The Liouville Equation and Its Potential Usefulness for the Prediction of Forecast Skill. Part I: Theory

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ABSTRACT

The Liouville equation provides the framework for the consistent and comprehensive treatment of the uncertainty inherent in meteorological forecasts. This equation expresses the conservation of the phase-space integral of the number density of realizations of a dynamical system originating at the same time instant from different initial conditions, in a way completely analogous to the continuity equation for mass in fluid mechanics. Its solution describes the temporal development of the probability density function of the state vector of a given dynamical model. Consideration of the Liouville equation ostensibly avoids in a natural way the problems inherent to more standard methodology for predicting forecast skill, such as the need for higher-moment closure within stochastic–dynamic prediction, or the need to generate a large number of realizations within ensemble forecasting. These benefits, however, are obtained only at the expense of considering high-dimensional problems.

The purpose of this work, presented in two parts, is to investigate the potential usefulness of the Liouville equation in the context of predicting forecast skill. After a review of the basic form of the Liouville equation, for the case that the dynamical system considered is represented by a set of coupled ordinary nonlinear first-order (nonstochastic) differential equations that are generic for meteorologically relevant situations, the general *analytical* solution of the Liouville equation is presented in this first part. This explicit solution allows one, at least in principle, to express in analytical terms the time evolution of the probability density function of the state vector of a given meteorological model.

Several properties of the general solution are discussed. As an illustration, the general solution is used to solve the Liouville equation relevant for a one-dimensional nonlinear dynamical system. The fundamental role of the Liouville equation in the context of predicting forecast skill is emphasized.

1. Introduction

Meteorological forecasts are inherently uncertain. This widely recognized fact has led to the statement that a forecast is incomplete unless it is accompanied by a predictive statement about the skill of the forecast (see, e.g., Cooke 1906; Tennekes et al. 1987). As a consequence, various efforts have been undertaken to quantify this uncertainty and thus improve the utility of the forecast for the user. Such quantification should ideally be expressed in the precise and unambiguous language of probability (Lindley 1987).

Among these efforts has been the specification of the likelihood of occurrence of specific events in terms of so-called *probability forecasts* (e.g., probability of precipitation forecasts) that are usually derived by statistical and/or subjective methods (see, e.g., Murphy 1985). More recently, methods appropriate to directly construct statements about the predictive skill of a forecast produced by means of a dynamical meteorological model have attracted much interest (see the overview by Tribbia 1991).

All the information that is necessary for the specification of the uncertainty of a given forecast is contained in the multivariate probability density function (pdf) ρ of the forecast variable (e.g., model state vector). Clearly, as predictive skill varies with the lead time of the forecast, this pdf is, in general, time dependent. Naturally, the structure and time evolution of ρ are strongly dependent upon the properties of the dynamical model under consideration, including the fact that the model may reflect the intrinsic instabilities and nonlinearities to which atmospheric flow is subject (see also, Palmer and Tibaldi 1988). In addition, ρ is influenced by the uncertainty in the initial model state as well as by errors in the model formulation (model errors).

Current practice for predicting the skill of forecasts made through numerical models is related to the concept of *stochastic–dynamic prediction* put forward by

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Epstein (1969). In this concept, the intrinsically unavoidable uncertainty in the initial conditions for a numerical model is acknowledged in a fundamental way, with regard to its importance for and its influence on the quality of the subsequent forecast (see also, Thompson 1957). The equations relevant for stochastic–dynamic prediction are derived from the general formulation of the continuity equation for probability, also known as the *Liouville equation* (Epstein 1969; Thompson 1985a). The Liouville equation (LE) is central to the question of predicting forecast skill in the sense that it governs the temporal evolution of the (multivariate) pdf ρ of the model state vector given information about the uncertainty of the initial state in terms of an initial pdf. The LE can be interpreted as a special case of the Fokker–Planck equation that arises if proper account is taken for model errors in the governing model equations in the form of random forcing terms; neglecting model errors reduces the Fokker–Planck equation to the LE. Since the LE describes the temporal evolution of the pdf of the model state vector, its solution permits the computation of the statistical properties of an ensemble of solutions of a dynamical system without the need to construct explicitly individual solutions. In addition, consideration of the LE as opposed to consideration of the stochastic–dynamic equations (SDEs) ostensibly avoids the notorious problem of higher-moment closure. The LE is a quasi-linear, inhomogeneous partial differential equation, and its explicit analytical solution may be given for a large class of dynamical systems (see section 3). However, mainly because of the high dimensionality of the state vector of realistic meteorological models and of the associated phase space, the actual evaluation of the solution of the LE at a reasonable resolution in phase space may pose substantial problems from a numerical viewpoint.

Thus, the approaches currently under investigation for the prediction of forecast skill in an operational environment concentrate on providing only partial information about the temporal development of the pdf without referring explicitly to the LE. The relevant methodology may be discussed in four main groups: (a) stochastic–dynamic prediction, (b) ensemble forecasting, (c) lagged averaged forecasting, and (d) statistical schemes.

Approach (a) involves the integration of the SDEs (i.e., the equations that describe the temporal development of the moments of the pdf) and thus leads directly to the temporal evolution of higher moments of the pdf. It can yield very useful results. It is, however, computationally expensive due to the consideration of the temporal development of higher moments and requires the derivation of the SDEs that in turn depend upon suitable closure assumptions (Epstein 1969). The question of closure, as well as the methods to reduce the computational cost of this approach have been addressed by Fleming (1971), Pitcher (1977), and Thompson (1985b, 1985c, 1986, 1988). In this context, it is noted that the Kalman filter (in its prognostic form) bears a strong relationship to this approach insofar as the Kalman filter deals explicitly with the (co)variances of the components of the model state vector (Jazwinski 1970; Cohn 1993).

Within approach (b), originally proposed by Leith (1974), characteristic features of the pdf are derived from an ensemble integration of the numerical model starting from randomly perturbed initial states (Monte Carlo forecasting). Questions of closure and derivation of additional equations are avoided, but the computational effort is substantial, because a large number of ensemble members may be necessary for the accurate estimation of higher moments, such as (co)variances. This approach is widely used to predict forecast skill (e.g., Kalnay and Dalcher 1987; Murphy 1988, 1990) and may be used as a standard to check the accuracy of closure assumptions (e.g., Epstein 1969; Fleming 1971; Thompson 1985c). Recently, more sophisticated approaches to ensemble forecasting have been described in an attempt to select ensemble members based upon dynamical information of error growth (see, e.g., Schubert et al. 1992; Tribbia and Baumhefner 1993; Mureau et al. 1993; Toth and Kalnay 1993; Tracton and Kalnay 1993; see also, Vukićević 1993).

Hoffman and Kalnay (1983) formulated the lagged average forecast technique that avoids the expensive production of additional forecasts by producing the ensemble from the collection of forecasts verifying at the same time but originating from different initial times. Results reported from the application of this technique emphasize the usefulness of this approach (e.g., Dalcher et al. 1988; Branković et al. 1990).

Finally, experiments based on statistical methods have been performed that directly seek relationships between a variety of predictors (e.g., the error in the estimate of the initial state, or specific features characterizing the initial state) and the skill of the forecast through multiple linear regression, for example (Molteni and Palmer 1991; Palmer and Tibaldi 1988; Colucci and Baumhefner 1992). While ideally suited for operational use due to their negligible cost, the results from the study of Molteni and Palmer (1991) clearly indicate the limitations of these empirical methods.

In the context of predicting the skill of model forecasts, it is important to account suitably for errors inherent in models describing atmospheric flow. It is common to approaches (a)–(c) that in their original form they do not account explicitly for model errors. Pitcher (1977) has considered the effect of model errors within stochastic–dynamic prediction. In the same context, in addition to studies concentrating directly on the skill of forecast models, a number of studies have been performed (i) to investigate diagnostically the characteristics of the atmospheric circulation, that is, to identify characteristic features of the pdf of the state vector of model atmospheres (e.g., Palmer et al. 1990;

Tibaldi et al. 1990; Toth 1991; Molteni et al. 1990; Molteni and Tibaldi 1990; Kimoto and Ghil 1993a,b) as well as (ii) to study the predictability of the atmosphere itself (e.g., Lorenz 1963, 1969, 1982, 1984; Leith 1983; Ghil 1987; Nicolis 1987, 1992; Palmer 1988, 1993; Tribbia and Baumhefner 1988; Farrell 1990; Moore and Farrell 1993; Molteni and Palmer 1993; Branstator et al. 1993). Comprehensive reviews of the state of predictability research may be found in Thompson (1985d) and Houghton (1991).

The preceeding discussion illustrates the central role of the LE for the question of predicting forecast skill. It is central in the sense that it provides the theoretical framework for the above approaches and summarizes completely the information provided only partially by these approaches. From this point of view, it is the purpose of this work to investigate in more detail the LE itself, together with its potential usefulness for and connection to the question of forecasting forecast skill. The work is presented in two parts; in this first part, theoretical aspects of the LE are discussed, whereas applications are considered in the second part of this paper (Ehrendorfer 1994a, hereafter referred to as Part II).

The general form of the LE is described in section 2. The explicit analytical solution of the LE for a large class of dynamical systems is presented in section 3. This solution can be derived using the method of characteristics, since the LE is a quasi-linear partial differential equation. In section 4, this general analytical solution is explicitly applied in the context of a one-dimensional nonlinear dynamical system to solve the Liouville equation relevant in this situation. More complicated, even though still low-dimensional, examples are considered in Part II (Ehrendorfer 1994a). A number of concluding remarks are made in section 5; a comprehensive summary and discussion is delayed until the final section of Part II. The two appendixes provide important technical details concerning the solution of the LE presented in section 3.

2. The Liouville equation

For the formal introduction of the LE, consider the situation that the state of a dynamical system at a particular instant is described by the values of a finite number N of parameters (or, variables) denoted by X_i ($i = 1, 2, \cdots, N$). For example, in the case of a model describing the atmosphere, these variables may be thought of as the coefficients of basis functions in a series expansion. Thus, in the corresponding N-dimensional *phase space* that is spanned by the variables X_i, the state of the system at a particular instant is fully described by a point and the temporal development of the system under consideration is described through a succession of such points. These points trace out a *trajectory* in phase space. [For a more detailed discussion of the concept of phase space, see also, Lorenz (1963) and Thompson (1985a).]

It is possible to derive the statistical properties of an *ensemble* of realizations in phase space without explicit construction of a large number of ensemble members (i.e., individual trajectories). This goal is achieved through the hypothetical consideration of a very large number of realizations—in analogy to statistical mechanics—such that the number density of realizations in phase space satisfies the continuum hypothesis (see, e.g., Batchelor 1967). Then, within a time interval during which no realizations are created or destroyed, which is the case if all realizations start at the same time instant, a continuity equation for the number density can be formulated. This basic continuity requirement is the LE (see also, Epstein 1969; Thompson 1983, 1985a). It is clear that the construction of a large number of individual members of the ensemble is avoided through dealing with the time-dependent number density of realizations in phase space. Appropriately normalized, this number density is a (multivariate) pdf. The pdf of the state vector of the dynamical system $\mathbf{X}(t)$ in phase space is denoted here by $\rho(\mathbf{X}, t)$.

For the mathematical formulation of these ideas, consider a dynamical system with state vector $\mathbf{X}(t)$—consisting of N components $X_i(t)$—whose temporal evolution is described in phase space by a set of N (nonautonomous) ordinary differential equations:

$$\dot{\mathbf{X}} = \mathbf{\Phi}[\mathbf{X}(t), t], \tag{2.1}$$

where the dot denotes the derivative with respect to time. Virtually all equations describing atmospheric flow can be brought into the form (2.1), through the usual approach of expanding unknown functions in partial differential equations in terms of suitably selected basis functions. Terminating the expansion at a large, but finite, degree then results in a set of ordinary differential equations for the coefficients in the expansion. Moreover, these equations usually are autonomous, indicating the time independence of the physical laws describing the atmosphere (see also, Thompson 1983, 1985a; Lorenz 1963).

The LE is introduced as the continuity equation for the pdf of the state vector $\mathbf{X}(t)$:

$$\frac{\partial \rho(\mathbf{X}, t)}{\partial t} + \sum_{k=1}^{N} \frac{\partial}{\partial X_k} [\rho(\mathbf{X}, t)\dot{X}_k(\mathbf{X}, t)] = 0. \tag{2.2}$$

In this form, the LE (2.2) is valid as long as no realizations are created or destroyed, because it basically expresses the conservation of the phase-space integral of the number density of realizations. [For a derivation of the LE from this conservation requirement, as well as for a brief historical account pointing out why the equation bears the name of Joseph Liouville, reference is made to Ehrendorfer (1994b).] In complete analogy to the conservation equation for mass (see, e.g., Batchelor 1967), 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 the small volume surrounding the point under consideration, which is equivalent to the requirement that realizations are neither created nor destroyed. [Note that the $\dot{X}_k$ are the known "velocity components" in phase space as given by (2.1).] In the differential form given in (2.2) certain assumptions concerning the differentiability of ρ must be satisfied that may, however, be relaxed at the more fundamental level of an integral formulation.

The LE describing the temporal development of the pdf $\rho(\mathbf{X}, t)$ in phase space is an inhomogeneous quasi-linear (in the sense that it is *linear* in the first derivatives of the dependent variable ρ) first-order partial differential equation in which the independent variables are time t and the components X_i of the state vector, and the *single* dependent variable is the density ρ. The fundamental importance of the LE within statistical mechanics—related to its (quasi-)linearity—as a tool for the investigation of complex dynamical systems has been emphasized by Balescu (1975). In particular, the LE plays a central role in the study of the statistical mechanical equilibrium of dynamical systems (see, e.g., Salmon et al. 1976).

Obviously, the solution of the LE (2.2) depends crucially on the form of the dynamical system (2.1) under consideration due to the direct insertion of the model dynamics into the LE. Thus, its solution must be expected to reflect qualitatively the characteristic behavior of the system. In addition, it may be seen from the generality of the formulation (2.1) and (2.2) that the inclusion of complex forcing terms and/or model error parameterizations does not present any difficulty in principle.

3. Solution of the Liouville equation

As a quasi-linear partial differential equation, the general form of the analytical solution of the LE described in the previous section can be given explicitly. This solution of the LE is discussed in this section. However, it is important to note that the solution of the LE presented requires implicitly that it is possible to solve in analytical and/or numerical terms the dynamical system being investigated.

Consider the following system of N first-order ordinary autonomous differential equations:

$$\dot{\mathbf{X}} = \mathbf{\Phi}(\mathbf{X}), \tag{3.1}$$

subject to the initial condition

$$\mathbf{X}(t = 0) = \mathbf{\Xi}. \tag{3.2}$$

System (3.1) is of the form of the equations presented in (2.1) with the restriction that the function $\mathbf{\Phi}$ is time independent. This restriction to autonomous systems is made for the remainder of the paper, since systems of ordinary differential equations developed in meteorological applications are usually autonomous. However, the results presented herein can easily be generalized to the nonautonomous case (see, e.g., Ehrendorfer 1994b).

It is well known that—under certain regularity conditions—the solution to (3.1) and (3.2) exists and is unique (see, e.g., Arnold 1992). This solution, namely, the state $\mathbf{X}$ at time t, is a (smooth) function of both time and initial condition, expressible in the form

$$\mathbf{X} = \mathbf{X}(\mathbf{\Xi}, t), \tag{3.3}$$

where this relationship between the state vector $\mathbf{X}$ at time t and the state vector $\mathbf{\Xi}$ at time $t = 0$ might be available either in analytical or numerical terms.

Making use of (3.1), the LE (2.2) is at this point reformulated as

$$\frac{\partial \rho(\mathbf{X}, t)}{\partial t} + \sum_{k=1}^{N} \Phi_k(\mathbf{X}) \frac{\partial \rho(\mathbf{X}, t)}{\partial X_k} + \rho(\mathbf{X}, t) \underbrace{\sum_{k=1}^{N} \frac{\partial \Phi_k(\mathbf{X})}{\partial X_k}}_{\equiv \psi(\mathbf{X})} = 0, \tag{3.4}$$

where $\Phi_k(\mathbf{X})$ denotes the kth component of $\mathbf{\Phi}(\mathbf{X})$. The scalar function $\psi(\mathbf{X})$, defined as indicated above, is the divergence of the vector field $\mathbf{\Phi}$ in phase space. Note that ψ has no explicit time dependence in the case of an autonomous dynamical system. To properly pose the problem of solving (3.4), the following initial condition is imposed:

$$\rho(\mathbf{X}, t = 0) = f(\mathbf{X}), \tag{3.5}$$

where f is an arbitrary, prespecified, nonnegative scalar function with unit integral over phase space Ω:

$$\int_{\Omega} f(\Omega') d\Omega' = 1. \tag{3.6}$$

Evidently, the initial condition (3.5), as well as constraint (3.6), are required in order to ensure that ρ possesses the basic properties of a pdf, namely, nonnegativeness and normalization to 1, at the initial time. Constraint (3.6) is consistent with the boundary condition of vanishing pdf ρ at infinity (see also appendix B).

To solve (3.4) and (3.5), the method of characteristics is advantageously used, which amounts to rewriting the partial differential equation (3.4) as $N + 2$ ordinary differential equations. In addition, the initial condition (3.5) must be expressed in parametric form (see, e.g., Zwillinger 1989; Kevorkian 1990). The solution to (3.4) and (3.5) is then found to be

$$\rho(\mathbf{X}, t) = f(\mathbf{\Xi}) \exp\left\{-\int_0^t \psi[\mathbf{X}(\mathbf{\Xi}, t')] dt'\right\}. \tag{3.7}$$

This result is to be interpreted in the context of the dynamical system (3.1) together with (3.2) in the following way. Given the arguments $\mathbf{X}$ and t, for which the value of the pdf ρ is desired, it is first necessary to find the point Ξ in phase space that—when used as initial condition for (3.1)—is taken to $\mathbf{X}$ at time t under the dynamics (3.1). This process amounts to inverting the solution (3.3) for fixed t in the form

$$\Xi = \Xi(\mathbf{X}, t). \quad (3.8)$$

This value of Ξ must be used as an argument to evaluate the function f as well as to determine $\mathbf{X}$ and, in turn, ψ, in the exponential term of (3.7). Obviously, the required inversion (3.8) may be difficult to obtain. However, at least theoretically, the inversion (3.8) always exists and is unique, because, for the type of dynamical systems considered here, trajectories starting at different initial conditions never intersect, or in other words, a certain point in phase space is uniquely connected to its initial condition.

These remarks imply that ρ, as given by (3.7), is in fact dependent only upon the arguments $\mathbf{X}$ and t, as may be seen from the fully explicit solution of the LE (3.4) subject to (3.5) that is obtained by substituting (3.8) into (3.7):

$$\rho(\mathbf{X}, t) = f[\Xi(\mathbf{X}, t)] \times \exp\left\langle -\int_0^t \psi\{\mathbf{X}[\Xi(\mathbf{X}, t), t']\}dt' \right\rangle. \quad (3.9)$$

In appendix A a proof is given for showing that (3.9) or, equivalently, (3.7), with the substitution of $\Xi = \Xi(\mathbf{X}, t)$, satisfies (3.4). It is immediately clear that (3.7) satisfies the initial condition (3.5). It is further necessary to verify that the solution (3.7) possesses the properties of a pdf. The nonnegativeness of ρ is evident. In appendix B a formal quantitative argument is presented to show that (3.7) is also appropriately normalized to 1 for all t, given that (3.6) is satisfied. This result may be easily understood intuitively from the physical point of view because the LE expresses the conservation of the phase-space integral of the number density of realizations. Thus, if the initial phase-space integral of the number density is equal to 1, it will be equal to 1 at any later time.

Investigation of the form of the solution (3.7) allows the general remark that the initial condition represented by f is in some sense damped out by the negative exponential term as time proceeds. However, this interpretation must be exercised with care due to the presence of Ξ representing the dynamical system. In addition, the function ψ when integrated over t' is bound to complicate the picture.

In this context, it is noted that this integration over t' appearing in the exponential term in (3.7)—to be performed analytically or numerically—is always one-dimensional (1D), independent of the dimension of phase space. Note, however, that since the integrand in (3.7) depends—through the appearance of Ξ [see (3.9)]—in a complicated way on the upper bound t of the integration, it is, in general, not possible to decompose this integration into several integrals spanning subintervals of the interval $(0, t)$. If such decomposition were possible, it could be advantageously used for the computation of the pdf ρ at a later time point, say, t_2, from the pdf at a preceeding time point, say t_1. However, due to the 1D nature of this integration, this fact is not considered to represent any major disadvantage in the context of evaluating the solution to the LE. Only after the actual computation of the phase-space point Ξ—according to (3.8)—the aforementioned decomposition becomes possible.

The above developments show that the solution to the general LE can be given explicitly in the form (3.7) for a large class of dynamical systems of the type (3.1). However, in order to use (3.7), the solution to (3.1) must be expressible in the form (3.3) in either analytical or numerical terms. In addition, a relationship like (3.8) must be available to connect a given state vector to its origin at the initial time. Both requirements do not limit generality in principle, due to existence and uniqueness theorems for ordinary autonomous differential equations. They may, however, limit the use of (3.7) in specific applications. A further discussion of these issues, as well as of the properties of the solution (3.7), is given in the context of illustrating (3.7) for three low-dimensional systems in the next section and in Part II, as well as in the final section of Part II.

Finally, it is noted that arbitrary statistics Θ_ϕ are readily evaluated through a multidimensional integration over (part of) phase space, once the solution ρ is available, since these statistics are defined as the expected value of specific scalar functions $\phi(\mathbf{X})$ of the state vector:

$$\Theta_\phi(t) \equiv \int_\Omega \phi(\mathbf{X})\rho(\mathbf{X}, t)d\mathbf{X}. \quad (3.10)$$

Even though the complexity of obtaining the pdf ρ seems to be larger when compared to the final evaluation of (3.10), it is worth emphasizing that, from the numerical point of view, this multidimensional integration may be quite challenging for larger dimensions of the phase space. (See the related remarks in section 5 of Part II.)

4. Illustration for a one-dimensional system

To illustrate the results presented in the previous section, a 1D Riccati equation is considered as a specific dynamical system of the form (3.1):

$$\dot{X} = aX^2 + bX + c, \quad (4.1)$$

with constant coefficients a, b, and c chosen such that

$$\Delta \equiv \frac{b^2}{4} - ac > 0. \quad (4.2)$$

For system (4.1), the general form of the LE (3.4) takes on the following specific form:

$$\frac{\partial \rho(X, t)}{\partial t} + (aX^2 + bX + c)\frac{\partial \rho(X, t)}{\partial X} + (2aX + b)\rho(X, t) = 0. \quad (4.3)$$

The solution of (4.3) subject to an initial condition of the form (3.5) is obtained by specializing the general solution (3.7) to system (4.1), for which relationships (3.3) and (3.8) are easily found analytically. In this respect, the solution of (4.1) is given by

$$X = X(\Xi, t) = \frac{r_1(a\Xi + r_2)e^{\gamma t} - r_2(a\Xi + r_1)}{-a(a\Xi + r_2)e^{\gamma t} + a(a\Xi + r_1)}, \quad (4.4)$$

where

$$r_1 \equiv \frac{b}{2} + \Delta^{1/2}, \quad r_2 \equiv \frac{b}{2} - \Delta^{1/2},$$
$$\gamma \equiv r_1 - r_2 \equiv 2\Delta^{1/2}. \quad (4.5)$$

Use of (4.4) in the general solution of the LE (3.7) leads to the following form of the solution of (4.3):

$$\rho(X, t) = f[\Xi(X, t)] \exp\left\langle -\int_0^t \left\{ 2a \frac{r_1[a\Xi(X, t) + r_2]e^{\gamma t'} - r_2[a\Xi(X, t) + r_1]}{-a[a\Xi(X, t) + r_2]e^{\gamma t'} + a[a\Xi(X, t) + r_1]} + b \right\} dt' \right\rangle, \quad (4.6)$$

where the dependence of Ξ on X and t has been indicated explicitly [see (3.9)]; this dependence is found from (4.4) as

$$\Xi = \Xi(X, t) = \frac{1}{a}\left[\frac{aX(r_2 e^{\gamma t} - r_1) + r_1 r_2(e^{\gamma t} - 1)}{aX(1 - e^{\gamma t}) - r_1 e^{\gamma t} + r_2}\right]. \quad (4.7)$$

Since the integration over t' in the exponential of (4.6) can be performed analytically, the result (4.6), that is, the solution to (4.3), can be written in the form

$$\rho(X, t) = \frac{f(\Xi)}{\gamma^2} \exp\left\{ bt + \frac{2r_1}{\gamma} \ln[\Xi a(e^{-\gamma t} - 1) - r_2 + r_1 e^{-\gamma t}] - \frac{2r_2}{\gamma} \ln[\Xi a(1 - e^{\gamma t}) + r_1 - r_2 e^{\gamma t}] \right\}, \quad (4.8)$$

where it is understood that (4.7) is used to express Ξ in terms of X and t. Note that (4.4) and (4.7) are the specific forms of relationships (3.3) and (3.8), respectively, relevant for the system considered here.

The significance of the analytical solution (4.8) of the LE (4.3) relevant for the 1D model (4.1) may be recognized by noting that (4.8) allows to identify the impact of any uncertainty in the initial state of the dynamical system—expressed through the initial pdf f—for any later time t without the need to perform a numerical integration of the LE (4.3) itself. Furthermore, the need to create an ensemble of solutions originating at different initial solutions is ostensibly avoided.

The structure of the solution (4.8) is shown in Fig. 1 for two truncated Gaussian initial pdfs (bold lines in Fig. 1) with means -2 (Fig. 1a), and 0 (Fig. 1b), respectively, and variance 0.1, for selected values of t. (These initial pdfs are nonzero only on the interval $-3 \leq X \leq -1$, and $-1 \leq X \leq 1$, respectively; the system parameters a, b, and c are specified as -1, 1, and 2, respectively.) It is clearly evident that the pdfs reflect the dynamical behavior of system (4.1) insofar as in the first case (Fig. 1a) the pdf evolves away from the unstable equilibrium point (at $X = -1$) of system (4.1), whereas in the second case (Fig. 1b) the pdf evolves toward the stable equilibrium point at $X = 2$. In addition, it is of interest to note the asymmetry in the pdfs at later times emerging from nonlinear effects, as well as—in the second case—the initial increase of the variance of the pdf followed by a decrease (note the comparatively broad shape of the pdf at $t = 0.3$ in Fig. 1b).

In concluding the discussion of this example, it is noted that in order to arrive at (4.8) the pertinent relationships (3.3) and (3.8) have been used in analytical form in the specification of the general form of the solution (3.7) of the LE. These relationships need to be evaluated numerically in the absence of analytical expressions. In addition, the 1D integration over t' in the exponential term, which might require numerical evaluation in more complicated situations, too, has also been performed analytically.

5. Concluding remarks

The LE represents the natural framework for dealing with imperfect initial conditions and model errors in the context of numerical weather forecasting and, specifically, in the context of forecasting forecast skill. Both of these sources for the increasing uncertainty of forecasts at increasing lead times can be accounted for within the LE that expresses the fact that the phase-space integral of the number density of realizations remains constant in time. As such, the LE describes the temporal evolution of the pdf of the model state vector in phase space. The LE is a quasi-linear, inhomogeneous partial differential equation, and its solution may

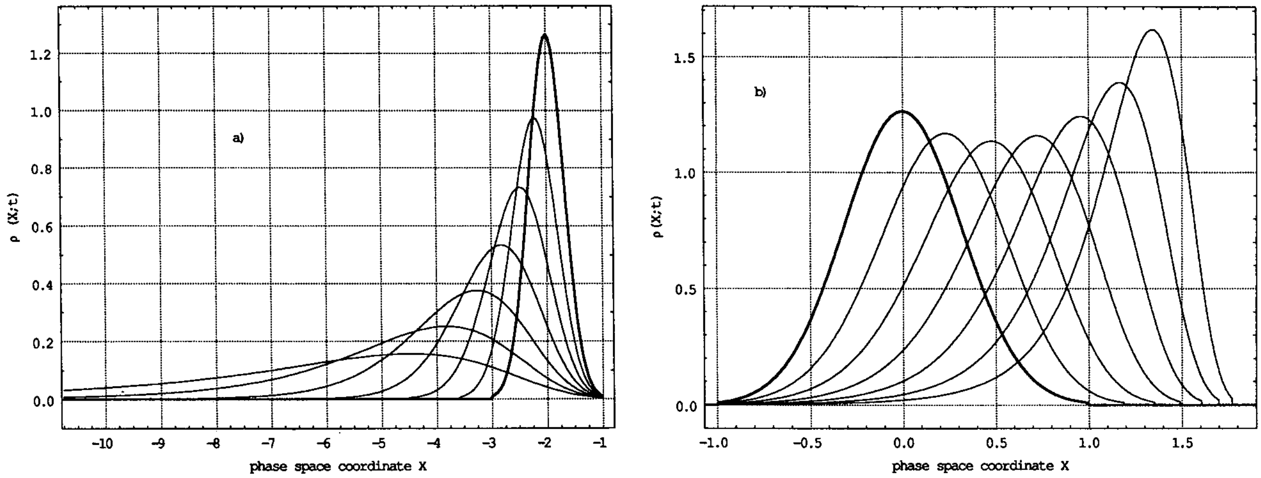

FIG. 1. Display of the analytical solution (4.8) of the LE (4.3) relevant for system (4.1) taking the initial pdf to be Gaussian with mean (a) −2, (b) 0, and variance 0.1 (marked bold). The pdf $\rho(\mathbf{X}, t)$ is plotted as a function of $\mathbf{X}$ with parameter t, taking on the values (a) 0.0–0.3 (step 0.05), and (b) 0.0–0.6 (step 0.1), respectively. For the values of the system parameters a, b, and c, see section 4.

be found by the method of characteristics. From its solution, basic information about the pdf of the state vector can be derived by integration over phase space. Such information about the pdf, as its mean, its (co)variance structure, and its higher moments, must be considered essential in the context of forecasting forecast skill.

In the first part of this work, the LE and its explicit analytical solution have been considered for the case that the dynamical system under consideration is described by a set of N autonomous, nonstochastic, ordinary differential equations (section 2). To arrive at the solution presented in section 3, it is assumed that the state vector $\mathbf{X}$ of the dynamical system at a particular time t can be related unambiguously to the state vector $\mathbf{\Xi}$ at the initial time $t = 0$. This relationship can be represented either in analytical or numerical terms. Thus, to evaluate the analytical solution of the LE, an analytical or numerical solution of the dynamical system considered must be available. This approach may be compared with the approach of Thompson (1983, 1985a), who solved the equilibrium form of the LE (more specifically, its associated Fokker–Planck equation) by a particular series expansion of the pdf ρ without requiring the availability of the solution of the dynamical system.

The usefulness of the general analytical solution presented for the process of solving the LE associated with a specific dynamical system has been illustrated here in the context of a one-dimensional example. In this example, the (one-dimensional) relationship between X and Ξ has been available in analytical form. In Part II of this work (Ehrendorfer 1994a), two three-dimensional examples are considered—in one, the relationship between $\mathbf{X}$ and $\mathbf{\Xi}$ is available only in numerical form. However, it is demonstrated in Part II that the solution presented in section 3 of this paper is equally well applicable.

A more extensive discussion of issues related to the applicability of the LE within the area of predicting forecast skill in more complicated contexts is also delayed until the end of the second part of this work. However, the fact that the solution of the LE provides detailed information about the time evolution of any uncertainty in the initial condition of the dynamical system considered emphasizes the central role of the LE in dealing with imperfect initial conditions in the context of predicting forecast skill. In turn, the central role of the LE requires the serious consideration of the LE in the context of developing and refining methods appropriate for the prediction of forecast skill.

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APPENDIX A

Verifying the Solution of the Liouville Equation

It is proved here that (3.7) satisfies (3.4). Use of the partial derivatives of $\rho(\mathbf{X}, t)$ [as given in (3.7)] with respect to **X** and t leads—after canceling the common nonzero exponential—to the following expression for the left-hand side of (3.4):

$$S \equiv \frac{\partial f(\Xi)}{\partial t} + f(\Xi)\frac{\partial g(\Xi,t)}{\partial t} + \sum_{k=1}^{N} \Phi_k(\mathbf{X})\left[\frac{\partial f(\Xi)}{\partial X_k} + f(\Xi)\frac{\partial g(\Xi,t)}{\partial X_k}\right] + \psi(\mathbf{X})f(\Xi), \quad (A.1)$$

where

$$g(\Xi,t) \equiv -\int_0^t \psi[\mathbf{X}(\Xi,t')]dt'. \quad (A.2)$$

Thus, for (3.7) to be the solution of (3.4), S, defined in (A.1), has to vanish identically. To show this, the derivatives of f occurring in (A.1) are evaluated using the chain rule and observing (3.8). Factoring common terms results in

$$S = \sum_{i=1}^{N} \frac{\partial f(\Xi)}{\partial \Xi_i}\underbrace{\left[\frac{\partial \Xi_i(\mathbf{X},t)}{\partial t} + \sum_{k=1}^{N}\Phi_k(\mathbf{X})\frac{\partial \Xi_i(\mathbf{X},t)}{\partial X_k}\right]}_{\equiv A} + f(\Xi)\underbrace{\left[\frac{\partial g(\Xi,t)}{\partial t} + \sum_{k=1}^{N}\Phi_k(\mathbf{X})\frac{\partial g(\Xi,t)}{\partial X_k} + \psi(\mathbf{X})\right]}_{\equiv B}. \quad (A.3)$$

Since $f(\Xi)$ is arbitrary and therefore, in general, nonzero, it is necessary in order for S to vanish that the bracketed terms in (A.3), denoted by A and B, both vanish identically.

To prove that A vanishes identically, consider the total differentials of X_j and Ξ_l:

$$dX_j(\Xi,t) = \sum_{m=1}^{N}\frac{\partial X_j(\Xi,t)}{\partial \Xi_m}d\Xi_m + \frac{\partial X_j(\Xi,t)}{\partial t}dt, \quad (A.4)$$

$$d\Xi_l(\mathbf{X},t) = \sum_{n=1}^{N}\frac{\partial \Xi_l(\mathbf{X},t)}{\partial X_n}dX_n + \frac{\partial \Xi_l(\mathbf{X},t)}{\partial t}dt. \quad (A.5)$$

Upon inserting (A.4) into (A.5) and rearranging terms, one obtains for the differential of Ξ_l:

$$d\Xi_l(\mathbf{X},t) = \sum_{n=1}^{N}\left\{\frac{\partial \Xi_l(\mathbf{X},t)}{\partial X_n}\left[\sum_{m=1}^{N}\frac{\partial X_n(\Xi,t)}{\partial \Xi_m}d\Xi_m + \frac{\partial X_n(\Xi,t)}{\partial t}dt\right]\right\} + \frac{\partial \Xi_l(\mathbf{X},t)}{\partial t}dt$$
$$= \sum_{n=1}^{N}\sum_{m=1}^{N}\frac{\partial \Xi_l(\mathbf{X},t)}{\partial X_n}\frac{\partial X_n(\Xi,t)}{\partial \Xi_m}d\Xi_m + \left[\sum_{n=1}^{N}\frac{\partial \Xi_l(\mathbf{X},t)}{\partial X_n}\frac{\partial X_n(\Xi,t)}{\partial t} + \frac{\partial \Xi_l(\mathbf{X},t)}{\partial t}\right]dt. \quad (A.6)$$

Since (A.6) is an identity, the following two relations are obtained from it:

$$\sum_{m=1}^{N}\sum_{n=1}^{N}\frac{\partial \Xi_l(\mathbf{X},t)}{\partial X_n}\frac{\partial X_n(\Xi,t)}{\partial \Xi_m}d\Xi_m = d\Xi_l, \quad (A.7)$$

$$\sum_{n=1}^{N}\frac{\partial \Xi_l(\mathbf{X},t)}{\partial X_n}\frac{\partial X_n(\Xi,t)}{\partial t} + \frac{\partial \Xi_l(\mathbf{X},t)}{\partial t} = 0. \quad (A.8)$$

[Note that (A.7), which is not needed in the remainder of the proof, just expresses the fact that the product of the Jacobians of a transformation and its inverse is unity.] At this point (A.8) may be used to rewrite A in the form:

$$A = -\sum_{n=1}^{N}\frac{\partial \Xi_i(\mathbf{X},t)}{\partial X_n}\frac{\partial X_n(\Xi,t)}{\partial t} + \sum_{k=1}^{N}\Phi_k(\mathbf{X})\frac{\partial \Xi_i(\mathbf{X},t)}{\partial X_k} = -\sum_{k=1}^{N}\frac{\partial \Xi_i(\mathbf{X},t)}{\partial X_k}$$
$$\times\left[\frac{\partial X_k(\Xi,t)}{\partial t} - \Phi_k(\mathbf{X})\right]. \quad (A.9)$$

Clearly, since **X** is a solution [see (3.3)] of the differential equation (3.1), the bracketed term in (A.9) vanishes identically, which in turn concludes the proof that A vanishes identically.

To prove that B vanishes identically, it is first necessary to note for the correct computation of required derivatives that (A.2) must be understood as [see also, (3.9)]

$$g(\Xi,t) = g[\Xi(\mathbf{X},t),t] = g(\mathbf{X},t)$$
$$\equiv -\int_0^t \psi[\mathbf{X}(\Xi,t')]dt'$$
$$= -\int_0^t \psi\{\mathbf{X}[\Xi(\mathbf{X},t),t']\}dt'. \quad (A.10)$$

Then, the partial derivative of g with respect to t is obtained as

$$\frac{\partial g(\Xi, t)}{\partial t} = -\frac{\partial}{\partial t}\int_0^t \psi\{\mathbf{X}[\Xi(\mathbf{X}, t), t']\}dt' = -\psi(\mathbf{X}) - \int_0^t \frac{\partial}{\partial t}\psi\{\mathbf{X}[\Xi(\mathbf{X}, t), t']\}dt'$$
$$= -\psi(\mathbf{X}) - \int_0^t \sum_{i=1}^N \frac{\partial\psi(\mathbf{X})}{\partial X_i}\frac{\partial X_i[\Xi(\mathbf{X}, t), t']}{\partial t}dt' = -\psi(\mathbf{X}) - \int_0^t \left[\sum_{i=1}^N \frac{\partial\psi(\mathbf{X})}{\partial X_i}\sum_{j=1}^N \frac{\partial X_i(\Xi, t')}{\partial \Xi_j}\frac{\partial \Xi_j(\mathbf{X}, t)}{\partial t}\right]dt'. \quad (A.11)$$

Similarly, the partial derivative of g with respect to X_k is obtained as

$$\frac{\partial g(\Xi, t)}{\partial X_k} = -\frac{\partial}{\partial X_k}\int_0^t \psi\{\mathbf{X}[\Xi(\mathbf{X}, t), t']\}dt' = -\int_0^t \frac{\partial}{\partial X_k}\psi\{\mathbf{X}[\Xi(\mathbf{X}, t), t']\}dt'$$
$$= -\int_0^t \sum_{l=1}^N \frac{\partial\psi(\mathbf{X})}{\partial X_l}\frac{\partial X_l[\Xi(\mathbf{X}, t), t']}{\partial X_k}dt' = -\int_0^t \left[\sum_{l=1}^N \frac{\partial\psi(\mathbf{X})}{\partial X_l}\sum_{m=1}^N \frac{\partial X_l(\Xi, t')}{\partial \Xi_m}\frac{\partial \Xi_m(\mathbf{X}, t)}{\partial X_k}\right]dt'. \quad (A.12)$$

Using expressions (A.11) and (A.12) in the definition of B [see (A.3)] yields

$$B = -\psi(\mathbf{X}) - \int_0^t \left[\sum_{i=1}^N \frac{\partial\psi(\mathbf{X})}{\partial X_i}\sum_{j=1}^N \frac{\partial X_i(\Xi, t')}{\partial \Xi_j}\frac{\partial \Xi_j(\mathbf{X}, t)}{\partial t}\right]dt'$$
$$- \sum_{k=1}^N \Phi_k(\mathbf{X})\int_0^t \left[\sum_{l=1}^N \frac{\partial\psi(\mathbf{X})}{\partial X_l}\sum_{m=1}^N \frac{\partial X_l(\Xi, t')}{\partial \Xi_m}\frac{\partial \Xi_m(\mathbf{X}, t)}{\partial X_k}\right]dt' + \psi(\mathbf{X}) = -\sum_{i=1}^N\sum_{j=1}^N \frac{\partial\psi(\mathbf{X})}{\partial X_i}\frac{\partial \Xi_j(\mathbf{X}, t)}{\partial t}$$
$$\times \int_0^t \frac{\partial X_i(\Xi, t')}{\partial \Xi_j}dt' - \sum_{k=1}^N \Phi_k(\mathbf{X})\sum_{i=1}^N\sum_{j=1}^N \frac{\partial\psi(\mathbf{X})}{\partial X_i}\frac{\partial \Xi_j(\mathbf{X}, t)}{\partial X_k}\int_0^t \frac{\partial X_i(\Xi, t')}{\partial \Xi_j}dt'$$
$$= -\sum_{i=1}^N\sum_{j=1}^N \frac{\partial\psi(\mathbf{X})}{\partial X_i}\left[\frac{\partial \Xi_j(\mathbf{X}, t)}{\partial t} + \sum_{k=1}^N \Phi_k(\mathbf{X})\frac{\partial \Xi_j(\mathbf{X}, t)}{\partial X_k}\right]\int_0^t \frac{\partial X_i(\Xi, t')}{\partial \Xi_j}dt'. \quad (A.13)$$

Note that in the computations in (A.13) several quantities independent of t' have been taken out of the integral and the order of integration and summation has been changed. Finally, note that the bracketed term in the last line of (A.13) is just the quantity A for which it was shown above that it vanishes identically [see (A.3) and (A.9)]. This, in turn, concludes the proof that B vanishes identically, too.

Thus, it has been shown that (3.7) is the general solution of the LE (3.4).

APPENDIX B

Normalization of the Solution (3.7)

It is demonstrated here that the solution of the LE given in (3.7) is appropriately normalized to 1 for all t (as necessary for the interpretation of ρ as a pdf), in the sense that

$$\int_{-\infty}^{\infty} \rho(\mathbf{X}, t)d\mathbf{X} = 1, \quad \forall t. \quad (B.1)$$

Note first, that relationship (B.1) is true for $t = 0$, since (3.7) satisfies the initial condition (3.5) and the function f is appropriately normalized [see (3.6)]. Further, since $\rho(\mathbf{X}, t)$ given by (3.7) satisfies the LE (3.4) identically (see appendix A), because it is the solution, integrating (3.4) with respect to $\mathbf{X}$ results in

$$\int_{-\infty}^{\infty} \left\{\frac{\partial\rho(\mathbf{X}, t)}{\partial t} + \sum_{k=1}^N \frac{\partial}{\partial X_k}[\rho(\mathbf{X}, t)\dot{X}_k(\mathbf{X}, t)]\right\}d\mathbf{X} = 0, \quad (B.2)$$

where it is understood that (3.7) is used for $\rho(\mathbf{X}, t)$. Equation (B.2) may be simplified to

$$\int_{-\infty}^{\infty} \frac{\partial\rho(\mathbf{X}, t)}{\partial t}d\mathbf{X} + \sum_{k=1}^N \int_{-\infty}^{\infty} \{[\rho(\mathbf{X}, t)\dot{X}_k(\mathbf{X}, t)]|_{-\infty}^{\infty}\} \times \prod_{\substack{i=1\\ i\neq k}}^N dX_i = 0. \quad (B.3)$$

It is now necessary to assume that the product $\rho\dot{X}_k$ tends to zero for $X_k \to \pm\infty$. This assumption may be easily justified by either the requirement that the mean value of ρ must remain finite (and thus ρ must vanish at infinity) or by the physical statement that there can be no flux of realizations at infinity. Under the above assumption, the bracketed term in (B.3) vanishes identically for each k, which, in turn, leads to a vanishing of the complete second term in (B.3). Thus, after reversing the order of differentiation and integration in (B.3), the result

$$\frac{\partial}{\partial t}\int_{-\infty}^{\infty}\rho(\mathbf{X},t)d\mathbf{X}=0 \qquad \text{(B.4)}$$

is obtained. Thus, the mean value (over phase space) of $\rho(\mathbf{X}, t)$ is independent of time and therefore constant. However, since the constant is 1 for $t = 0$ (see above), it follows immediately that (B.1) is true.

Note that for the proof given, reference to the specific form of the solution (3.7) is made only insofar as (3.7) is required to satisfy (3.5). However, when integrating the LE (3.4) over phase space, the arguments deduced for (3.7) are valid only if $\rho(\mathbf{X}, t)$ satisfies the LE identically. This, in turn, is the case (see appendix A), and therefore the solution (3.7) is correctly normalized to unity for all t.

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