The Liouville Equation in Atmospheric Predictability

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1 Introduction and Motivation

It is widely recognized that weather forecasts made with dynamical models of the atmosphere are inherently uncertain. Such uncertainty of forecasts produced with numerical weather prediction (NWP) models arises primarily from two sources: namely, from imperfect knowledge of the initial model conditions and from imperfections in the model formulation itself. The recognition of the potential importance of accurate initial model conditions and an accurate model formulation dates back to times even prior to operational NWP (Bjerknes 1904; Thompson 1957). In the context of NWP, the importance of these error sources in degrading the quality of forecasts was demonstrated to arise because errors introduced in atmospheric models, are, in general, growing (Lorenz 1982; Lorenz 1963; Lorenz 1993), which at the same time implies that the predictability of the atmosphere is subject to limitations (see, Errico et al. 2002). An example of the amplification of small errors in the initial conditions, or, equivalently, the divergence of initially nearby trajectories is given in Fig. 1, for the system discussed by Lorenz (1984). The uncertainty introduced into forecasts through uncertain initial model conditions, and uncertainties in model formulations, has been the subject of numerous studies carried out in parallel to the continuous development of NWP models (e.g., Leith 1974; Epstein 1969; Palmer 2000).

In addition to studying the intrinsic predictability of the atmosphere (e.g., Lorenz 1969a; Lorenz 1969b; Thompson 1985a; Thompson 1985b), efforts have been directed at the quantification or prediction of forecast uncertainty that arises due to the sources of uncertainty mentioned above (see the review papers by Ehrendorfer 1997 and Palmer 2000, and Ehrendorfer 1999). In the context of predicting uncertainty, the Liouville equation (LE) arises as the general framework to describe in a probabilistic manner the time–dependent behavior of an ensemble of solutions of a numerical model started from different initial conditions. It carries the name of Joseph Liouville (for an extensive biographical account, see, Lützen 1990), since its formulation can be traced back to a mathematical result that Liouville published in 1838 (see section 2). The generality of the LE arises from the fact that the LE governs the time evolution of the probability density function (pdf) of the model's state vector $\mathbf{X}$ given the corresponding model dynamics. Closely analogous to the mass conservation equation in hydrodynamics, the LE is the mathematical formulation of the statement that realizations (i.e., members of the ensemble) cannot spontaneously appear or disappear which, in turn, implies that the phase–space integral of the density of realizations is constant in time. These properties of the LE imply that it contains all (statistical) information about time–

evolving model solutions, and as such is the basis for studying uncertainty prediction and state–dependent predictability of weather and climate phenomena.

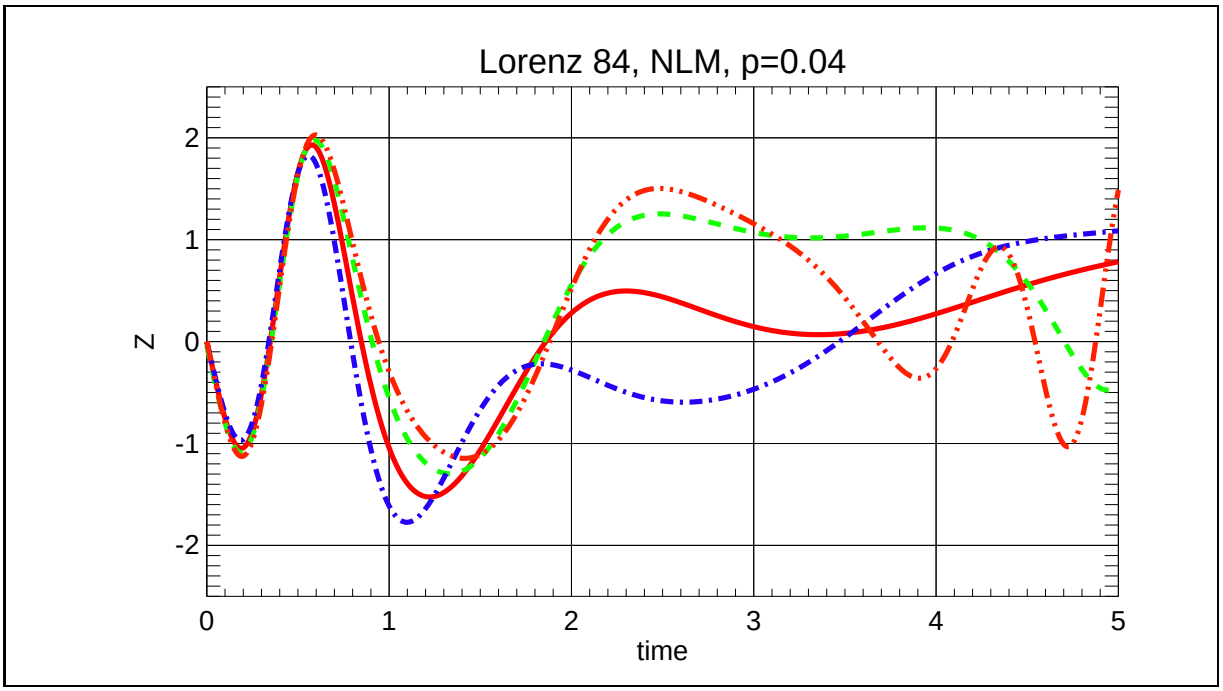


Figure 1: Time evolution of Z component of Lorenz (1984) model. Initial perturbation size is 0.04. Dashed indicates negative perturbation, dash–dot plus SV1 perturbation, and dash–dot–dot minus SV1 perturbation (see also, sections 4.2 and 5.2).

The purpose of this paper is to review the LE and its relation to atmospheric predictability. Following an overview of the LE, together with its various connections to mathematical physics (section 2), the general solution to the LE is described (section 3). The relationship of various aspects of the LE to operational ensemble prediction, to the stochastic–dynamic equations, and to classical and statistical mechanics, is discussed in section 4. The paper is concluded with a summarizing outlook.

2 The Liouville Equation: Background

2.1 Historical Background

The LE is apparently named after Joseph Liouville, since it can be related to a result that he proved in 1838 on the material derivative of the "Jacobian" of the transformation exerted by the solution of an ordinary differential equation on its initial condition (see section 2.2). Subsequently, this result can be used in deriving the so–called Transport Theorem. Further, the LE, the Fokker–Planck Equation (FPE) and the Liouville Theorem (LT) of statistical mechanics can all be viewed as special cases of the Transport Theorem. Comprehensive accounts on the historical details may be found in Lützen (1990) who mentions that Liouville's *Nachlass* contains 340 notebooks, consisting of more than 40,000 pages.

In view of the fundamental nature of Liouville's results, references to his name are found in various

areas of physics, and in the atmospheric sciences. Some selected areas are briefly discussed here.

In *classical mechanics*, Liouville is referred to with regard to the LT (see, section 5.6) that expresses the conservation of phase space *volume* for Hamiltonian systems (see, e.g., Abraham and Marsden 1978, Arnold 1989, Goldstein 1980, Marion and Thornton 1988; see also, section 5.6). The importance of the LT for *statistical mechanics* is emphasized, for example, by Landau and Lifschitz (1979) who state that *the pdf remains constant along trajectories* (for a Hamiltonian system; see also, eq. (5.6.5)). Balescu (1991) points out that the LE is the most important equation of statistical mechanics and emphasizes that the most important feature of the LE is its linearity. Lindenberg and West (1990) mention the LE as describing the conservation of phase–space points (their p. 21). Penrose (1989) refers to the LT as "a very beautiful theorem, due to the distinguished French mathematician Joseph Liouville (1809–1882), that tells us that the *volume* of any region of the phase space must remain constant under any Hamiltonian evolution" (his p. 181; see also section 5.6; see, also Penrose 1970). In the literature on *stochastic processes*, the LE plays an important role in its connection with the Fokker–Planck equation (Risken 1989, Gardiner 1990, van Kampen 1992; see also, section 5.4). In that context, these equations are also referred to as the Chapman–Kolmogorov equation, or the Master equation (Gardiner 1990). Also, as a further remark on terminology, Nicolis (1995) refers to a time–discrete version of a pdf–governing equation as Frobenius–Perron equation.

In the meteorological and in the turbulence literature, the LE has been used as starting point for various investigations, among them the problem of deriving equilibrium statistics of geophysical flows (see, Holloway 1986, for an excellent overview), described, for example, in Thompson (1972), Salmon et al. (1976), Thompson 1983, Thompson 1985b, and Merryfield et al. (2001) (see also, Hasselmann 1976, Penland and Matrosova 1994, Stanišić 1988, McComb 1991, Hu and Pierrehumbert 2001, Chu et al. 2002, Weiss 2003). More specifically, with regard to the time evolution of uncertainty in atmospheric models, the LE was considered as a fundamental tool for approaching that question by Epstein (1969), Gleeson (1966), Tatarskiy (1969), and Fortak (1973).

Given the above brief (and necessarily incomplete) overview of some of the implications of Liouville's work, a more detailed inspection of his result is discussed in the next section.

2.2 Theoretical Background

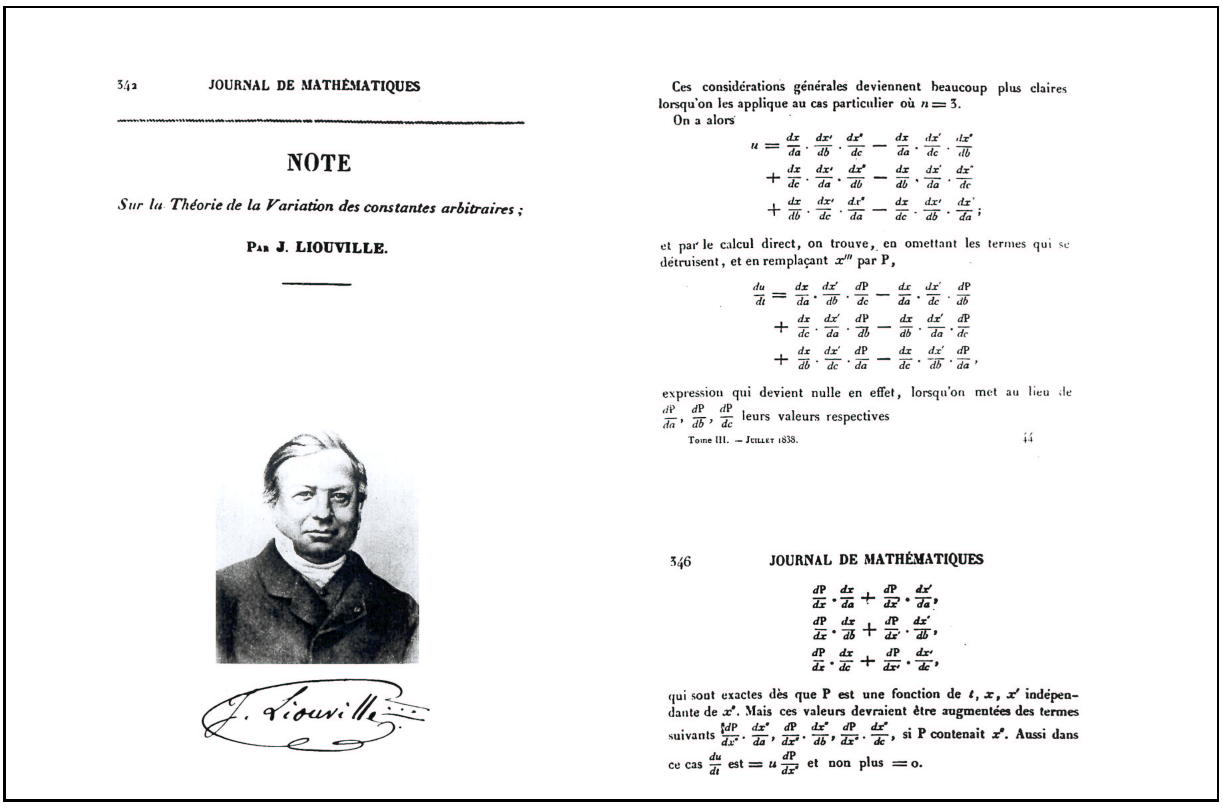
2.2.1 The Result of J. Liouville in 1838

In the paper that may be considered to contain the basic result for the LE and the LT, Liouville (1838) first discussed the general result for an Nth order ordinary differential equation and then considered the particular case $N = 3$ by illustrating in terms of a third–order ordinary differential equation of the following form:

$$x''' = P(t, x, x', x'') \,, \tag{2.2.1.1}$$

subsequently assuming the solution to be of the form:

$$x = x(t, a, b, c) \,. \tag{2.2.1.2}$$



342 JOURNAL DE MATHÉMATIQUES

NOTE

Sur la Théorie de la Variation des constantes arbitraires ;

PAR J. LIOUVILLE.

Ces considérations générales deviennent beaucoup plus claires lorsqu'on les applique au cas particulier où $n = 3$.

On a alors

$$u = \frac{dx}{da}\cdot\frac{dx'}{db}\cdot\frac{dx''}{dc} - \frac{dx}{da}\cdot\frac{dx'}{dc}\cdot\frac{dx''}{db} + \frac{dx}{dc}\cdot\frac{dx'}{da}\cdot\frac{dx''}{db} - \frac{dx}{db}\cdot\frac{dx'}{da}\cdot\frac{dx''}{dc} + \frac{dx}{db}\cdot\frac{dx'}{dc}\cdot\frac{dx''}{da} - \frac{dx}{dc}\cdot\frac{dx'}{db}\cdot\frac{dx''}{da};$$

et par le calcul direct, on trouve, en omettant les termes qui se détruisent, et en remplaçant x''' par P,

$$\frac{du}{dt} = \frac{dx}{da}\cdot\frac{dx'}{db}\cdot\frac{dP}{dc} - \frac{dx}{da}\cdot\frac{dx'}{dc}\cdot\frac{dP}{db} + \frac{dx}{dc}\cdot\frac{dx'}{da}\cdot\frac{dP}{db} - \frac{dx}{db}\cdot\frac{dx'}{da}\cdot\frac{dP}{dc} + \frac{dx}{db}\cdot\frac{dx'}{dc}\cdot\frac{dP}{da} - \frac{dx}{dc}\cdot\frac{dx'}{db}\cdot\frac{dP}{da},$$

expression qui devient nulle en effet, lorsqu'on met au lieu de $\frac{dP}{da}, \frac{dP}{db}, \frac{dP}{dc}$ leurs valeurs respectives

Tome III. — JUILLET 1838. 44

346 JOURNAL DE MATHÉMATIQUES

$$\frac{dP}{dx}\cdot\frac{dx}{da} + \frac{dP}{dx'}\cdot\frac{dx'}{da},$$
$$\frac{dP}{dx}\cdot\frac{dx}{db} + \frac{dP}{dx'}\cdot\frac{dx'}{db},$$
$$\frac{dP}{dx}\cdot\frac{dx}{dc} + \frac{dP}{dx'}\cdot\frac{dx'}{dc},$$

qui sont exactes dès que P est une fonction de t, x, x' indépendante de x''. Mais ces valeurs devraient être augmentées des termes suivants $\frac{dP}{dx''}\cdot\frac{dx''}{da}, \frac{dP}{dx''}\cdot\frac{dx''}{db}, \frac{dP}{dx''}\cdot\frac{dx''}{dc}$, si P contenait x''. Aussi dans ce cas $\frac{du}{dt}$ est $= u\frac{dP}{dx''}$ et non plus $= 0$.

Figure 2: Reproduction of (parts of) original proof by J. Liouville (photograph from Lützen 1990).

He defined u, the determinant of the Jacobian of the mapping the solution of the differential equation exerts on the initial condition as:

$$u = u(a,b,c,t) = \det\begin{pmatrix} \frac{\partial x(t,a,b,c)}{\partial a} & \frac{\partial x(t,a,b,c)}{\partial b} & \frac{\partial x(t,a,b,c)}{\partial c} \\ \frac{\partial x'(t,a,b,c)}{\partial a} & \frac{\partial x'(t,a,b,c)}{\partial b} & \frac{\partial x'(t,a,b,c)}{\partial c} \\ \frac{\partial x''(t,a,b,c)}{\partial a} & \frac{\partial x''(t,a,b,c)}{\partial b} & \frac{\partial x''(t,a,b,c)}{\partial c} \end{pmatrix}. \tag{2.2.1.3}$$

He then showed that it is true that:

$$\boxed{\frac{\partial u}{\partial t} = u\frac{\partial P}{\partial x''}} \tag{2.2.1.4}$$

when the chain rule of differentiation is observed to rewrite, for example, the following partial derivative in the form:

$$\frac{\partial x'''}{\partial a} = \frac{\partial P}{\partial a} = \frac{\partial P}{\partial x}\frac{\partial x}{\partial a} + \frac{\partial P}{\partial x'}\frac{\partial x'}{\partial a} + \frac{\partial P}{\partial x''}\frac{\partial x''}{\partial a}. \tag{2.2.1.5}$$

As already mentioned, the result was generalized to Nth order equations and to systems of first–order equations. A part of the original paper from 1838 is reproduced in Fig. 2.

2.2.2 Generalization of Liouville's Result

The generalization of Liouville's result is known as the *material derivative of the Jacobian*, or as the *Euler expansion formula* (see, e.g., chapter 13.4 in Lin and Segel 1988). To illustrate that extension, an

N–dimensional system of first–order ordinary differential equations:

$$\dot{\mathbf{X}} = \mathbf{\Phi}(\mathbf{X}, t) \tag{2.2.2.1}$$

is considered with the solution $\mathbf{X}$ being a function of both the initial condition $\mathbf{\Xi}$ and time t:

$$\mathbf{X} = \mathbf{X}(\mathbf{\Xi}, t)\,. \tag{2.2.2.2}$$

Under the assumption of continuous dependence on the initial condition (e.g., Nicolis 1995, p. 51), the Jacobian J may be defined as the determinant of the transformation that the solution exerts on the initial condition:

$$J = J(\mathbf{\Xi}, t) = \det\Big(\frac{\partial \mathbf{X}(\mathbf{\Xi}, t)}{\partial \mathbf{\Xi}}\Big|_{\mathbf{\Xi}}\Big)\,. \tag{2.2.2.3}$$

At the same time it is implied that $\mathbf{\Xi}$ can be recovered from knowledge of $\mathbf{X}$ and t, through "inverting" eq. (2.2.2.2):

$$\mathbf{\Xi} = \mathbf{\Xi}(\mathbf{X}, t)\,. \tag{2.2.2.4}$$

In that situation, two equivalent formulations of the generalization of Liouville's result are:

$$\frac{\partial J(\mathbf{\Xi}, t)}{\partial t} = \Big(\sum_{i=1}^{N} \frac{\partial \Phi_i(\mathbf{X}, t)}{\partial X_i}\Big|_{\mathbf{X}(\mathbf{\Xi}, t)}\Big) J(\mathbf{\Xi}, t) \tag{2.2.2.5}$$

and:

$$\Big(\frac{\partial}{\partial t} + \sum_{i=1}^{N} \dot{X}_i \frac{\partial}{\partial X_i}\Big) J(\mathbf{X}, t) = \Big(\sum_{i=1}^{N} \frac{\partial \Phi_i(\mathbf{X}, t)}{\partial X_i}\Big) J(\mathbf{X}, t)\,. \tag{2.2.2.6}$$

Here, in the first formulation ("material" formulation), eq. (2.2.2.5), J is considered as a function of $\mathbf{\Xi}$ and t, and the partial derivative with respect to time t is taken for fixed $\mathbf{\Xi}$, and the divergence expression (in parentheses) must be written as a function of $\mathbf{\Xi}$, too. In the second formulation ("spatial" formulation), eq. (2.2.2.6), however, J is considered as a function of $\mathbf{X}$ and t, and an advective term appears. An illustration of these concepts appears in the next subsection.

2.2.3 A One–dimensional Example

To illustrate the result on the material derivative of the Jacobian in the two versions (2.2.2.5) and (2.2.2.6), consider the following Riccati equation (see, e.g., Zwillinger 1989):

$$\dot{X} = -X^2 \tag{2.2.3.1}$$

with the solution written in the form (2.2.2.2) as:

$$X(\Xi, t) = \frac{\Xi}{1 + t\Xi} \tag{2.2.3.2}$$

and the "inverse" mapping of the form (2.2.2.4) written as:

$$\Xi(X, t) = \frac{X}{1 - tX}\,. \tag{2.2.3.3}$$

From (2.2.3.2), J is obtained as a function of Ξ and t through the defining equation (2.2.2.3) as:

$$J(\Xi,t) = \frac{\partial X}{\partial \Xi} = \frac{1}{(1+t\Xi)^2}\,. \tag{2.2.3.4}$$

Further, $J(X,t)$ may be found by expressing Ξ in (2.2.3.4) through its dependence on X as given in (2.2.3.3) in the form:

$$J(X,t) = \frac{1}{[1+t\Xi(X,t)]^2} = \frac{1}{(1+t\frac{X}{1-tX})^2} = (1-tX)^2\,. \tag{2.2.3.5}$$

To see the correctness of the first formulation (2.2.2.5), the derivative of J using (2.2.3.4):

$$\frac{\partial J(\Xi,t)}{\partial t} = (-2)\underbrace{(1+t\Xi)^{-2}}_{=J(\Xi,t)}(1+t\Xi)^{-1}\Xi \tag{2.2.3.6}$$

is compared to the right–hand–side of (2.2.2.5) written in the form:

$$\frac{\partial \Phi(X,t)}{\partial X}\Big|_{X(\Xi,t)} J(\Xi,t) = (-2)X(\Xi,t)J(\Xi,t)\,. \tag{2.2.3.7}$$

Clearly, on the basis of (2.2.3.2), results (2.2.3.6) and (2.2.3.7) are the same, establishing Liouville's result in the formulation (2.2.2.5) for the example under consideration here. Similarly, for the second formulation, the left–hand–side of (2.2.2.6) is, for the example under consideration here, found to be:

$$\Big(\frac{\partial}{\partial t} + \dot{X}\frac{\partial}{\partial X}\Big)J(X,t) = (-2X)(1-tX) + (-X^2)(-2t)(1-tX)\,, \tag{2.2.3.8}$$

or, equivalently:

$$\Big(\frac{\partial}{\partial t} + \dot{X}\frac{\partial}{\partial X}\Big)J(X,t) = (-2X)\underbrace{(1-tX)^2}_{=J(X,t)}, \tag{2.2.3.9}$$

which, on the basis of (2.2.3.5), is equal to the right–hand–side of (2.2.2.6), thus establishing Liouville's result in the second formulation.

2.3 The Transport Theorem

The Transport Theorem (TT) describes how to rewrite the time derivative of the phase space integral of some quantity χ over a material region. This result is briefly derived below. In the derivation of the TT, Liouville's result is used in the formulation (2.2.2.5). Consequently, the TT may be viewed as one of the main implications of Liouville's result. In turn, all the consequences derivable from the TT, especially the LE and the LT, relate through this dependence back to the work of Liouville.

Consider the integral of χ over a material region $R(t)$ (see, e.g., chapter 14.1 in Lin and Segel 1988), with the material points subject to the dynamics (2.2.2.1):

$$I(t) \equiv \int_{R(t)} \chi(\mathbf{X},t)d\mathbf{X}\,. \tag{2.3.1}$$

The time derivative of $I(t)$ is:

$$\begin{aligned} \frac{dI(t)}{dt} &= \frac{d}{dt}\int_{R(t)} \chi(\mathbf{X},t)d\mathbf{X} = \\ &= \frac{d}{dt}\int_{R(0)} \chi\Big(\mathbf{X}(\boldsymbol{\Xi},t),t\Big)J(\boldsymbol{\Xi},t)d\boldsymbol{\Xi}, \end{aligned} \tag{2.3.2}$$

where the integral has been transformed to the initial region $R(0)$ and $J(\boldsymbol{\Xi},t)$ is defined in eq. (2.2.2.3). Since $R(0)$ does not depend on time, the time derivative can be taken inside the integral, noting that $\boldsymbol{\Xi}$ has to be held fixed:

$$\begin{aligned} \frac{dI(t)}{dt} &= \int_{R(0)} \frac{d}{dt}\Big|_{\boldsymbol{\Xi}}\Big[\chi\Big(\mathbf{X}(\boldsymbol{\Xi},t),t\Big)J(\boldsymbol{\Xi},t)\Big]d\boldsymbol{\Xi} = \\ &= \int_{R(0)} \Big\{J(\boldsymbol{\Xi},t)\frac{d\chi\big(\mathbf{X}(\boldsymbol{\Xi},t),t\big)}{dt}\Big|_{\boldsymbol{\Xi}} + \chi\Big(\mathbf{X}(\boldsymbol{\Xi},t),t\Big)\underbrace{\frac{dJ(\boldsymbol{\Xi},t)}{dt}\Big|_{\boldsymbol{\Xi}}}\Big\}d\boldsymbol{\Xi}, \end{aligned} \tag{2.3.3}$$

where the bracketed term has been differentiated according to the product rule. In the next step, the first term of the integrand is differentiated according to the chain rule, whereas result (2.2.2.5) is used to express the underbraced time derivative of the Jacobian:

$$\begin{aligned} \frac{dI(t)}{dt} &= \int_{R(0)} J(\boldsymbol{\Xi},t)\Big\{\frac{\partial\chi\big(\mathbf{X}(\boldsymbol{\Xi},t),t\big)}{\partial t} + \sum_{j=1}^{N}\frac{\partial\chi\big(\mathbf{X}(\boldsymbol{\Xi},t),t\big)}{\partial X_j}\frac{dX_j(\boldsymbol{\Xi},t)}{dt}\Big|_{\boldsymbol{\Xi}}\Big\}d\boldsymbol{\Xi} + \\ &\quad + \int_{R(0)} \chi\Big(\mathbf{X}(\boldsymbol{\Xi},t),t\Big)\underbrace{\Big(\sum_{i=1}^{N}\frac{\partial\dot{X}_i}{\partial X_i}\Big|_{\mathbf{X}=\mathbf{X}(\boldsymbol{\Xi},t)}\Big)J(\boldsymbol{\Xi},t)}\,d\boldsymbol{\Xi}. \end{aligned} \tag{2.3.4}$$

At this point, the Jacobian appears as common factor in both terms of the integrand and is factored out:

$$\begin{aligned} \frac{dI(t)}{dt} &= \int_{R(0)} \Big\{\frac{\partial\chi\big(\mathbf{X}(\boldsymbol{\Xi},t),t\big)}{\partial t} + \sum_{j=1}^{N}\frac{\partial\chi\big(\mathbf{X}(\boldsymbol{\Xi},t),t\big)}{\partial X_j}\frac{dX_j(\boldsymbol{\Xi},t)}{dt}\Big|_{\boldsymbol{\Xi}} + \\ &\quad + \chi\Big(\mathbf{X}(\boldsymbol{\Xi},t),t\Big)\Big(\sum_{i=1}^{N}\frac{\partial\dot{X}_i}{\partial X_i}\Big|_{\mathbf{X}=\mathbf{X}(\boldsymbol{\Xi},t)}\Big)\Big\}J(\boldsymbol{\Xi},t)d\boldsymbol{\Xi}. \end{aligned} \tag{2.3.5}$$

Finally, the integration over $R(0)$ is reverted back to integration over $R(t)$, analogously to (2.3.2), through which step the dependencies on $\mathbf{X}$ reappear:

$$\boxed{\frac{d}{dt}\int_{R(t)} \chi(\mathbf{X},t)d\mathbf{X} = \int_{R(t)} \Big\{\frac{\partial\chi(\mathbf{X},t)}{\partial t} + \sum_{j=1}^{N}\dot{X}_j\frac{\partial\chi(\mathbf{X},t)}{\partial X_j} + \chi(\mathbf{X},t)\sum_{i=1}^{N}\frac{\partial\dot{X}_i}{\partial X_i}\Big\}d\mathbf{X}.} \tag{2.3.6}$$

The result (2.3.6) is known as the TT. The above derivation has clearly shown the central role of Liouville's result (2.2.2.5) in order to arrive at the TT. The consequences of the TT are manifold. For example, if χ is set to the density of realizations in phase space $\rho(\mathbf{X},t)$ and it is required that the phase space integral over any material region of that density cannot change (i.e., realizations cannot leave the material region or the probability mass in the material region must remain constant):

$$\frac{d}{dt}\int_{R(t)} \rho(\mathbf{X},t)d\mathbf{X} = 0, \tag{2.3.7}$$

which is the natural analogy to mass conservation in hydrodynamics, then the integrand in (2.3.6) has to vanish, which in turn is the LE (see section 2.4). Equally important is the special case $\chi = 1$, that makes $I(t)$ equal to the *volume* $V(t)$ of a material region:

$$\chi \equiv 1 \qquad \rightarrow \qquad I(t) = \int_{R(t)} d\mathbf{X} \equiv V(t)\,. \tag{2.3.8}$$

In this situation, the TT implies the result:

$$\frac{dV(t)}{dt} = \int_{R(t)} \Big(\sum_{i=1}^{N} \frac{\partial \dot{X}_i}{\partial X_i} \Big) d\mathbf{X}\,, \tag{2.3.9}$$

stating that the time derivative of the volume of a material region is equal to the integral of the phase–space divergence (see also, section 5.6). It is finally noted that setting $\chi \equiv \rho F$ in the TT, where ρ satisfies the requirement (2.3.7), leads, on the basis of (2.3.6), to the result:

$$\frac{d}{dt} \int_{R(t)} \rho(\mathbf{X},t) F(\mathbf{X},t) d\mathbf{X} = \int_{R(t)} \rho(\mathbf{X},t) \Big\{ \frac{\partial F(\mathbf{X},t)}{\partial t} + \sum_{j=1}^{N} \dot{X}_j \frac{\partial F(\mathbf{X},t)}{\partial X_j} \Big\} d\mathbf{X}\,, \tag{2.3.10}$$

which, similar to the TT, gives a description on how to interchange the time derivative and the phase–space integration. It is noted in passing that combining the second and the third of the terms on the right–hand–side in eq. (2.3.6) into a "divergence" expression, and subsequently rewriting the integral over that divergence expression through the Gauß divergence theorem as a surface integral, leads to a reformulation of result (2.3.6) that is sometimes known as the *Reynolds transport theorem* (e.g., Lin and Segel 1988).

2.4 Formulation of the Liouville Equation

The LE is the continuity equation for the pdf ρ of the state vector $\mathbf{X}$ of a dynamical system. On the basis of the requirement (2.3.7), by setting $\chi = \rho$ in the TT, the LE is obtained as:

$$\boxed{\frac{\partial \rho(\mathbf{X},t)}{\partial t} + \sum_{k=1}^{N} \frac{\partial}{\partial X_k} \Big[\rho(\mathbf{X},t) \dot{X}_k(\mathbf{X},t) \Big] = 0\,,} \tag{2.4.1}$$

where the flow $\dot{\mathbf{X}}$ of the dynamical system in phase space is given by (2.2.2.1); that is, the time evolution of the state $\mathbf{X}$ is governed by the (non–autonomous) dynamical system specified through $\boldsymbol{\Phi}$. Another formulation of the LE that is completely equivalent to (2.4.1) is given by expanding the phase–space derivative:

$$\frac{\partial \rho(\mathbf{X},t)}{\partial t} + \sum_{k=1}^{N} \Phi_k(\mathbf{X},t) \frac{\partial \rho(\mathbf{X},t)}{\partial X_k} = -\psi(\mathbf{X},t) \rho(\mathbf{X},t)\,, \tag{2.4.2}$$

where:

$$\psi(\mathbf{X},t) \equiv \sum_{k=1}^{N} \frac{\partial \Phi_k(\mathbf{X},t)}{\partial X_k} \tag{2.4.3}$$

is the divergence of the flow in phase space. Evidently, since derived from (2.3.7), the LE expresses the conservation of the phase–space integral of the number density of realizations of the dynamical system

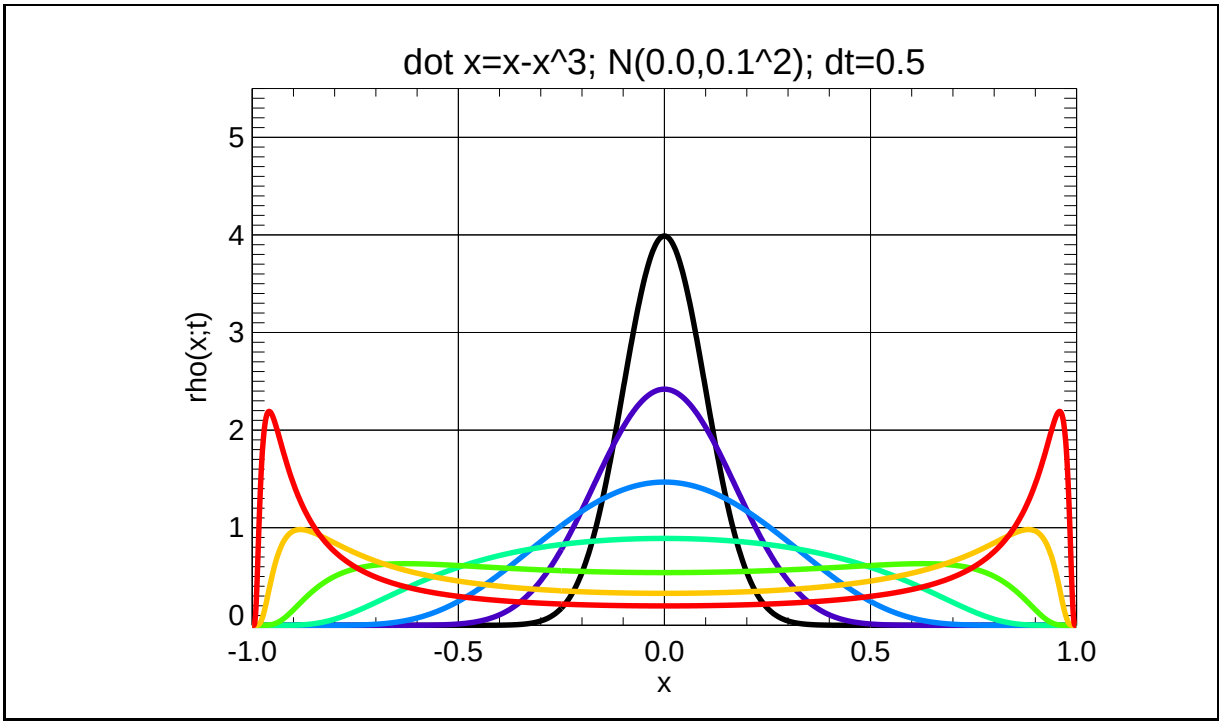


Figure 3: Solution of LE for system $\dot{x} = x - x^3$; initial pdf is $\mathtt{N}(0, 0.1^2)$; $\rho(x,t)$ is shown at time increments of 0.5. Initial pdf is colored black, pdf for last time point shown is red.

(2.2.2.1). As a continuity equation, it is entirely analogous to the continuity equation in hydrodynamics. In the case of the LE, however, the phase space velocity is a known function at every point in phase space through (2.2.2.1), whereas when the continuity equation is considered in physical space in hydrodynamics the flow velocity has to be determined through the momentum equation.

Physically, the LE states that the local change of ρ – at a particular point in phase space – must be exactly balanced by the net flux of realizations across the faces of a small volume surrounding the point under consideration (see, Thompson 1983). In the balance equation for the pdf, given by the LE (2.4.1), no source terms or non–convective fluxes appear. The absence of source terms is equivalent to the requirement that realizations are neither created nor destroyed in phase space. Inspection of the LE in the form (2.4.3) shows that the LE is a linear (in ρ), inhomogeneous partial differential equation with the single dependent variable being the pdf ρ. The independent variables in the LE are time t and the phase space coordinates $\mathbf{X}$. Finally, it is apparent that the solution to the LE is fundamentally dependent on the model dynamics $\mathbf{\Phi}(\mathbf{X}, t)$.

3 Solution of the Liouville Equation

Given the one–to–one relationship between the initial state $\mathbf{X}(t = 0) \equiv \mathbf{\Xi}$ and the state $\mathbf{X}(t)$ of the dynamical system (2.2.2.1) at time t, as expressed through eqs. (2.2.2.2) and (2.2.2.4) (see section 2.2.2), it is possible to formulate an analytical solution to the LE. For obtaining the solution to the LE, written in the

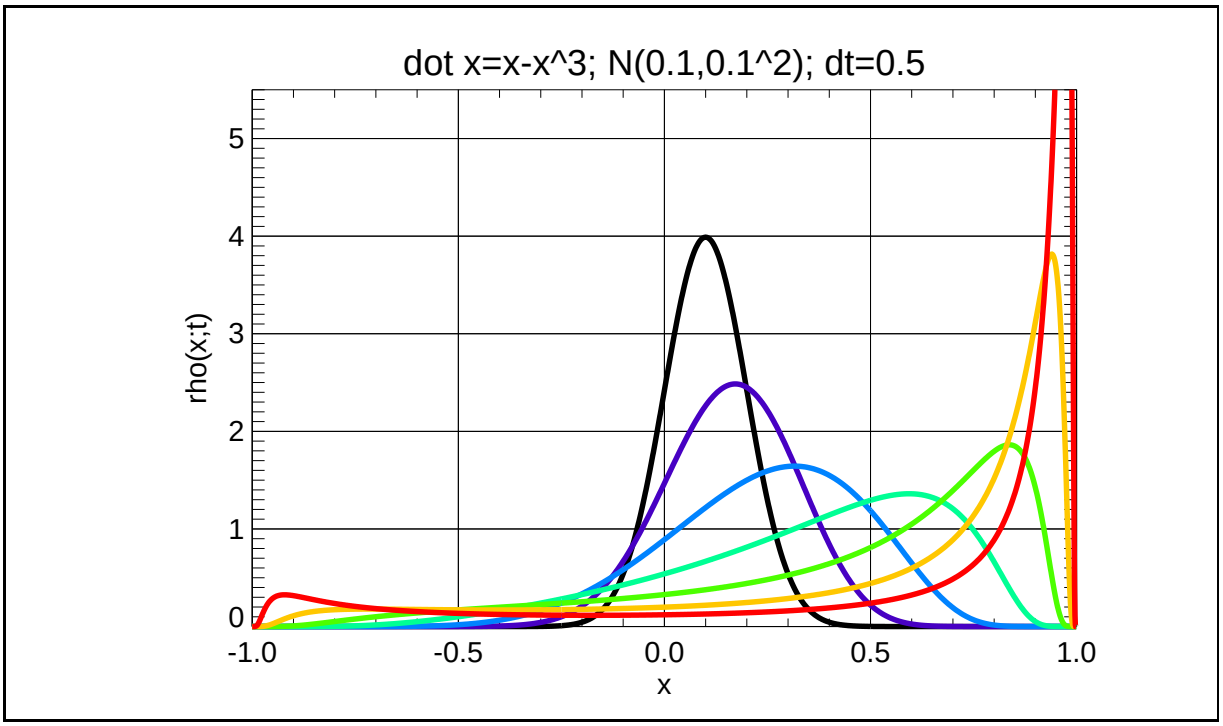


Figure 4: Solution of LE for system $\dot{x} = x - x^3$; initial pdf is $\mathtt{N}(0.1, 0.1^2)$; $\rho(x,t)$ is shown at time increments of 0.5. Initial pdf is colored black, pdf for last time point shown is red.

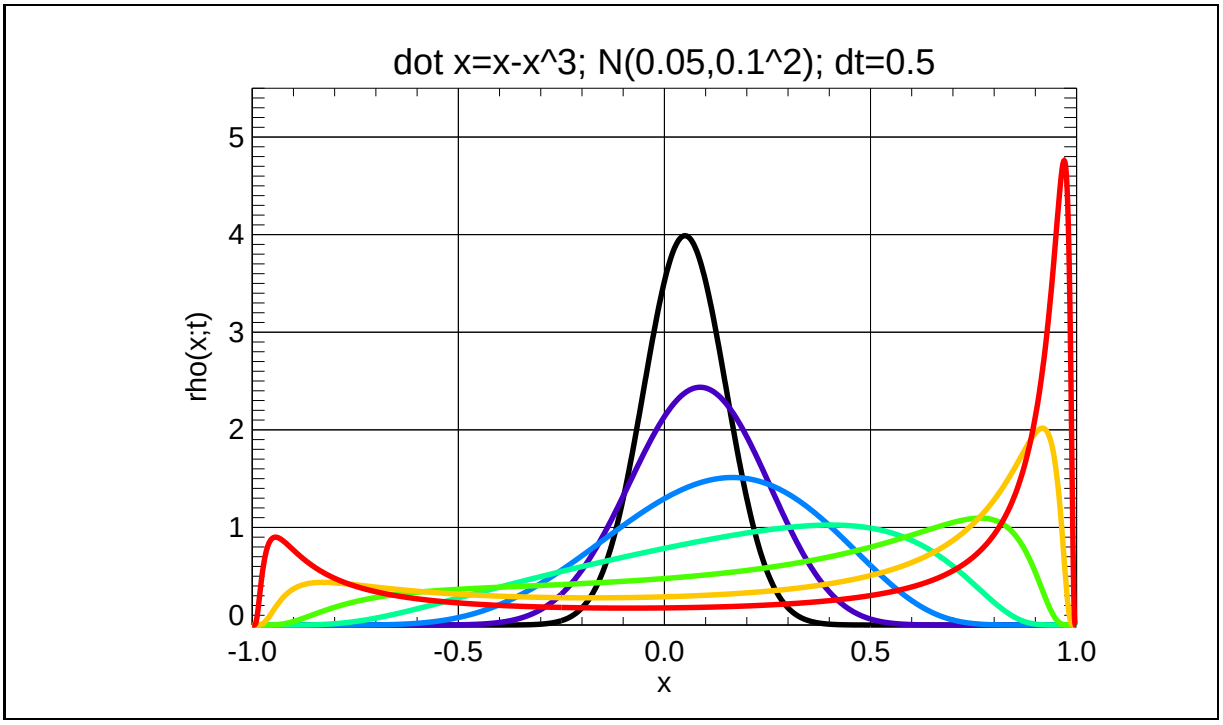


Figure 5: Solution of LE for system $\dot{x} = x - x^3$; initial pdf is $\mathtt{N}(0.05, 0.1^2)$; $\rho(x,t)$ is shown at time increments of 0.5. Initial pdf is colored black, pdf for last time point shown is red.

form (2.4.2), the method of characteristics is used (e.g., Zwillinger 1989) together with the fact that the LE is linear. For an initial condition prescribed through ρ_0:

$$\rho(\mathbf{X}, t=0) = \rho_0(\mathbf{X}), \tag{3.1}$$

the solution is:

$$\rho(\mathbf{X}, t) = \rho_0(\boldsymbol{\Xi}) \underbrace{\exp\left[-\int_0^t \psi\Big(\mathbf{X}(\boldsymbol{\Xi}, t'), t'\Big) dt'\right]}_{\equiv h(\mathbf{X}, t)}. \tag{3.2}$$

In this formulation of the solution (see, Ehrendorfer 1994a; Ehrendorfer 1994b), for a given point $\mathbf{X}$ in phase space and time t, it is necessary to compute $\boldsymbol{\Xi}$ according to (2.2.2.4). Subsequently, $\boldsymbol{\Xi}$ is used for evaluating the solution (3.2) by computing $\rho_0(\boldsymbol{\Xi})$ and referring to the definition of ψ in eq. (2.4.3). An illustration of such a computation is given in section 4.1. It is therefore also evident that the function h is indeed a function of $\mathbf{X}$ and t; for a discussion of h, see section 5, and especially section 5.1. It is further apparent that the solution (3.2) satisfies the initial condition (3.1) and is both non–negative and – essentially through requirement (2.3.7) – correctly normalized. Solution (3.2) does indeed satisfy the LE (2.4.2) (see, Ehrendorfer 1994a).

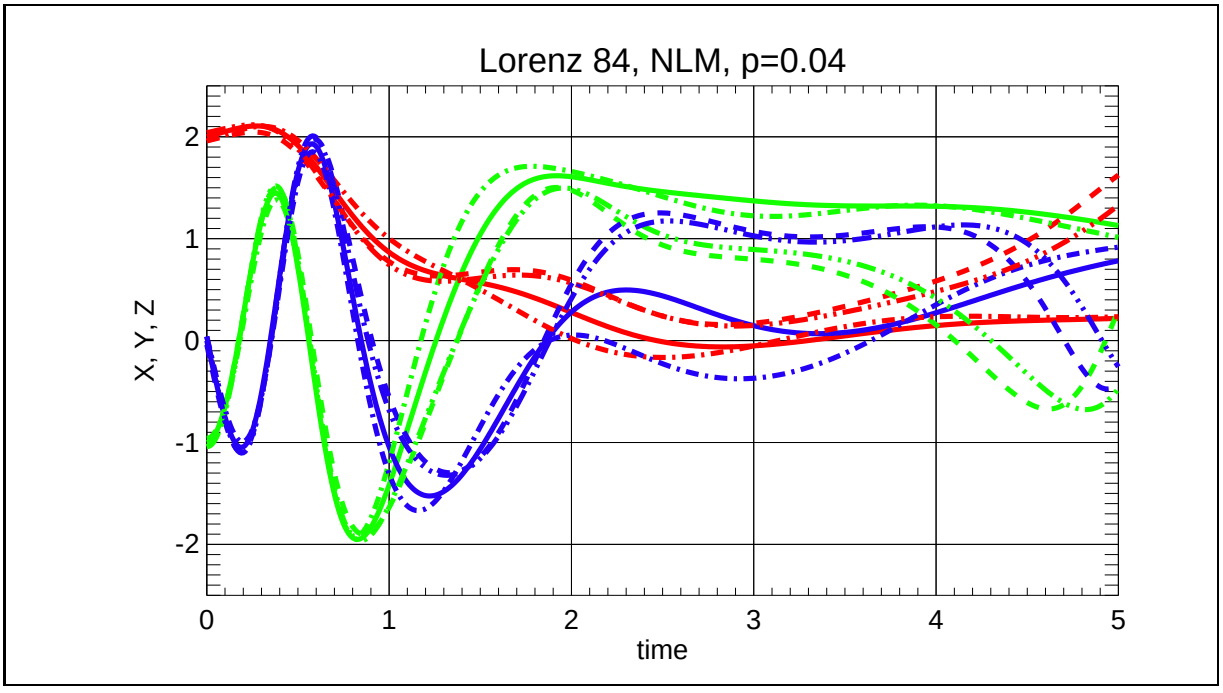


Figure 6: Nonlinear evolution of states in Lorenz (1984) system. Reference initial state is defined by $(2, -1, 0)$. Red X, green Y, blue Z. Perturbation sizes are 0.04, with dashed $(-,-,-)$ perturbation, dash–dot $(-,+,+)$ perturbation, and dash–dot–dot $(+,-,+)$ perturbation on reference initial state.

4 Illustrations

4.1 A one–dimensional autonomous example

As an illustration of the LE and its solution, as expressed in eq. (3.2), the one–dimensional autonomous dynamical system:

$$\frac{d}{dt}x = x - x^3 \tag{4.1.1}$$

is considered, with the functions Φ and ψ (see eqs. (2.2.2.1) and (2.4.3)) given as:

$$\Phi(x) = x - x^3\,, \qquad \psi(x) = 1 - 3x^2\,. \tag{4.1.2}$$

System (4.1.1) has two stable equilibrium points at $x_s = \pm 1$ and one unstable equilibrium point at $x_u = 0$. The LE specific for this system is given by (see eq. (2.4.2)):

$$\frac{\partial \rho(x,t)}{\partial t} + (x - x^3)\frac{\partial \rho(x,t)}{\partial x} = -(1 - 3x^2)\rho(x,t)\,. \tag{4.1.3}$$

The solution to the LE (4.1.3) for an arbitrary initial condition ρ_0 is obtained on the basis of (3.2) as:

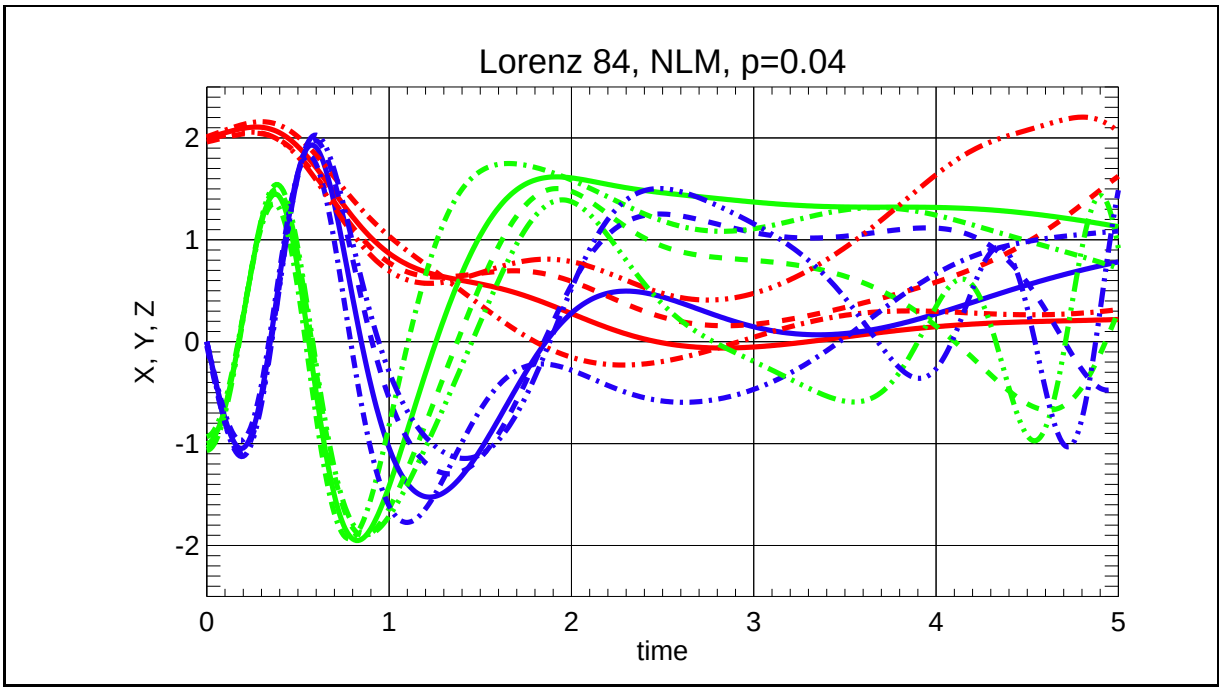


Figure 7: Nonlinear evolution of states in Lorenz (1984) system. As in Fig. 6, except for dash–dot denoting positive SV1 perturbation, and dash–dot–dot negative SV1 perturbation. SV optimized for $t = 1$. For perturbation sizes compare TLD/NLD picture in Fig. 8.

$$\rho(x,t) = \rho_0\Big(\xi[x,t]\Big)\exp\Big[-\int_0^t \underbrace{\Big\{1 - 3\Big(x\{\xi[x,t],t'\}\Big)^2\Big\}}_{=\psi(x)} dt'\Big]\,. \tag{4.1.4}$$

Here, the function ψ is indicated for clarity; note that for the present autonomous system ψ possesses no *explicit* time dependence (time dependence enters only implicitly through the dependence of x on t).

In the more general formulation of a non–autonomous system used in sections 2.4 and 3, ψ possesses an explicit time dependence, as indicated in eq. (2.4.3). For the present system, conditions (2.2.2.2) and (2.2.2.4) – explicitly solving (4.1.1) – are:

$$x = x(\xi,t) = \xi e^t \left(1 - \xi^2 + \xi^2 e^{2t}\right)^{-\frac{1}{2}} \quad \Leftrightarrow \quad \xi(x,t) = x e^{-t} \left(1 - x^2 + x^2 e^{-2t}\right)^{-\frac{1}{2}} . \tag{4.1.5}$$

Illustrations of the functional form of the time evolution of the pdf, given the dynamics (4.1.1), are shown in Figs. 3 – 5. The initial pdf is taken as normal with the same variance in all three illustrations, but with different means. It is apparent that the pdf decreases at the unstable equilibrium point x_u as realizations are attracted to the stable equilibrium points x_s. Depending on how much initial probability mass lies on either side of x_u, the pdf becomes differently asymmetric at later times; for example, in Fig. 4 the pdf at the last time point shown (colored red) is much more strongly peaked at $x_s = +1$ than in Fig. 5, since the initial pdf is centered at 0.1 in the former case, whereas it is centered at 0.05 in the latter case. The pdfs shown in Fig. 3 are entirely symmetric, as the initial pdf is centered at zero.

An example code for carrying out the actual computation for evaluating the solution (4.1.4) is given below. Here `x` denotes x and `time` denotes t. Note that the time integral that appears in (4.1.4) is approximated in this code through an approximate trapezoidal rule (even though the integration could – presumably – be carried out analytically in the present situation).

```
xi = x*exp(-time)/sqrt(1.-x*x+x*x*exp(-2.*time))   ; find xi

a1 = (xi-smean)/sdev
y1 (i) = 1./(sqrt(2.*!pi)*sdev)* exp(-0.5*a1*a1)  ; rho_0 (xi)

xint=0.0
for k = 1 , 100 do begin
tp=k*time/100.0
b=xi*exp(tp)/sqrt(1.0-xi*xi+xi*xi*exp(2.*tp))  ; finding x(xi,t')
c=1.0-3.0*b*b   ; psi (x)
xint=xint+c & endfor

y1 (i) = y1 (i) * exp ( -xint*time/100.0 ) ; apply h(x,t)
```

4.2 A three–dimensional autonomous example

To illustrate the LE in a somewhat higher–dimensional context, the prototypical chaotic model for atmospheric flow proposed by Lorenz (1984) is used. This model consists of three coupled, nonlinear ordinary differential equations for the variables X, Y and Z, written as:

$$\begin{pmatrix} \dot{X} \\ \dot{Y} \\ \dot{Z} \end{pmatrix} = \begin{pmatrix} -Y^2 - Z^2 - aX + aF \\ XY - bXZ - Y + G \\ bXY + XZ - Z \end{pmatrix} , \tag{4.2.1}$$

where the parameters a, b, F, and G take on the values $a = 0.25, b = 4.0, F = 8.0, G = 1.25$. Since this

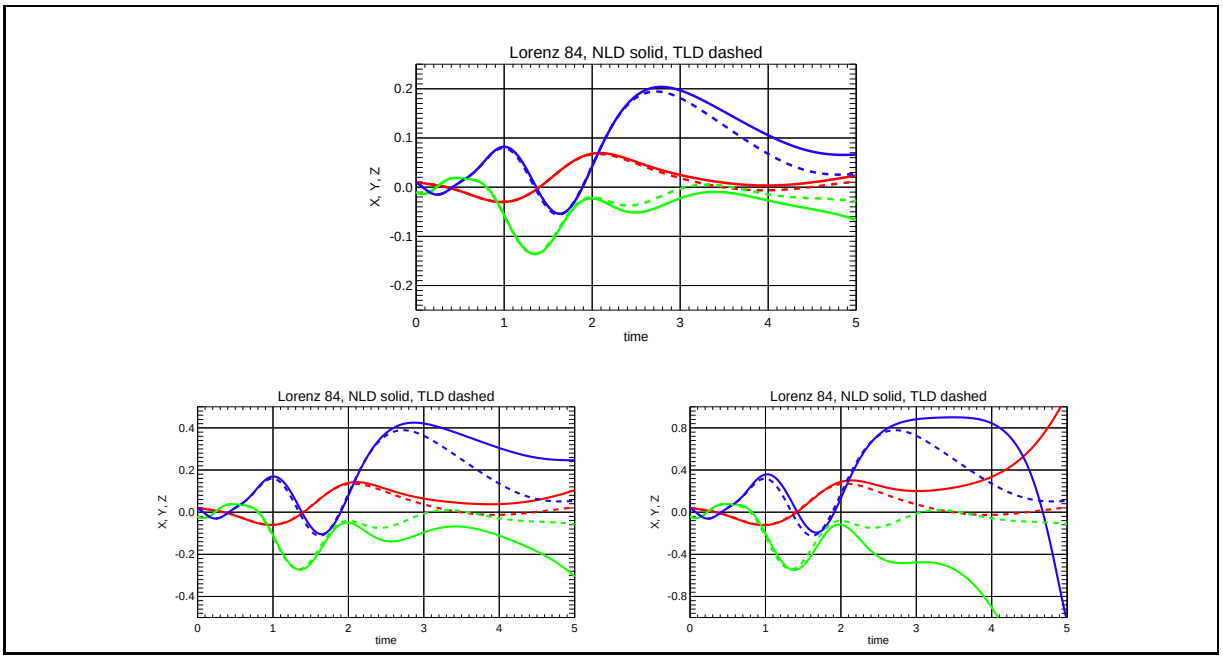


Figure 8: Evolution of perturbations in Lorenz (1984) system. Basic state is defined by $(2, -1, 0)$. Red X, green Y, blue Z. Perturbation size increases by factor of 2. Solid is nonlinear difference (NLD), dashed is tangent–linear difference (TLD). Note that TLD scales exactly.

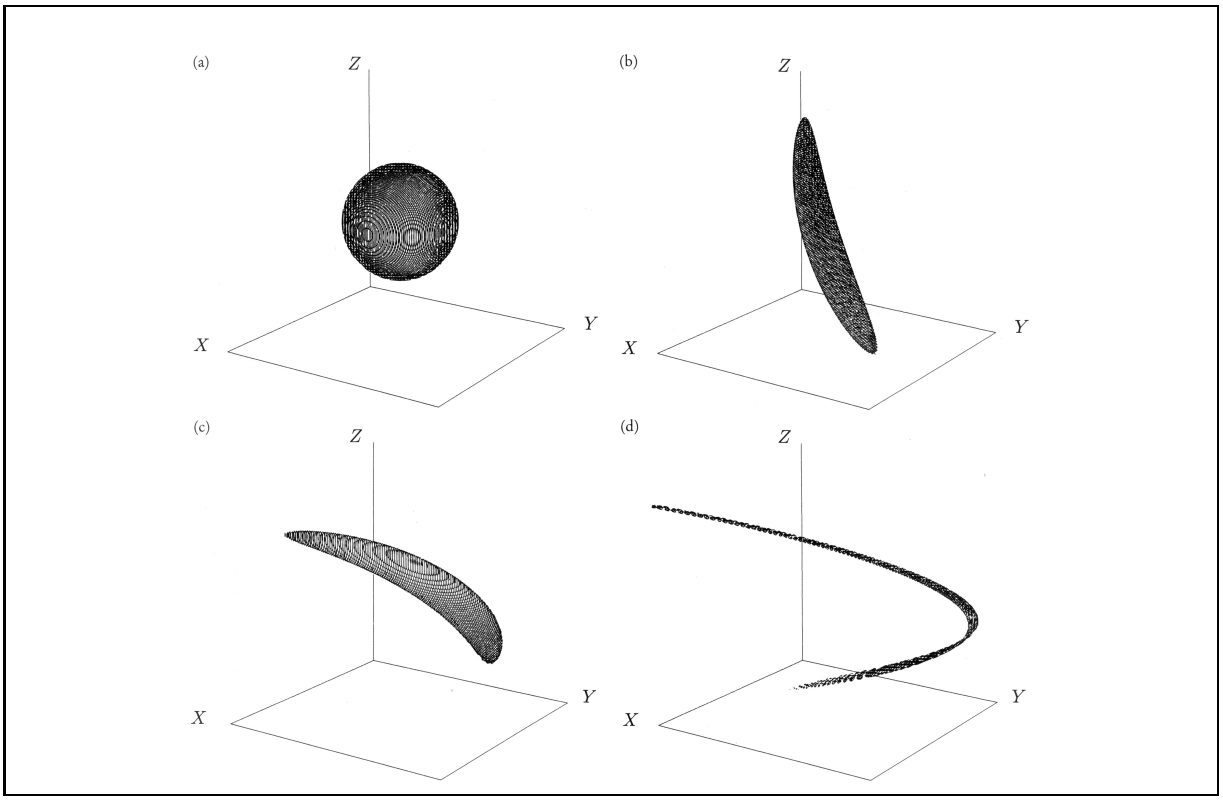


Figure 9: Solution of the Liouville equation for the Lorenz (1984) system.

system will be used later for illustrating other properties of the LE, the tangent–linear system corresponding to (4.2.1) for primed perturbation variables is recorded here, too:

$$\begin{pmatrix} \dot{X}' \\ \dot{Y}' \\ \dot{Z}' \end{pmatrix} = \underbrace{\begin{pmatrix} -a & -2\overline{Y} & -2\overline{Z} \\ \overline{Y} - b\overline{Z} & \overline{X} - 1 & -b\overline{X} \\ b\overline{Y} + \overline{Z} & b\overline{X} & \overline{X} - 1 \end{pmatrix}}_{\mathsf{L}_{\overline{\mathbf{X}}(t)}} \begin{pmatrix} X' \\ Y' \\ Z' \end{pmatrix} , \tag{4.2.2}$$

where L denotes the tangent–linear model operator that depends on the time–dependent basic state $\overline{\mathbf{X}}(t)$ that is used for linearizing the nonlinear model (4.2.1). The tangent–linear system to any nonlinear system is obtained by retaining the term linear in the perturbation quantities in a Taylor series expansion of the nonlinear model dynamics along $\overline{\mathbf{X}}(t)$:

$$\frac{d}{dt}\underbrace{(\mathbf{X} - \overline{\mathbf{X}})}_{\equiv \mathbf{X}'} = \mathbf{\Phi}(\mathbf{X}) - \mathbf{\Phi}(\overline{\mathbf{X}}) \approx \mathsf{L}_{\overline{\mathbf{X}}}\underbrace{(\mathbf{X} - \overline{\mathbf{X}})}_{\equiv \mathbf{X}'} , \tag{4.2.3}$$

where the tangent–linear model operator (illustrated here in eq. (4.2.2) above) is given as:

$$\mathsf{L}_{\overline{\mathbf{X}}} \equiv \left(\frac{\partial \Phi_i(\mathbf{X})}{\partial X_j} \right)_{\overline{\mathbf{X}}} , \tag{4.2.4}$$

and the tangent–linear resolvent $\mathsf{M}_{\Xi,t}$ connects an initial perturbed state to a perturbed state at time t:

$$\mathbf{X}'(t) = \mathsf{M}_{\Xi,t}\mathbf{X}'(t=0) . \tag{4.2.5}$$

An approximation to the dynamics of perturbations made in the form of the linear model (4.2.3) will obviously be valid only to the degree that the perturbations are in some sense small. In the absence of analytical model solutions, numerical solutions to the nonlinear and the tangent–linear Lorenz (1984) model, eqs. (4.2.1) and (4.2.2), respectively, are obtained here with a predictor–corrector method to connect $\mathbf{X}$ and Ξ (see eqs. (2.2.2.2) and (2.2.2.4)). Illustrations of the behavior of the nonlinear system are shown in Figs. 6 and 7. In Fig. 8, the evolution of perturbations is shown, as obtained by both the fully nonlinear difference (solid) in eq. (4.2.3), as well as through (numerically) solving the tangent–linear model, as given in (4.2.5) (dashed). In the three panels in Fig. 8, the size of the initial perturbation increases by a factor of two by going from panel to panel; it is apparent that the tangent–linear solution scales exactly, whereas the nonlinear differences deviate from the tangent–linear solution earlier when the initial perturbation size becomes larger.

In the situation of system (4.2.1), the pdf with its time evolution described through the LE is a function of the three model variables and time, given as $\rho(X,Y,Z,t)$. Stating the LE in the form (2.4.2) is straightforward noting that ψ, defined in (2.4.3), takes on the form:

$$\psi(X,Y,Z) \equiv \frac{\partial \dot{X}}{\partial X} + \frac{\partial \dot{Y}}{\partial Y} + \frac{\partial \dot{Z}}{\partial Z} = -a + (X-1) + (X-1) = 2X - 2 - a . \tag{4.2.6}$$

As in section 4.1, ψ contains no explicit time dependence as the dynamical system under consideration is autonomous. Referring back to the general solution of the LE given in eq. (3.2), the solution of the LE

relevant for the system (4.2.1) can be written in the form:

$$\rho(\mathbf{X},t) = \rho_0(\boldsymbol{\Xi}) \underbrace{\exp\Big[-\int_0^t \psi\Big(\mathbf{X}(\boldsymbol{\Xi},t')\Big)\,dt'\Big]}_{\equiv h(\mathbf{X},t)} . \tag{4.2.7}$$

In stating this form of the solution, the fact that ψ is not explicitly time dependent has been used. Also, as in section 4.1, it is necessary to find $\boldsymbol{\Xi}$ through the (numerical) implementation of eq. (2.2.2.4) appropriate for system (4.2.1) given $\mathbf{X}$ and t. The form of the solution stated in (4.2.7) is shown in Fig. 9. Since, in the present situation, the pdf lives in a three–dimensional phase space, it is obviously necessary to somehow contour three–dimensional regions of the same values of the pdf. An attempt to visualize the pdf is shown in Fig. 9 by showing the surface (as a contour in three–dimensional space) that encloses all pdf values that are greater than one at a given time. At the initial time (Fig. 9(a)) that surface is a sphere, since the initial pdf ρ_0 is specified to be multivariate normal with the same variance for all three variables. At a somewhat later time (Fig. 9(b)) that surface becomes elongated along the direction of preferred error growth in the model (4.2.1), and still later (Figs. 9(c), (d)) acquires some curvature and clearly nonlinear features. It is noted that this surface (defined through the equation "ρ equal to some specified constant") is clearly not a material surface, since realizations on that surface clearly do not have to remain connected to that particular value of ρ (see also, Ehrendorfer 1997).

5 Comments on the Liouville Equation

In this chapter various comments relating to the LE and atmospheric predictability are brought together.

5.1 A Likelihood Ratio

It is noted that the quantity h, defined in eq. (3.2), may be referred to as likelihood ratio, as it is the ratio of two pdfs:

$$h(\mathbf{X},t) = \frac{\rho(\mathbf{X},t)}{\rho_0(\boldsymbol{\Xi})} \equiv \exp\Big[-\int_0^t \psi\Big(\mathbf{X}(\boldsymbol{\Xi},t'),t'\Big)\,dt'\Big] . \tag{5.1.1}$$

On the other hand, since, on the basis of (2.2.2.2), $\mathbf{X}$ can be viewed as the time–dependent transform of $\boldsymbol{\Xi}$, it is possible to ascertain that the pdf of $\mathbf{X}$ (viewed as the transformed $\boldsymbol{\Xi}$) may be specified in terms of the pdf of $\boldsymbol{\Xi}$ in the form (see, e.g., Theorem 4.6.18 in Dudewicz and Mishra 1988):

$$\frac{\rho(\mathbf{X},t)}{\rho_0(\boldsymbol{\Xi})} = \frac{1}{|J|} , \tag{5.1.2}$$

where J – already defined in eq. (2.2.2.3) – is the determinant of the Jacobian of the transformation:

$$J \equiv \det\Big(\frac{\partial \mathbf{X}(\boldsymbol{\Xi},t)}{\partial \boldsymbol{\Xi}}\Big|_{\boldsymbol{\Xi}}\Big) = \det\Big(\mathsf{M}_{\boldsymbol{\Xi},t}\Big) . \tag{5.1.3}$$

The second equality in the above equation (5.1.3) represents expressing the Jacobian in terms of the resolvent $\mathsf{M}_{\boldsymbol{\Xi},t}$ of the tangent–linear model, defined in eq. (4.2.5) as the operator that maps an initial

perturbation into a perturbation at time t. The identification used in eq. (5.1.3) becomes clear by, referring to (2.2.2.2), taking the following Taylor series expansion:

$$\mathbf{X}(\boldsymbol{\Xi}+\boldsymbol{\Xi}',t) = \mathbf{X}(\boldsymbol{\Xi},t) + \frac{\partial \mathbf{X}(\boldsymbol{\Xi},t)}{\partial \boldsymbol{\Xi}}\Big|_{\boldsymbol{\Xi}}\boldsymbol{\Xi}' + hot\,. \tag{5.1.4}$$

It is evident from eq. (5.1.4) that $\mathsf{M}_{\boldsymbol{\Xi},t}$ – the resolvent of the tangent–linear model that linearizes the mapping $\mathbf{X} = \mathbf{X}(\boldsymbol{\Xi},t)$ around a trajectory starting at $\boldsymbol{\Xi}$ up to time t – is precisely the same as $\frac{\partial \mathbf{X}(\boldsymbol{\Xi},t)}{\partial \boldsymbol{\Xi}}\big|_{\boldsymbol{\Xi}}$, as already indicated in eq. (5.1.3).

Consequently, on the basis of the results (5.1.1), (5.1.2), and (5.1.3), the likelihood ratio h can be expressed in the two different, but exactly equivalent formulations as follows:

$$\boxed{h(\mathbf{X},t) = \exp\Big[-\int_0^t \psi\Big(\mathbf{X}(\boldsymbol{\Xi},t'),t'\Big)\,dt'\Big] = \Big[\big|\det\Big(\mathsf{M}_{\boldsymbol{\Xi},t}\Big)\big|\Big]^{-1}.} \tag{5.1.5}$$

The important result (5.1.5) will be referred to in subsequent sections. Fig. 10 shows the (almost) exact agreement of computing h by the two methods indicated in eq. (5.1.5), for five different initial conditions $\boldsymbol{\Xi}$, for the Lorenz (1984) system (4.2.1).

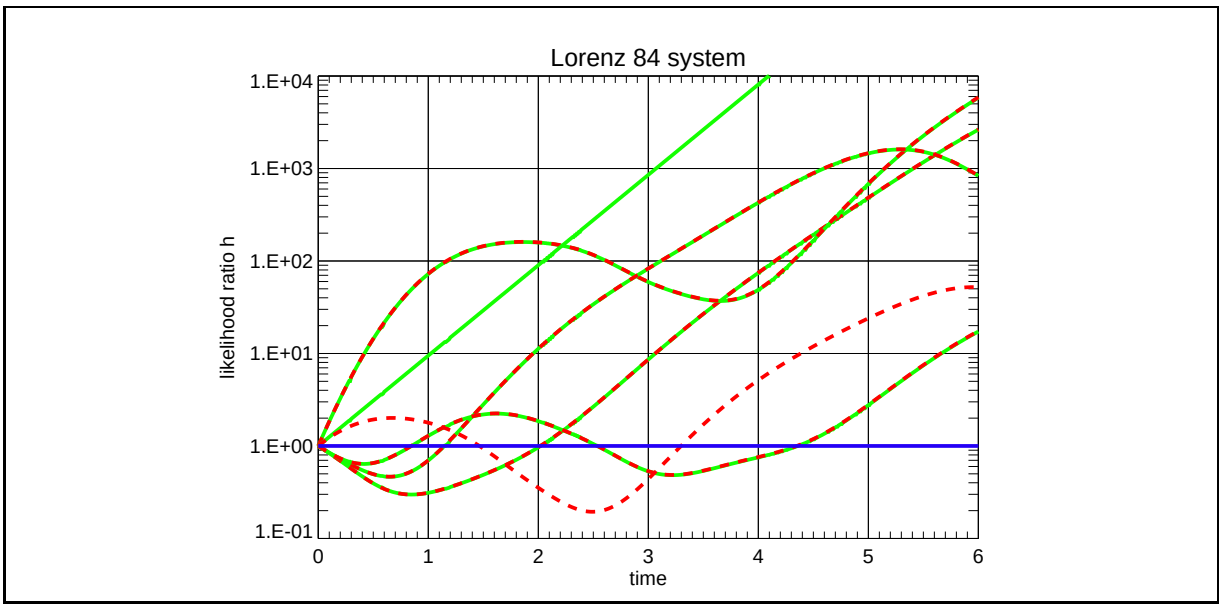


Figure 10: Likelihood ratio h, defined in (3.2), for the Lorenz (1984) system (4.2.1), for five different initial conditions. Overplotted green and red curves show results computed by determinant of resolvent (red), and by evaluating ψ (green) in (5.1.5). The dashed red curve shows h for $F = G = 0$, with $\boldsymbol{\Xi} = 0$; the solid green curve shows h when computed for a "resting" basic state; in that case $h(t) = \exp[-(-a-2)t]$.

5.2 The Liouville Equation and Singular Vectors

To illustrate a connection between the LE and the computation of singular vectors (SVs), consider the linear non–autonomous system (see also, e.g., eq. (4.2.2)):

$$\dot{\mathbf{X}} = \mathsf{L}(t)\mathbf{X} \tag{5.2.1}$$

as the dynamics (2.2.2.1) relevant for the LE (2.4.1). In that situation the phase space divergence ψ, defined in (2.4.3), is independent of the position in phase space, but remains to be a function of time t:

$$\psi(\mathbf{X},t) = \psi(t) = \sum_{k=1}^{N} (\mathsf{L}(t))_{k,k} \equiv \sigma(t)\,. \tag{5.2.2}$$

In the autonomous situation, L and σ become time–independent, and, consequently, the eigendecomposition of L (assumed to exist) has the time–independent eigenvalues l_k. In that situation, ψ may be written as the sum of the eigenvalues l_k of L (e.g., Strang 1993):

$$\psi = \mathrm{trace}(\mathsf{L}) = \sum_{k=1}^{N} l_k\,. \tag{5.2.3}$$

Through the solution of the autonomous version of (5.2.1) in the form:

$$\mathbf{X}(t) = e^{\mathsf{L}t}\boldsymbol{\Xi} \tag{5.2.4}$$

the resolvent M_t (see, eq. (4.2.5)) is identified as:

$$\mathsf{M}_t = e^{\mathsf{L}t}\,, \tag{5.2.5}$$

which yields the following relation between l_k and the eigenvalues m_k of M_t:

$$m_k = e^{l_k t}\,, \qquad k = 1,\ldots,N\,. \tag{5.2.6}$$

Referring back to the definition of the likelihood ratio, eq. (3.2), relation (5.1.5) becomes explicit in the present autonomous situation as follows:

$$h^{-1}(t) = \exp\Big(\int_0^t \sum_{k=1}^{N} l_k dt'\Big) = \exp\Big(t\sum_{k=1}^{N} l_k\Big) = \prod_{k=1}^{N} e^{l_k t} = \prod_{k=1}^{N} m_k = \det \mathsf{M}_t\,. \tag{5.2.7}$$

Eq. (5.2.7) is an explicit illustration of the general result (5.1.5) for the special situation of the linear system (5.2.1) considered in autonomous form, where relation (5.2.6) was used, as well as the fact that the determinant of a matrix may be written as the product of its eigenvalues.

Referring back to the non–autonomous situation, it is evident that the LE (2.4.2) may be written on the basis of (5.2.1) and (5.2.2) as:

$$\frac{\partial\rho}{\partial t} + \sum_{k=1}^{N} (\mathsf{L}(t)\mathbf{X})_k \frac{\partial\rho}{\partial X_k} + \sigma(t)\rho = 0\,, \tag{5.2.8}$$

with the explicit solution given on the basis of (3.2) and (5.2.2) as follows:

$$\rho(\mathbf{X},t) = \rho_0(\boldsymbol{\Xi}) \exp\Big[-\int_0^t \sigma(t')dt'\Big]\,, \tag{5.2.9}$$

or, more explicitly, by denoting the resolvent of the non–autonomous system (5.2.1) as M_t:

$$\rho(\mathbf{X},t) = \rho_0(\mathsf{M}_t^{-1}\mathbf{X}) \exp\Big[-\int_0^t \sigma(t')dt'\Big]\,. \tag{5.2.10}$$

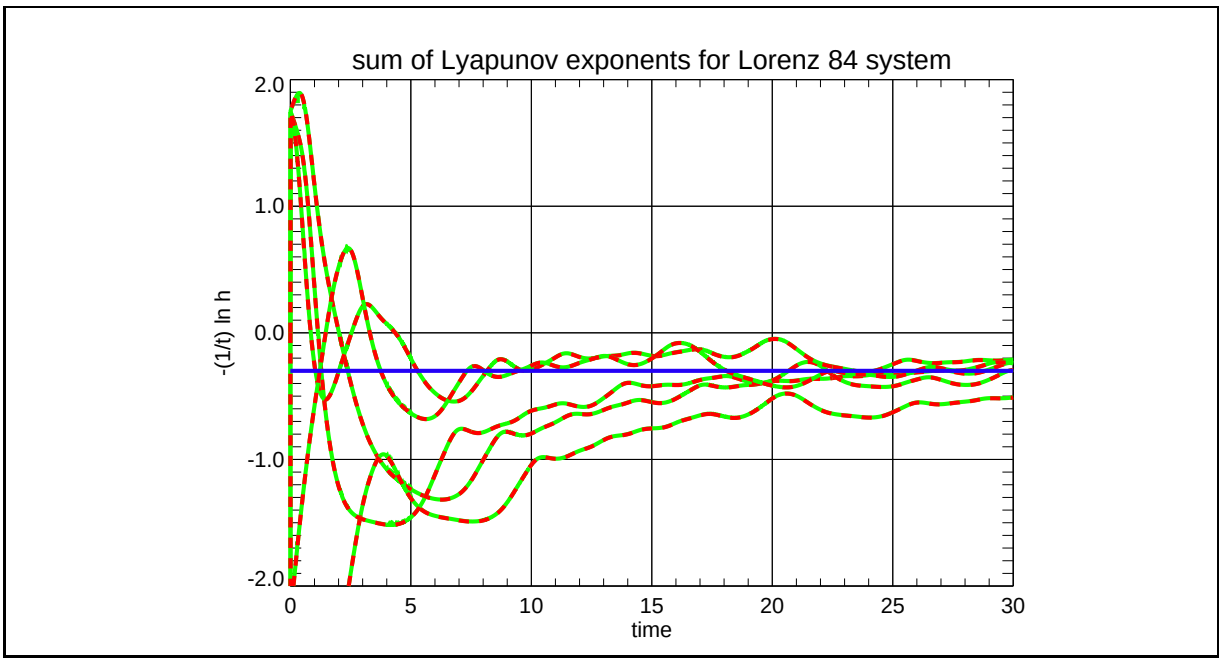


Figure 11: Sum of Lyapunov exponents as defined in (5.3.1), computed via the likelihood ratio h, defined in (3.2), for the Lorenz (1984) system (4.2.1), for five different initial conditions (as in Fig. 10). Overplotted green and red curves show results for $\sum_k \hat{\gamma}$ (see eq. (5.3.2)) obtained from h that is computed either through the determinant of resolvent (red), or by evaluating ψ (green) according to eq. (5.1.5).

Equation (5.2.10) is the solution to the LE (5.2.8) appropriate for the non–autonomous system (5.2.1) using the definition (5.2.2). It clearly allows for computing the time evolution of the pdf associated with a linear system for an arbitrary ρ_0 given knowledge about L and the associated resolvent M_t (see also, Tribbia and Baumhefner 1993).

As a next step the following SV problem using the same norm – described through $\mathsf{C}^{\mathrm{T}}\mathsf{C}$ – at initial and final times, is considered (see, e.g., Ehrendorfer and Tribbia 1997, Errico et al. 2001):

$$\left(\mathsf{C}^{\mathrm{T}}\mathsf{C}\right)^{-1}\mathsf{M}_t^{\mathrm{T}}\left(\mathsf{C}^{\mathrm{T}}\mathsf{C}\right)\mathsf{M}_t\mathbf{z}_0 = \lambda\mathbf{z}_0 \quad \text{subject to}: \ \mathbf{z}_0^{\mathrm{T}}\left(\mathsf{C}^{\mathrm{T}}\mathsf{C}\right)\mathbf{z}_0 = 1\,. \tag{5.2.11}$$

Given the (squared) singular value spectrum λ_k, the product of the λ_k determines the likelihood ratio h through:

$$\prod_{k=1}^{N}\lambda_k = \det\left[\left(\mathsf{C}^{\mathrm{T}}\mathsf{C}\right)^{-1}\mathsf{M}_t^{\mathrm{T}}\left(\mathsf{C}^{\mathrm{T}}\mathsf{C}\right)\mathsf{M}_t\right] = \left(\det\mathsf{M}_t\right)^2 = \left[h(\mathbf{X},t)\right]^{-2}, \tag{5.2.12}$$

where (5.1.5) has been used (omitting the subscript $_{\Xi}$) together with relations between determinants and eigenvalues of matrices (e.g., Strang 1993). Result (5.2.12) implies the following relation between the likelihood ratio h and the eigenvalue spectrum λ_k:

$$\boxed{h^2(\mathbf{X},t) = \left(\prod_{k=1}^{N}\lambda_k\right)^{-1}.} \tag{5.2.13}$$

Retracing the steps that lead to result (5.2.13), it is evident that (5.2.13) is valid for resolvents M_t that correspond to non–autonomous (and autonomous) linear systems systems. Clearly, result (5.2.13) may be used to reexpress the solution (5.2.10) of the LE for system (5.2.1) in the form:

$$\boxed{\rho(\mathbf{X},t) = \rho_0(\mathsf{M}_t^{-1}\mathbf{X})\Big(\prod_{k=1}^{N}\lambda_k\Big)^{-1/2}}\,, \tag{5.2.14}$$

so that knowledge of the resolvent M_t and its singular value spectrum is sufficient to determine the time evolution of the pdf.

Referring back to (5.1.5), it is seen that a consequence of (5.2.13) is that for tangent–linear systems with vanishing phase space divergence (i.e., $\psi = 0$) the product of the squared singular values is one:

$$\psi = 0 \qquad \Rightarrow \qquad \prod_{k=1}^{N}\lambda_k = 1\,. \tag{5.2.15}$$

It is obvious that condition (5.2.15) does not necessarily imply that the singular value spectrum is symmetric in the sense that $\lambda_k = \lambda_{N-k+1}^{-1}$ $(k = 1,2,...,\frac{N}{2})$ even though it is interesting to ask under what circumstances such symmetry will exist; it should be expected that these circumstances will be closely related to properties of the basic state used to define the resolvent M_t. Further, it is clear that (5.2.15) implies that the averaged sum of the squared singular values is greater (or equal) than one:

$$\prod_{k=1}^{N}\lambda_k = 1 \qquad \Rightarrow \qquad \frac{1}{N}\sum_{k=1}^{N}\lambda_k \geq 1\,, \tag{5.2.16}$$

essentially, because the arithmetic mean is greater (or equal) than the geometric mean (with equality only if all λ_k are equal).

5.3 Lyapunov Exponents

The Lyapunov exponents relevant for a nonlinear dynamical system of the form (2.2.2.1) may be defined as (see, e.g., Parker and Chua 1989):

$$\gamma_k \equiv \lim_{t\to\infty} \underbrace{\frac{1}{t}\ln\Big|m_k\Big(\mathsf{M}_{\boldsymbol{\Xi},t}\Big)\Big|}_{\equiv\hat{\gamma}_k}\,, \qquad k = 1,2,...,N\,, \tag{5.3.1}$$

where the resolvent $\mathsf{M}_{\boldsymbol{\Xi},t}$ is defined in the context of eq. (4.2.5), and m_k denotes the eigenvalues of $\mathsf{M}_{\boldsymbol{\Xi},t}$ (see, section 5.2). Clearly, through the relationship between h and M discussed in section 5.1, especially through eq. (5.1.5), the following relationship may be derived between the likelihood ration h and the sum of the (unconverged) Lyapunov exponents $\hat{\gamma}_k$:

$$\sum_{k=1}^{N}\hat{\gamma}_k = \frac{1}{t}\sum_{k=1}^{N}\ln\Big|m_k\Big| = \frac{1}{t}\ln\Big|\prod_{k=1}^{N}m_k\Big| = \frac{1}{t}\ln\Big|\det\mathsf{M}_{\boldsymbol{\Xi},t}\Big| = \frac{1}{t}\ln\Big[h(\mathbf{X},t)\Big]^{-1}\,. \tag{5.3.2}$$

On the basis of (5.3.2), it follows that the sum of the Lyapunov exponents may be expressed in terms of the likelihood ratio as:

$$\boxed{\sum_{k=1}^{N} \gamma_k = -\lim_{t\to\infty} \frac{1}{t} \ln h(\mathbf{X}, t)\,.} \tag{5.3.3}$$

Alternatively, by reexpressing h through the result (5.2.13) in terms of the product of λ_k, and inserting into (5.3.2), the following relationship between the sum of the (unconverged) Lyapunov exponents $\hat{\gamma}_k$ and the logarithms of the squared singular values λ_k is obtained:

$$\sum_{k=1}^{N} \hat{\gamma}_k = \sum_{k=1}^{N} \frac{1}{2t} \ln \lambda_k\,, \tag{5.3.4}$$

or, for the sum of the Lyapunov exponents themselves:

$$\sum_{k=1}^{N} \gamma_k = \lim_{t\to\infty} \frac{1}{2t} \sum_{k=1}^{N} \ln \lambda_k\,. \tag{5.3.5}$$

Even though both eqs. (5.3.4) and (5.3.5) are written in terms of sums over k, the relation between an individual γ_k and λ_k should hold analogously. For the chaotic attractor of the Lorenz (1984) system, the sum of the three Lyapunov exponents is *negative* (about -0.3 for the parameters used; see section 4.2, and Fig. 11). Thus, in the limit, h *grows* exponentially (see Fig. 10). Fig. 11 illustrates how $-t^{-1} \ln h$ converges to $\sum_k \hat{\gamma}$ (eq. (5.3.3)) as a function of t for five different initial conditions.

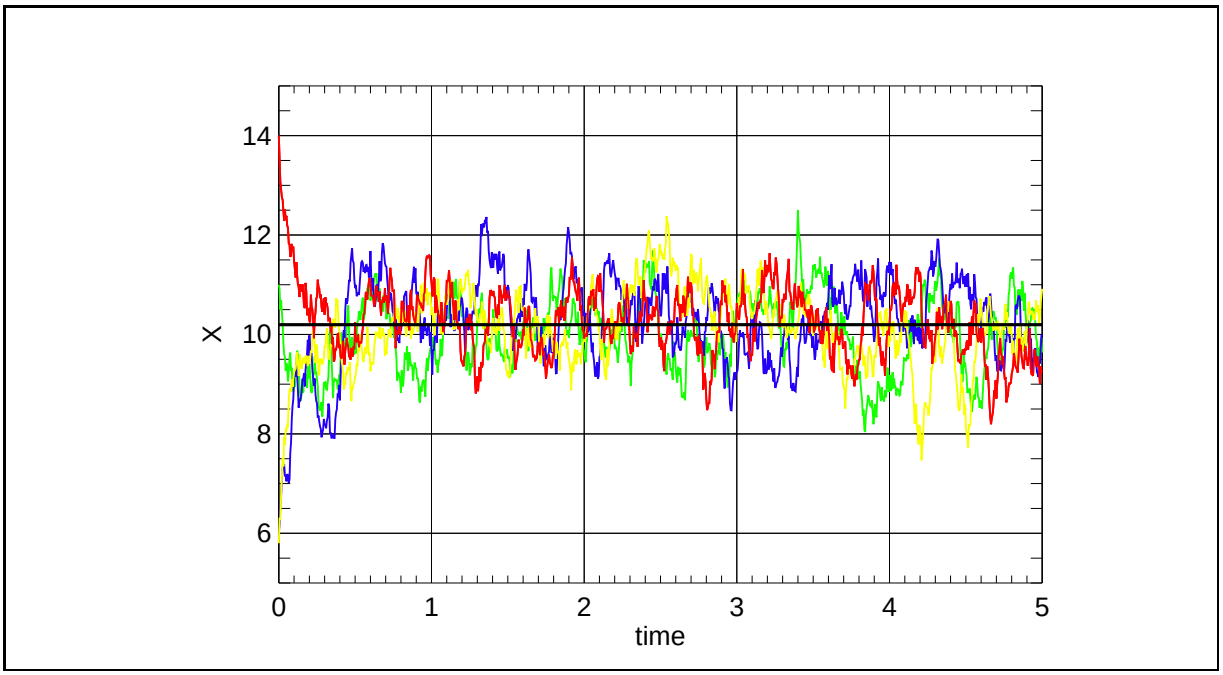


Figure 12: Numerical solution of one-dimensional stochastic differential equation (5.4.1) with $\Gamma = 10$ for system (5.4.4) and four different initial conditions. The equilibrium pdf is not normal, its mean close to, but not equal to $X_{s,1} = 10.19615$ (black, solid).

5.4 The Fokker–Planck Equation

Random processes added to the governing dynamics (2.2.2.1) appear in the equation governing the evolution of the pdf, namely the LE, as a diffusion term, since the transport of phase space points by random motions is a diffusive process (see, e.g., Thompson 1972, Thompson 1983, de Groot and Mazur 1984). The LE written for such a dynamical system that includes random processes to account for, for example, model error, is generally referred to as Fokker–Planck equation (FPE). As in the case of the LE, the FPE (see, e.g., Risken 1989, Gardiner 1990, Soize 1994) has only one dependent variable, namely the probability density function ρ, and it is a linear equation (Thompson 1972).

Selected references to the FPE include the work by Hasselmann (1976), Thompson (1983) and Thompson (1985b), accounting by random processes for unknown forcings in the equations, and investigating the problem of determining equilibrium statistics of the atmosphere/climate system under such circumstances. It is worth pointing out that the FPE is – quite analogously to the LE – governing the time evolution of the pdf, and, as such, also contains all information about the equilibrium statistics of the forced dynamical system, as well as all relevant information regarding the predictability of that system (Hasselmann 1976). The statistical equilibrium between forcing and dissipation has been referred to as fluctuation–dissipation relation (see, e.g., Penland 1989 and Penland and Matrosova 1994). Thompson (1983) has discussed the problem of finding analytical solutions to the stationary form of the FPE (see also, Thompson 1985b).

As an example, consider the one–dimensional dynamical system that includes δ–correlated (white) noise:

$$\dot{X} = \Phi(X) + \eta(t) \qquad \text{with:} \qquad < \eta(t)\eta(t') >= \Gamma\delta(t-t')\,, \tag{5.4.1}$$

where $\eta(t)$ is a normal random variable, with mean zero and variance Γ. The FPE for system (5.4.1) is obtained by inserting $\dot{X}$ into the LE (2.4.1) as:

$$\boxed{\frac{\partial\rho(X,t)}{\partial t} + \frac{\partial}{\partial X}\Big[\Phi(X)\rho(X,t) - \underbrace{\frac{\Gamma}{2}\frac{\partial\rho(X,t)}{\partial X}}_{=\eta\rho}\Big] = 0\,,} \tag{5.4.2}$$

where the first term in brackets results from the deterministic component in (5.4.1) and the second (diffusive) term results from the stochastic component in (5.4.1). Clearly, for a stationary (equilibrium) solution of (5.4.2) it is necessary that the bracketed term is a constant.

As an alternative to solving analytically for the stationary solution of (5.4.2), a numerical integration of the stochastic differential equation (5.4.1) may be carried out as, for example:

$$X(t+\Delta t) = X(t) + \Phi(X)\Delta t + \sqrt{\Gamma} * \sqrt{\Delta t} * g \qquad \text{with:} \qquad g \sim \mathtt{N}(0,1)\,, \tag{5.4.3}$$

where g is a standard–normal random variable (see, e.g. Penland 1989). Fig. 12 shows the result of four integrations of eq. (5.4.1) according to (5.4.3) with different initial conditions with the deterministic dynamics specified as:

$$\Phi(X) = -X^2 + 10X + 2\,. \tag{5.4.4}$$

Note that the two stationary solutions of the *unforced* system (5.4.1), given the dynamics (5.4.4), are given by $X_{s,1} = 10.19615$ and $X_{s,2} = -0.19615$. It is noted that the equilibrium pdf of the forced system has a mean close to, but not equal to, $X_{s,1}$. For a detailed discussion of the impact of forcing on the equilibrium statistics of nonlinear dynamical systems see Palmer (1999) and Palmer (2000).

5.5 The Stochastic–Dynamic Equations

The LE was used by Epstein (1969) as the starting point to derive the so–called stochastic–dynamic equations. The stochastic–dynamic equations describe the time evolution of the statistical moments of a state vector governed by a nonlinear dynamical system such as eq. (2.2.2.1). The statistical moments are the expectations of various functions of powers of the state vector.

To review the computation of expectations consider the random variable X with pdf $f(x)$, that is, $X \sim f(x)$, and the random variable Y that is related to X through the deterministic function r:

$$Y = r(X)\,. \tag{5.5.1}$$

One possibility for the computation of the expectation of Y is given through determining the pdf $g(y)$ of Y (from the known pdf of X), essentially through equation (5.1.2), and then directly compute $E(Y)$ as (e.g. DeGroot 1986, p. 184):

$$E[r(X)] = E[Y] = \int yg(y)dy\,. \tag{5.5.2}$$

In analogy to eq. (5.5.2), the expectation of the model state $\mathbf{x}_t$ at time t is computed from the pdf ρ_t for the random variable $\mathbf{x}_t$, as:

$$E[\mathbf{x}_t] = \int \mathbf{x}\rho_t(\mathbf{x})d\mathbf{x}\,. \tag{5.5.3}$$

As an extension, the expectation of any function s of $\mathbf{x}_t$ (e.g., any power of $\mathbf{x}_t$) is computed as:

$$E[s(\mathbf{x}_t)] = \int s(\mathbf{x})\rho_t(\mathbf{x})d\mathbf{x}\,. \tag{5.5.4}$$

It is noted that result (5.5.4) accomplishes the computation of the expectation of the random variable $s(\mathbf{x}_t)$ *without* actually computing its associated pdf (see, e.g., DeGroot 1986), as is the case in eq. (5.5.2). Eq. (5.5.4), more abstractly rewritten as:

$$E[r(X)] = \int r(x)f(x)dx\,, \tag{5.5.5}$$

is, in fact, the fundamental basis of ensemble prediction, in which the Monte Carlo approach is used to compute (among other things) the expectation of the state $\mathbf{x}_t$ at time t:

$$E[\mathbf{x}_t] = E[\mathtt{M}_t(\mathbf{x}_0)] = \int \mathtt{M}_t(\mathbf{x})\rho_0(\mathbf{x})d\mathbf{x}\,, \tag{5.5.6}$$

on the basis of the pdf ρ_0 of the initial state variable $\mathbf{x}_0$, where the nonlinear model $\mathtt{M}_t$ takes on the role of the function r in eq. (5.5.5) (see also, Paegle and Robl 1977).

Evidently, from (5.5.6), or (5.5.4), the expectation of the variable $s(\mathbf{x}_t)$ is time dependent. That time dependence is described by the stochastic–dynamic equations that govern the time evolution of expectations. An appropriate starting point for deriving these equations is given by taking the time derivative of

eq. (5.5.4), and subsequently using the transport theorem (2.3.6) to obtain the second line in eq. (5.5.7), where ψ is defined in eq. (2.4.3), and the operator $\frac{d}{dt}$ inside the integral is simply the sum of the first two operators inside the integral on the right–hand–side of eq. (2.3.6):

$$\begin{aligned}
\frac{d}{dt}E[s(\mathbf{x})] &\equiv \frac{d}{dt}\int s(\mathbf{x})\rho_t(\mathbf{x})d\mathbf{x} = \\
&\overset{\text{TT}}{=} \int\Big(\frac{d}{dt}(s\rho_t)+(s\rho_t)\psi\Big)d\mathbf{x} = \\
&= \int\Big(\rho_t\frac{ds}{dt}+s\frac{d\rho_t}{dt}+s\rho_t\psi\Big)d\mathbf{x} = \\
&= \int\Big(\rho_t\frac{ds}{dt}+s\Big[\frac{d\rho_t}{dt}+\rho_t\psi\Big]\Big)d\mathbf{x} = \\
&\overset{\text{LE}}{=} \int\rho_t\frac{ds}{dt}d\mathbf{x} = \\
&= E\Big[\frac{ds(\mathbf{x})}{dt}\Big]. \qquad (5.5.7)
\end{aligned}$$

The third and fourth line in eq. (5.5.7) are obtained by simple rearrangements, whereas the fifth line is obtained by observing that the bracketed term in the fourth line is zero on the basis of the LE in the form (2.4.1). The last line in eq. (5.5.7) is obtained by recognizing that the integral in the fifth line is simply the expectation of the time derivative of s. Note also the close analogy between result (2.3.10) and the equality expressed through the fifth line in eq. (5.5.7). The important result eq. (5.5.7) relates the time derivative of the expectation to the expectation of time derivatives and is therefore at the basis of deriving the stochastic–dynamic equations (see also, Epstein 1969, and Fortak 1973):

$$\boxed{\frac{d}{dt}E[s(\mathbf{x})] = E\Big[\frac{ds(\mathbf{x})}{dt}\Big].} \qquad (5.5.8)$$

To illustrate the implications of eq. (5.5.8) consider the following one–dimensional example with governing dynamics given by:

$$\dot{X} = aX^2+bX+c\,. \qquad (5.5.9)$$

Consider the function s_1 as:

$$s_1(X) = X\,, \qquad (5.5.10)$$

with the notations:

$$E[s_1(X)] = E[X] \equiv \mu\,, \qquad \sigma^2 \equiv E[(X-\mu)^2]\,. \qquad (5.5.11)$$

For the function s_1, result (5.5.8) implies:

$$\frac{d\mu}{dt} = E[\dot{X}]\,, \qquad (5.5.12)$$

or, on the basis of (5.5.9):

$$\frac{d\mu}{dt} = E[aX^2 + bX + c]\,. \tag{5.5.13}$$

Using the identity:

$$E(X^2) = \sigma^2 + \mu^2\,, \tag{5.5.14}$$

the stochastic–dynamic equation (5.5.13) for the mean μ may be written as:

$$\dot{\mu} = a\mu^2 + b\mu + c + a\sigma^2\,. \tag{5.5.15}$$

It is obvious from eq. (5.5.15) that the equation for the mean μ is *not* obtained by replacing X by μ in the governing dynamics (5.5.9). An additional term appears in the stochastic–dynamic equation (5.5.15) that contains the variance σ^2. Clearly, (5.5.15) can only be evaluated if σ^2 is available as a function of time. The stochastic–dynamic equation for σ^2 can be derived by considering the function s_2:

$$s_2(X) = (X - \mu)^2\,, \tag{5.5.16}$$

with:

$$E[s_2(X)] = \sigma^2\,. \tag{5.5.17}$$

For the function s_2, result (5.5.8) implies:

$$\frac{d\sigma^2}{dt} = E\left[\frac{d}{dt}(X-\mu)^2\right], \tag{5.5.18}$$

which may be rewritten as:

$$\frac{d\sigma^2}{dt} = E\left[2(X-\mu)(\dot{X}-\dot{\mu})\right], \tag{5.5.19}$$

or, due to eqs. (5.5.11) and (5.5.12) as:

$$\frac{1}{2}\frac{d\sigma^2}{dt} = E(X\dot{X}) - \mu\dot{\mu}\,. \tag{5.5.20}$$

Since, on the basis of (5.5.9) and (5.5.15), the two terms on the right–hand–side of (5.5.20) can be rewritten as:

$$\begin{aligned} E(X\dot{X}) &= aE(X^3) + bE(X^2) + c\mu = \\ &= a\Big(E(X-\mu)^3 + 3\mu\sigma^2 + \mu^3\Big) + b\sigma^2 + b\mu^2 + c\mu\,, \\ \mu\dot{\mu} &= \mu\Big(a\mu^2 + b\mu + c + a\sigma^2\Big)\,, \end{aligned} \tag{5.5.21}$$

the stochastic–dynamic equation (5.5.20) for σ^2 may be brought in the form:

$$\frac{1}{2}\frac{d\sigma^2}{dt} = aE(X-\mu)^3 + 2a\mu\sigma^2 + b\sigma^2\,. \tag{5.5.22}$$

Summarizing, the stochastic–dynamic equations for the mean μ and the variance σ^2 for the dynamical system (5.5.9) are given as:

$$\boxed{\frac{d\mu}{dt} = a\mu^2 + b\mu + c + a\sigma^2\,, \qquad \frac{d\sigma^2}{dt} = 4a\mu\sigma^2 + 2b\sigma^2 + 2a\underbrace{E(X-\mu)^3}_{\equiv\vartheta}\,.} \tag{5.5.23}$$

As in the context of eq. (5.5.15), the stochastic–dynamic equation for the variance σ^2 contains a higher–order moment term that needs to be specified somehow in order for eqs. (5.5.23) to be useful. It is clearly possible to derive an equation for the evolution of $\vartheta \equiv E(X-\mu)^3$ by defining the function:

$$s_3(X) = (X-\mu)^3, \tag{5.5.24}$$

and obtaining, on the basis of (5.5.8), and with the definition of ϑ:

$$\frac{d\vartheta}{dt} = E\left[\frac{d}{dt}(X-\mu)^3\right]. \tag{5.5.25}$$

Using steps analogous to those necessary to obtain eq. (5.5.22), it is possible to rewrite (5.5.25) as:

$$\frac{d\vartheta}{dt} = 6a\mu\vartheta + 3b\vartheta - 3a\sigma^4 + 3aE(X-\mu)^4. \tag{5.5.26}$$

As expected, the equation for ϑ is unclosed again, containing a fourth–order term. The basic principle

It is very convenient to write Eq. (2.2.12) in differential form:

$$\frac{\partial F(q,p;t)}{\partial t} \equiv \partial_t F(q,p;t) = -[e^{-(H)t}F(q,p), H]_P$$

or else

$$\partial_t F(q,p;t) = [H(q,p), F(q,p;t)]_P \tag{2.2.14}$$

This is called the *Liouville equation* and is, beyond any doubt, the most important equation of statistical mechanics, just as the Schrödinger equation is the central equation of quantum mechanics.

The most important feature of the Liouville equation is its *linearity*. This property introduces an important touch of simplicity into an otherwise very complex theory and should be exploited as thoroughly as possible. To stress this feature, it is often convenient to write Eq. (2.2.14) in a slightly different form*:

$$\partial_t F(t) = LF(t) \tag{2.2.15}$$

where we introduced the linear operator L naturally defined as follows:

$$LF \equiv [H, F]_P = \sum_{n=1}^{N}\left\{\frac{\partial H}{\partial q_n}\frac{\partial F}{\partial p_n} - \frac{\partial H}{\partial p_n}\frac{\partial F}{\partial q_n}\right\} \tag{2.2.16}$$

The fundamental operator L will be called the *Liouvillian* of the system.

Figure 13: Reference from Balescu (1991, p. 41) concerning the LE for Hamiltonian dynamics.

of how to obtain the stochastic–dynamic equations is now evident. For a nonlinear governing dynamical system, such as (5.5.9), these equations are nonlinear themselves, as well as coupled, and unclosed. No finite closed hierarchy of stochastic–dynamic equations will be derivable for nonlinear dynamics. This situation is very similar to the closure problem in turbulence work (e.g., McComb 1991, Stanišić 1988). This property is also very clearly stated by Epstein (1969) as: " ... as long as the deterministic prognostic

equations are nonlinear it is impossible to write a closed finite set of prognostic equations for the moments. In other words, to predict exactly the future behavior of even the mean of the distribution, all the moments of the distribution (or, equivalently, the entire distribution itself) must be known." Nevertheless, when a closure assumption is utilized, the stochastic–dynamic equations provide the means to determine moments of the pdf without the need to integrate the governing dynamics multiple times, as necessary when a Monte Carlo approach is taken.

5.6 Classical and Statistical Mechanics

As already mentioned in sections 2.1 and 2.3 (see, eq. (2.3.9)), the LE takes on a particularly simple form for Hamiltonian dynamics. In addition, Liouville's results imply conditions on the evolution of phase space volume for Hamiltonian dynamics that may be written as (e.g., Marion and Thornton 1988):

$$\dot{q}_k = \frac{\partial H}{\partial p_k} \tag{5.6.1}$$

and:

$$\dot{p}_k = -\frac{\partial H}{\partial q_k} \tag{5.6.2}$$

for coordinates q_k and momenta p_k. The formulation eqs. (5.6.1) and (5.6.2) specifies, for a given Hamiltonian H, a dynamical system of the form (2.2.2.1). Apparently it follows with eqs. (5.6.1) and (5.6.2) that the phase space divergence ψ, defined in (2.4.3), vanishes, since:

$$\psi = \frac{\partial \dot{q}_k}{\partial q_k} + \frac{\partial \dot{p}_k}{\partial p_k} = \frac{\partial}{\partial q_k}\frac{\partial H}{\partial p_k} + \frac{\partial}{\partial p_k}\Big(-\frac{\partial H}{\partial q_k}\Big) = 0\,. \tag{5.6.3}$$

The fact that the phase space divergence vanishes for Hamiltonian systems leads to the following two implications. First, the LE (2.4.2) takes on the simplified form:

$$\frac{\partial \rho}{\partial t} + \sum_k \dot{q}_k \frac{\partial \rho}{\partial q_k} + \sum_k \dot{p}_k \frac{\partial \rho}{\partial p_k} = 0\,, \tag{5.6.4}$$

which may be expressed by saying, sometimes referred to as *Liouville theorem*, that the pdf remains constant during (along) the motion (see, e.g., Landau and Lifschitz 1979, and Marion and Thornton 1988, p. 235). Clearly, $\psi = 0$ implies, by (5.1.5), that the likelihood ratio h is one, so that the above statement can be seen in terms of the solution of the LE (3.2) as:

$$\rho(\mathbf{X}, t) = \rho_0(\Xi)\,. \tag{5.6.5}$$

Further, by inserting the dynamics into (5.6.4), Balescu (1991) expresses the LE in the form:

$$\frac{\partial \rho}{\partial t} = \underbrace{\sum_k \Big(-\frac{\partial H}{\partial p_k}\frac{\partial \rho}{\partial q_k} + \frac{\partial H}{\partial q_k}\frac{\partial \rho}{\partial p_k}\Big)}_{\equiv [H,\rho]}\,, \tag{5.6.6}$$

or:

$$\frac{\partial \rho}{\partial t} = [H, \rho] \tag{5.6.7}$$

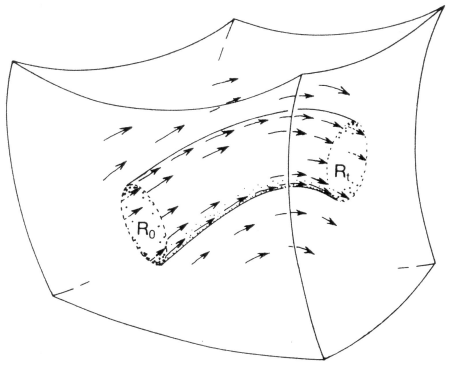


Fig. 5.13. As time evolves, a phase state region R_o is dragged along by the vector field to a new region R_t. This could represent the time-evolution of a particular alternative for our device.

What can be said about Hamiltonian systems generally? Do regions in phase space tend to spread with time or do they not? It might seem that for a problem of such generality, very little could be said. However, it turns out that there is a very beautiful theorem, due to the distinguished French mathematician Joseph Liouville (1809–1882), that tells us that the *volume* of any region of the phase space must remain constant under any Hamiltonian evolution. (Of course, since our phase space has some high dimension, this has to be a 'volume' in the appropriate high-dimensional sense.) Thus the volume of each R_t must be the *same* as the volume of the original R_0. At first sight this would seem to answer our stability question in the affirmative. For the *size*—in the sense of this phase-space volume—of our region *cannot grow*, so it would seem that our region cannot spread itself out over the phase space.

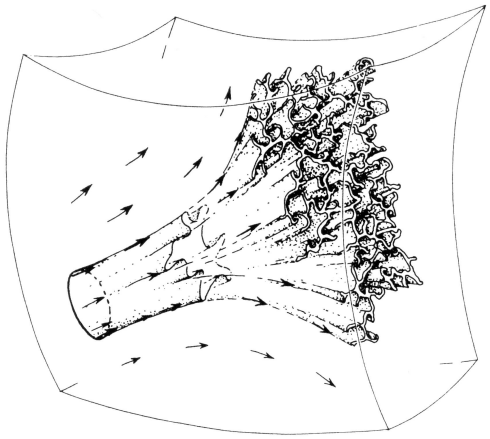


Fig. 5.14. Despite the fact that Liouville's theorem tells us that phase-space volume does not change with time-evolution, this volume will normally *effectively* spread outwards because of the extreme complication of this evolution.

Figure 14: Reference from Penrose (1989, pp. 181) concerning the LT on phase space volume.

by defining the *linear* operator $[H,...]$ as the *Liouvillian* of the system (5.6.1) and (5.6.2). Referring to the central role of the LE in statistical mechanics, Balescu (1991) emphasizes the need to exploit the linearity of the LE as thoroughly as possible (see also, Fig. 13).

Second, the property $\psi = 0$ for Hamiltonian systems implies on the basis of the general result eq. (2.3.9) that the time derivative of a *material* volume in phase space is zero:

$$\frac{dV(t)}{dt} = 0\,. \tag{5.6.8}$$

Consequently, for Hamiltonian evolution (with $\psi = 0$) one has $V(t)$=const, which is also referred to as Liouville Theorem (e.g., Arnold 1989, Penrose 1989; see also section 2.1). The importance of the aspect of volume conservation for Hamiltonian systems has been discussed by Penrose (1989) (see also the quote in section 2.1, as well as Fig. 14). Penrose (1989) points out that in a way similar to how a small drop of ink placed in a large container of water spreads over the entire contents of the container (while preserving the volume of ink), an initially "reasonably" shaped region in phase space will distort and stretch in a very complicated way and can get very thinly spread out over huge regions of the phase space (this effect is also illustrated in Fig. 14).

In addition, through eq. (5.3.3), implications exist for the Lyapunov exponents in case of Hamiltonian evolution (with $\psi = 0$).

5.7 A Spectral Barotropic Model

As a final illustration of the LE it will be demonstrated below that a spectral formulation of the barotropic model has zero divergence in phase space. The consequences for the LE are discussed.

The model equation in physical space is the barotropic quasigeostrophic potential vorticity equation with free surface and bottom topography h_B:

$$\frac{\partial}{\partial t}\underbrace{\left[\nabla^2\psi - \Delta R^{-2}\psi\right]}_{\equiv \mathrm{L}\psi} + J(\psi, \underbrace{\nabla^2\psi + f - \Delta R^{-2}\psi + \Delta f_0 \frac{h_B}{\overline{h}}}_{\equiv q}) = 0\,, \tag{5.7.1}$$

where ψ is the streamfunction for the geostrophic flow, R is the Rossby deformation radius, defined by $R^2 = g^*\overline{h}/f_0^2$, f is the Coriolis parameter indicating the rotation rate of the fluid, with reference value f_0, g^* is gravity, h_B is the bottom topography (positive above a $z = 0$ reference level), and $\overline{h}$ is the mean depth of the fluid. The operator J denotes the Jacobian operator defined as ($\mathbf{k}$ is the unit vector in the vertical):

$$J(\psi, q) = \mathbf{k} \cdot (\nabla\psi \times \nabla q)\,, \tag{5.7.2}$$

and the parameter Δ is included to allow for a divergent $(\Delta = 1)$ or a non–divergent $(\Delta = 0)$ model (in physical space). Eq. (5.7.1) results from approximating the full shallow–water equations for a homogeneous rotating fluid assuming nearly geostrophic flow, with q being the geostrophically approximated shallow–water potential vorticity (for further details, see Salmon 1998). It is important to note that flow subject to (5.7.1) conserves (for appropriate boundary conditions) a form of total energy given as $\frac{1}{2}[(\nabla\psi)^2 + \Delta R^{-2}\psi^2]$. The spectral formulation of eq. (5.7.1) for flow on a sphere with radius a, in

spherical coordinates λ (longitude) and μ (sine of latitude), assuming an expansion of $\psi(\lambda,\mu,t)$ in terms of the spherical harmonics $Y_n^m(\lambda,\mu)$, may be written as:

$$\dot{\psi}_n^m = \alpha_n J_n^m\,, \qquad \text{with:} \qquad \alpha_n \equiv \frac{a^2}{n(n+1)+\Delta(a/R)^2}\,, \tag{5.7.3}$$

where $\psi_n^m(t)$ are the time–dependent expansion coefficients (observe the dot on top of ψ_n^m in eq. (5.7.3) indicating time differentiation), the factor α_n results from inverting the linear operator L in eq. (5.7.1), and the spectral Jacobian J_n^m is given as:

$$J_n^m = \frac{1}{4\pi}\int_0^{2\pi}\int_{-1}^{+1} J(\psi,q)(Y_n^m)^* d\mu d\lambda\,, \tag{5.7.4}$$

where $(Y_n^m)^*$ denotes the complex conjugate spherical harmonic. The spectral formulation (5.7.3) describes one of the simplest geophysical flow examples for an N–dimensional system of first–order autonomous differential equations of the form (2.2.2.1), as it represents a set of nonlinear coupled ordinary differential equations. The number N of equations depends on the type and degree of spectral truncation.

The special property of zero phase space divergence of system (5.7.3) results by first inserting the spectral expansions for ψ and q into the Jacobian formulation (5.7.4):

$$J_n^m = \frac{1}{4\pi}\int_0^{2\pi}\int_{-1}^{+1} J\Big\{\sum_{m'}\sum_{n'}\psi_{n'}^{m'}(t)Y_{n'}^{m'}(\lambda,\mu),\sum_{m''}\sum_{n''}q_{n''}^{m''}(t)Y_{n''}^{m''}(\lambda,\mu)\Big\}(Y_n^m)^* d\mu d\lambda\,, \tag{5.7.5}$$

and subsequently rearranging integrals and summations as:

$$J_i = \sum_j\sum_k \psi_j q_k \underbrace{\frac{1}{4\pi}\int_0^{2\pi}\int_{-1}^{+1} Y_i^* J(Y_j,Y_k)d\mu d\lambda}_{\equiv A_{ijk}} = \sum_{j,k} A_{ijk}\psi_j q_k\,. \tag{5.7.6}$$

In eq. (5.7.6), the summation indices j and k (as well as the free index i) must be understood to stand for the index pair (n,m) in the previous eq. (5.7.5). Note that the interaction coefficients A_{ijk}, defined in (5.7.6), are independent of the actual fields and may be precomputed; it is noted in passing that (5.7.6) forms the basis of the fully spectral (but computationally highly inefficient) interaction coefficient method (see, Bourke 1972, for a comparison of that method to the so–called transform method). The spectral expansion of q may be found from the spectral expansion of ψ as:

$$q_n^m = -\alpha_n^{-1}\psi_n^m + g_n^m\,, \qquad \text{with:} \qquad g_n^m \equiv (f+\Delta f_0\frac{h_B}{\overline{h}})_n^m\,, \tag{5.7.7}$$

where g_n^m denotes the spectral coefficients of the expansion of the term in parenthesis in (5.7.7). In the more symbolic notation used in (5.7.6), eq. (5.7.7) reads:

$$q_k = -\alpha_k^{-1}\psi_k + g_k\,. \tag{5.7.8}$$

On the basis of (5.7.6) and (5.7.8), the spectral equation (5.7.3) may be written in the form:

$$\dot{\psi}_i = \underbrace{\alpha_i\sum_{j,k} A_{ijk}\psi_j\Big(-\alpha_k^{-1}\psi_k + g_k\Big)}_{\equiv f_i(\psi_l)}\,. \tag{5.7.9}$$

Obviously, a function f_i may be defined, as done in eq. (5.7.9), that defines the right–hand–side of eq. (5.7.3), or, equivalently, eq. (5.7.9), in terms of ψ_l and precomputed coefficients. Eq. (5.7.9) most clearly demonstrates the analogy between the geophysical example eq. (5.7.1) and the prototypical system eq. (2.2.2.1). At this point the property of the interaction coefficients to vanish if two indices are equal:

$$A_{iik} = A_{iji} = 0 \tag{5.7.10}$$

is observed that is basically a consequence of properties of the Jacobian operator (5.7.2) and the definition of the interaction coefficients in (5.7.6). It therefore follows that f_i, defined in (5.7.9), does not depend on ψ_i. This result clearly implies that the divergence in phase space (defined as ψ in eq. (2.4.3)) of system (5.7.9) is zero, even though the flow may evidently be divergent in physical space (for $\Delta = 1$). In other words, the dynamics (5.7.1) has no divergence in phase space (see also, Salmon et al. 1976). Using the symbolic notation that the vector $\mathbf{X}$ contains the ordered real and imaginary expansion coefficients:

$$\mathbf{X} = \begin{pmatrix} \dots \\ {}_r(\psi)_n^m \\ {}_i(\psi)_n^m \\ \dots \end{pmatrix}, \tag{5.7.11}$$

the dynamics (5.7.9) are written as:

$$\dot{\mathbf{X}} = \mathbf{f}(\mathbf{X}), \tag{5.7.12}$$

(see eq. (2.2.2.1)) with divergence–free $\mathbf{f}$. As a consequence the LE, as written in section 2.4, takes on the form:

$$\frac{\partial \rho}{\partial t} + \dot{\mathbf{X}} \cdot \nabla \rho = 0, \tag{5.7.13}$$

with solution (see eq. (3.2)) given by $\rho(\mathbf{X}, t) = \rho_0(\Xi)$; all the consequences discussed in section 5.6 for a system with vanishing phase space divergence apply. Due to the phase–space non–divergence condition of the barotropic dynamics (5.7.1), the *stationary* solution ρ_s to the LE (5.7.13) is determined by:

$$\dot{\mathbf{X}} \cdot \nabla \rho_s = 0, \qquad \text{or:} \qquad \sum_k f_k(\mathbf{X}) \frac{\partial \rho_s}{\partial X_k} = 0, \tag{5.7.14}$$

with the definitions introduced above, in particular through eqs. (5.7.11) and (5.7.9). This linear last equation (5.7.14) determines the stationary pdf ρ_s (see also, Thompson 1983). For further discussion, reference is made to Holloway (1986), Salmon et al. (1976), and Salmon (1998).

6 Conclusions

The Liouville equation governs the time evolution of the pdf of the state of a dynamical system. Since such dynamical systems play a prominent role as prediction models in the atmospheric sciences in general, and in NWP in particular, the LE, governing the relevant pdfs, plays a fundamental role in atmospheric predictability. As the continuity equation for probability, the LE contains all the relevant information about the predictability of a (forced) dynamical system.

The LE is demonstrably linear and it is a partial differential equation. As the LE describes the entire pdf, closure problems typical for nonlinear dynamical systems are avoided, as is the need for obtaining many realizations of the system, if specific values of the pdf are of interest. The LE provides the basis for making probabilistic statements about specific forecasts, as well as about atmospheric predictability in general.

In the context considered here, an "analytical" solution to the LE (see, eq. (3.2)) was given for arbitrary governing dynamics. This solution avoids the fully numerical solution of an initial–value problem for a partial differential equation with very many independent variables. In the context of that solution, various considerations related to singular vectors, Lyapunov exponents, stochastic differential equations, the Fokker–Planck equation, the stochastic–dynamic equations, and statistical mechanics were considered in this paper.

It is clear that a fundamental difficulty in dealing with the LE is related to the extremely high dimensionality of phase space that must be considered in contexts of realistic NWP models. Nevertheless, its theoretical attractiveness makes the LE a fundamental tool for exploring various aspects and relationships in the area of atmospheric predictability.

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References

Abraham, R., and J.E. Marsden, 1978: *Foundations of Mechanics*. Addison–Wesley, 806 pp.

Arnold, V.I., 1989: *Mathematical Methods of Classical Mechanics*. Springer, 508 pp.

Balescu, R., 1991: *Equilibrium and Nonequilibrium Statistical Mechanics*. Krieger Publishing Company, 742 pp.

Bjerknes, V., 1904: Das Problem der Wettervorhersage, betrachtet vom Standpunkte der Mechanik und der Physik. *Meteorol.Z.*, **21**, 1–7.

Bourke, W., 1972: An efficient, one–level, primitive–equation spectral model. *Mon. Wea. Rev.*, **100**, 683–689.

Chu, P.C., L.M. Ivanov, T.M. Margolina, and O.V. Melnichenko, 2002: Probabilistic stability of an atmospheric model to various amplitude perturbations. *J. Atmos. Sci.*, **59**, 2860–2873.

de Groot, S.R., and P. Mazur, 1984: *Non–Equilibrium Thermodynamics*. Dover, 510 pp.

DeGroot, M.H., 1986: *Probability and Statistics*. Addison-Wesley, 723 pp.

Dudewicz, E.J., and S.N. Mishra, 1988: *Modern Mathematical Statistics*. Wiley, 838 pp.

Ehrendorfer, M., 1994a: The Liouville equation and its potential usefulness for the prediction of forecast skill. Part I: Theory. *Mon. Wea. Rev.*, **122**, 703–713.

Ehrendorfer, M., 1994b: The Liouville equation and its potential usefulness for the prediction of forecast skill. Part II: Applications. *Mon. Wea. Rev.*, **122**, 714–728.

Ehrendorfer, M., 1997: Predicting the uncertainty of numerical weather forecasts: a review. *Meteorol. Z., N.F.*, **6**, 147–183.

Ehrendorfer, M., 1999: Prediction of the uncertainty of numerical weather forecasts: Problems and approaches. In: *Proceedings ECMWF Workshop on Predictability, 20 – 22 October 1997*, pp. 27–99.

Ehrendorfer, M., and J.J. Tribbia, 1997: Optimal prediction of forecast error covariances through singular vectors. *J. Atmos. Sci.*, **54**, 286–313.

Epstein, E.S., 1969: Stochastic dynamic prediction. *Tellus*, **21**, 739–759.

Errico, R.M., M. Ehrendorfer, and K. Raeder, 2001: The spectra of singular values in a regional model. *Tellus*, **53A**, 317–332.

Errico, R.M., R. Langland, and D.P. Baumhefner, 2002: The workshop in atmospheric predictability. *Bull. Amer. Meteorol. Soc.*, **83**, 1341–1343.

Fortak, H., 1973: Prinzipielle Grenzen der deterministischen Vorhersagbarkeit atmosphärischer Prozesse. *Ann. Metorol., N.F.*, **6**, 111–120.

Gardiner, C.W., 1990: *Handbook of Stochastic Methods for Physics, Chemistry and the Natural Sciences*. Springer, 442 pp.

Gleeson, T.A., 1966: A causal relation for probabilities in synoptic meteorology. *J. Appl. Meteor.*, **5**, 365–368.

Goldstein, H., 1980: *Classical Mechanics*. Addison–Wesley, 672 pp.

Hasselmann, K., 1976: Stochastic climate models. Part I. Theory. *Tellus*, **28**, 473–485.

Holloway, G., 1986: Eddies, waves, circulation, and mixing: Statistical geofluid mechanics. *Ann. Rev. Fluid Mech.*, **18**, 91–147.

Hu, Y., and R.T. Pierrehumbert, 2001: The advection–diffusion problem for stratospheric flow. Part I: Concentration probability distribution function. *J. Atmos. Sci.*, **58**, 1493–1510.

Landau, L.D., and E.M. Lifschitz, 1979: *Lehrbuch der Theoretischen Physik. Band V Statistische Physik, Teil 1*. Akademie–Verlag, Berlin, 517 pp.

Leith, C.E., 1974: Theoretical skill of Monte Carlo forecasts. *Mon. Wea. Rev.*, **102**, 409–418.

Lin, C.C., and L.A. Segel, 1988: *Mathematics Applied to Deterministic Problems in the Natural Sciences*. Society for Industrial and Applied Mathematics, 609 pp.

Lindenberg, K., and B.J. West, 1990: *The Nonequilibrium Statistical Mechanics of Open and Closed Systems*. VCH Publishers, 448 pp.

Liouville, J., 1838: Sur la Théorie de la Variation des constantes arbitraires. *Journal de Mathématiques pures et appliquées*, **3**, 342–349.

Lorenz, E.N., 1963: Deterministic nonperiodic flow. *J. Atmos. Sci.*, **20**, 130–141.

Lorenz, E.N., 1969a: The predictability of a flow which possesses many scales of motion. *Tellus*, **21**, 289–307.

Lorenz, E.N., 1969b: Three approaches to atmospheric predictability. *Bull. Amer. Meteorol. Soc.*, **50**, 345–349.

Lorenz, E.N., 1982: Atmospheric predictability experiments with a large numerical model. *Tellus*, **34**, 505–513.

Lorenz, E.N., 1984: Irregularity: a fundamental property of the atmosphere. *Tellus*, **36A**, 98–110.

Lorenz, E.N., 1993: *The Essence of Chaos*. University of Washington Press, 227 pp.

Lützen, J., 1990: *Joseph Liouville (1809–1882): Master of Pure and Applied Mathematics*. Springer, 884 pp.

Marion, J.B., and S.T. Thornton, 1988: *Classical Dynamics*. Harcourt Brace Jovanovich, 602 pp.

McComb, W.D., 1991: *The Physics of Fluid Turbulence*. Oxford University Press, 572 pp.

Merryfield, W.J., P.F. Cummins, and G. Holloway, 2001: Equilibrium statistical mechanics of barotropic flow over finite topography. *J. Phys. Oceanogr.*, **31**, 1880–1890.

Nicolis, G., 1995: *Introduction to nonlinear science*. Cambridge University Press, 254 pp.

Paegle, J., and E. Robl, 1977: The time behavior of the probability density function of some simplified atmospheric flows. *J. Atmos. Sci.*, **34**, 979–990.

Palmer, T.N., 1999: A nonlinear dynamical perspective on climate prediction. *J. Climate*, **12**, 575–591.

Palmer, T.N., 2000: Predicting uncertainty in forecasts of weather and climate. *Rep. Prog. Phys.*, **63**, 71–116.

Parker, T.S., and L.O. Chua, 1989: *Practical Numerical Algorithms for Chaotic Systems*. Springer–Verlag, 348 pp.

Penland, C., 1989: Random forcing and forecasting using principal oscillation pattern analysis. *Mon. Wea. Rev.*, **117**, 2165–2185.

Penland, C., and L. Matrosova, 1994: A balance condition for stochastic numerical models with application to the El Niño–Southern Oscillation. *J. Climate*, **7**, 1352–1372.

Penrose, O., 1970: *Foundations of Statistical Mechanics*. Pergamon Press, 260 pp.

Penrose, R., 1989: *The Emperor's New Mind: Concerning Computers, Minds, and the Laws of Physics*. Penguin Books, 466 pp.

Risken, H., 1989: *The Fokker–Planck Equation – Methods of Solution and Applications*. Springer, 472 pp.

Salmon, R., 1998: *Lectures on Geophysical Fluid Dynamics*. Oxford University Press, 378 pp.

Salmon, R., G. Holloway, and M.C. Hendershott, 1976: The equilibrium statistical mechanics of simple quasi–geostrophic models. *J. Fluid Mech.*, **75**, 691–703.

Soize, C., 1994: *The Fokker–Planck Equation for Stochastic Dynamical Systems and its Explicit Steady State Solutions*. World Scientific, 321 pp.

Stanišić, M.M., 1988: *The Mathematical Theory of Turbulence*. Springer, 501 pp.

Strang, G., 1993: *Introduction to Linear Algebra*. Wellesley–Cambridge Press, 472 pp.

Tatarskiy, V.I., 1969: The use of dynamic equations in the probability prediction of the pressure field. *Izv., Atmospheric and Oceanic Physics*, **5**, 293–297.

Thompson, P.D., 1957: Uncertainty of initial state as a factor in the predictability of large scale atmospheric flow patterns. *Tellus*, **9**, 275–295.

Thompson, P.D., 1972: Some exact statistics of two–dimensional viscous flow with random forcing. *J. Fluid Mech.*, **55**, 711–717.

Thompson, P.D., 1983: Equilibrium statistics of two–dimensional viscous flows with arbitrary random forcing. *Phys. Fluids*, **26**, 3461–3470.

Thompson, P.D., 1985a: Prediction of probable errors of predictions. *Mon. Wea. Rev.*, **113**, 248–259.

Thompson, P.D., 1985b: A statistical–hydrodynamical approach to problems of climate and its evolution. *Tellus*, **37A**, 1–13.

Tribbia, J., and D. Baumhefner, 1993: On the problem of prediction beyond the deterministic range. In: *Prediction of Interannual Climate Variations*, J. Shukla (Ed.), NATO ASI Series, Vol. 16, pp. 251–265. Springer.

van Kampen, N.G., 1992: *Stochastic Processes in Physics and Chemistry*. North–Holland, 465 pp.

Weiss, J.B., 2003: Coordinate invariance in stochastic dynamical systems. *Tellus*, **55A**, 208–218.

Zwillinger, D., 1989: *Handbook of Differential Equations*. Academic Press, 673 pp.