Local predictability and information flow in complex dynamical systems

X. San Liang, *

Courant Institute of Mathematical Sciences
New York, New York, USA

Abstract

Predictability is by observation a local notion in complex dynamical systems. Its spatio-temporal structure is associated with a flow, or transfer in discrete cases, of information that redistributes the local predictability within the state space of concern. This flow or transfer is formalized with respect to relative entropy within a framework of a system with many components, each signifying a location or a structure. Given a component, the mechanism governing the evolution of its predictability can be classified into two groups, one due to the component itself, another due to a transfer of information from its peers. A measure of the transfer is rigorously derived, and an explicit expression obtained. This measure possesses a form remniscent of that we have obtained before with respect to absolute entropy in Liang and Kleeman (2007b). Properties have been explored and discussed; particularly discussed is the property of asymmetry or causality, which states that information transfer from one component to another carries no hint about the transfer in the other direction, in contrast to the transfer of other quantities such as energy. This formalism has been applied to the study of the scale-scale interaction and information transfer between the first two modes of the truncated Burgers equation. It is found that all the 12 transfers are essentially zero or negligible, save for a strong transfer between the sine components from the low-frequency mode to the high-frequency mode. That is to say, the predictability of the high-frequency mode is controlled by the knowledge of the low-frequency mode. This result, though from a highly idealized system, has interesting implications about the dynamical closure problem in turbulence research and atmosphere-ocean science, i.e., the subgrid processes may to some extent be parameterized by the large-scale dynamics. We have also discussed how this study can be adopted to investigate the propagation of uncertainties in fluid flows, which has important applications in problems such as atmospheric observing platform design.

Key words: Information transfer, predictability, causality, relative entropy, Frobenius-Perron operator, dynamical closure, ensemble prediction

1 Introduction

In his pioneering work, Lorenz (1963) shows that prediction of the state of a nonlinear dynamical system is impossible beyond a certain time limit if the system is intrinsically chaotic. This raises a severe issue in philosophy (e.g. Leiber, 1998), and since then the problem of predictability has received enormous attention, in both theoretical dynamical systems (see Lichtenberger and Liberman, 1992, and references therein) and applied fields such as atmosphere-ocean science (e.g., Carnevale and Holloway 1982; Farrell 1990; Schneider and Griffies 1999; Smith et al. 1999; Shukla 1998; Kleeman 2002; Kleeman et al. 2002; Kalnay 2003; Tribbia and Baumhefner 2004; Kleeman and Majda 2005; Kleeman 2007). The past deacades have seen a surge of interest in ensemble forecast (e.g. Leith, 1974; Epstein, 1969; Ehrendorfer and Tribbia, 1997; Palmer, 2000; Miller and Ehret, 2002; Kalnay, 1997; Moore, 1999; Kirwan et al., 2003; Lermusiaux, 2006; Kleeman, 2007); the fundamental scientific thrust is predictability.

Classically predictability is a global concept over the whole system. But in realistic problems, particularly in problems with high dimensional systems, people have observed that it generally varies from place to place. For example, Palmer (1988) finds that his numerical weather model has different predictability for different flow regimes; Farrell(1990) shows that predictability is structure dependent, and in the linear limit the most unpredictable structure can be identified; Kleeman (2002) realizes the predictability difference between the El Niño modes; Tribbia (2005) and Kleeman (2002, 2005, 2007) have studied the predictability evolution in physical space. In other words, predictability is by observation a local concept, varying in physical space and/or phase space as it evolves in time.

The spatio-temporal structure of predictability implies a flow, or transfer in discrete cases, of information that redistributes predictability from one place to another within the dynamical system of concern. This flow or transfer is important in that it determines how predictability in one place is altered due to other places, how uncertainties propagate in the system, and hence helps to identify the source region(s) of unpredictability. An immediate application is in observing platform design. In atmospheric science, for example, it has been argued that observations should target at these source locations (Tribbia 2005; Kleeman 2007), in order for a weather forecast system to increase its forecast skill.

The above problem may be formalized within a framework of dynamical systems with many components, each component standing for a physical location

* Courant Institute of Mathematical Sciences, 251 Mercer St, New York, NY 10012
Email address: sanliang@cims.nyu.edu (X. San Liang,).

or a structure. This way what we are discussing is essentially about the information transfer between dynamical system components, a concept which has been of interest for decades in communication, nonlinear time series coherence analysis, neuroscience, to name a few (Kaneko 1986; Vastano and Swinney 1988; Rosenblum et al. 1996; Arnhold et al. 1999; Schreiber 2000; Abarbanel et al. 2001; Kaiser and Schreiber 2002). The available formalisms include the delayed mutual information (Vastano and Swinney 1988) and the more sphisticated transfer entropy by Schreiber (2000). In relation to this study, these empirical/half-empirical formalisms have been applied to the investigation of the information flow in weather forecasts (Kleeman, 2007). Recently the notion of information transfer has been put on a rigorous footing in the context of dynamical systems (Liang and Kleeman 2005; Liang and Kleeman 2007a,b; hereafter LK05, LK07a, LK07b, respectively). The resulting measure of the transfer is qualitatively consistent with the classical formalisms but is based on rigorous derivations. Explicit expressions have been obtained for continuous dynamical systems, and for two well-studied mappings, the baker transformation and the Hénon map. These results, most of them unique to the Liang and Kleeman formalism, agree well with what one may expect by physical intuition.

The Liang and Kleeman formalism is with respect to Shannon entropy, or absolute entropy as one may refer to. The predictability of a dynamical system, however, is measured by relative entropy. Relative entropy is also called Kullback-Leibler divergence; it is a measure of the difference between two probability distributions. Kleeman (2002) points out that, in order to measure the utility of a forecast, one should ask how much additional information is added rather than how much information it has. Relative entropy provides a very natural measure of this information addition, should one probability is set as the initial distribution. Kleeman (2002) also argues in favor of relative entropy becuase of its appealing properties, such as its invariance on nonlinear transformations, its nonnegativity (Cover and Thomas, 1991). In the context of a Markov chain, it has been proved that it always drecreases monotonically with time, a property usually referred to as the generalized second law of thermodynamics (*ibid*). The concept of relative entropy is now a well accepted measure of predictability (e.g., Kleeman, 2002; Kleeman et al., 2002; Tang et al. 2006; Barlas et al., 2006).

Our problem here is therefore fundamentally on how information is transferred with respect to relative entropy. The purpose of this study is to develop a formalism for this information transfer. The development parallels what we have done in LK06b, and the resulting transfer will be referred to as *information transfer with respect to relative entropy*, or simply *information transfer* when no confusion arises. In the literature the term "information flow" is also seen (e.g. Tribbia 2005; Kleeman 2007; Majda and Harlim 2007) for the same meaning. We recognize that it might be more appropriate to use "transfer" for discrete systems, but it indeed forms a flow when the system components are associated with locations in physical space. We will use the two in the text without distinguishment.

In the following section, we first present a conceptual framework for this study, then give the concept a formal definition. An explicit formula is derived for the information transfer of concern; the detailed derivations are supplied in sections 3, 4, and 5. Properties of the formulation are investigated and discussed (section 6), and an application presented (section 7). This study is summarized in section 8.

2 Definition and mathematical framework

The problem can be put in the framework of an n-dimensional dynamical system:

$$\frac{dx_1}{dt} = F_1(x_1, x_2, ..., x_n), \tag{1}$$
$$\frac{dx_2}{dt} = F_2(x_1, x_2, ..., x_n), \tag{2}$$
$$\vdots \qquad\qquad \vdots$$
$$\frac{dx_n}{dt} = F_n(x_1, x_2, ..., x_n). \tag{3}$$

for state variables $\underline{\mathbf{x}} = (x_1, x_2, ..., x_n)$. We want to understand how the predictability of one component of $\underline{\mathbf{x}}$ is altered by another, namely, how information is transferred between two components with respect to relative entropy. Here $\underline{\mathbf{F}} = (F_1, F_2, ..., F_n)$ is written in an autonomous form, but as one will see through the derivations henceforth, autonomy is not essential. For simplicity, the above equation set may also appear in the text in a vectorial form,

$$\frac{d\underline{\mathbf{x}}}{dt} = \underline{\mathbf{F}}(\underline{\mathbf{x}}). \tag{4}$$

Denote by $\underline{\mathbf{X}} = (X_1, X_2, ..., X_n) \in \Omega$ the random variables corresponding to $(x_1, x_2, ..., x_n)$, where Ω is the sample space, and let $\rho = \rho(x_1, x_2, ..., x_n)$ be the joint probability density of $\underline{\mathbf{X}}$. Assume

$$\Omega = \Omega_1 \times \Omega_2 \times ... \times \Omega_n, \tag{5}$$

(Ω_i is the sample spaces of X_i, $i = 1, 2, ..., n$), and write

$$\Omega_{jn} \equiv \Omega_j \times \Omega_{j+1} \times ... \times \Omega_n, \qquad j = 1, 2, ..., n-1 \tag{6}$$

throughout for notational convenience. Further assume that ρ vanishes at the boundaries of Ω, i.e., the extreme events have a measure of zero in the probability space. These assumptions have been justified for real problems in our previous studies (LK05, LK07b). For many problems of interest, $\Omega = \mathbb{R}^n$. In this case, the assumption of vanishing ρ at boundaries automatically holds, since ρ is compactly supported.

In LK05, LK07a,b, we have developed a formalism of information transfer with respect to absolute entropy

$$H = -\int_{\Omega} \rho \log \rho \; d\underline{\mathbf{x}}. \tag{7}$$

In this study, we will follow the same route of development but with respect to relative entropy

$$D = D(\rho \| q) = \int_{\Omega} \rho \log \frac{\rho}{q} d\underline{\mathbf{x}} = -H - \int_{\Omega} \rho \log q \; d\underline{\mathbf{x}}. \tag{8}$$

In the definition, q is a density at some fixed time. Usually it is the initial density or density in the equilibrium state; in this study, let it be the initial density to avoid any confusion that may arise. With respect to D, we are concerned with the information transfer between two components. Without loss of generality, one need only consider the transfer from X_2 to X_1; if not, the variables may always be reordered to make so. We hence need the marginal relative entropy of X_1:

$$D_1 = \int_{\Omega_1} \rho_1 \log \frac{\rho_1}{q_1} dx_1 = -H_1 - \int_{\Omega_1} \rho_1 \log q_1 \; dx_1, \tag{9}$$

where

$$\rho_1 = \int_{\Omega_{2n}} \rho \; dx_2 dx_3 ... dx_n, \qquad q_1 = \int_{\Omega_{2n}} q \; dx_2 dx_3 ... dx_n, \tag{10}$$

are the marginal densities, and

$$H_1 = -\int_{\Omega_1} \rho_1 \log \rho_1 \; dx_1 \tag{11}$$

the marginal absolute entropy. Following the argument of LK07b, the mechanisms governing the time evolution of D_1 can be classified exclusively into two groups: one from a modified system with the effect of X_2 excluded, another from the component X_2. This latter mechanism is the very information transfer from X_2 to X_1. Correspondingly $\frac{dD_1}{dt}$, the time rate of change of D_1, can be decomposed as the change of D_1 with x_2 frozen instantaneously as a parameter, denoted as $\frac{dD_{1\not{2}}}{dt}$, plus the time rate of information transfer, $T_{2\to1}$. We thence have the following definition.

Definition 1 *For system (4), the information transfer from X_2 to X_1 with respect to relative entropy, $T_{2\to1}$, is defined as the difference between the time rate of change of the marginal relative entropy of X_1, $\frac{dD_1}{dt}$, and the time rate of change of the marginal entropy of X_1 with x_2 frozen instantaneously as a parameter, $\frac{dD_{1\not{2}}}{dt}$, i.e.,*

$$T_{2\to1} = \frac{dD_1}{dt} - \frac{dD_{1\not{2}}}{dt}. \tag{12}$$

The units of $T_{2\to1}$ vary, depending on the base of the logarithm in D_1 that is used. The common units are nats per second for base e and bits per second for base 2.

The whole problem is now converted to the derivation of $\frac{dD_1}{dt}$ and $\frac{dD_{1\not{2}}}{dt}$. In the following section $\frac{dD_1}{dt}$ is derived. The challenge comes from the derivative of $D_{1\not{2}}$, which we defer to section 4. For convenience, the notation $\not{2}$ in the subscript of $D_{1\not{2}}$ will be extended to any $\not{j}$ to signify that component j is frozen, or that component j is excluded from a set of n independent variables. For example,

$$\rho_{\not{2}} = \rho_{\not{2}}(x_1, x_3, ..., x_n) = \int_{\Omega_2} \rho(\underline{\mathbf{x}})\ dx_2, \tag{13}$$

$$\rho_{\not{1}\not{2}} = \rho_{\not{1}\not{2}}(x_3, ..., x_n) = \int_{\Omega_1\times\Omega_2} \rho(\underline{\mathbf{x}})\ dx_1 dx_2. \tag{14}$$

This convention will be used throughout the paper without further clarification.

3 Time rate of change of D_1

Theorem 2 *For the system described in section 2,*

$$
\begin{aligned}
\frac{dH}{dt} &= E(\nabla \cdot \underline{\mathbf{F}}), && (15)\\
\frac{dH_1}{dt} &= \int_{\Omega} \log \rho_1 \cdot \frac{\partial(F_1\rho)}{\partial x_1}\ d\underline{\mathbf{x}}, && (16)\\
\frac{dD_1}{dt} &= -\int_{\Omega} \log \frac{\rho_1}{q_1} \cdot \frac{\partial(F_1\rho)}{\partial x_1}\ d\underline{\mathbf{x}}, && (17)
\end{aligned}
$$

where E is the operator of expectation with respect to the density ρ.

Proof
See Appendix A.

Eq. (15) was obtained in LK05; it states that the change of absolute entropy in a system is totally controlled by the divergence of the flow, or the contraction/expansion of the phase space. Notice that $\int_\Omega \frac{\partial(F_1\rho)}{\partial x_1}\ d\underline{\mathbf{x}} = 0$ by the assumptions introduced before (vanishing density at boundaries and cartesian product form for Ω). So Eq. (17) can be be equivalently written as

$$
\frac{dD_1}{dt} = -\int_{\Omega} \left(1 + \log \frac{\rho_1}{q_1}\right) \cdot \frac{\partial(F_1\rho)}{\partial x_1}\ d\underline{\mathbf{x}}. \qquad (18)
$$

Later on we will have opportunity to use (18).

4 Time rate of change of D_1 with x_2 as a parameter

Theorem 3 *For the dynamical system described in section 2, the time rate of change of the marginal relative entropy of X_1 with x_2 frozen instantaneously as a parameter is*

$$
\frac{dD_{1\not{2}}}{dt} = -\int_{\Omega} \left(1 + \log \frac{\rho_1}{q_1}\right) \frac{\partial(F_1\rho_{\not{2}})}{\partial x_1} \Theta_{2|1}\ d\underline{\mathbf{x}} + \int_{\Omega} \frac{\partial(F_1\rho_1 \log \frac{\rho_1}{q_1})}{\partial x_1} \theta_{2|1}\ d\underline{\mathbf{x}}, \qquad (19)
$$

where

$$
\begin{aligned}
\theta_{2|1} &= \theta_{2|1}(x_1, x_2, x_3, ..., x_n) = \frac{\rho}{\rho_{\not{2}}} \rho_{\not{1}\not{2}}, && (20)\\
\Theta_{2|1} &= \Theta_{2|1}(x_1, x_2) = \int_{\Omega_{3n}} \theta_{2|1}\ dx_3 ... dx_n, && (21)
\end{aligned}
$$

This theorem cannot be proved as that for Theorem 2 using the Liouville equation (cf. Lasota and Mackey, 1994) corresponding to (4), as the dynamics is changed upon freezing x_2. In LK07b, we approach the problem by discretizing (1)-(3) or (4), finding how $D_{1\not 2}$ increases from time t to time $t+\Delta t$, and then take the limit as $\Delta t \to 0$. In the following the same strategy is adopted.

Discretization of the continuous system (4) results in a mapping $\Phi : \Omega \longrightarrow \Omega$, $\underline{\mathbf{x}} \mapsto \underline{\mathbf{y}}$ such that

$$\Phi : \underline{\mathbf{y}} = \underline{\mathbf{x}} + \Delta t \ \underline{\mathbf{F}}(\underline{\mathbf{x}}), \tag{22}$$

i.e., an approximation of (4) up to the first order of Δt. To avoid confusion, here $\underline{\mathbf{x}}(t+\Delta t)$ has been written as $\underline{\mathbf{y}} = (y_1, y_2, ..., y_n)$; this convention will be kept throughout. In component form, the mapping is

$$\Phi = (\Phi_1, \Phi_2, ..., \Phi_n) : \begin{cases} y_1 = x_1 + \Delta t \cdot F_1(\underline{\mathbf{x}}), \\ y_2 = x_2 + \Delta t \cdot F_2(\underline{\mathbf{x}}), \\ \vdots \qquad\qquad \vdots \\ y_n = x_n + \Delta t \cdot F_n(\underline{\mathbf{x}}). \end{cases} \tag{23}$$

Corresponding to Φ that maps the state from t to $t+\Delta t$, there is an operator sending the density of the state variables from t to $t+\Delta t$. This is the Frobenius-Perron operator, or F-P operator for short. Formally, the F-P operator, written as $\mathcal{P}$, corresponding to a transformation $\Phi : \Omega \mapsto \Omega$ is a map $\mathcal{P} : L^1(\Omega) \mapsto L^1(\Omega)$ such that, for any $\omega \subset \Omega$,

$$\int_\omega \mathcal{P}\rho(\underline{\mathbf{x}}) \ d\underline{\mathbf{x}} = \int_{\Phi^{-1}(\omega)} \rho(\underline{\mathbf{x}}) \ d\underline{\mathbf{x}}.$$

It can be viewed as the discrete form of the Liouville equation for density ρ. See Lasota and Mackey (1992) for more details. Liang and Kleeman (LK07b) have showed that the mapping Φ and its associated F-P operator $\mathcal{P}$ possess some interesting properties, which here we briefly summarize.

(1) As Δt goes to zero, Φ and its individual components are always invertible, and

$$\Phi^{-1} : \begin{cases} x_1 = y_1 - \Delta t \cdot F_1(\underline{\mathbf{y}}) + O(\Delta t^2), \\ x_2 = y_2 - \Delta t \cdot F_2(\underline{\mathbf{y}}) + O(\Delta t^2), \\ \vdots \qquad\qquad \vdots \\ x_n = y_n - \Delta t \cdot F_n(\underline{\mathbf{y}}) + O(\Delta t^2). \end{cases} \tag{24}$$

(2) The Jacobian of Φ, J, and its inverse, are

$$J = \det \left[\frac{\partial(y_1, y_2, ..., y_n)}{\partial(x_1, x_2, ..., x_n)} \right] = 1 + \Delta t \nabla \cdot \underline{\mathbf{F}} + O(\Delta t^2); \tag{25}$$

$$J^{-1} = 1 - \Delta t \nabla \cdot \underline{\mathbf{F}} + O(\Delta t^2). \tag{26}$$

(3) The F-P operator $\mathcal{P}$ can be explicitly written out:

$$\begin{aligned} \mathcal{P}\rho(y_1, ..., y_n) &= \rho\left(\Phi^{-1}(y_1, ...y_n)\right) \ \left|J^{-1}\right| \\ &= \rho(x_1, x_2, ..., x_n) \ \left|J^{-1}\right|, \end{aligned} \tag{27}$$

because of the invertibility of Φ (cf. Lasota and Mackey, 1994).

When x_2 is frozen, the mapping Φ is modified, resulting in a new transformation:

$$\Phi_{\not 2} : \begin{cases} y_1 = x_1 + \Delta t \cdot F_1(\underline{\mathbf{x}}) \\ y_3 = x_3 + \Delta t \cdot F_3(\underline{\mathbf{x}}) \\ \vdots \qquad\qquad \vdots \\ y_n = x_n + \Delta t \cdot F_n(\underline{\mathbf{x}}) \end{cases} \tag{28}$$

which maps $(x_1, x_3, x_4, ..., x_n)$ to $(y_1, y_3, y_4, ..., y_n)$ with x_2 as a parameter. Corresponding to $\Phi_{\not 2}$ there is an F-P operator. Write it as $\mathcal{P}_{\not 2}$. $\mathcal{P}_{\not 2}\rho$ is the joint density at time $t + \Delta t$ with x_2 frozen as a parameter at time t, and

$$(\mathcal{P}_{\not 2}\rho)_1(y_1) = \int_{\Omega_{3n}} \mathcal{P}_{\not 2}\rho(y_1, y_3, ..., y_n) \ dy_1 dy_3 ... dy_n$$

the corresponding marginal density of $Y_1 = X_1(t + \Delta t)$. (Note $(\mathcal{P}_{\not 2}\rho)_1$ has dependence on the parameter x_2.) From LK07a and LK07b, the marginal absolute entropy for X_1 evolved from H_1 with contribution from X_2 excluded since time t is

$$\begin{aligned} H_{1\not 2}(t + \Delta t) = \int_{\Omega} & (\mathcal{P}_{\not 2}\rho)_1(y_1) \log (\mathcal{P}_{\not 2}\rho)_1(y_1) \\ & \cdot \ \rho(x_2 | x_1, x_3, ..., x_n) \cdot \rho_{3...n}(x_3, ..., x_n) \ dy_1 dx_2 ... dx_n, \end{aligned}$$

where $y_1 = x_1 + \Delta t \ F_1(\underline{\mathbf{x}})$, $\rho_{3...n} = \rho_{\not 1 \not 2}$, $\rho(x_2 | x_1, x_3, ..., x_n)$ the conditional density of X_2 on $(X_1, X_3, ..., X_n)$. By the same argument, we have

$$D_{1\not 2}(t + \Delta t) = \int_{\Omega} (\mathcal{P}_{\not 2}\rho)_1(y_1) \log \frac{(\mathcal{P}_{\not 2}\rho)_1(y_1)}{q_1(y_1)}$$

$$\cdot\ \rho(x_2|x_1,x_3,...,x_n)\cdot\rho_{3...n}(x_3,...,x_n)\ dy_1dx_2...dx_n \tag{29}$$

To evaluate $D_{1\not 2}(t+\Delta t)$, the key is the evaluation of the F-P operator associated with the modified mapping $\Phi_{\not 2}$:

Proposition 4

$$(\mathcal{P}_{\not 2}\rho)_1(y_1) = \rho_1(y_1) - \Delta t\cdot\int\limits_{\Omega_{3n}} \frac{\partial F_1\rho_{\not 2}}{\partial y_1}\ dx_3...dx_n + O(\Delta t^2). \tag{30}$$

Proof
See Appendix B. With this proposition, we are ready to prove the Theorem of this section.

Outline of the proof of Theorem 3
Substitute (30) into (29), and express the x_1 in $\rho(x_2|x_1,x_3,...,x_n)$ as a function of y_1 (from the inverse map $\Phi_{\not 2}^{-1}$). Then compute $\frac{D_{1\not 2}(t+\Delta t)-D_1(t)}{\Delta t}$. Eq. (19) follows as $\Delta t\to 0$. Refer to Appendix C for the lengthy detailed derivation.

5 Information transfer with respect to relative entropy

Theorem 5 *For the system described in section 2, the information transfer with respect to relative entropy from X_2 to X_1 is*

$$\begin{aligned} T_{2\to 1} = &-\int\limits_{\Omega}\left(1+\log\frac{\rho_1}{q_1}\right)\cdot\left(\frac{\partial F_1\rho}{\partial x_1} - \frac{\partial F_1\rho_{\not 2}}{\partial x_1}\Theta_{2|1}\right)\ d\underline{\mathbf{x}} \\ &-\int\limits_{\Omega}\frac{\partial}{\partial x_1}\left(F_1\rho_1\log\frac{\rho_1}{q_1}\right)\cdot\theta_{2|1}\ d\underline{\mathbf{x}}, \end{aligned} \tag{31}$$

where

$$\theta_{2|1} = \theta_{2|1}(x_1,x_2,x_3,...,x_n) = \frac{\rho}{\rho_{\not 2}}\rho_{\not 1\not 2},$$

$$\Theta_{2|1} = \Theta_{2|1}(x_1,x_2) = \int\limits_{\Omega_{3n}}\theta_{2|1}\ dx_3...dx_n,$$

and $\Theta_{2|1}$ may be viewed as a generalized conditional density of X_2 on X_1.

Proof
Subtract (19) from (18) and the result follows.

Note the transfer rate of relative entropy is in a form similar to that for absolute entropy. One changes $\log \rho_1$ in the equation (50) of LK07b into $\log \frac{\rho_1}{q_1}$ and multiplies the whole formula by (-1), and he obtains Eq. (31). Recalling the definition of relative entropy (8), this is just one may expect.

Above is the transfer from X_2 to X_1. Following the same procedure, it is easy to arrive at the transfer from X_j to X_i, for any $i, j = 1, 2, ..., n$, $i \neq j$. One may replace the index 2 by j, and 1 by i in (31), and make the corresponding modification for $\theta_{2|1}$ and $\Theta_{2|1}$ to obtain the formula. But the easiest way is to re-arrange the order of (1)-(3) such that j is in the second slot and i in the first. This way the rate of transfer is expressed in the same form as (31).

6 Properties

The rate of information transfer (31) possesses some interesting properties. The first one is the concretization of the transfer asymmetry as emphasized by Schreiber (2000). It reads

Theorem 6 *For the system defined in section 2, if F_1 is independent of x_2, then $T_{2\to 1} = 0$. In the mean time, $T_{1\to 2}$ does not need to be zero, unless F_2 is independent of x_1.*

Proof
If F_1 is independent of x_2, in (31) the ρ, $\Theta_{2|1}$, and $\theta_{2|1}$ can be integrated separately with respect to x_2. Observe that

$$\begin{aligned}
\int \rho dx_2 &= \rho_{\not 2}, \\
\int \theta_{2|1} dx_2 &= \int \frac{\rho}{\rho_{\not 2}} \rho_{\not 1 \not 2} dx_2 = \rho_{\not 1 \not 2}, \\
\int \Theta_{2|1} dx_2 &= \int \left(\int \theta_{2|1} dx_3 ... dx_n \right) \, dx_2 = \int \rho_{\not 1 \not 2} dx_3 ... dx_n = 1.
\end{aligned}$$

So integrating (31) once with respect to x_2 gives

$$\begin{aligned}
T_{2\to 1} &= -\int \left(1 + \log \frac{\rho_1}{q_1}\right) \cdot \left(\frac{\partial F_1 \rho_{\not 2}}{\partial x_1} - \frac{\partial F_1 \rho_{\not 2}}{\partial x_1} \right) \, dx_1 dx_3 ... dx_n \\
&\quad - \int \frac{\partial}{\partial x_1} \left(F_1 \rho_1 \log \frac{\rho_1}{q_1} \right) \cdot \rho_{\not 1 \not 2} \, dx_1 dx_3 ... dx_n \\
&= -\int \frac{\partial}{\partial x_1} \left(F_1 \rho_1 \log \frac{\rho_1}{q_1} \rho_{\not 1 \not 2} \right) \, dx_1 dx_3 ... dx_n \\
&= 0.
\end{aligned} \tag{32}$$

The following theorem relates Theorem 3 to the 2D results of LK05:

Theorem 7 *When* $n = 2$, $\frac{dD_{1\not 2}}{dt} = -E\left(\frac{\partial F_1}{\partial x_1}\right) - E\left(F_1 \frac{\partial \log q_1}{\partial x_1}\right)$.

Proof
By definition, when $n = 2$,

$$\Theta_{2|1} = \theta_{2|1} = \rho(x_2|x_1) = \frac{\rho}{\rho_1},$$

and

$$\rho_{\not 2} = \rho_1,$$

So

$$\begin{aligned}
\frac{dD_{1\not 2}}{dt} &= -\int_\Omega \left(1 + \log\frac{\rho_1}{q_1}\right) \frac{\partial F_1 \rho_{\not 2}}{\partial x_1} \Theta_{2|1}\ d\underline{\mathbf{x}} + \int_\Omega \frac{\partial (F_1 \rho_1 \log\frac{\rho_1}{q_1})}{\partial x_1} \theta_{2|1}\ d\underline{\mathbf{x}} \\
&= -\int_\Omega \left(1 + \log\frac{\rho_1}{q_1}\right) \frac{\partial F_1 \rho_1}{\partial x_1} \frac{\rho}{\rho_1}\ d\underline{\mathbf{x}} + \int_\Omega \frac{\partial (F_1 \rho_1 \log\frac{\rho_1}{q_1})}{\partial x_1} \frac{\rho}{\rho_1}\ d\underline{\mathbf{x}} \\
&= -\int \left[-\rho \frac{F_1}{q_1} \frac{\partial q_1}{\partial x_1} - \rho \frac{\partial F_1}{\partial x_1}\right]\ d\underline{\mathbf{x}} \\
&= -E\left(\frac{\partial F_1}{\partial x_1}\right) - E\left(F_1 \frac{\partial \log q_1}{\partial x_1}\right).
\end{aligned}$$

Q.E.D.

7 Application with the truncated Burgers-Hopf system

As an example of application, we re-consider the truncated Burgers-Hopf system (TBS) examined in LK07b, a system first introduced by Majda and Timofeyev (2000; 2002) to study a stochastic scheme of parameterization of the unresolved processes in numerical weather forecasts. It is obtained through a Galerkin truncation of the inviscid Burgers equation. If only two modes are retained, the TBS is reduced to the following 4-dimensional autonomous system (see LK07b):

$$\frac{dx_1}{dt} = F_1(x_1, x_2, x_3, x_4) = x_1 x_4 - x_3 x_2 \tag{33}$$

$$\frac{dx_2}{dt} = F_2(x_1, x_2, x_3, x_4) = -x_1 x_3 - x_2 x_4, \tag{34}$$

$$\frac{dx_3}{dt} = F_3(x_1, x_2) = 2x_1 x_2, \tag{35}$$

$$\frac{dx_4}{dt} = F_4(x_1, x_2) = -x_1^2 + x_2^2, \tag{36}$$

where (x_1, x_2) are the cosine and sine components of the first mode, and (x_3, x_4) the components of the second mode, respectively. This system is intrinsically chaotic, with a low-dimensional attractor; see Majda and Timofeyev (2000; 2002) and Abramov et al. (2003) for details. We now study the information transfers with respect to relative entropy between the four components, and compare the results to those in LK07b.

The key to the computation of the information transfer (31) is the estimation of the joint density of $(X_1,\ X_2,\ X_3,\ X_4)$ as a function of time. This may be obtained through solving

$$\frac{\partial \rho}{\partial t} + \frac{\partial (F_1 \rho)}{\partial x_1} + \frac{\partial (F_2 \rho)}{\partial x_2} + \frac{\partial (F_3 \rho)}{\partial x_3} + \frac{\partial (F_4 \rho)}{\partial x_4} = 0, \tag{37}$$

the Liouville equation corresponding to Eqs. (33)-(36). A more efficient way is, instead of solving ρ directly, estimating the density with the ensembles generated at each time step from ensemble prediction of (33)-(36), as schematized in Fig. 1. The ensemble is formed with the trajectories randomly distributed in

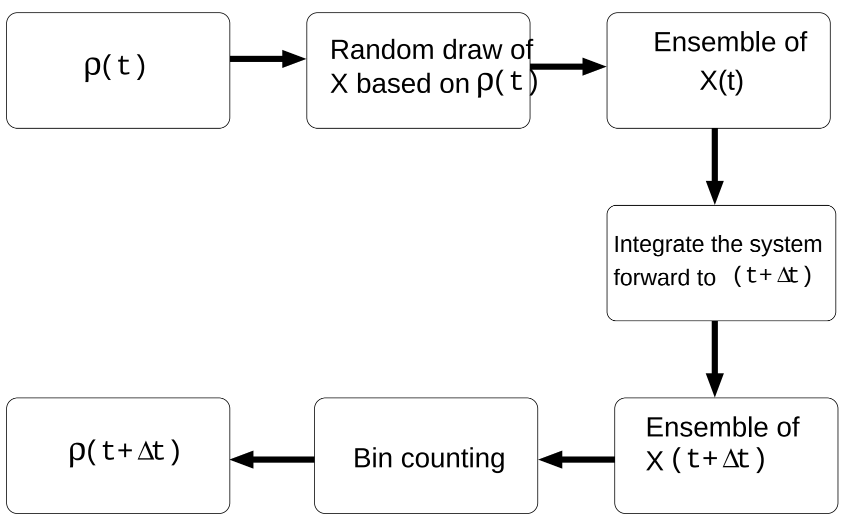

Fig. 1. Numerical scheme to solve the joint density ρ. Instead of obtaining $\rho(t+\Delta t)$ directly from $\rho(t)$ by solving the Liouville equation, a detour is made through ensemble prediction of the TBS system.

the beginning, through solving (33)-(36) using the second order Runge-Kutta method with a time step size $\Delta t = 0.01$. A typical computed trajectory is plotted in Figs. 2 and 3; it shows an invariant manifold or strange attractor limited within some finite domain. If we write $\Omega_d = [-d, d] \times [-d, d] \times [-d, d] \times [-d, d]$,

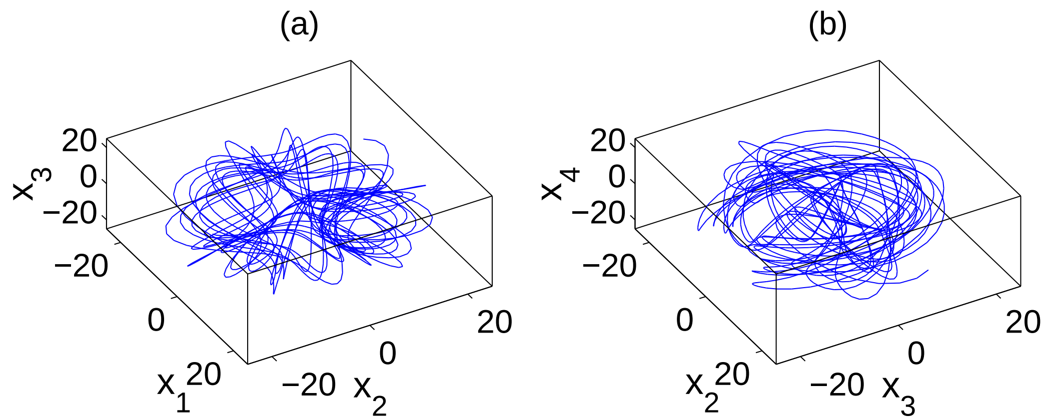

Fig. 2. A trajectory of (33)-(36) starting from from $t = 0$ at $\underline{\mathbf{x}}(0) = (40, 40, 40, 40)$. It is attracted into a domain as shown after $t = 1.5$ (the part prior to $t = 1.5$ not plotted). (a) and (b) are projections in subspaces x_1-x_2-x_3 and x_2-x_3-x_4, respectively.

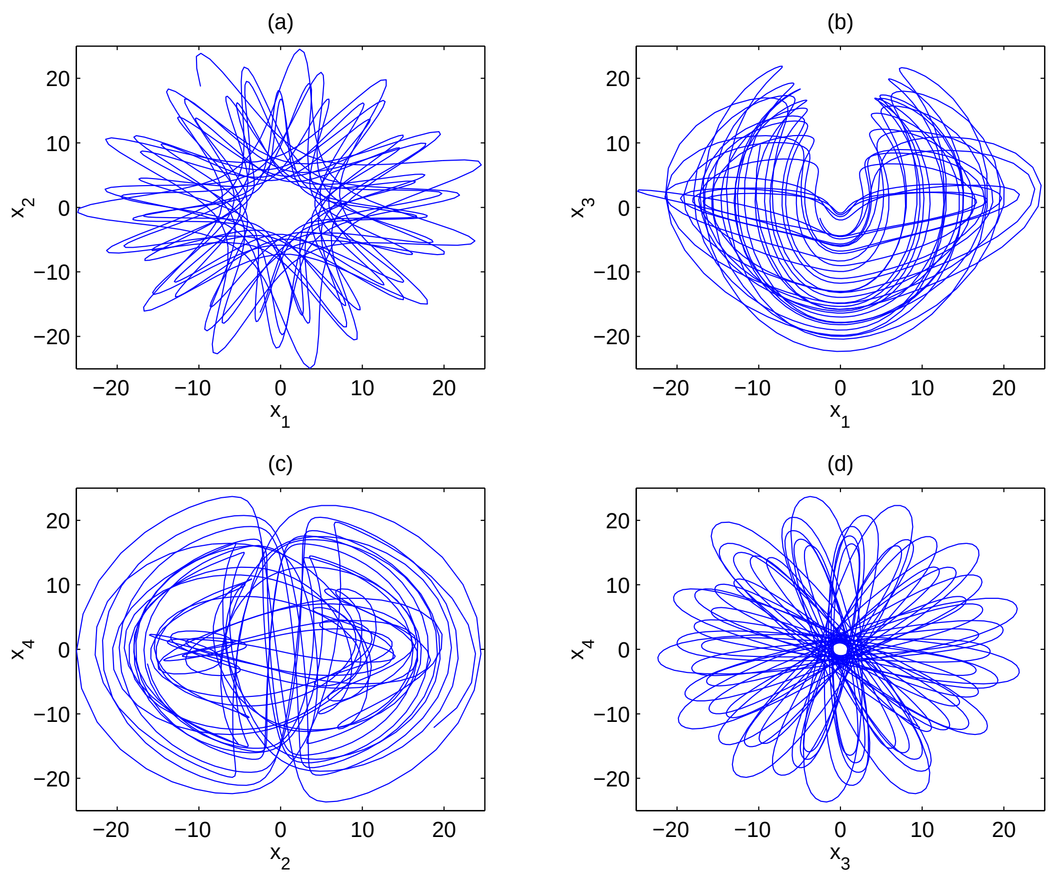

Fig. 3. As Fig. 2, but for projections on 2D planes.

the strange attractor lies within Ω_{25}. So a finite domain may be chosen for the computation, albeit ρ is defined on $\mathbb{R}^4$. We choose it be Ω_{30}, a domain slightly larger than Ω_{25}. This domain is then uniformly partitioned into $30\times 30\times 30\times 30$ bins, with a spacing of 2 in each dimension. A huge ensemble of initial conditions of size $40^4 = 2.56\times 10^6$ is first generated, through drawing randomly according to a preset distribution $\rho_0(\underline{\mathbf{x}})$. We adopt an ensemble size of 40^4 instead of 30^4 to ensure more than one draw per bin on average. Suppose $\underline{\mathbf{x}}$ is initially distributed as a Gaussian $N(\underline{\mu}, \underline{\underline{\mathbf{\Sigma}}})$, with a mean $\underline{\mu} = (\mu_i)$ and a covariance matrix $\underline{\underline{\mathbf{\Sigma}}} = (\sigma_{ij})$, $i, j = 1, 2, 3, 4$, and suppose $\sigma_{ii} = \sigma_i^2$, and $\sigma_{ij} = 0$ if $i \neq j$. The parameters μ_i and σ_i^2 $(i = 1, 2, 3, 4)$ are open for experiments. With these initial conditions, Eqs. (33)-(36) are integrated forward. At every time step we obtain an ensemble of $\underline{\mathbf{X}}$, and therefrom a joint density ρ through bin-counting.

The transfers $T_{j\to i}$, $i, j = 1, 2, 3, 4, i \neq j$, now can be computed straightforwardly by evaluating (31). As in LK07b, there are 12 series to compute. Notice that in (35) and (36), the evolutions of x_3 and x_4 do not depend on x_3 and x_4, so $T_{3\to 4} = T_{4\to 3} = 0$ by Theorem 6. The computed results agree with this inference. The other transfers have only numerical solutions, and may vary with the initial distribution. We have conducted experiments for different σ_i^2 and $\underline{\mu}_i$ in generating the initial ensemble. It is found that the variances σ_i^2 do not affect much the final results, so in these experiments we keep $\sigma_i^2 = 9$ fixed, only allowing $\underline{\mu}$ to vary. Fig. 4 displays the results for the experiment with $\underline{\mu} = (9, 9, 9, 9)$. They correspond to those shown in the Figure 3 of LK07b. Like the latter, most of the transfers are essentially zero. One of the nonzero transfer is $T_{3\to 2}$. See Fig. 4b; also see Fig. 5 for a close-up. It is negative through the time, with a time average of -3.8. This is in consistent with the $T_{3\to 2}$ in LK07b, which is positive (refer to the definition of relative entropy (8) for a relation between D and H). The difference is that here it is not a constant, but oscillates throughout; another difference is that it is far smaller in magnitude than its counterpart in LK07b.

The largest difference between the result here and that in LK07b is that there are two nonzero transfers here, and the dominant one is $T_{2\to 4}$, as shown in Fig. 4d. In fact, $T_{3\to 2}$ is almost negligible in comparison with $T_{2\to 4}$, which averages to 20 and is nearly constant through the time. So it is $T_{2\to 4}$ that makes the counterpart of the $T_{3\to 2}$ in LK07b. This is remarkable, as $T_{2\to 4}$ and $T_{3\to 2}$ stand for information flow in the opposite direction between the two modes—components (x_1, x_2) stand for the lower frequency mode in the truncation, while (x_3, x_4) for the higher mode (refer to LK07b for the derivation of (33)-(36)). In the present study, the computed results shows that information flows primarily from the lower mode to the higher mode, though weak information flow in the opposite direction has also been identified ($T_{3\to 2}$).

The above result is very robust. Experiments with different $\underline{\mu}$ on $[-9, 9]\times[-9, 9]\times[-9, 9]\times[-9, 9]$ have been conducted, all yielding a $T_{2\to 4}$ large in magnitude, except that $\underline{\mu} = 0$ which makes all the transfers vanish. $T_{2\to 4}$

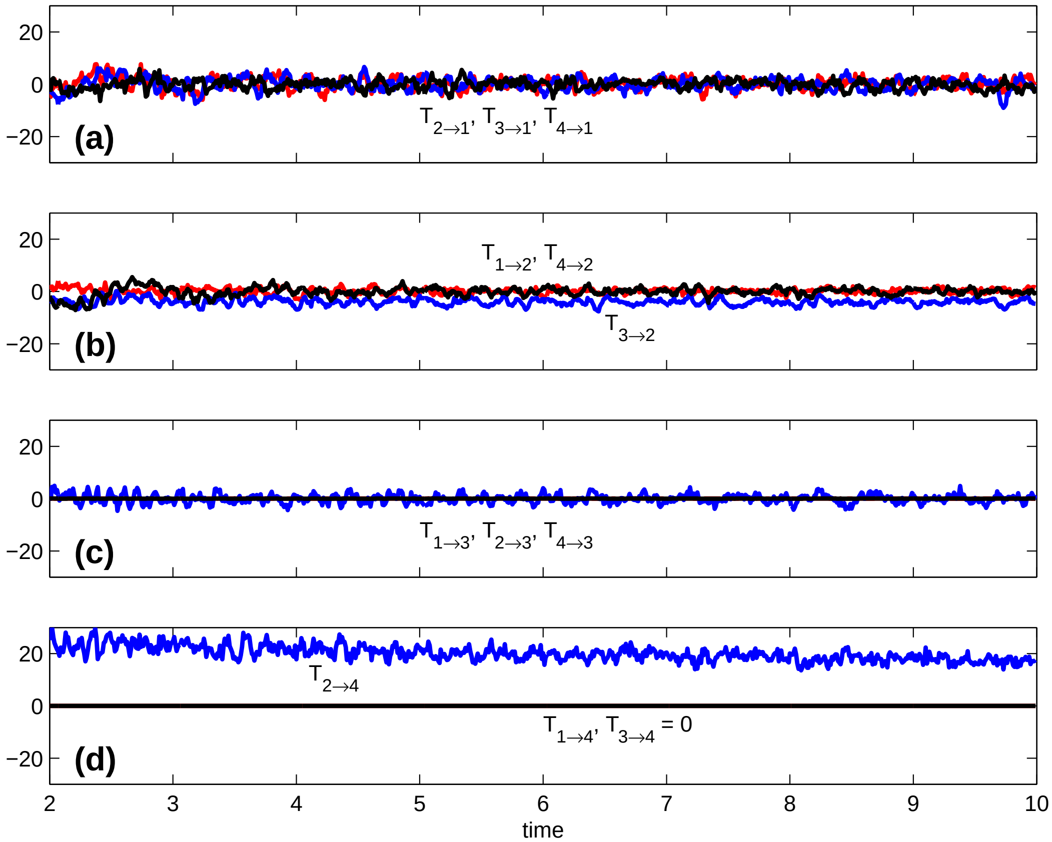

Fig. 4. Information transfer between different pairs of components with $\underline{\mu} = (9, 9, 9, 9)$. The series prior to $t = 2$ are not shown because some trajectories are still outside the computational domain by that time.

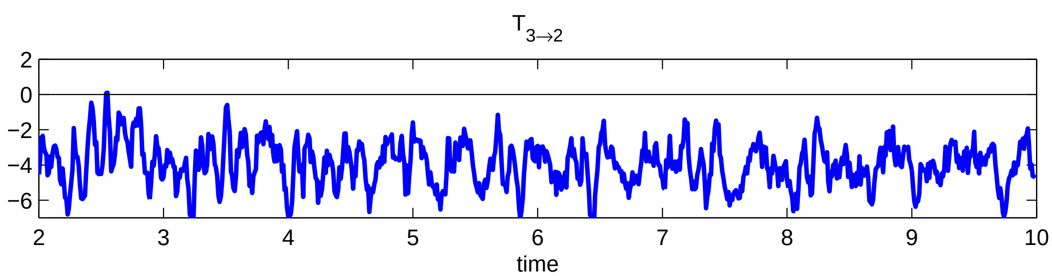

Fig. 5. A Close-up of $T_{3\to2}$ in Fig. 4b.

may be positive or negative, indicating that X_2 may increase or decrease the predictability of X_4. Plotted in Fig. 6 is the result of an experiment with $\underline{\mu} = (9, 9, -9, -9)$. The computed $T_{2\to4}$ is approximately -20. In some of the experiments, discernible small $T_{3\to2}$ as that in Fig. 5 may also be identified; in others it is not significantly different from zero. For example, in both Figs. 4b and 6 they are not zero (±4 on average), though very small in comparison to $T_{2\to4}$; By observation it is found that when $\mu_1 = \mu_2 < 0$, $T_{3\to2}$ vanishes, leaving $T_{2\to4}$ the only transfer. An interesting observation is that, if $T_{3\to2}$ is not zero, it always appears with a sign opposite to $T_{2\to4}$. Figs. 4 and 6 give two such examples. That is to say, if the lower frequency mode increases the predictability of the higher frequency mode, then the latter decreases the predictability of the former; vice versa. This result is very interesting and has important implications for realistic problems, though the TBS is just a highly idealized model. We will give some discussion in the following section.

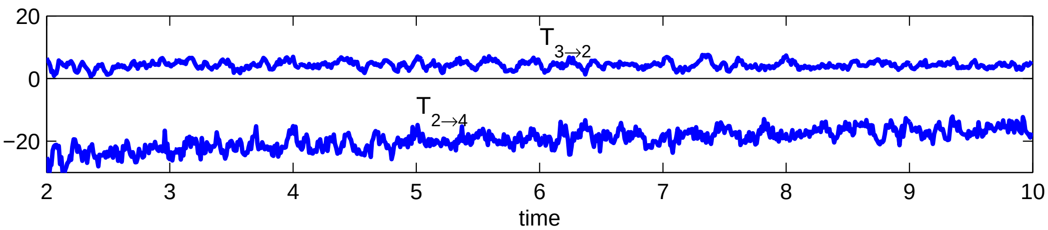

Fig. 6. Same as Fig. 4, but with $\underline{\mu} = (9, 9, -9, -9)$. Transfers other than $T_{2\to 4}$ and $T_{3\to 2}$ are not significantly different from zero.

8 Discussion and conclusions

Information transfer, or information flow as called, with respect to relative entropy was formulated to study how predictability varies locally as a dynamical system evolves. The resulting measure of transfer (31) is in a form similar to that with respect to absolute entropy, but for two terms modified in the formula. Properties have been explored and discussed. Given a component, if its evolution is independent of another, then there is no information flowing from the latter, while in the same time the transfer in the opposite direction need not be zero. In other words, between two components, information transfer in one direction carries no implication of that in the other direction, in contrast to the transfer of other physical properties such as energy [28]. This is the very property of asymmetry or property of causality emphasized in [44].

The formalism was applied to the study of the information flow between the first two modes of a truncated Burgers equation. It is found that all the 12 transfers are essentially zero, save for a strong transfer between the sine components from the low-frequency mode to the high-frequency mode ($T_{2\to 4}$), plus a weak transfer from the high-frequency cosine component to the low-frequency sine component ($T_{3\to 2}$). The latter is very small in comparison to the former, and may vanish in some cases. But, interestingly, if it does not vanish, it always carries a sign in opposite to that of the former. In other words, if knowledge of the low-frequency mode increases the predictability of the high-frequency mode, the feedback, if any, is always to reduce the predictability of the low-frequency mode, and vice versa. As a whole, the information flow from the low-frequency mode is dominantly important; the flow in the opposite direction is in general negligible. That is to say, the predictability of the high-frequency mode is controlled by the low-frequency mode.

The above causal relation between processes on different frequencies or scales is very important in that it gives implication on one of the major problems in turbulence research and atmosphere-ocean science, i.e., the parameterization of unresolved or sugrid processes in numerical models. In a turbulent flow, there is a continuous spectrum of processes of all scales, but even with the most powerful computers to date it is impossible to resolve all the scales. The system is therefore not closed. The unresolved processes must be represented, or parameterized, with the resolved dynamics to fulfill the closure. The above result with the TBS implies that this kind of parameterization seems to work, as the predictability of the small-scale (high-frequency) mode is controlled by the large-scale (low-frequency) mode. Of course, one cannot draw conclusions from such a highly idealized system, although originally the TBS was introduced as a prototype of the atmosphere for the study of dynamical closure (see Majda and Timofeyev, 2000; 2002).

The importance of the inter-scale information transfer is not only out of the above practical concern; it is also an important physical problem in nature. For example, the North Atlantic Oscillation (NAO), the dominant mode controlling the wintertime climate of the North America and Europe, is believed to be driven by the synoptic eddies with a time scale of several days to weeks. How the NAO interacts with the eddies in the stormy boreal winters is a continuing challenging problem in the atmospheric research because it is highly nonlinear in nature. Compounding the problem is that the interaction is essentially two-way. That is to say, while the eddy-driven origin is an issue, the NAO also causes the growth and decay of the eddies. This work is expected to be useful in the investigation of these problems, particularly in the investigation of the causal relation in a quantitative way.

Another important problem concerns how uncertainty, and hence predictability, propagates in physical space. This is a problem naturally arising in fields such as material science, nanotechnology, and atmosphere-ocean science where ensemble prediction is used. This question actually may be posed for any problems governed by a partial differential equation (PDE). To illustrate how it may be approached, consider a Burgers equation. A dynamical system of large dimensionality can be formed by discretizing the space. The differencing may be fulfilled using a three point scheme. The resulting ODEs are thence connected to each other through the grid. Each ODE is tagged with the location in physical space, as well as a component in the system. The information transfer between the components then form a flow of information in the space. Specifically, an ODE is connected to two other ODEs in the immediate neighborhood; it does not depend on other components. So for each point in the space, there are two transfers from ahead and back. By drawing these transfers, one obtains a flow forward and a flow backward, revealing how predictability changes due to uncertainty propagation. Theoretically this can be done, but practically it is hampered by the formidable computational job in evaluating the joint density in (31). For example, consider a five-dimensional joint density. Allowing 10 draws for each dimension, this totals to 10^5 ensemble members. While ensembles of this size might be feasible for Burgers equation, in dealing with realistic problems usually one can only handle ensembles of size in the order hundreds or even tens. To overcome this difficulty, we need simplify the rigorously derived formula (31), usually through problem-specific approximation. In a forthcoming paper, a systematic simplification will be reported in the context of geophysical fluid dynamics, and an example of realistic ocean problem presented on how this study may be applied (Liang and Kleeman, 2007).

Acknowledgments The author learned about the concept of information flow from Richard Kleeman. Richard also read through an early version of this manuscript and his comments are sincerely appreciated.

A Proof of Theorem 2

Eqs. (15) was originally obtained in LK05. It can be proved with the aid of the Liouville equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\underline{\mathbf{F}}\rho) = 0 \tag{A.1}$$

corresponding to the dynamical system (4) (cf. Lasota and Mackey 1994). Multiplication of (A.1) by $-(1 + \log \rho)$ gives

$$\begin{aligned}
-\frac{\partial \rho \log \rho}{\partial t} &= \underline{\mathbf{F}} \cdot \nabla(\rho \log \rho) + \rho(1 + \log \rho)\nabla \cdot \underline{\mathbf{F}} \\
&= [\log \rho \nabla \cdot (\underline{\mathbf{F}}\rho) + \underline{\mathbf{F}} \cdot \nabla \rho] + \rho \nabla \cdot \underline{\mathbf{F}} \\
&= \nabla \cdot (\rho \log \rho \underline{\mathbf{F}}) + \rho \nabla \cdot \underline{\mathbf{F}}.
\end{aligned}$$

Integrate over $\Omega = \Omega_1 \times \Omega_2 \times ... \times \Omega_n$ and notice the assumption of vanishing ρ at the boundaries. This results in

$$\frac{dH}{dt} = \int_\Omega \rho \nabla \cdot \underline{\mathbf{F}} \, d\underline{\mathbf{x}} = E(\nabla \cdot \underline{\mathbf{F}}).$$

To prove (16), first integrate (A.1) with respect to $(x_2, x_3, ..., x_n)$ over Ω_{2n} to get the evolution equation for ρ_1:

$$\frac{\partial \rho_1}{\partial t} + \int\limits_{\Omega_{2n}} \frac{\partial (F_1 \rho)}{\partial x_1}\ dx_2 ... dx_n = 0. \tag{A.2}$$

Multiplying $-(1+\log \rho_1)$ and following the same procedure as above, one easily obtains (16).

By definition the marginal relative entropy of X_1 is

$$D_1 = -H_1 - \int\limits_{\Omega_1} \rho_1 \log q_1 \ dx_1,$$

where q_1 is independent of time. Take derivative on both sides with respect to t to get

$$\frac{dD_1}{dt} = -\frac{dH_1}{dt} - \int\limits_{\Omega_1} \frac{\partial \rho_1}{\partial t} \log q_1 \ dx_1.$$

Substitute (A.2) for $\frac{\partial \rho_1}{\partial t}$ and (17) follows. Q.E.D.

B Proof of Proposition 4

This is a result obtained in LK07b; we rewrite the proof here for completeness.

We know from section 4 that Φ and its components are invertible. $\Phi_{\not 2}$ is hence also invertible, and its inverse is

$$\Phi_{\not 2}^{-1} : \begin{cases} x_1 = y_1 - \Delta t \cdot F_1(y_1, x_2, y_3, ..., y_n) + O(\Delta t^2), \\ x_3 = y_3 - \Delta t \cdot F_3(y_1, x_2, y_3, ..., y_n) + O(\Delta t^2), \\ \vdots \qquad\qquad\qquad \vdots \\ x_n = y_n - \Delta t \cdot F_n(y_1, x_2, y_3, ..., y_n) + O(\Delta t^2), \end{cases} \tag{B.1}$$

and

$$\begin{aligned} J_{\not 2}^{-1} &= \det \left[\frac{\partial (x_1, x_3, ..., x_n)}{\partial (y_1, y_3, ..., y_n)} \right] \\ &= 1 - \Delta t \sum_{i \neq 2} \frac{\partial F_i}{\partial x_i} + O(\Delta t^2). \end{aligned} \tag{B.2}$$

By (27),

$$\mathcal{P}_{\jupiter}\rho(y_1, y_3, ..., y_n) = \rho\left(\Phi_{\jupiter}^{-1}(y_1, y_3, ..., y_n)\right)\left|J_{\jupiter}^{-1}\right|. \tag{B.3}$$

So

$$\begin{aligned}
(\mathcal{P}_{\jupiter}\rho)_1(y_1) &= \int\limits_{\Omega_{3n}} \rho_{\jupiter}(y_1 - \Delta t\ F_1, y_3 - \Delta t\ F_3, ..., y_n - \Delta t\ F_n)\times \\
&\qquad \times \left|J_{\jupiter}^{-1}\right|\ dy_3...dy_n + O(\Delta t^2) \\
&= \int\limits_{\Omega_{3n}} \rho_{\jupiter}(\underline{\mathbf{y}}_{\jupiter} - \Delta t\ \underline{\mathbf{F}}_{\jupiter})\left|J_{\jupiter}^{-1}\right|\ dy_3...dy_n + O(\Delta t^2),
\end{aligned} \tag{B.4}$$

where $\underline{\mathbf{F}}_{\jupiter} = (F_1, F_3, ..., F_n)$ is understood as functions of $(y_1, x_2, y_3, ..., y_n)$. Make change of variables, $x_i = y_i - \Delta t \cdot F_i(y_1, x_2, y_3, ..., y_n)$, for $i = 3, 4, ..., n$. The Jacobian associated with this transformation is

$$\begin{aligned}
J_{3n} &= \det\left[\frac{\partial(y_3, y_4, ..., y_n)}{\partial(x_3, x_4, ..., x_n)}\right] \\
&= 1 + \Delta t \sum_{i=3}^{n} \frac{\partial F_i}{\partial x_i} + O(\Delta t^2),
\end{aligned} \tag{B.5}$$

which gives

$$\left|J_{\jupiter}^{-1}\right| \cdot |J_{3n}| = 1 - \Delta t \frac{\partial F_1}{\partial x_1} + O(\Delta t^2). \tag{B.6}$$

With these substituted (B.4) becomes

$$\begin{aligned}
(\mathcal{P}_{\jupiter}\rho)_1(y_1) &= \int\limits_{\Omega_{3n}} \rho_{\jupiter}(y_1 - \Delta t\ F_1(y_1, x_2, x_3, ..., x_n) \cdot \left|J_{\jupiter}^{-1}\right| \cdot |J_{3n}|\ \ dx_3...dx_n \\
&= \int\limits_{\Omega_{3n}} \rho_{\jupiter}(y_1 - \Delta t\ F_1(y_1, x_2, x_3, ..., x_n) \cdot \left(1 - \Delta t \frac{\partial F_1}{\partial x_1}\right)\ dx_3...dx_n + O(\Delta t^2) \\
&= \left[\rho_{\jupiter}(y_1, x_3, ..., x_n) - \Delta t \frac{\partial \rho_{\jupiter}}{\partial y_1} F_1\right]\left(1 - \Delta t \frac{\partial F_1}{\partial x_1}\right)\ dx_3...dx_n + O(\Delta t^2) \\
&= \rho_1(y_1) - \Delta t \cdot \int\limits_{\Omega_{3n}} \left[\frac{\partial F_1}{\partial x_1}\rho_{\jupiter}(y_1, x_3, ..., x_n) + F_1 \frac{\partial \rho_{\jupiter}(y_1, x_3, ..., x_n)}{\partial y_1}\right]\ dx_3...dx_n \\
&\qquad + O(\Delta t^2).
\end{aligned} \tag{B.7}$$

Since x_1 and y_1 are interchangeable up to an order of Δt, the two terms in the bracket can be combined, with the residual going to the higher order terms. That is to say,

$$(\mathcal{P}_{\mercury}\rho)_1(y_1) = \rho_1(y_1) - \Delta t \cdot \int_{\Omega_{3n}} \frac{\partial F_1 \rho_{\mercury}}{\partial y_1}\ dx_3 ... dx_n + O(\Delta t^2).$$

Q.E.D.

C Proof of Theorem 3

Subtract $D_1(t)$ from (29) to get

$$\begin{aligned}
\Delta D_{1\mercury} &= D_{1\mercury}(t + \Delta t) - D_1(t) \\
&= -\Delta H_{1\mercury} - \int_{\Omega} (\mathcal{P}_{\mercury}\rho)_1(y_1) \log q_1(y_1) \cdot \rho(x_2|x_1, x_3, ..., x_n) \\
&\qquad \cdot \rho_{3...n}(x_3, ..., x_n)\ dy_1 dx_2 ... dx_n + \int_{\Omega} \rho_1(x_1) \log q_1(x_1)\ dx_1 \\
&\equiv -\Delta H_{1\mercury} - D_* + \int_{\Omega} \rho_1 \log q_1\ dx_1. \qquad \text{(C.1)}
\end{aligned}$$

In this equation, $\Delta H_{1\mercury}$ has already been obtained in LK07b. We need to compute D_*. Note x_1 and y_1 coexist in the expression, the latter being $x_1 + F_1 \Delta t$. Perform a Taylor series expansion around $(y_1, x_2, x_3, ..., x_n)$ to get rid of x_1:

$$\begin{aligned}
\rho(x_2|x_1, x_3, ..., x_n) &= \frac{\rho}{\rho_{\mercury}}(x_1, x_2, ..., x_n) = \frac{\rho}{\rho_{\mercury}} + \frac{\partial \frac{\rho}{\rho_{\mercury}}}{\partial y_1} \cdot (-F_1 \Delta t) + O(\Delta t^2) \\
&= \rho(x_2|y_1, x_3, ..., x_n) + \frac{\rho}{{\rho_{\mercury}}^2} \frac{\partial \rho_{\mercury}}{\partial y_1} F_1 \Delta t - \frac{1}{\rho_{\mercury}} \frac{\partial \rho}{\partial y_1} F_1 \Delta t + O(\Delta t^2) \\
&= \rho(x_2|y_1, x_3, ..., x_n) + \rho(x_2|y_1, x_3, ..., x_n) \cdot \frac{\partial \log \rho_{\mercury}}{\partial y_1} F_1 \Delta t \\
&\qquad - \frac{1}{\rho_{\mercury}} \frac{\partial \rho}{\partial y_1} F_1 \Delta t + O(\Delta t^2), \qquad \text{(C.2)}
\end{aligned}$$

where the variables without independent variables explicitly written out are tacitly supposed to be functions of $(y_1, x_2, x_3, ..., x_n)$ With this expansion and (30) from Proposition 4,

$$\begin{aligned}
D_* = \int_{\Omega} \log q_1(y_1) \cdot &\left(\rho_1(y_1) - \Delta t \int_{\Omega_{3n}} \frac{\partial F_1 \rho_{\mercury}}{\partial y_1} dx_3 ... dx_n \right) \\
&\cdot \left(\rho(x_2|y_1, x_3, ..., x_n) + \rho(x_2|y_1, x_3, ..., x_n) \cdot \frac{\partial \log \rho_{\mercury}}{\partial y_1} F_1 \Delta t - \frac{1}{\rho_{\mercury}} \frac{\partial \rho}{\partial y_1} F_1 \Delta t \right)
\end{aligned}$$

$$
\begin{aligned}
&\qquad \cdot \rho_{3\ldots n}(x_3,...,x_n)\ dy_1 dx_2 ... dx_n + O(\Delta t^2) \\
&= \int\limits_{\Omega} \log q_1(y_1) \rho_1(y_1) \cdot \rho(x_2|y_1,x_3,...,x_n)\ dy_1 dx_2 ... dx_n \\
&\qquad + \Delta t \int\limits_{\Omega} \log q_1(y_1) \cdot \rho_1(y_1) \cdot \left[\rho(x_2|y_1,x_3,...,x_n) \frac{\partial \log \rho_{\not 2}}{\partial y_1} F_1 - \frac{1}{\rho_{\not 2}} \frac{\partial \rho}{\partial y_1} F_1 \right] \\
&\qquad\quad \cdot \rho_{3\ldots n}(x_3,...,x_n)\ dy_1 dx_2 ... dx_n \\
&\qquad - \Delta t \int\limits_{\Omega} \log q_1(y_1) \cdot \left(\int\limits_{\Omega_{3n}} \frac{\partial F_1 \rho_{\not 2}}{\partial y_1} dx_3 ... dx_n \right) \cdot \rho(x_2|y_1,x_3,...,x_n) \\
&\qquad\quad \cdot \rho_{3\ldots n}(x_3,...,x_n)\ dy_1 dx_2 ... dx_n \\
&\qquad + O(\Delta t^2) \\
&\equiv (I) + (II) + (III) + O(\Delta t^2).
\end{aligned}
$$

Now evaluate the three terms one by one. For convenience, all the y_1 are replaced by x_1. This is legitimate as now y_1 is an dummy variable. The first term is

$$
\begin{aligned}
(I) &= \int\limits_{\Omega} \log q_1 \cdot \rho_1 \cdot \frac{\rho}{\rho_{\not 2}} \cdot \rho_{\not 1 \not 2}\ d\underline{\mathbf{x}} \\
&= \int\limits_{\Omega_1} \rho_1(x_1) \log q_1(x_1)\ dx_1.
\end{aligned} \tag{C.3}
$$

At the second step, we first integrate $\frac{\rho(\underline{\mathbf{x}})}{\rho_{\not 2}}$ with respect to x_2 (all other parts are independent of x_2) to get 1, then take the integral with respect to $x_3, ..., x_n$ and eliminate $\rho_{\not 1 \not 2}$.

For the second part,

$$
\begin{aligned}
(II) &= \Delta t \int\limits_{\Omega} \log q_1(x_1) \rho_1(x_1) \left[\frac{\rho}{\rho_{\not 2}} \frac{\partial \log \rho_{\not 2}}{\partial x_1} F_1 - \frac{1}{\rho_{\not 2}} \frac{\partial \rho}{\partial x_1} F_1 \right] \rho_{\not 1 \not 2}\ d\underline{\mathbf{x}} \\
&= -\Delta t \int\limits_{\Omega} \rho_1 \log q_1 \cdot \frac{\rho_{\not 2}}{\rho} \cdot \frac{\partial \rho / rho_{\not 2}}{\partial x_1} \cdot F_1 \cdot \frac{\rho \rho_{\not 1 \not 2}}{\rho_{\not 2}}\ d\underline{\mathbf{x}} \\
&= -\Delta t \int\limits_{\Omega} F_1 \rho_1 \log q_1 \cdot \frac{\partial}{\partial x_1} \left(\frac{\rho_{\not 1 \not 2} \rho}{\rho_{\not 2}} \right)\ d\underline{\mathbf{x}}.
\end{aligned} \tag{C.4}
$$

Using the notations (20) and (21):

$$
\begin{aligned}
\theta_{2|1} &= \frac{\rho_{\not 1 \not 2} \rho}{\rho_{\not 2}}, \\
\Theta_{2|1} &= \int\limits_{\Omega_{3n}} \theta_{2|1}(\underline{\mathbf{x}})\ dx_3 ... dx_n
\end{aligned}
$$

simplifies the above formula to be

$$
\begin{aligned}
(II) &= -\Delta t \int_{\Omega} F_1 \rho_1 \log q_1 \cdot \frac{\partial \theta_{2|1}}{\partial x_1} \; d\underline{\mathbf{x}} \\
&= \Delta t \int_{\Omega} \frac{\partial (F_1 \rho_1 \log q_1)}{\partial x_1} \cdot \theta_{2|1} \; d\underline{\mathbf{x}}.
\end{aligned}
\tag{C.5}
$$

The third term (III) may be equally simplified,

$$
(III) = -\Delta t \int_{\Omega} \underbrace{\left[\log q_1(x_1) \cdot \left(\int_{\Omega_{3n}} \frac{\partial F_1 \rho_{\not{2}}}{\partial x_1} dx_3 ... dx_n \right) \right]}_{\text{(integration by parts)}} \cdot \theta_{2|1}(\underline{\mathbf{x}}) \; d\underline{\mathbf{x}}.
$$

The part in the square brackets is independent of $(x_3, ..., x_n)$. So integration can be performed on $\theta_{2|1}$ with respect to $(x_3, ..., x_n)$, which gives

$$
\begin{aligned}
(III) &= -\Delta t \int_{\Omega_1 \times \Omega_2} \log q_1(x_1) \cdot \left(\int_{\Omega_{3n}} \frac{\partial F_1 \rho_{\not{2}}}{\partial x_1} dx_3 ... dx_n \right) \cdot \Theta_{2|1}(x_1, x_2) \; d\underline{\mathbf{x}} \\
&= -\Delta t \int_{\Omega} \log q_1 \cdot \frac{\partial F_1 \rho_{\not{2}}}{\partial x_1} \cdot \Theta_{2|1} \; d\underline{\mathbf{x}}.
\end{aligned}
\tag{C.6}
$$

Combining (I), (II), and (III), one has

$$
\begin{aligned}
D_* = \int_{\Omega_1} \rho_1 \log q_1 \; dx_1 &+ \Delta t \int_{\Omega} \frac{\partial (F_1 \rho_1 \log q_1)}{\partial x_1} \theta_{2|1} \; d\underline{\mathbf{x}} \\
&- \Delta t \int_{\Omega} \log q_1 \frac{\partial F_1 \rho_{\not{2}}}{\partial x_1} \Theta_{2|1} \; d\underline{\mathbf{x}} + O(\Delta t^2).
\end{aligned}
$$

So

$$
\begin{aligned}
\Delta D_{1\not{2}} &= -\Delta H_{1\not{2}} - D_* + \int_{\Omega} \rho_1 \log q_1 \; dx_1 \\
&= -\Delta H_{1\not{2}} - \Delta t \int_{\Omega} \frac{\partial F_1 \rho_1 \log q_1}{\partial x_1} \theta_{2|1} \; d\underline{\mathbf{x}} \\
&\quad + \Delta t \int_{\Omega} \log q_1 \frac{\partial F_1 \rho_{1\not{2}}}{\partial x_1} \Theta_{2|1} \; d\underline{\mathbf{x}} + O(\Delta t^2).
\end{aligned}
$$

Letting $\Delta t \to 0$, it becomes

$$\frac{dD_{1\not{2}}}{dt} = -\frac{dH_{1\not{2}}}{dt} - \int_{\Omega} \frac{\partial F_1 \rho_1 \log q_1}{\partial x_1} \theta_{2|1} \; d\underline{\mathbf{x}} + \int_{\Omega} \log q_1 \frac{\partial F_1 \rho_{1\not{2}}}{\partial x_1} \Theta_{2|1} \; d\underline{\mathbf{x}}. \qquad \text{(C.7)}$$

By the Eq. (48) of LK07b,

$$\begin{aligned}
\frac{dH_{1\not{2}}}{dt} &= \int_{\Omega} (1 + \log \rho_1) \frac{\partial F_1 \rho_{\not{2}}}{\partial x_1} \Theta_{2|1} \; d\underline{\mathbf{x}} + \int_{\Omega} F_1 \rho_1 \log \rho_1 \frac{\partial \rho / \rho_{\not{2}}}{\partial x_1} \rho_{\not{1}\not{2}} \; d\underline{\mathbf{x}} \\
&= \int_{\Omega} (1 + \log \rho_1) \frac{\partial F_1 \rho_{\not{2}}}{\partial x_1} \Theta_{2|1} \; d\underline{\mathbf{x}} + \int_{\Omega} F_1 \rho_1 \log \rho_1 \frac{\partial \theta_{2|1}}{\partial x_1} \; d\underline{\mathbf{x}} \\
&= \int_{\Omega} (1 + \log \rho_1) \frac{\partial F_1 \rho_{\not{2}}}{\partial x_1} \Theta_{2|1} \; d\underline{\mathbf{x}} - \int_{\Omega} \frac{\partial (F_1 \rho_1 \log \rho_1)}{\partial x_1} \theta_{2|1} \; d\underline{\mathbf{x}}. \qquad \text{(C.8)}
\end{aligned}$$

In arriving at the last step, integration by parts has been performed together with the assumption of vanishing boundary density. Substituting (C.8) back to (C.7), one finally arrives at (19). Q.E.D.

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