{aligned}
U_{i \rightarrow -m, l} &\equiv \langle Y_l^{-m} | i \rangle \\
&= \sum_{\theta, \phi} \langle Y_l^{-m} | \theta, \phi \rangle \langle \theta, \phi | i \rangle \\
&= \sum_{\theta, \phi} \langle \theta, \phi | Y_l^m \rangle \langle \theta, \phi | i \rangle \quad (C.3.7)
\end{aligned}$$

$$\begin{aligned}
U_{i \rightarrow ml}^* &\equiv \langle i | Y_l^m \rangle \\
&= \sum_{\theta, \phi} \langle i | \theta, \phi \rangle \langle \theta, \phi | Y_l^m \rangle. \quad (C.3.8)
\end{aligned}$$

So $U_{i \rightarrow m, l}^* = U_{i \rightarrow -m, l}$ if and only if $\langle \theta, \phi | i \rangle$ is real.

Therefore $C_{ipn}^{(+)} = C_{inp}^{(+)}$ and $C_{ipn}^{(-)*} = C_{inp}^{(-)}$ if and only if $\langle \theta, \phi | i \rangle$ is real.

Appendix D

Conserved Quantities in Ensemble CE2

D.1 Lemmas

D.1.1 Vanishing area integrals of a Jacobian

The Jacobian is defined such that $J[A, B] = \hat{n} \cdot (\nabla A \times \nabla B)$. Thus $J[a, bc] = bJ[a, c] + cJ[a, b]$ since $\nabla(AB) = A\nabla B + B\nabla A$.

The convective term of any material derivative can be written as a Jacobian as follows:

$$\begin{aligned}\vec{u} \cdot \nabla A &= (\hat{n} \times \nabla \psi) \cdot \nabla A \\ &= \hat{n} \cdot (\nabla \psi \times \nabla A) \\ &= J[\psi, A]\end{aligned}\tag{D.1.1}$$

Thus the material derivative of an arbitrary scalar A can be expressed as a sum of its explicit time derivative and a Jacobian term, $\frac{D}{Dt}A = \frac{\partial}{\partial t}A - J[A, \psi]$.

The convective term of the material derivative can be expressed as $\vec{u} \cdot \nabla A = \nabla \cdot$

$(A\vec{u}) - A\nabla \cdot \vec{u}$. But $\nabla \cdot \vec{u} = 0$ for incompressible flow and $\int_A \nabla \cdot (A\vec{u}) d^2r = \oint_C A\vec{u} \cdot d\vec{l} = 0$ on a boundaryless surface by the divergence theorem. Therefore the area integral of the convective term of the material derivative vanishes for incompressible flow on a boundaryless surface.

Consequently this also means that the area integral of $J[A, \psi]$ vanishes as well. For the case of an ensemble average, if $\nabla \cdot \vec{u} = 0$ then $\nabla \cdot \overline{\vec{u}} = 0$ too and so the area integrals of $J[A, \overline{\psi}]$ and $J[A, \psi']$ must also vanish.

Similarly, it can be shown that the area integral of $J[A, \psi^n]$ also vanishes because:

$$\begin{aligned} J[\psi^n, A] &= n\psi^{n-1}J[\psi, A] \\ &= n\psi^{n-1}\vec{u} \cdot \nabla A \\ &= \nabla \cdot (n\psi^{n-1}\vec{u}A) - A\vec{u} \cdot \nabla (n\psi^{n-1}) - An\psi^{n-1}\nabla \cdot \vec{u} \end{aligned}$$

The first term vanishes under an area integral over a boundaryless surface by Stokes theorem. The third term vanishes for incompressible flow. As for the second term, it can be re-expressed as $-AnJ[\psi, \psi^{n-1}]$ and so it too vanishes.

D.1.2 Surface integral in spherical coordinates

Let $A = A(\theta, \phi)$ and $B = B(\theta, \phi)$ be scalars. Then in spherical coordinates:

$$\begin{aligned} J[A, B] &= \hat{n} \cdot (\nabla A \times \nabla B) \\ &= \frac{1}{r^2 \sin \theta} \left(\frac{\partial A}{\partial \theta} \frac{\partial B}{\partial \phi} - \frac{\partial A}{\partial \phi} \frac{\partial B}{\partial \theta} \right). \end{aligned} \tag{D.1.2}$$

Now define S as the following surface area integral:

$$\begin{aligned} S &= \int \int \cos(\theta) * J[A, B] d^2r \\ &= \int \int \cos(\theta) \left(\frac{\partial A}{\partial \theta} \frac{\partial B}{\partial \phi} - \frac{\partial A}{\partial \phi} \frac{\partial B}{\partial \theta} \right) d\theta d\phi. \end{aligned} \tag{D.1.3}$$

Now let $B = \nabla^2 A$. In spherical coordinates, the laplacian is given by:

$$B = \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial A}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 A}{\partial \phi^2}. \quad (\text{D.1.4})$$

Thus the integrand I of integral S is:

$$\begin{aligned} Ir^2 = & \frac{\cos \theta}{\sin^2 \theta} \frac{\partial^3 A}{\partial \phi^3} \frac{\partial A}{\partial \theta} + \frac{\cos^2 \theta}{\sin \theta} \frac{\partial^2 A}{\partial \theta \partial \phi} \frac{\partial A}{\partial \theta} + \cos \theta \frac{\partial^3 A}{\partial \theta^2 \partial \phi} \frac{\partial A}{\partial \theta} \\ & + 2 \frac{\cos^2 \theta}{\sin^3 \theta} \frac{\partial^2 A}{\partial \phi^2} \frac{\partial A}{\partial \phi} + \frac{\cos \theta}{\sin^2 \theta} \frac{\partial A}{\partial \theta} \frac{\partial A}{\partial \phi} - \frac{\cos \theta}{\sin^2 \theta} \frac{\partial^3 A}{\partial \theta \partial \phi^2} \frac{\partial A}{\partial \phi} \\ & - \frac{\cos^2 \theta}{\sin \theta} \frac{\partial^2 A}{\partial \theta^2} \frac{\partial A}{\partial \phi} - \cos \theta \frac{\partial^3 A}{\partial \theta^3} \frac{\partial A}{\partial \phi}. \end{aligned} \quad (\text{D.1.5})$$

Integration by parts on the first term can cancel out two terms:

$$\int \frac{\cos \theta}{\sin^2 \theta} \frac{\partial^3 A}{\partial \phi^3} \frac{\partial A}{\partial \theta} d\phi = \int -\frac{\cos \theta}{\sin^2 \theta} \frac{\partial^3 A}{\partial \theta \partial \phi^2} \frac{\partial A}{\partial \phi} d\phi. \quad (\text{D.1.6})$$

Note that here we have made use of the periodic boundary conditions on the surface of a sphere. Hence, for example, $\left[\frac{\cos \theta}{\sin^2 \theta} \frac{\partial^2 A}{\partial \phi^2} \frac{\partial A}{\partial \theta} \right]_{\phi=0}^{\phi=2\pi} = 0$. Similarly, the last term can be rewritten by integration by parts as:

$$\int -\cos \theta \frac{\partial^3 A}{\partial \theta^3} \frac{\partial A}{\partial \phi} d\theta = \int \left(\cos \theta \frac{\partial^2 A}{\partial \theta \partial \phi} \frac{\partial^2 A}{\partial \theta^2} - \sin \theta \frac{\partial^2 A}{\partial \theta^2} \frac{\partial A}{\partial \phi} \right) d\theta. \quad (\text{D.1.7})$$

So now the integrand I simplifies to:

$$\begin{aligned} Ir^2 = & \frac{\cos^2 \theta}{\sin \theta} \frac{\partial^2 A}{\partial \theta \partial \phi} \frac{\partial A}{\partial \theta} + \cos \theta \frac{\partial^3 A}{\partial \theta^2 \partial \phi} \frac{\partial A}{\partial \theta} \\ & + 2 \frac{\cos^2 \theta}{\sin^3 \theta} \frac{\partial^2 A}{\partial \phi^2} \frac{\partial A}{\partial \phi} + \frac{\cos \theta}{\sin^2 \theta} \frac{\partial A}{\partial \theta} \frac{\partial A}{\partial \phi} \\ & - \frac{1}{\sin \theta} \frac{\partial^2 A}{\partial \theta^2} \frac{\partial A}{\partial \phi} + \cos \theta \frac{\partial^2 A}{\partial \theta \partial \phi} \frac{\partial^2 A}{\partial \theta^2}. \end{aligned} \quad (\text{D.1.8})$$

Now the last term can be expressed as:

$$\int \cos \theta \frac{\partial^2 A}{\partial \theta \partial \phi} \frac{\partial^2 A}{\partial \theta^2} d\theta = \int \left(\sin \theta \frac{\partial^2 A}{\partial \theta \partial \phi} \frac{\partial A}{\partial \theta} - \cos \theta \frac{\partial^3 A}{\partial \theta^2 \partial \phi} \frac{\partial A}{\partial \theta} \right) d\theta, \quad (\text{D.1.9})$$

and the second last term can be expressed as:

$$\int -\frac{1}{\sin \theta} \frac{\partial^2 A}{\partial \theta^2} \frac{\partial A}{\partial \phi} d\theta = \int \left(-\frac{\cos \theta}{\sin^2 \theta} \frac{\partial A}{\partial \theta} \frac{\partial A}{\partial \phi} + \frac{1}{\sin \theta} \frac{\partial^2 A}{\partial \theta \partial \phi} \frac{\partial A}{\partial \theta} \right) d\theta. \quad (\text{D.1.10})$$

Thus the integrand further simplifies to:

$$\begin{aligned} Ir^2 &= \frac{2}{\sin \theta} \frac{\partial^2 A}{\partial \theta \partial \phi} \frac{\partial A}{\partial \theta} + 2 \frac{\cos^2 \theta}{\sin^3 \theta} \frac{\partial^2 A}{\partial \phi^2} \frac{\partial A}{\partial \phi} \\ &= \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} \left(\frac{\partial A}{\partial \theta} \right)^2 + \frac{\cos^2 \theta}{\sin^3 \theta} \frac{\partial}{\partial \phi} \left(\frac{\partial A}{\partial \phi} \right)^2. \end{aligned} \quad (\text{D.1.11})$$

Performing an integral, this time over ϕ , gives zero for periodic boundary conditions.

Therefore the surface integral on a sphere of $\int \cos(\theta) * J[A, \nabla^2 A] d^2 r$ vanishes for an arbitrary A such that $A = A(\theta, \phi)$.

D.2 General proof for conserved quantities

Consider the following ensemble average of a Jacobian:

$$\begin{aligned} \overline{\nabla \psi \times \nabla A} &= \overline{\nabla(\bar{\psi} + \psi') \times \nabla(\bar{A} + A')} \\ &= \overline{\nabla \bar{\psi} \times \nabla \bar{A}} + \overline{\nabla \psi' \times \nabla A'}. \end{aligned} \quad (\text{D.2.1})$$

Therefore $\overline{J[\psi, A]} = J[\bar{\psi}, \bar{A}] + \overline{J[\psi', A']}$.

Now define the quantity $\chi = \int A dr^2$. Then $\frac{d}{dt} \chi = \int \frac{D}{Dt} A dr^2$. The material

derivative of $\bar{\chi}$ is then given by:

$$\begin{aligned}
\frac{d}{dt}\bar{\chi} &= \frac{d}{dt} \int \bar{A} d^2r \\
&= \int \frac{D}{Dt} \bar{A} d^2r \\
&= \int \left(\frac{\partial}{\partial t} \bar{A} + J[\psi, \bar{A}] \right) d^2r = \\
&= \int \left(\overline{\frac{\partial}{\partial t} A} + \overline{J[\psi, A]} - \overline{J[\bar{\psi}, \bar{A}]} - \overline{J[\psi', A']} + J[\psi, \bar{A}] \right) d^2r \\
&= \int \left(\overline{\frac{D}{Dt} A} \right) d^2r + \int \left(J[\psi, \bar{A}] - \overline{J[\bar{\psi}, \bar{A}]} - \overline{J[\psi', A']} \right) d^2r \\
&= \overline{\frac{d}{dt} \chi} + \int J[\psi', \bar{A}] d^2r - \overline{J[\psi', A']} d^2r.
\end{aligned} \tag{D.2.2}$$

Therefore the material derivative and ensemble average in general do not commute. But as shown in Appendix D.1.1, the area integral $J[A, \psi']$ vanishes for arbitrary A in the case of incompressible flow on a boundaryless surface, giving $\frac{d}{dt}\bar{\chi} = \overline{\frac{d}{dt}\chi}$ and so the ensemble average of a conserved quantity is also a conserved quantity.

This can also be seen by neglecting the convective portion of the material derivative (because its area integral is zero) and thus $\frac{d}{dt}\bar{\chi} = \int \left(\frac{\partial}{\partial t} \bar{A} + J[\psi, \bar{A}] \right) d^2r = \overline{\int \left(\frac{\partial}{\partial t} A \right) d^2r} = \overline{\frac{d}{dt} \chi}$.

However, this is true assuming no approximation is made and the full hierarchy of cumulants is retained (i.e. an exact theory). In the case of a cumulant expansion closure assumption it is still possible that the quantity in question will not be conserved and therefore it must be checked that the neglected cumulants have no contribution. But this check is simplified since only the explicit time derivative portion of the material derivative can contribute as $\frac{d}{dt}\bar{\chi} = \int \left(\frac{\partial}{\partial t} \bar{A} + J[\psi, \bar{A}] \right) d^2r = \int \left(\frac{\partial}{\partial t} \bar{A} \right) d^2r$. This is done next for the cases of angular momentum, enstrophy and energy.

D.2.1 Angular momentum

In the case of angular momentum, $\overline{L_z} = \int \nu \overline{\xi(\vec{r}_1)} d^2 r_1 = \int \nu c(\vec{r}_1) d^2 r_1$ and therefore:

$$\frac{d}{dt} \overline{L_z} = \int \nu \frac{\partial}{\partial t} c(\vec{r}_1) d^2 r_1. \quad (\text{D.2.3})$$

But since the EOM of $c(\vec{r}_1)$ contains only the first and second cumulant, the CE2 closure has no effect on the $\frac{\partial}{\partial t} c(\vec{r}_1)$ term which appears in the $\frac{d}{dt} \overline{L_z}$ term and therefore the ensemble angular momentum is conserved.

D.2.2 Enstrophy

In the case of enstrophy, $\overline{\Gamma_2} = \int \overline{q(\vec{r}_1)^2} d^2 r_1$ where $\overline{q(\vec{r}_1)^2} = c(\vec{r}_1, \vec{r}_1) + (c(\vec{r}_1) + f(\vec{r}_1))^2$ and therefore:

$$\begin{aligned} \frac{d}{dt} \overline{\Gamma_2} &= \int \frac{\partial}{\partial t} (c(\vec{r}_1, \vec{r}_1) + (c(\vec{r}_1) + f(\vec{r}_1))^2) d^2 r_1 \\ &= \int \frac{\partial}{\partial t} c(\vec{r}_1, \vec{r}_1) + 2(c(\vec{r}_1) + f(\vec{r}_1)) \frac{\partial}{\partial t} (c(\vec{r}_1) + f(\vec{r}_1)) d^2 r_1. \end{aligned} \quad (\text{D.2.4})$$

This time there is the appearance of the EOM of the second cumulant and this contains the third cumulant. Since CE2 neglects this third cumulant, we need to explicitly check that its area integral is zero.

Inspecting the EOMs of the second cumulant (derived above), it can be seen that the third cumulant appears in the form of a Jacobian, $\int J_1 [p(\vec{r}_1, \vec{r}_2, \vec{r}_3), \delta(\vec{r}_1 - \vec{r}_3)] d^2 r_3$ which can be re-expressed as $\int J_1 [\zeta'(\vec{r}_1) \zeta'(\vec{r}_2), \psi'(\vec{r}_1)] d^2 r_3$. But since the area integral $J[A, \psi']$ vanishes for arbitrary A in the case of incompressible flow on a boundaryless surface, the ensemble enstrophy is conservative under CE2.

D.2.3 Energy

The ensemble-averaged energy can be expressed as $\overline{E} = -\frac{1}{2} \int \overline{\xi(\vec{r}_1) \psi(\vec{r}_1)} d^2 r_1 = -\frac{1}{2} \int c(\vec{r}_1) p(\vec{r}_1) + p(\vec{r}_1, \vec{r}_1) d^2 r_1$ and therefore:

$$\frac{d}{dt} \overline{E} = -\frac{1}{2} \int \frac{\partial}{\partial t} (c(\vec{r}_1) p(\vec{r}_1) + p(\vec{r}_1, \vec{r}_1)) d^2 r_1 \quad (\text{D.2.5})$$

So $\frac{d}{dt} \overline{E}$ contains the EOMs of $c(\vec{r}_1)$, $p(\vec{r}_1)$ and $p(\vec{r}_1, \vec{r}_1)$. But $\frac{\partial}{\partial t} c(\vec{r}_1)$ and $\frac{\partial}{\partial t} p(\vec{r}_1)$ contain at most a second order cumulant which is not truncated at CE2 level. On the other hand, $\frac{\partial}{\partial t} p(\vec{r}_1, \vec{r}_1)$ can be rewritten as:

$$\begin{aligned} \frac{\partial}{\partial t} p(\vec{r}_1, \vec{r}_1) &= \frac{\partial}{\partial t} \overline{\xi'(\vec{r}_1) \psi'(\vec{r}_1)} \\ &= \left\{ \overline{\psi'(\vec{r}_1) \frac{\partial}{\partial t} \xi'(\vec{r}_1)} \right\}_{\xi, \psi} \\ &= \left\{ \overline{\psi'(\vec{r}_1) \frac{\partial}{\partial t} \xi(\vec{r}_1)} \right\}_{\xi, \psi} \\ &= \left\{ \overline{\left(\psi(\vec{r}_1) - \overline{\psi(\vec{r}_1)} \right) J[\xi(\vec{r}_1) + f(\vec{r}_1), \psi(\vec{r}_1)]} \right\}_{\xi, \psi} \\ &= \frac{1}{2} \left\{ \overline{J[\xi(\vec{r}_1) + f(\vec{r}_1), \psi^2(\vec{r}_1)]} \right\}_{\xi, \psi} \\ &\quad - \left\{ \overline{\psi(\vec{r}_1) J[\xi(\vec{r}_1) + f(\vec{r}_1), \psi(\vec{r}_1)]} \right\}_{\xi, \psi}. \end{aligned} \quad (\text{D.2.6})$$

The first term, which contains a third-order cumulant, is the ensemble average of a Jacobian and therefore vanishes over an area integral, as proven in Appendix D.1.1. The second term contains nothing higher than a second cumulant. Thus the ensemble-averaged energy is conserved.

D.3 An explicit proof for conserved quantities

An alternative way of proving the conservation laws is by explicitly evaluating the integrals for angular momentum, enstrophy and energy. This is what follows.

D.3.1 Angular Momentum

DNS

Now consider the angular momentum $L_z = \int \nu \xi d^2r$. Its time derivative is:

$$\begin{aligned} \frac{d}{dt} L_z &= \int \nu \frac{\partial}{\partial t} \xi d^2r \\ &= \int (\nu J[\xi + f, \psi]) d^2r \\ &= \int \left(\nu J[\xi, \psi] + \frac{1}{2\beta} J[f^2, \psi] \right) d^2r. \end{aligned} \quad (\text{D.3.1})$$

The area integral of the second term obviously vanishes. The first term can be expressed in spherical coordinates as $\int \cos(\theta) * J[\psi, \nabla^2 \psi] d^2r$. But this term vanishes on the surface of a sphere, by the proof given in Appendix D.1.1. Thus angular momentum is conserved on a sphere.

Ensemble CE2

Consider the ensemble average of the angular momentum $\overline{L_z} = \int c(\vec{r}_1) \nu d^2r$. Its time derivative is given by $\frac{d}{dt} \overline{L_z} = \int \nu \frac{\partial}{\partial t} c(\vec{r}_1) d^2r$ where:

$$\begin{aligned} \nu \frac{\partial}{\partial t} c(\vec{r}_1) &= \nu \int J_1[p(\vec{r}_1, \vec{r}_2), \delta(\vec{r}_1 - \vec{r}_2)] d^2r_2 \\ &\quad + \nu J_1[c(\vec{r}_1) + f(\vec{r}_1), p(\vec{r}_1)] \\ &= \overline{\nu J_1[\xi'(\vec{r}_1), \psi'(\vec{r}_1)]} \\ &\quad + \nu J_1[c(\vec{r}_1), p(\vec{r}_1)] + \frac{1}{2\beta} J_1[f(\vec{r}_1)^2, p(\vec{r}_1)]. \end{aligned} \quad (\text{D.3.2})$$

The last term vanishes under an area integral. Therefore $\frac{d}{dt} \overline{L_z}$ is given by:

$$\begin{aligned} \frac{d}{dt} \overline{L_z} &= \overline{\int \cos \theta J[\xi'(\vec{r}), \psi'(\vec{r})] d^2r} \\ &\quad + \int \cos \theta J[c(\vec{r}), p(\vec{r})] d^2r. \end{aligned} \quad (\text{D.3.3})$$

But $\xi'(\vec{r}) = \nabla^2 \psi'(\vec{r})$ and $c(\vec{r}) = \nabla^2 p(\vec{r})$. Therefore by the “Surface Integral” proof at the end, both terms vanish. Thus $\overline{L_z}$ is conserved under CE2.

D.3.2 Enstrophy

DNS

Now consider the material derivative of the vorticity squared, $\frac{D}{Dt}q^2 = \frac{\partial}{\partial t}q^2 + J[\psi, q^2]$, where:

$$\begin{aligned}\frac{\partial}{\partial t}q^2 &= \frac{\partial}{\partial t}(\xi + f)^2 \\ &= \frac{\partial}{\partial t}\xi^2 + 2f\frac{\partial}{\partial t}\xi \\ &= 2(f + \xi)\frac{\partial}{\partial t}\xi \\ &= 2qJ[q, \psi],\end{aligned}\tag{D.3.4}$$

and

$$J[\psi, q^2] = 2qJ[\psi, q].\tag{D.3.5}$$

Therefore $\frac{D}{Dt}q^2 = 0$. But enstrophy is given by $\Gamma_2 = \int q^2 dA$ so $\frac{d}{dt}\Gamma_2 = 0$ and thus enstrophy is conserved.

Ensemble CE2

The ensemble average enstrophy is $\overline{\Gamma_2} = \int \overline{q(\vec{r}_1)^2} d^2r_1$ where $\overline{q(\vec{r}_1)^2} = c(\vec{r}_1, \vec{r}_1) + (c(\vec{r}_1) + f(\vec{r}_1))^2$. Therefore the time derivative of the ensemble-averaged enstrophy is given by $\frac{d}{dt}\overline{\Gamma_2} = \int \frac{\partial}{\partial t}\overline{q(\vec{r}_1)^2} d^2r_1$ where:

$$\begin{aligned}
\frac{\partial}{\partial t} \left(\overline{q^2} \right) &= \frac{\partial}{\partial t} c(\vec{r}_1, \vec{r}_1) + 2(c(\vec{r}_1) + f(\vec{r}_1)) \frac{\partial}{\partial t} c(\vec{r}_1) \\
&= 2 \int (p(\vec{r}_1, \vec{r}_2)) J_1 [c(\vec{r}_1) + f(\vec{r}_1), \delta(\vec{r}_1 - \vec{r}_2)] d^2 r_2 \\
&\quad + J[c(\vec{r}_1, \vec{r}_1), p(\vec{r}_1)] \\
&\quad + 2(c(\vec{r}_1) + f(\vec{r}_1)) \left(\int J_1 [p(\vec{r}_1, \vec{r}_2), \delta(\vec{r}_1 - \vec{r}_2)] d^2 r_2 + J_1 [c(\vec{r}_1) + f(\vec{r}_1), p(\vec{r}_1)] \right) \\
&= 2 \int J_1 [p(\vec{r}_1, \vec{r}_2) (c(\vec{r}_1) + f(\vec{r}_1)), \delta(\vec{r}_1 - \vec{r}_2)] d^2 r_2 \\
&\quad + J [c(\vec{r}_1, \vec{r}_1) + (c(\vec{r}_1) + f(\vec{r}_1))^2, p(\vec{r}_1)] \\
&= 2 \int J_1 [p(\vec{r}_1, \vec{r}_2) (c(\vec{r}_1) + f(\vec{r}_1)), \delta(\vec{r}_1 - \vec{r}_2)] d^2 r_2 \\
&\quad + J [\overline{q^2}, p(\vec{r}_1)].
\end{aligned} \tag{D.3.6}$$

The area integral of the second Jacobian term vanishes straight-forwardly. As for the first Jacobian term, it can be rewritten as:

$$\begin{aligned}
&\int J_1 [p(\vec{r}_1, \vec{r}_2) (c(\vec{r}_1) + f(\vec{r}_1)), \delta(\vec{r}_1 - \vec{r}_2)] d^2 r_2 \\
&= \int J_1 [\overline{\xi'(\vec{r}_1) \psi'(\vec{r}_2)} (c(\vec{r}_1) + f(\vec{r}_1)), \delta(\vec{r}_1 - \vec{r}_2)] d^2 r_2
\end{aligned} \tag{D.3.7}$$

$$\begin{aligned}
&= \overline{\int J_1 [\xi'(\vec{r}_1) \psi'(\vec{r}_2) (c(\vec{r}_1) + f(\vec{r}_1)), \delta(\vec{r}_1 - \vec{r}_2)] d^2 r_2} \\
&= \overline{J_1 [\xi'(\vec{r}_1) (c(\vec{r}_1) + f(\vec{r}_1)), \psi'(\vec{r}_1)]},
\end{aligned} \tag{D.3.8}$$

and thus its area integral too vanishes straight-forwardly. Thus $\overline{\Gamma_2}$ is conserved.

D.3.3 Energy

Define the $\{\dots\}$ averaging operator such that $\{f(\xi, \psi)\} = \frac{1}{2} (f(\xi, \psi) + f(\psi, \xi))$.

DNS

The time derivative of energy is given by:

$$\begin{aligned}
\frac{d}{dt}\overline{E} &= -\frac{1}{2} \int \frac{\partial}{\partial t}(\xi\psi) d^2r \\
&= -\frac{1}{2} \int \left(\frac{\partial \xi}{\partial t}\psi + \xi \frac{\partial \psi}{\partial t} \right) d^2r \\
&= -\int \left\{ \frac{\partial \xi}{\partial t}\psi \right\} d^2r \\
&= -\int \{J[\xi + f, \psi]\psi\} d^2r \\
&= -\frac{1}{2} \left\{ \int J[\xi + f, \psi^2] d^2r \right\}, \tag{D.3.9}
\end{aligned}$$

which vanishes because $\int J[\psi^2, A] d^2r = 0$ where A is an arbitrary scalar because $\hat{n} \times \nabla \psi^2$ is divergence-free just like $\vec{u}$. This can be seen by recognizing that $\vec{u}$ is perpendicular to $\nabla \psi$. Thus total energy is conserved in DNS.

Ensemble CE2

The ensemble-averaged energy is given by $\overline{E} = -\frac{1}{2} \int \overline{\xi(\vec{r}_1)\psi(\vec{r}_1)} d^2r_1$ where $\overline{\xi(\vec{r}_1)\psi(\vec{r}_1)} = c(\vec{r}_1)p(\vec{r}_1) + p(\vec{r}_1, \vec{r}_1)$. Therefore its time derivative is given by $\frac{d}{dt}\overline{E} = -\frac{1}{2} \int \frac{\partial}{\partial t} \overline{\xi(\vec{r}_1)\psi(\vec{r}_1)} d^2r_1 = -\frac{1}{2} \int \frac{\partial}{\partial t} (c(\vec{r}_1)p(\vec{r}_1) + p(\vec{r}_1, \vec{r}_1)) d^2r_1$. The first term can be rewritten as:

$$\begin{aligned}
\left\{ p(\vec{r}_1) \frac{\partial}{\partial t} c(\vec{r}_1) \right\} &= 2 \left\{ p(\vec{r}_1) \left(\int J_1[p(\vec{r}_1, \vec{r}_2), \delta(\vec{r}_1 - \vec{r}_2)] d^2r_2 + J_1[c(\vec{r}_1) + f(\vec{r}_1), p(\vec{r}_1)] \right) \right\} \\
&= \left\{ 2p(\vec{r}_1) \overline{J_1[\xi'(\vec{r}_1), \psi'(\vec{r}_1)]} + J_1[c(\vec{r}_1) + f(\vec{r}_1), p^2(\vec{r}_1)] \right\}. \tag{D.3.10}
\end{aligned}$$

And the second term can be rewritten as:

$$\begin{aligned}
\frac{d}{dt}p(\vec{r}_1, \vec{r}_1) &= \frac{\partial}{\partial t} \overline{\xi'(\vec{r}_1) \psi'(\vec{r}_1)} \\
&= 2 \left\{ \overline{\psi'(\vec{r}_1) \frac{d}{dt} \xi'(\vec{r}_1)} \right\} \\
&= 2 \left\{ \overline{\psi'(\vec{r}_1) \frac{d}{dt} \xi(\vec{r}_1)} \right\} \\
&= 2 \left\{ \overline{\psi'(\vec{r}_1) J[\xi(\vec{r}_1) + f(\vec{r}_1), \psi(\vec{r}_1)]} \right\} \\
&= 2 \left\{ \overline{\psi'(\vec{r}_1) J[\xi(\vec{r}_1) + f(\vec{r}_1), p(\vec{r}_1) + \psi'(\vec{r}_1)]} \right\} \\
&= \left\{ \overline{J[\xi(\vec{r}_1) + f(\vec{r}_1), (\psi'(\vec{r}_1))^2]} + 2 \overline{\psi'(\vec{r}_1) J[\xi'(\vec{r}_1), p(\vec{r}_1)]} \right\} \\
&= \left\{ \overline{J[c(\vec{r}_1) + f(\vec{r}_1), \overline{\psi'(\vec{r}_1) \psi'(\vec{r}_1)}]} \right\} \tag{D.3.11}
\end{aligned}$$

$$+ 2 \left\{ \overline{\psi'(\vec{r}_1) J[\xi'(\vec{r}_1), p(\vec{r}_1)]} \right\}, \tag{D.3.12}$$

where $\overline{\xi'(\vec{r}_1) (\psi'(\vec{r}_1))^2} = 0$ under CE2. Therefore:

$$\begin{aligned}
\frac{\partial}{\partial t} \overline{\xi(\vec{r}_1) \psi(\vec{r}_1)} &= \left\{ \overline{J[c(\vec{r}_1) + f(\vec{r}_1), \overline{\psi'(\vec{r}_1) \psi'(\vec{r}_1)} + p^2(\vec{r}_1)]} + 2 \overline{J[\xi'(\vec{r}_1), \psi'(\vec{r}_1) p(\vec{r}_1)]} \right\} \\
&= \left\{ \overline{J[c(\vec{r}_1) + f(\vec{r}_1), \psi(\vec{r}_1)^2]} + 2 \overline{J[\xi'(\vec{r}_1), \psi'(\vec{r}_1) p(\vec{r}_1)]} \right\}. \tag{D.3.13}
\end{aligned}$$

The first term vanishes straight-forwardly. The second term also vanishes as $\hat{n} \times \nabla(\psi'(\vec{r}_1) p(\vec{r}_1))$ is divergence-free:

$$\begin{aligned}
\hat{n} \times \nabla(\psi'(\vec{r}_1) p(\vec{r}_1)) &= \psi'(\vec{r}_1) \hat{n} \times \nabla(p(\vec{r}_1)) + p(\vec{r}_1) \hat{n} \times \nabla(\psi'(\vec{r}_1)) \\
&= \psi'(\vec{r}_1) \overline{\vec{u}(\vec{r}_1)} + p(\vec{r}_1) \vec{u}'(\vec{r}_1) \tag{D.3.14}
\end{aligned}$$

$$\begin{aligned}
\Rightarrow \nabla \cdot (\hat{n} \times \nabla(\psi'(\vec{r}_1) p(\vec{r}_1))) &= \nabla \cdot (\psi'(\vec{r}_1) \overline{\vec{u}(\vec{r}_1)}) + \nabla \cdot (p(\vec{r}_1) \vec{u}'(\vec{r}_1)) \\
&= \overline{\vec{u}(\vec{r}_1)} \cdot \nabla(\psi'(\vec{r}_1)) + \vec{u}'(\vec{r}_1) \cdot \nabla(p(\vec{r}_1)) \\
&= \hat{n} \cdot (\nabla(\psi'(\vec{r}_1)) \times \nabla(p(\vec{r}_1)) + \nabla(p(\vec{r}_1)) \times \nabla(\psi'(\vec{r}_1))) \\
&= 0. \tag{D.3.15}
\end{aligned}$$

Thus ensemble-averaged energy $\overline{E}$ is conserved in ensemble CE2.

Appendix E

Code

E.1 Power spectrum of the Lorenz attractor

This code is also available at:

https://bitbucket.org/altan_allawala/power-spectrum-of-the-lorenz-attractor

```
1 #!/usr/bin/python
2
3 # Integrates the equations of motion of the stochastically-forced Lorenz
   attractor via a fourth-order Runge-Kutta time step. Then constructs
   and plots its power spectrum by performing a Fourier transform on
   the time series of its x-values. Written by Altan Allawala.
4
5 import math
6 from numpy import *
7 from pylab import *
8 from scipy import weave
9 import scipy.interpolate
10 import scipy.ndimage.interpolation
11 from scipy.weave import converters
12 from scipy.integrate import odeint
13 from matplotlib.colors import LogNorm
```

```

14 from scipy.interpolate import interp1d
15 from mpl_toolkits.axes_grid1 import make_axes_locatable
16
17 import time
18
19 class Lorenz (object):
20
21     def __init__(self, x=0.0, y=0.0, z=0.0, gamma = 10., endTime = 100.0,
22                 dt = 0.01, N = 100):
23         self.dt = dt
24         self.gamma = gamma
25         self.endTime = endTime
26         self.phaseSpace = array([x, y, z])
27         self.phaseSpacestore = np.zeros((int(self.endTime/self.dt),3))
28         self.N = N
29         self.Nt = int(self.endTime/self.dt)
30
31     def CreateStochasticForcing(self): # Require that dt<<deltaT<<T
32         print "Creating random gaussian array"
33
34         T = 1. #T = 0.1 # Time-scale of the system (this is set by the
35             attractor itself)
36         deltaT = sqrt(T*self.dt) # Time-scale over which to vary the
37             stochastic forcing
38         Nt = self.Nt # Number of time steps
39         coursex = arange(0.,self.endTime+deltaT,deltaT) # Create stochastic
40             points seperated by deltaT
41         nt = len(coursex)
42         coursef = sqrt(2.0 * self.gamma/deltaT) * np.random.normal(loc=0.,
43                             scale=1., size = (nt,3))
44
45         print "Interpolating"

```

```

42     finex = arange(0., self.endTime, self.dt)
43     finefx = np.interp(finex, coursex, coursef[:,0])
44     finefy = np.interp(finex, coursex, coursef[:,1])
45     finefz = np.interp(finex, coursex, coursef[:,2])
46
47     self.f = concatenate((finefx, finefy, finefz), axis=0)
48     self.f = reshape(self.f, (Nt,3), order='F')
49
50
51     def RHS(self, xarray, f):
52
53         x = xarray[0]
54         y = xarray[1]
55         z = xarray[2]
56
57         sigma = 3.#10.
58         rho = 26.5#28.
59         beta = 0.16#1.#8./3.
60
61         xdot = sigma * (y - x) + f[0]
62         ydot = x * (rho - z) - y + f[1]
63         zdot = x * y - beta * z + f[2]
64
65         return array([xdot, ydot, zdot])
66
67
68     def integrate(self): # Fourth Order Runge-Kutta method
69         print "Integrating"
70         t = 0.
71         i = 0
72         Nt = self.Nt
73
74         f = self.f

```

```

75
76     for i in range(Nt):
77         self.k1 = self.dt * self.RHS(self.phaseSpace, f[i,:])
78         self.k2 = self.dt * self.RHS(self.phaseSpace+0.5*self.k1, f[i,:])
79         self.k3 = self.dt * self.RHS(self.phaseSpace+0.5*self.k2, f[i,:])
80         self.k4 = self.dt * self.RHS(self.phaseSpace+self.k3, f[i,:])
81         self.phaseSpace = self.phaseSpace + self.k1/6. + self.k2/3. + self
            .k3/3. + self.k4/6.
82         self.phaseSpacestore[i]=self.phaseSpace
83         i = i + 1
84         if (i%100000==0):
85             print "Time = ", i*self.dt
86
87         self.TimeSeries = self.phaseSpacestore[:,0] # SELECT x VALUES
88
89
90 def FFT(self): # Fast Fourier transform
91     import numpy.fft
92     ft = rfft(self.TimeSeries) # Take the FT
93     self.PowerSpectrum = np.abs(ft)**2
94
95
96 def Binning(self): # Bin the data points into a histogram
97
98     print "Taking FT, ", time.clock()
99     freqs = rfftfreq(len(self.PowerSpectrum)*2-2, d=self.dt)
100
101     print "Binning data, ", time.clock()
102     bins = int(freqs[-1]/self.dt)+1
103     from scipy.stats import binned_statistic
104     self.PowerSpectrum = binned_statistic(freqs, self.PowerSpectrum,
            bins=bins)[0]
105     self.freqs = np.linspace(0, freqs[-1], num=bins)

```

```

106
107     print "Combining data, ", time.clock()
108     self.Data = array([ self.freqs , self.PowerSpectrum])
109
110
111     def SaveData(self):
112         # print "Saving time series"
113         # np.savetxt('TimeSeries', self.TimeSeries)
114
115         print "Saving binned power spectrum, ", time.clock()
116         np.savetxt('PowerSpectrum', self.Data)
117
118
119     def LoadData(self): # Load data of the same form as is saved
120         print "Loading data, ", time.clock()
121         self.Data = np.loadtxt('PowerSpectrum')
122         # self.TimeSeries = np.loadtxt('TimeSeries')
123
124
125     def Plot(self): # Plot the power spectrum of the Lorenz attractor
126         # print "Plotting time series"
127         # plot(self.TimeSeries)#, color='black', linestyle='--', linewidth=2.)
128         #, vmin=0., vmax=4., c=c1, cmap=cmap)
129
130         print "Plotting frequency spectrum, ", time.clock()
131         figure() # Plot the Power Spectrum
132         plot(self.Data[0,:], self.Data[1,:], 'b-')
133         xlim(0,1.5)
134         xlabel('Frequency')
135         ylabel('Power Spectrum')
136         savefig('PowerSpectrum.pdf')
137

```

```

138 p = Lorenz(x=1., y=1., z=25., gamma=0.01, endTime=1000., dt=.01, N=478)
139 p.CreateStochasticForcing()
140 p.integrate()
141 p.FFT()
142 p.Binning()
143 p.SaveData()
144 p.LoadData()
145 p.Plot()
146 show()

```

E.2 Zero mode of FPE operator

```

1 % Constructs the FPE operator for the Lorenz attractor as a sparse
   matrix representation. Then solves for its zero mode using the JDQR
   package. Then computes & saves the three axial projections of the
   PDF (eigenvector). Written by Altan Allawala.
2 clear
3
4 Nx = 160;
5 Lx = 14.;
6 Ly = 20.;
7 Lz = 20.;
8
9 dx = Lx/(Nx-1);
10 dy = Ly/(Nx-1);
11 dz = Lz/(Nx-1);
12
13 vx = linspace(-Lx/2.,Lx/2.,Nx);
14 vy = linspace(-Ly/2.,Ly/2.,Nx);
15 vz = linspace(25.-Lz/2.,25.+Lz/2.,Nx);
16
17 sigma = 3.;

```

```

18 rho = 26.5;
19 beta = 0.16;%8./3.;
20 gamma = 0.02
21
22 iden = speye(Nx);
23
24 N = linspace(1,Nx,Nx);
25 xcoord = sparse(N,N,vx,Nx,Nx);
26 ycoord = sparse(N,N,vy,Nx,Nx);
27 zcoord = sparse(N,N,vz,Nx,Nx);
28
29 A = zeros(1,Nx);
30 A(2) = 1;
31 D1 = toeplitz(-A,A);
32 D1 = sparse(D1);
33
34 B = zeros(1,Nx);
35 B(1) = -2;
36 B(2) = 1;
37 D2 = toeplitz(B,B);
38 D2 = sparse(D2);
39
40 identity = kron(kron(iden, iden), iden);
41
42 x = kron(kron(xcoord, iden), iden);
43 y = kron(kron(iden, ycoord), iden);
44 z = kron(kron(iden, iden), zcoord);
45
46 Dx = kron(kron(D1, iden), iden)/(2.*dx);
47 Dy = kron(kron(iden, D1), iden)/(2.*dy);
48 Dz = kron(kron(iden, iden), D1)/(2.*dz);
49
50 D2x = kron(kron(D2, iden), iden)/dx^2;

```

```

51 D2y = kron(kron(iden , D2) , iden)/dy^2;
52 D2z = kron(kron(iden , iden) , D2)/dz^2;
53
54 laplacian = D2x + D2y + D2z;
55
56 Loperator = Dx*(sigma*(x-y)) + Dy*(y-rho*x+x*z) + Dz*(beta*z-x*y) +
    gamma*laplacian;
57
58 zeromatrix = sparse(Nx^3,Nx^3);
59
60 H = Loperator;
61
62 disp('Number of non-zero entries is'), disp(nnz(H));
63
64 opts.jmin = 2;
65 opts.jmax = 4;
66 opts.MaxIt = 100; % Default 100
67 opts.LS_MaxIt = 5; % Default 5
68 opts.Disp = 1; % Display shiznit
69 opts.Tol = 1.e-5;
70 opts.Precond = H;
71
72 tic;
73 [V,E] = jdqr(H, 1, 0, opts);
74 toc;
75 saveas(gca, 'iter.jpg')
76 size(V)
77 disp('Tic toc time is'), disp(toc);
78
79 E = diag(E)
80 [energy , index] = min(abs(E));
81
82 disp('Selected energy is'), disp(energy);

```



```

83
84 psi = V(:, index);
85
86 psi = real(psi);
87 psi = psi/sum(psi);
88 psi = reshape(psi, Nx, Nx, Nx);
89
90 psixy = sum(psi, 1);
91 psixz = sum(psi, 2);
92 psiyz = sum(psi, 3);
93
94 psixy = reshape(psixy, Nx*Nx, 1);
95 psixz = reshape(psixz, Nx*Nx, 1);
96 psiyz = reshape(psiyz, Nx*Nx, 1);
97
98 save psixy psixy -ASCII;
99 save psixz psixz -ASCII;
100 save psiyz psiyz -ASCII;

```

E.3 TR-BDF2

```

1 // Relevant portion from the GCM code (available on Mac App Store) for
  // the TR-BDF2 solver and Krylov subspace iterative solver.
2
3 - (void)semiImplicitIntegration // Written by Altan Allawala.
4   {
5       const long blockOfSteps = 4;
6       const double targetError = _precision;
7       double maxDt = 1.0;
8       double gama = 1. - pow(2., -0.5); // Optimal value for time
      // stepping parameter. Ref: Hosea, M.E. and Shampine, L.F.,
      // 1996. Analysis and implementation of TR-BDF2. Applied

```

```
9      cumulants qdot, kstar, RHS2, DX, AX, r1, r2;
10
11      for (long j = 0; j < blockOfSteps; j++) {
12          qdot = [self tendency:_q];
13          kstar = [self increment:_q forRHS:qdot forTimeStep:_dt*gama
14                  ]; // First implicit step of TR-BDF2
15          RHS2 = _dt * (gama * qdot + (1 - gama) * kstar);
16          _dq = [self increment:_q forRHS:RHS2 forTimeStep:_dt*gama];
17              // Second implicit step of TR-BDF2
18          DX = _dq - _dt * gama * [self jacobian:_q forCumulant:_dq];
19              // DX where DDX=B
20          AX = DX - _dt * gama * [self jacobian:_q forCumulant:DX]; //
21              AX=DDX=B
22          r1 = kstar - qdot - _dt * gama * [self jacobian:_q
23              forCumulant:kstar];
24          r2 = _dq - _dt * (gama * qdot + gama * [self jacobian:_q
25              forCumulant:_dq] + (1. - gama) * kstar);
26          _q += _dq;
27
28          dispatch_sync(_drawingQueue, ^{
29              @autoreleasepool {
30                  [self sampleCumulants];
31                  [self zonalRecord];
32              }
33          });
34
35          _t += _dt;
36          //NSLog(@"dt is %g", _dt);
37
38          double error = relativeError(_q + r1, _q) + relativeError(_q
39              + r2, _q);
```

```

33         if (error < targetError) _dt = _dt * pow(targetError/error ,
34             0.2);
35         else _dt = _dt * pow(targetError/error , 0.25);
36         if (_dt > maxDt) _dt = maxDt;
37     }
38 }
39
40 - (cumulants)increment:(cumulants &)q forRHS:(cumulants &)BB forTimeStep
    :(const double)dt // Solves  $A x = B$  for  $x$ . Modified by Altan
    Allawala .
41 {
42     long dim = [[NSUserDefaults standardUserDefaults] integerForKey:
        KrylovSubspaceDimension];
43     cumulants w;
44     cumulants *v = new cumulants[dim];
45     double h[dim*dim];
46     bzero(h, dim*dim*sizeof(double));
47     v[0] = BB; // This is the RHS (B)
48     double beta = norm(v[0]);
49     v[0] = v[0] / beta;
50
51     for (long j = 0; j < dim; j++) {
52         w = v[j] - dt * [self jacobian:q forCumulant:v[j]]; // This is A
            v where  $A x = B$ 
53
54         for (long i = 0; i <= j; i++) {
55             h[i*dim+j] = real(inner(w, v[i]));
56             w -= h[i*dim+j] * v[i];
57         }
58
59         if (j+1 < dim) { // add vector to subspace
60             double nw = norm(w);

```

```

61         h[(j+1)*dim+j] = nw;
62         v[j+1] = w / nw;
63     }
64 }
65
66 invert(h, dim);
67 cumulants dq;
68 for (long i = 0; i < dim; i++) dq += (h[i*dim+0] * beta) * v[i];
69 delete[] v;
70 _iterations = 1;
71
72 return dq;
73 }

```