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Approximating Stationary Statistical Properties**

Xiaoming WANG*

(*Dedicated to Professor Andrew Majda on the Occasion of his* 60*th Birthday with Admiration and Friendship*)

Abstract It is well-known that physical laws for large chaotic dynamical systems are revealed statistically. Many times these statistical properties of the system must be approximated numerically. The main contribution of this manuscript is to provide simple and natural criterions on numerical methods (temporal and spatial discretization) that are able to capture the stationary statistical properties of the underlying dissipative chaotic dynamical systems asymptotically. The result on temporal approximation is a recent finding of the author, and the result on spatial approximation is a new one. Applications to the infinite Prandtl number model for convection and the barotropic quasi-geostrophic model are also discussed.

Keywords Stationary statistical property, Invariant measure, Global attractor, Dissipative system, Time discretization, Spatial discretisation, Uniformly dissipative scheme, Infinite Prandtl number model for convection, Barotropic quasi-geostrophic equations

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1 Introduction

Many dynamical systems arising in physical applications possess very complex behavior with abundant instability and sensitive dependence on initial data and parameters (see [2, 23, 33]). The complex/chaotic/turbulent behaviors are not necessarily related to the possible loss of regularity of the solution to the underlying equation (say the three dimensional Navier-Stokes equations). Even the simple logistic map $T(x) = 4x(1-x)$ on the unit interval, the Lorenz 63 and Lorenz 96 model possess intrinsic chaotic behavior which renders approximation of single trajectory extremely difficult over a long time. On the other hand, it is well-known that the statistical properties of these kind of systems are much more important, physically relevant and stable than single trajectories (see [10, 18, 20, 24, 25, 36]). Indeed, much of the classical turbulence theories are formulated in statistical forms (via spatial and temporal averages), for instance, the famous Kolmogorov $\frac{U^3}{L}$ scaling law of the energy dissipation rate per unit mass as well as the Kolmogorov $k^{-\frac{5}{3}}$ energy spectrum in the inertial range in three dimensional homogeneous isotropic turbulence (see [10, 11, 25]).

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*Department of Mathematics, Florida State University, Tallahassee, FL 32306-4510, USA. E-mail: wxm@math.fsu.edu
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Therefore, for complex physical processes, due to the intrinsic stochasticity, it is necessary to consider statistical properties (averaged quantities) of the system instead of properties of individual orbit (see, for instance, [10, 11, 20, 24, 25, 36]). Then it is obvious that we need probability measures on the phase space that respects the dynamics in order to discuss statistical properties (statistical averages).

For a given abstract autonomous continuous in time dynamical system determined by a semi-group $\{S(t), t \geq 0\}$ on a separable metric space H, we recall that if the system reaches a statistical equilibrium in the sense that the statistics are time independent (stationary statistical properties), the probability measure μ on H that describes the stationary statistical properties can be characterized via either the strong (pull-back) or weak (push-forward) formulation (see [10, 20, 24, 36, 37]).

Definition 1.1 (Invariant Measure (Stationary Statistical Solution)) *Let $\{S(t), t \geq 0\}$ be a continuous semi-group on a metric space H which generates a dynamical system on H. A Borel probability measure μ on H is called an invariant measure (stationary statistical solution) of the dynamical system if*

$$\mu(E) = \mu(S^{-1}(t)(E)), \quad \forall\, t \geq 0,\ \forall\, E \in \mathcal{B}(H), \tag{1.1}$$

where $\mathcal{B}(H)$ represents the σ-algebra of all Borel sets on H. Equivalently, the invariant measure μ can be characterized through the following push-forward weak invariance formulation

$$\int_H \Phi(\mathbf{u}) \mathrm{d}\mu(\mathbf{u}) = \int_H \Phi(S(t)\mathbf{u}) \mathrm{d}\mu(\mathbf{u}), \quad \forall\, t \geq 0, \tag{1.2}$$

for all bounded continuous test functionals Φ.

Invariant measure (stationary statistical solution) for a discrete dynamical system generated by a map S_{discrete} on a metric space H is defined in a similar fashion with the continuous time t replaced by discrete time $n = 0, 1, 2, \cdots$.

Another popular object utilized below associated with long time behavior of a dissipative dynamical system is the global attractor. Recall that a compact set $\mathcal{A}$ is called the global attractor of the dynamical system if it is invariant and attracts all bounded sets in the phase space H (see [10, 13, 33]).

A dynamical system is called dissipative if it possesses a global attractor. It is easy to see, thanks to the invariance and the attracting property, that the global attractor, when it exists, is unique (see [13, 33]). The reader is cautioned that our definition of dissipativity may be slightly different (weaker) from the traditional notation (see [13, 33]).

We are usually interested in $\int_H \Phi(\mathbf{u}) \mathrm{d}\mu(\mathbf{u})$ (statistical average) for various test functionals Φ. These averaged quantities are also called observables in physics literatures. One approach to estimate these observables is to estimate the invariant measure μ directly. This is the so-called directly approach (see [20, 30]). If the phase space is a finite dimensional Euclidean space, one can try to approximate the probability density function (pdf) p associated with the invariant measure by solving the Liouville equation (see [20])

$$\frac{\partial}{\partial t} p(\mathbf{u}, t) + \nabla \cdot (F(\mathbf{u}) p(\mathbf{u}, t)) = 0, \tag{1.3}$$

where the forcing term $F(\mathbf{u})$ defines the dynamical system in the sense that $\frac{\mathrm{d}}{\mathrm{d}t} S(t)\mathbf{u} = F(S(t)\mathbf{u})$. However, computing the invariant measure (or the associated pdf in the finite dimensional case) is usually very hard and costly if the spatial dimension is high. One of the commonly used alternative methods in calculating the statistical quantity is to substitute spatial average by long time average under Boltzmann's assumption of ergodicity (see [10, 20, 24, 37]),

$$\int_H \Phi(\mathbf{u})\mathrm{d}\mu(\mathbf{u}) = \lim_{t\to\infty} \frac{1}{t}\int_0^t \Phi(S(s)\mathbf{u})\mathrm{d}s.$$

This is usually termed indirect method. Although the above relationship is true for each ergodic invariant measure μ and almost all initial data with respect to μ, the relationship is in general false for non-ergodic invariant measure since the long time average which exists for almost all initial data (with respect to the given invariant measure) may depend on the initial data and hence may not be a constant (the spatial average) (see [20, 37]). One way to circumvent this difficulty is to replace the long time limit by Banach (generalized) limits (see [21, §4.2]), which are bounded linear functionals on the space of bounded functions that agree with the usual long time limit on those functions whenever the long time limit exists. One may show via the so-called Bogliubov-Krylov argument that these generalized long time averages over trajectory lead to invariant measures (may depend on the chosen Banach limit and initial datum $\mathbf{u}$) of the system for appropriate dissipative dynamical systems, and the spatial and temporal averages are equivalent (see, for instance, [10, §4.3] or [40, Theorem 2]).

Due to the presumed complexity of the dynamics, the physically interesting stationary statistical properties need to be calculated using numerical methods in generic case. Even under the ergodicity assumption, it is not at all clear that classical numerical schemes which provide accurate approximation on finite time interval will remain meaningful for stationary statistical properties (long time properties) since small error will be amplified and accumulated over long time except in the case that the underlying dynamics is asymptotically stable (see [12, 14, 19]) where statistical approach is not necessary since there is no chaos. Indeed, let S_k be the solution operator of a one-step scheme with time step $k = \Delta t$ and assume that the scheme is of order m so that the following type of error estimate holds: $\mathrm{dist}_H(S(nk)\mathbf{u}, S_k^n\mathbf{u}) \le C\exp(\alpha nk)k^m$ where $C > 0$ and α are constants, which would induce on a time interval $[0, T]$, an a priori error bound on the long time average of the order of $k^m\frac{\exp(\alpha T)-\exp(\alpha k)}{\exp(\alpha k)-1}$ which diverges for positive α as T approaches infinity. The positivity of α follows from the existence of at least one positive Lyapunov exponent (the existence of chaotic behavior). Even if the long time averages of the scheme converge, the limit is not necessarily that of the original dynamical system under approximation since the two limits of letting the time interval go to infinity and the limit of letting the time step approach zero are not commutative in general. Extra work is needed to verify that the limit is the desired one. Addressing issues like this is of great importance in many real life applications such as numerical study of climate change since the climate is customary estimated via long time integration of the system. Therefore, it is of great importance and a challenge to search for numerical methods that are able to capture stationary statistical properties of infinite dimensional complex dynamical system. We will focus on dissipative systems and discuss both temporal and spatial discretisation.

There have been a lot of work in terms of approximating statistical properties of finite dimensional dynamical systems (see [30] for a recent survey on the finite dimensional case, and [31] for general questions related to approximating finite dimensional dynamical systems). Of course, infinite dimensional dynamical systems may be approximated by finite dimensional ones (spatial discretisation of PDE for example). However, the associated question of convergence of statistical properties for these approximation has not been addressed in the literature so far (see Theorem 2.2 below for the case of dissipative system).

On the other hand, there are few results on the convergence of stationary statistical properties of numerical schemes for chaotic PDEs (see [4, 5, 41]), although there have been a lot of work on temporal/spatial approximation of dissipative dynamical systems, such as the two dimensional incompressible Navier-Stokes system and the one-dimensional Kuramoto-Sivashinsky equation (see [8, 9, 12, 15, 17, 28, 29, 34] among others). These authors were mostly interested in the long time stability of the scheme in the sense of deriving uniform in time bounds on the scheme (sometimes bound in the phase space H only which is not sufficient for uniform dissipativity, although it may be sufficient for the convergence of the global attractors), and approximation of various invariant sets (such as steady states, time periodic orbits, global attractors, inertial manifolds, etc., see [15, 16, 28, 31–33] and the references therein). We would like to point out that the convergence of invariant sets and the convergence of stationary statistical properties are two related but very different issues associated with the long time behavior. It is easy to construct two dynamical systems with exactly the same global attractor or inertial manifold but with totally different dynamics or stationary statistical properties.

It seems that the common theme of algorithms that are good at approximating long time behavior is the faithfulness to the original continuous dynamical system. In the finite dimensional conservative Hamiltonian system case, the key is to preserve the geometric structure, which implies the conservation of a slightly perturbed Hamiltonian and other conserved quantities, so that the scheme is symplectic (see [22, 27] and the references therein). Indeed, we can show that the preservation of the energy/Hamiltonian and the finite time convergence of the scheme imply the convergence of stationary statistical properties (see Proposition 2.1 below) provided that all the energy surfaces are bounded. In the case of dissipative dynamical system, the key ingredient in the convergence of stationary statistical properties is again the faithfulness to the original system in the sense that the numerical scheme must be uniformly dissipative for small enough time step and/or spatial mesh size, and the scheme must converge on any finite time interval (see the main theorems in the next section for more precise statement). These criterions seem natural and the proof of our main results are straightforward. The criterion must be verified in each application which itself may be nontrivial (this is a part of the design of the algorithms). We hope that the main results here will provide clear guideline on how to construct schemes that are able to capture the invariant measures or stationary statistical properties of infinite dimensional dynamical systems. Many questions, such as convergence rate, efficient approximation and selection of physically relevant ones, remain open.

The author learned much of the statistical way of thinking through collaborative work with Andrew Majda. Hence it seems fit to dedicate this work to Andy on this special occasion with sincere gratitude.

The rest of the manuscript is organized as follows. In Section 2, we present the main results, namely the convergence of stationary statistical properties of numerical schemes (both temporal and spatial discretization) for dissipative infinite dimensional system. In Section 3, we discuss an application of the main results to the infinite Prandtl number model for convection and the barotropic quasi-geosrophic equation with damping and forcing. We then provide conclusion and remarks in Section 4.

2 Main Results

Here we present our main results, namely, uniform dissipativity plus finite time uniform convergence imply convergence of the stationary statistical properties/invariant measures.

Throughout this section, all semigroups are assumed to be continuous in the sense that $S(t), t \geq 0$, $S_N(t), t \geq 0$ and S_k are continuous operators on H.

We first recall the following convergence result on temporal approximation (see [41]).

Theorem 2.1 (Temporal Approximation) *Let $\{S(t), t \geq 0\}$ be a continuous semi-group on a separable Hilbert space H which generates a continuous dissipative dynamical system in the sense of possessing a compact global attractor $\mathcal{A}$. Let $\{S_k, 0 < k \leq k_0\}$ be a family of continuous maps on H which generates a family of discrete dissipative dynamical system (with global attractor $\mathcal{A}_k$). Suppose that the following three conditions are satisfied.*

(1) (Uniform Dissipativity) *There exists a $k_1 \in (0, k_0)$ such that $\{S_k, 0 < k \leq k_1\}$ is uniformly dissipative in the sense that*

$$K = \bigcup_{0<k\leq k_1} \mathcal{A}_k \tag{2.1}$$

is pre-compact in H.

(2) (Uniform Convergence on the Unit Time Interval) *S_k uniformly converges to S on the unit time interval (modulo an initial layer) and uniformly for initial data from the global attractor of S_k in the sense that for any $t_0 \in (0, 1)$,*

$$\lim_{k\to 0} \sup_{\substack{\mathbf{u}\in\mathcal{A}_k \\ nk\in[t_0,1]}} \|S_k^n \mathbf{u} - S(nk)\mathbf{u}\|_H = 0. \tag{2.2}$$

(3) (Uniform Continuity of the Continuous System) *$\{S(t), t \geq 0\}$ is uniformly continuous on K on the unit time interval in the sense that for any $T^* \in [0, 1]$,*

$$\lim_{t\to T^*} \sup_{\mathbf{u}\in K} \|S(t)\mathbf{u} - S(T^*)\mathbf{u}\|_H = 0. \tag{2.3}$$

Then the invariant measures of the discrete dynamical system $\{S_k, 0 < k \leq k_0\}$ converge to invariant measures of the continuous dynamical system S. More precisely, let $\mu_k \in \mathcal{IM}_k$ where $\mathcal{IM}_k$ denotes the set of all invariant measures of S_k. There must exist a subsequence, still denoted by $\{\mu_k\}$, and $\mu \in \mathcal{IM}$ (an invariant measure of $S(t)$), such that μ_k weakly converges to μ, i.e.,

$$\mu_k \rightharpoonup \mu, \quad \text{as } k \to 0. \tag{2.4}$$

Moreover, extremal statistics converge in upper-semi-continuous fashion in the sense that for any bounded continuous functional Φ on the phase space H, there exist ergodic invariant measures $\mu_k \in \mathcal{IM}_k$ and an ergodic invariant measure $\mu \in \mathcal{IM}$, such that

$$\begin{aligned}\sup_{\mathbf{u}_0\in H} \limsup_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \Phi(S_k^n(\mathbf{u}_0)) &= \int_H \Phi(\mathbf{u}) \mathrm{d}\mu_k(\mathbf{u}) \\ &= \lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \Phi(S_k^n(\mathbf{v}_0)), \quad a.s.\ w.r.t.\ \mu_k,\end{aligned} \tag{2.5}$$

$$\sup_{\mathbf{u}_0\in H}\limsup_{T^*\to\infty}\frac{1}{T^*}\int_0^{T^*}\Phi(S(t)\mathbf{u}_0)\mathrm{d}t=\int_H\Phi(\mathbf{u})\mathrm{d}\mu(\mathbf{u})$$
$$=\lim_{T^*\to\infty}\frac{1}{T^*}\int_0^{T^*}\Phi(S(t)\mathbf{v}_0)\mathrm{d}t,\quad a.s.\ w.r.t.\ \mu, \tag{2.6}$$
$$\limsup_{k\to 0}\sup_{\mathbf{u}_0\in H}\limsup_{N\to\infty}\frac{1}{N}\sum_{n=1}^{N}\Phi(S_k^n(\mathbf{u}_0))\le\sup_{\mathbf{u}_0\in H}\limsup_{T^*\to\infty}\frac{1}{T^*}\int_0^{T^*}\Phi(S(t)\mathbf{u}_0)\mathrm{d}t. \tag{2.7}$$

The proof of this result is relatively straightforward. Roughly speaking, the uniform dissipativity ensures the tightness of the set of invariant measures $\{\mu_k\}$ while the unit time uniform convergence and the uniform continuity of the underlying system ensure that the limit is an invariant measure of the underlying dynamical system. The interested reader is referred to [41] for the details of this result and a related result on the convergence of global attractors.

Remark 2.1 In general, we only have an inequality in (2.7) rigorously although the equality is expected for most system with enough mixing, such as the infinite Prandtl number model for convection at large Rayleigh number (yet to be proved). However, if the system under approximation is uniquely ergodic, i.e., there exists only one invariant measure, the equality holds. This follows easily from the proof and the fact that the unique invariant measure must be ergodic (since it is an extremal point). This also covers the case when the system has only one ergodic invariant measure, since in this case the set of all invariant measures must consist of one element only as all extremal points of the set must be ergodic (see [37, 40]). In the generic case of a system with multiple ergodic invariant measures, it seems mathematically difficult to separate the physically relevant ergodic invariant measures from the others, due to the lack of Lebesgue measure in this infinite dimensional setting. One idea is to consider their stability under random perturbation. But the concept of generic noise in this infinite dimensional setting is also up to debate.

In application, the time discrete dynamical systems $\{S_k\}$ are usually generated by one time step discretization (numerical scheme) with time step k. In other words, $\mathbf{u}^{n+1}=S_k(\mathbf{u}^n)$ is the solution to the numerical scheme. The uniform dissipativity of the numerical scheme is customary established via the existence of a uniform (in time step) absorbing ball in another separable Hilbert space V which is compactly imbedded in H in the case of strongly dissipative system (see the next section for an example). However, this may not be feasible for weakly dissipative systems, such as the Darcy-Boussinesq system for convection in fluid saturated porous media, or weakly damped driven Schrödinger equation. The finite time uniform convergence comes with classical numerical analysis for reasonable schemes (see next section for an example). The uniform continuity of the underlying continuous dynamical system is also easily verified for reasonable systems.

Notice that boundedness implies pre-compactness in the finite dimensional case. An easy consequence of the result above is the following convergence result for finite dimensional conservative system.

Proposition 2.1 *Let $\{S(t)\}$ be a continuous semi-group on a finite dimensional Riemannian manifold $\mathbb{M}^N$ which conserves a continuous energy E. We also assume that all constant energy surfaces $E_C:=\{\mathbf{u}\in\mathbb{M}^N \mid E(\mathbf{u})=C\}$ are bounded. Let $\{S_k, 0<k\le k_0\}$ be a family of continuous maps on $H=\mathbb{M}^N$ which generates a family of discrete dynamical systems.*

Suppose that the following three conditions are satisfied.

(1) (Conservative of the Scheme) *S_k conserves an approximate energy E_k such that $E_k(\mathbf{u}) \to E(\mathbf{u})$, $\forall\, \mathbf{u} \in \mathbb{M}^N$.*

(2) (Uniform Conservancy) *There exists a $k_1 \in (0, k_0)$ such that following set is bounded in $\mathbb{M}^N$ for all C,*

$$K_C := \bigcup_{0<k\le k_1} E_{k,C}, \quad E_{k,C} := \{\mathbf{u} \in \mathbb{M}^N \mid E_k(\mathbf{u}) = C\}. \tag{2.8}$$

(3) (Uniform Convergence on the Unit Time Interval) *S_k uniformly converges to S on the unit time interval (modulo an initial layer) and uniformly for initial data from any bounded ball from $\mathbb{M}^N$,*

$$\lim_{k\to 0} \sup_{\substack{\mathbf{u}\in B_R(\mathbb{M}^N)\\ nk\in[t_0,1]}} \mathrm{dist}_M(S_k^n\mathbf{u}, S(nk)\mathbf{u}) = 0, \quad \forall\, t_0 \in (0,1). \tag{2.9}$$

Then the invariant measures of the discrete dynamical system $\{S_k, 0 < k \le k_0\}$ converge to invariant measures of the continuous dynamical system S. More precisely, let $\mu_k \in \mathcal{IM}_k^C$ where $\mathcal{IM}_k^C$ denotes the set of all invariant measures of S_k with energy level C. There must exist a subsequence, still denoted by $\{\mu_k\}$, and $\mu \in \mathcal{IM}^C$ (an invariant measure of $S(t)$ with energy level C), such that μ_k weakly converges to μ, i.e.,

$$\mu_k \rightharpoonup \mu, \quad \textit{as } k \to 0. \tag{2.10}$$

Proof Since the discrete dynamical system S_k conserves approximate energy E_k (see condition (1)), we see that the S_k must possess invariant measures for each nontrivial energy level ($E_{k,C} \ne \emptyset$) via a Bogliubov-Krylov argument. Let μ_k be a microcanonical invariant measure of S_k with energy level C, where C is a fixed arbitrary constant. Thanks to the uniform conservancy assumption (2), we see that $\{\mu_k, k \in (0, k_1)\}$ is tight in the space of all Borel probability measures on H thanks to Prokhorov's theorem (see [1, 10, 21]), since

$$\mathrm{supp}(\mu_k) \subset E_{k,C} \subset K_C, \quad \forall\, k \in (0, k_1)$$

is pre-compact. Hence it must contain a weakly convergent subsequence (still denoted by $\{\mu_k\}$) which weakly converges to a Borel probability measure μ on H, i.e.,

$$\int_H \varphi(\mathbf{u})\mathrm{d}\mu_k(\mathbf{u}) \to \int_H \varphi(\mathbf{u})\mathrm{d}\mu(\mathbf{u}), \quad \text{as } k \to 0,$$

for all bounded and continuous functionals φ on $H = \mathbb{M}^N$.

It is easy to see that μ must be supported on E_C. Indeed, if this were not true, we would have a $\delta > 0$ neighborhood of E_C such that there exists $\mathbf{u}_k \in E_{k,C}$ with $\mathrm{dist}_M(\mathbf{u}_k, E_C) \ge \delta$, $\forall\, k$. Without loss of generality, we may assume $\mathbf{u}_k \to \mathbf{u}_\infty$ since $\mathbf{u}_k \in K_C$ is pre-compact. Now

$$E(\mathbf{u}_\infty) = \lim_{k\to 0} E(\mathbf{u}_k) = \lim_{k\to 0} E_k(\mathbf{u}_k) + \lim_{k\to 0}(E(\mathbf{u}_k) - E_k(\mathbf{u}_k)) = C,$$

where we have utilized the uniform convergence of E_k to E on the pre-compact set K_C. This implies $\mathbf{u}_\infty \in E_C$, which is a contradiction.

Our goal now is to show that μ is invariant under $S(t)$. For this purpose, we fix a $T^* \in (0, 1]$ and let $n_k = \lfloor \frac{T^*}{k} \rfloor$ be the floor of $\frac{T^*}{k}$ $\big($the largest integer dominated by $\frac{T^*}{k}\big)$, and let φ be any smooth (C^1) test functional (observable). We have

$$\begin{aligned}\Big|\int_H(\varphi(S(T^*)\mathbf{u})-\varphi(\mathbf{u}))\mathrm{d}\mu(\mathbf{u})\Big| &= \lim_{k\to 0}\Big|\int_H(\varphi(S(T^*)\mathbf{u})-\varphi(\mathbf{u}))\mathrm{d}\mu_k(\mathbf{u})\Big| \\ &\le \lim_{k\to 0}\Big|\int_H(\varphi(S(T^*)\mathbf{u})-\varphi(S(n_k k)\mathbf{u}))\mathrm{d}\mu_k(\mathbf{u})\Big| \\ &\quad+\lim_{k\to 0}\Big|\int_H(\varphi(S(n_k k)\mathbf{u})-\varphi(\mathbf{u}))\mathrm{d}\mu_k(\mathbf{u})\Big| \\ &\le \lim_{k\to 0}\sup_{\mathbf{u}\in K_C}\|\varphi'(\mathbf{u})\|\sup_{\mathbf{u}\in K_C}\mathrm{dist}_M(S(T^*)\mathbf{u},S(n_k k)\mathbf{u}) \\ &\quad+\lim_{k\to 0}\Big|\int_H(\varphi(S(n_k k)\mathbf{u})-\varphi(S_k^{n_k}\mathbf{u}))\mathrm{d}\mu_k(\mathbf{u})\Big| \\ &\le \lim_{k\to 0}\sup_{\mathbf{u}\in K_C}\|\varphi'(\mathbf{u})\|\sup_{\mathbf{u}\in K_C}\mathrm{dist}_M(S_k^{n_k}\mathbf{u},S(n_k k)\mathbf{u}) \\ &\le \lim_{k\to 0}\sup_{\mathbf{u}\in K_C}\|\varphi'(\mathbf{u})\|\sup_{\substack{\mathbf{u}\in K_C\\ nk\in[\frac{T^*}{2},T^*]}}\mathrm{dist}_M(S_k^{n}\mathbf{u},S(nk)\mathbf{u}) \\ &=0,\end{aligned}$$

where we have utilized the continuity of φ and $\varphi\circ S$, and the weak convergence in the first step, the triangle inequality in the second step, the mean value theorem and the invariance of μ_k under S_k in the third step, the uniform continuity of the solution semigroup S on $E_C\times[0,1]$ and the mean value theorem in the fourth step, and condition (3) in the last step.

This is exactly the weak invariance (1.2) for the smooth (C^1) test functional (observable) with $T^*\in(0,1]$. A general bounded continuous test functional φ can be approximated by smooth Friedrich's mollifier as usual. This proves the short time weak invariance (1.2) for any bounded continuous test functional ϕ and $T^*\in(0,1]$.

Now for a general $T^{**}>1$, there exists a unique positive integer n and $T_*\in(0,1]$ such that $T^{**}=n+T_*$. Hence

$$\int_H\varphi(S(T^{**})\mathbf{u})\mathrm{d}\mu(\mathbf{u})=\int_H\varphi(S^n(1)S(T_*)\mathbf{u})\mathrm{d}\mu(\mathbf{u})=\int_H\varphi(S(T_*)\mathbf{u})\mathrm{d}\mu(\mathbf{u})=\int_H\varphi(\mathbf{u})\mathrm{d}\mu(\mathbf{u}),$$

where we have utilized the semi-group property of $S(t)$, the strong continuity of $S(t)$ and the short time weak invariance that we proved above with $T^*=1$ n times and $T^*=T_*$ once.

This completes the proof of the theorem.

Next, we consider spatial discretization. The essential idea is similar: be faithful to the original system. In the dissipative case, retain dissipativity. We have the following result which may be suitable for spectral and finite element type discretization but would require more work for finite difference type approximation.

Theorem 2.2 (Spatial Discretisation) *Let $\{S(t),t\ge 0\}$ be a dissipative dynamical system on a Hilbert space H with global attractor $\mathcal{A}$. Let $\{S_N(t),t\ge 0\}$ be a family of dissipative dynamical systems on Hilbert spaces H_N with global attractors $\mathcal{A}_N\subset H_N$. Suppose that the following three assumptions are satisfied:*

(1) (Embedding) *There is a continuous embedding of $E_N:H_N\hookrightarrow H$.*

(2) (Uniform Dissipativity)

$$K=\bigcup_{\infty>N\ge N_0}E_N(\mathcal{A}_N)$$

is pre-compact in H.

(3) (Finite Time Uniform Convergence) *For any $t \in (0,1]$, we have*

$$\lim_{N\to\infty} \sup_{\mathbf{u}\in\mathcal{A}_N} \|E_N(S_N(t)\mathbf{u}) - S(t)(E_N\mathbf{u})\| \to 0.$$

Then for any sequence of invariant measures $\mu_N \in \mathcal{IM}_N$ of the dynamical system S_N, there must exist a subsequence, still denoted by $\{\mu_N\}$, and an invariant measure $\mu \in \mathcal{IM}$ of the $S(t)$ such that

$$E_N^*\mu_N \rightharpoonup \mu,$$

where E_N^* is the lift operator induced by the continuous embedding E_N in the sense that for any bounded continuous test functional φ on H,

$$\int_H \varphi(\mathbf{u})\mathrm{d}(E_N^*\mu_N)(\mathbf{u}) := \int_{H_N} \varphi(E_N(\mathbf{u}))\mathrm{d}\mu_N(\mathbf{u}). \tag{2.11}$$

Proof Thanks to the definition of the lift of invariant measures of S_N (2.11), the continuity of the embedding operator E_N (see assumption (1)), the uniform dissipativity assumption (2), and the Kakutani-Riesz representation theorem (see [21]), we see that $\{E_N^*\mu_N\}$ must be a sequence of Borel probability measures on H. Moreover, this sequence must be tight by Prokhorov's theorem (see [1, 21]) since the support of $E_N^*\mu_N$ must be included in the compact set $\overline{K}$. Hence it must have a convergent subsequence, still denoted by $\{E_N^*\mu_N\}$, and a Borel probability measure μ on H such that

$$E_N^*\mu_N \rightharpoonup \mu.$$

Our goal is to show that $\mu \in \mathcal{IM}$, i.e., it is invariant under $S(t)$.

For each $t \in (0,1]$ and each C^1 test functional φ with compact support, we have

$$\begin{aligned}
\Big|\int_H (\varphi(S(t)\mathbf{u}) - \varphi(\mathbf{u}))\mathrm{d}\mu(\mathbf{u})\Big| &= \lim_{N\to\infty}\Big|\int_{H_N} (\varphi(S(t)E_N\mathbf{u}) - \varphi(E_N\mathbf{u}))\mathrm{d}\mu_N(\mathbf{u})\Big| \\
&\le \lim_{N\to\infty}\Big|\int_{H_N} (\varphi(S(t)E_N\mathbf{u}) - \varphi(E_N S_N(t)\mathbf{u}))\mathrm{d}\mu_N(\mathbf{u})\Big| \\
&\quad + \lim_{N\to\infty}\Big|\int_{H_N} (\varphi(E_N S_N(t)\mathbf{u}) - \varphi(E_N\mathbf{u}))\mathrm{d}\mu_N(\mathbf{u})\Big| \\
&\le \lim_{N\to\infty} \sup_{\mathbf{u}\in H} \|\varphi'(\mathbf{u})\| \sup_{\mathbf{u}\in\mathcal{A}_N} \|S(t)E_N\mathbf{u} - E_N S_N(t)\mathbf{u}\| \\
&= 0,
\end{aligned}$$

where we have utilized the weak convergence of $E_N^*\mu_N$, the lift (2.11), and the continuity of φ and $\varphi \circ S(t)$ in the first step, the triangle inequality in the second step, the mean value theorem, the fact that μ_N is supported on $\mathcal{A}_N$, the invariance of μ_N under S_N in the third step, the finite time uniform convergence assumption (3) and the assumption that φ is C^1 with compact support in the last step. A general bounded continuous test functional φ can be approximated by C^1 test functional with compact support through classical finite dimensional approximation and mollifier technique. The interested reader is referred to [10, 41] for more details. This proves the weak invariance of μ for $t \in (0,1]$. For a general time t, we decompose t as $t = n + t^*$, where n is a non-negative integer and $t^* \in (0,1)$. We apply the semigroup property of $S(t)$ and the weak invariance n times with $t = 1$ and one time with $t = t^*$. We deduce the weak invariance for arbitrary time.

This ends the proof of the theorem.

In application, the spatial discrete dynamical systems $\{S_N\}$ are usually generated by spatial discretization (numerical scheme, with finite dimensional phase space H_N) of the original infinite dimensional dynamical system (generated by a time-dependent PDE). In other words, $S_N(\mathbf{u})$ is the solution to the numerical scheme. For the case of spectral or finite element discretisation, the embedding operator can be taken as the natural inclusion operator but the case with finite difference discretisation is more challenging. The uniform dissipativity of the numerical scheme can be established via the existence of a uniform (in mesh size) absorbing ball in discrete form in another separable Hilbert space V which is compactly imbedded in H in the case of strongly dissipative system (see the next section for an example). Similar difficulty exists for weakly dissipative systems just as in the temporal discretisation case. The finite time uniform convergence comes with classical numerical analysis for reasonable schemes (see next section for an example).

3 Application

3.1 Infinite Prandtl number model for convection

Here we illustrate an application of the main result on temporal approximation to the following (non-dimensional) infinite Prandtl number model for convection (see [3, 6, 7, 35, 38, 39]):

$$\nabla p = \Delta \mathbf{u} + \mathrm{Ra}\,\mathbf{k}T, \quad \nabla \cdot \mathbf{u} = 0, \quad \mathbf{u}|_{z=0,1} = 0, \tag{3.1}$$

$$\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = \Delta T, \quad T|_{z=0} = 1, \quad T|_{z=1} = 0, \tag{3.2}$$

where $\mathbf{u}$ is the Eulerian velocity of the fluid, p represents the kinematic pressure of the fluid, T is the temperature of the fluid, $\mathbf{k}$ is the unit vector in the z direction, Ra is the Rayleigh number measuring the ratio of differential heating over overall dissipation, and we assume that the fluids occupy the (non-dimensionalized) region $\Omega = [0, L_x] \times [0, L_y] \times [0, 1]$ with periodicity imposed in the horizontal directions for simplicity.

Since the temperature field T satisfies inhomogeneous boundary conditions, it is mathematically convenient to consider a perturbative temperature field

$$\theta = T - \tau(z), \quad \tau(0) = 1, \quad \tau(1) = 0,$$

where $\tau(z)$ is an appropriate smooth fixed background temperature profile (see [6, 7, 39]). This decomposition is also in accordance with the mean (τ) and fluctuation (θ) decomposition commonly used in the study of turbulent flows.

The system can be also written in terms of the perturbative temperature field θ as

$$\frac{\partial \theta}{\partial t} + \mathrm{Ra}\, A^{-1}(\mathbf{k}\theta) \cdot \nabla \theta + \mathrm{Ra}\, A^{-1}(\mathbf{k}\theta)_3 \tau'(z) = \Delta \theta + \tau''(z), \quad \theta|_{z=0,1} = 0,$$

where A denotes the Stokes operator with the associated boundary conditions and viscosity one, and $A^{-1}(\mathbf{k}\theta)_3$ represents the third component (vertical velocity) of $A^{-1}(\mathbf{k}\theta)$.

The phase space of the problem is set to be $H = L^2(\Omega)$. We then propose the following family of semi-implicit (linear) schemes for the infinite Prandtl number model

$$\frac{\theta_k^{n+1}-\theta_k^n}{k}+\mathrm{Ra}\,A^{-1}(\mathbf{k}\theta_k^n)\cdot\nabla\theta_k^{n+1}+\mathrm{Ra}\,A^{-1}(\mathbf{k}(\lambda\theta_k^n+(1-\lambda)\theta^{n+1}))_3\tau'(z)=\Delta\theta_k^{n+1}+\tau''(z), \quad (3.3)$$

where $\lambda \in [0,1]$ is a free parameter. It can be verified that the conditions in Theorem 2.1 are satisfied for these schemes (see [4, 5, 41]), so that the stationary statistical properties of the time discrete scheme converge to those of the infinite Prandtl number model as the time step approaches zero.

3.2 Barotropic quasi-geostrophic equation

Here we consider an application of the spatial discretisation method to the following barotropic quasi-geostrophic equation with dissipation and external forcing (see [24]):

$$\frac{\partial q}{\partial t}+\nabla^{\perp}\psi\cdot\nabla q=\mathcal{D}\psi+f, \quad (3.4)$$

$$q=-\Delta\psi+F\psi+\beta y, \quad F\geq 0,\ \beta>0, \quad (3.5)$$

$$\mathcal{D}=-\sum_{j=1}^{k}d_j(-\Delta)^j, \quad d_j\geq 0,\ \forall j,\ \sum_{j=2}^{k}d_j>0. \quad (3.6)$$

Here $\psi(x,y;t)$ represents the stream-function of the barotropic flow, q is the potential vorticity, $F>0$ is the F-plane constant related to the stratification of the fluid, $\beta>0$ is the beta-plane constant, d_1 is the Ekman damping coefficient, d_2 is the eddy/Newtonian viscosity coefficient, d_j, $j\geq 3$ are the coefficients of various hyper-viscosity, and f represents external forcing.

The phase space for the system is $H=\dot{H}^1_{\mathrm{per}}([0,2\pi]\times[0,2\pi])$, i.e. all H^1 periodic functions with period 2π in each direction and with average zero. The phase space can be characterized easily via Fourier series as

$$\dot{H}^1_{\mathrm{per}}([0,2\pi]\times[0,2\pi]):=\Big\{\psi=\sum_{\mathbf{k}\neq 0}\widehat{\psi}_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{x}}\ \Big|\ \sum_{\mathbf{k}}|\mathbf{k}|^2|\widehat{\psi}_{\mathbf{k}}|^2<\infty\Big\}.$$

It is obvious that Fourier spectral discretisation is the natural spatial discretisation for this problem. We define the finite dimensional space

$$H_N:=\Big\{\psi_N=\sum_{N\geq|\mathbf{k}|^2>0}\widehat{\psi}_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{x}}\Big\}.$$

We also define the truncated dynamics on this finite dimensional space H_N as

$$\frac{\partial q_N}{\partial t}+P_N(\nabla^{\perp}\psi_N\cdot\nabla q_N)=\mathcal{D}\psi_N+P_N(f), \quad (3.7)$$

$$q_N=-\Delta\psi_N+F\psi_N+\beta y, \quad (3.8)$$

where the projection operator P_N is defined as

$$P_N(\psi)=\sum_{N\geq|\mathbf{k}|^2>0}\widehat{\psi}_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{x}}, \quad \text{if } \psi=\sum_{\mathbf{k}\neq 0}\widehat{\psi}_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{x}}.$$

In this case, the embedding operator E_N can be taken as the identity operator (natural inclusion). The uniform convergence of the scheme on finite time interval as well as the uniform dissipativity of it are essentially the same as those of the two dimensional incompressible Navier-Stokes equations and their spectral Galerkin approximation (see [32, 33]). In fact, one can show the existence of an absorbing ball in $\dot{H}^2_{\rm per}$ which attracts all bounded sets in $\dot{H}^1_{\rm per}$ for the original dynamical system and the truncated systems uniformly in the truncation number N. We leave the detail to the interested reader. Therefore the stationary statistical properties of the finite dimensional system converge to those of the barotropic quasi-geostrophic equation as the truncation number N approaches infinity according to Theorem 2.2.

4 Conclusions and Remarks

We have presented simple and natural criterions on the convergence of stationary statistical properties of temporal and spatial approximations of infinite dimensional dissipative dynamical systems. The key ingredient that ensures the convergence of the invariant measures is the faithfulness to the original system. In the case of dissipative systems under investigating, the most important and natural assumption is the uniform dissipativity of the scheme. We have also illustrated the application of the abstract results to the infinite Prandtl number model for convection (temporal approximation) and the barotropic quasi-geostrophic equation (spatial discretisation).

Despite the progress reported here, much remains to be done in terms of finding efficient numerical methods that are able to capture the stationary statistical properties of infinite dimensional dissipative dynamical systems.

(1) First, we should test and further validate our general approach on a few simple models with known exact stationary statistical properties.

(2) For each application, we have to develop schemes that satisfy the postulated criterions. In the temporal approximation case, fully implicit approach may not work since the scheme may not generate a discrete dynamical system due to possible non-uniqueness of the solution to the scheme (this is on top of the potential high computational cost associated with fully implicit schemes). In the spatial approximation case, the finite difference approach may require significant work.

(3) Many dissipative systems are small perturbation of conservative systems. What would be the pros and cons of designing algorithms that are conservative for the conservative part and dissipative for the dissipative part?

(4) Since we are interested in long time asymptotic statistical properties of large chaotic dynamical systems, efficiency of the scheme is very important. The stability/dissipativity criterion favors implicit approach while efficiency prefers explicit time stepping. How do we balance the stability and efficiency?

(5) Related to efficiency, are there any efficient higher order schemes with guaranteed convergence of the stationary statistical properties?

(6) Many applications involve disparate temporal and/or spatial scales. How do we develop efficient schemes that take advantage of the separation of scales?

(7) We do not have a convergence rate here. It is perhaps not expected in general. Under what circumstances, do we have convergence rate? Which scheme has better convergence rate? How do we balance the accuracy and efficiency?

(8) The underlying physical system might have multiple invariant measures. How do we

design numerical schemes that select the physically relevant ones? Would noise perturbation work? What kind of noise perturbation works better?

(9) Many physical systems are under periodic or quasi-periodic influence of the environment. How do we generalize the current theory to the non-autonomous case?

(10) We encounter uncertainty in many parameters and data of the underlying dynamical system in application. How do we utilize the current theory to quantify the uncertainty in long time statistics (the climate)? Would a combination with linear response/fluctuation dissipation theory (FDT) be useful? Is there any implication to the study of model errors?

(11) Can we further develop this theory and combine it with fluctuation dissipation theory to study climate change in climate models?

(12) Many physical models involve randomness. How do we generalize the current theory to infinite dimensional dissipative random dynamical systems?

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