ERROR IN APPROXIMATION OF LYAPUNOV EXPONENTS
ON INERTIAL MANIFOLDS:
THE KURAMOTO-SIVASHINSKY EQUATION

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Abstract. We provide an analysis of the error in approximating Lyapunov exponents of dissipative PDEs on inertial manifolds using QR techniques. The reduction in the number of modes needed for an inertial form facilitates the error analysis. Numerical computations on the Kuramoto-Sivashinsky equation illustrate the results.

1. **Introduction.** In this work we provide bounds on the approximation error in Lyapunov exponents and Sacker-Sell spectrum for some dissipative nonlinear partial differential equations. Our key assumptions are that we have a good finite dimensional approximation in terms of an inertial manifold reduction together with shadowing type error bounds for the approximation of the nonlinear problem. The techniques we employ are C^1 convergence results for inertial manifolds of semilinear and quasilinear PDEs and an error analysis for Lyapunov exponents computed by the so-called discrete QR technique.

Although our approach and analysis applies to a larger class of dissipative nonlinear PDEs, we apply it here to the Kuramoto-Sivashinsky equation. This equation exhibits rich and complex dynamics, while still allowing for a low dimensional system to capture the complexity of the full PDE. This is due to the presence of symmetry [3, 2] and to the existence of a low-dimensional inertial manifold [16]. For this reason, the Kuramoto-Sivashinsky equation (KSE) continues to receive attention, both

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mathematically and computationally, see [7, 17, 22, 23, 41]. Moreover, the KSE has proven to be amenable also to computer verified proofs ([43, 44, 9]). These computer assisted verifications have so far been restricted to dynamically simple, though very important, sets: equilibria and (attracting) periodic orbits. Yet, one of the most interesting features of the KSE is given by the chaotic dynamics which take place on the low dimensional attractor, and this is the regime we consider in this work.

Lyapunov exponents are routinely used as a computational means for detecting chaotic dynamics. For example, for the KSE, they have been used to this end in [29, 6, 39], and see also [40]. Lyapunov exponents are also used in many other contexts; e.g., see [34] for the use of Lyapunov exponents in estimating the entropy of a system, see [8] for their use in estimating dimension of attractors, or see [4] for use of the Lyapunov exponents as a tool for studying the bifurcations of random dynamical systems.

Example 1.1. Here we exemplify how the Kaplan-Yorke dimension, $\dim_{\mathrm{KY}}$, of the KSE attractor, can be used to determine bifurcations of an attractor. We take the KSE in the form (6.1)– for values of ξ in [0.299 , 0.3], see (6.3). See Sections 5,6 for justification on the form of the equation and meaning of ξ.

Recall that, if $\lambda_1 \geq \lambda_2 \geq \ldots$ are the Lyapunov exponents of the system, and the system is dissipative (the sum of all Lyapunov exponents is negative), $\dim_{\mathrm{KY}}$ is defined as follows:

$$\text{Let } k : \sum_{i=1}^{k} \lambda_i \geq 0 \ , \quad \text{but} \quad \sum_{i=1}^{k+1} \lambda_i < 0 \ . \quad \text{Then} \quad \dim_{\mathrm{KY}} \ = \ k + \frac{\sum_{i=1}^{k} \lambda_i}{|\lambda_{k+1}|} \ .$$
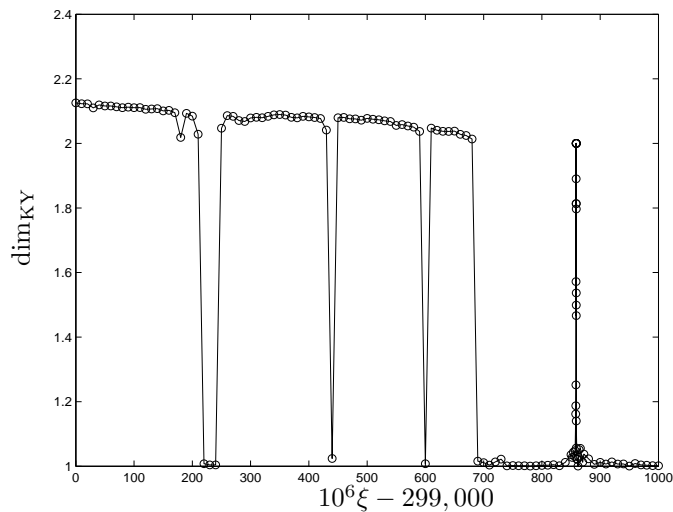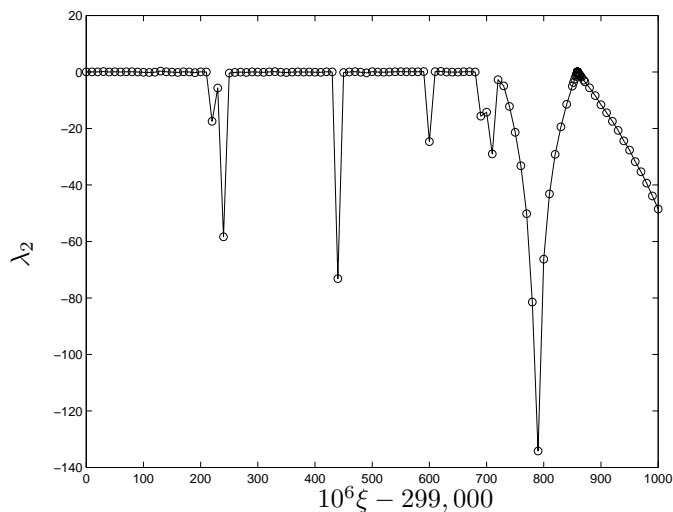
For example, if the trajectory is following an attracting periodic orbit, then $\lambda_1 = 0$, $\lambda_2 < 0$, and $\dim_{\mathrm{KY}} = 1$.

In Figure 1, we show a plot of $\dim_{\mathrm{KY}}$ against ξ, while in Figure 2 we show a plot of λ_2 against ξ. For plotting purposes, the values of ξ have been rescaled as $10^6 \xi - 299,000$. For later reference, we notice that the value $\xi = 0.02991$ corresponds to an abscissa of 100 in the plots below.

These figures were obtained performing a 16 modes truncation of the Fourier expansion of the KSE, integrating the nonlinear system and computing the Lyapunov exponents up to time 100, after having passed the initial transient for the trajectory and having settled on the attractor.

Based on these Figures, we see that the trajectories either move on a chaotic attractor with $\dim_{\mathrm{KY}}$ slightly larger than 2, or on an attracting periodic orbit. Notice that we have $\lambda_2 \approx 0$ on the chaotic attractor, while $\lambda_2 < 0$ on the periodic orbit. These are nontrivial computations, since there are several periodic windows within the given range of ξ-values and an exhaustive search has not been attempted. Furthermore, there are values of ξ for which we are not confident that our computations are sufficiently accurate; e.g., for abscissas between 850 and 900 in the plots. However, the performed computations betray well the bifurcation scenario. Moreover, our results confirm (see [6]) that at the value $\xi = 0.02991$ there is chaotic behavior. This is the value on which we will focus in Section 6.

It is important to remark that, in spite of the chaotic dynamics, the Lyapunov exponents are often robust quantities and can be reliably computed. For this to be true, one basically needs that the underlying linearized system enjoys the property of integral separation; we review this in Section 4. For example, in [10], for the well known Lorenz system, this property was verified to hold. In the present work,

PSfrag replacements

FIGURE 1. Kaplan-Yorke dimension of attractor, versus ξ.

PSfrag replacements

FIGURE 2. Second Lyapunov exponent λ_2, versus ξ.

we will infer that the property of integral separation also holds for the KSE at a particular value of the parameter; the "abscissa 100" in the Figures above.

This paper is organized as follows. We begin with background on inertial manifold, followed by C^1 convergence results. Then, after background on the computation of Lyapunov exponents and the error analysis developed in [11, 12, 14], we give our main theorem quantifying the error in the Lyapunov exponents (or Sacker-Sell spectrum). The error in the Lyapunov exponents is based upon the error in the QR techniques, the magnitude of the upper triangular R-factors, the error in the

perturbed linear variational problem, and the degree to which the given linearized system is integrally separated. To illustrate our analysis, we give numerical results with Galerkin and nonlinear Galerkin truncations for the Kuramoto-Sivashinsky equation with periodic boundary conditions.

We verify that Lyapunov exponents of this dissipative PDE can be accurately computed by using a good approximation to the inertial manifold. This is not to imply that this is the most efficient means to do so. Indeed, to compute the manifold accurately requires much more work than using an accurate Galerkin truncation with more modes. It is the error analysis that benefits from the reduction of system size brought by the inertial manifold.

2. **Background on Inertial Manifolds.** We consider an evolutionary equation in a Hilbert space H

$$\frac{du}{dt} + Au = f(u) \, , u \in H \, . \tag{2.1}$$

The linear operator A has a complete set of eigenvectors $w_1, w_2, w_3, \ldots$ associated with a sequence of positive eigenvalues $\mu_1, \mu_2, \mu_3, \ldots$, defining projectors P_n onto the span of $\{w_1, \ldots, w_n\}$, and the function $f : G \to H$ is globally Lipschitz

$$|f(u) - f(v)|_H \leq \ell_f |u - v|_G, \qquad \forall \, u, v \in H \, , \tag{2.2}$$

where G is a subspace of H (with perhaps a different norm). Under certain further assumptions, for large enough n, an inertial manifold $\mathcal{M}$ for (2.1) can be realized as the graph of a function $\Phi : P_n H \to (I - P_n)H$. The inertial form

$$\frac{dp}{dt} + Ap = P_n f(p + \Phi(p)) \, , p \in P_n H \, , \tag{2.3}$$

captures all the long-time behavior of (2.1).

For the sake of clarity, we emphasize that (2.3) is a finite dimensional system, of dimension n.

As in [38] we assume there holds an exponential dichotomy

$$\|e^{-tA}P_n\|_{\mathcal{L}(H,H)} \leq K_1 e^{-\mu_n t}, \quad \forall \, t \leq 0,$$
$$\|e^{-tA}P_n\|_{\mathcal{L}(G,H)} \leq K_1 \mu_n^\alpha e^{-\mu_n t}, \quad \forall \, t \leq 0, \tag{2.4}$$

$$\|e^{-tA}(I - P_n)\|_{\mathcal{L}(H,H)} \leq K_2 e^{-\mu_{n+1} t}, \quad \forall \, t \geq 0,$$
$$\|e^{-tA}(I - P_n)\|_{\mathcal{L}(G,H)} \leq K_2 (t^{-\alpha} + \mu_{n+1}^\alpha) e^{-\mu_{n+1} t}, \quad \forall \, t > 0, \tag{2.5}$$

where $K_1, K_2 \geq 1$, $0 \leq \alpha < 1$, and $\| \cdot \|_{\mathcal{L}(G,H)}$ is the operator norm from G to H. The critical assumption is that the *spectral gap condition*

$$\mu_{n+1} - \mu_n > 3\ell_f K_1 K_2 [\mu_n^\alpha + (1 + \gamma_\alpha)\mu_{n+1}^\alpha], , \tag{2.6}$$

where

$$\gamma_\alpha = \begin{cases} \int_0^{+\infty} e^{-r} r^{-\alpha} dr, & \text{if } 0 < \alpha < 1, \\ 0, & \text{if } \alpha = 0, \end{cases}$$

holds for some $n \in \mathbb{N}$.

If (2.6) holds, one can choose σ such that

$$\mu_n + 2\ell_f K_1 \mu_{n+1}^\alpha < \sigma < \mu_{n+1} - 2\ell_f K_1 K_2 (1 + \gamma_\alpha) \mu_{n+1}^\alpha. \tag{2.7}$$

This σ is used to define the Banach space

$$\mathcal{F}_\sigma = \{\varphi \in C\left((-\infty, 0], E\right) ; |\varphi|_{\mathcal{F}_\sigma} = \sup_{t \leq 0} e^{\sigma t} |\varphi(t)|_H < \infty\}.$$

A trajectory on the inertial manifold can be found as the fixed point $\varphi = \varphi(p)$ of a mapping $\mathcal{T}(\cdot, p) : \mathcal{F}_\sigma \to \mathcal{F}_\sigma$ given by

$$\mathcal{T}(\varphi, p)(t) = e^{-tA}p - \int_t^0 e^{-(t-s)A}P_n f(\varphi(s))ds \\ + \int_{-\infty}^t e^{-(t-s)A}(I - P_n)f(\varphi(s))ds \ . \tag{2.8}$$

The inertial manifold $\mathcal{M} = \text{graph}\Phi$ is the collection of all such trajectories, where $\Phi : P_n H \to (I - P_n)H$ is defined by the fixed point φ of (2.8),

$$\Phi(p) = (I - P_n)\varphi(p)(0), \qquad \forall \, p \in P_n H.$$

The spectral gap condition (2.6) ensures not only that $\mathcal{T}$ has a contraction rate

$$\theta_{n,\sigma} = \frac{\ell_f K_1 \mu_n^\alpha}{\sigma - \mu_n} + \frac{\ell_f K_2 (1 + \gamma_\alpha)\mu_{n+1}^\alpha}{\mu_n - \sigma} < 1 \ , \tag{2.9}$$

but also that the resulting manifold is *exponentially tracking*, i.e. corresponding to any initial condition $u_0 \in H$ there exists a particular solution *on* the manifold, to which the trajectory through u_0 is attracted at an exponential rate.

The mapping $\mathcal{T}$ was discretized in [37] by replacing the function space $\mathcal{F}_\sigma$ with

$$\tilde{\mathcal{F}}_0 = \{\psi : (-\infty, 0] \to H; \psi \text{ piecewise constant w/ finite number of discontinuities}\} \ .$$

Given a time step $\tau > 0$, number of steps $N \in \mathbb{N}$, and base point $p_0 \in P_n H$, a mapping $\mathcal{T}_\tau^N : \tilde{\mathcal{F}}_0 \times PE \to \tilde{\mathcal{F}}_0$ is defined for $k = 0, 1, \ldots, N$ by

$$\mathcal{T}_{\tau,0}^N(\psi, p)(t) = e^{k\tau A}P_n p - \int_{-k\tau}^0 e^{-(-k\tau - s)A}P_n f(\psi(s))ds \\ + \int_{-\infty}^{-k\tau} e^{-(-k\tau - s)A}(I - P_n)f(\psi(s))ds, \tag{2.10}$$

for $t \in (-(k+1)\tau, -k\tau]$, if $k < N$, or $t \in (-\infty, -N\tau]$, if $k = N$. Since ψ is piecewise constant on intervals, the integrals can be calculated exactly, and are thus reduced to summations over the intervals. It was shown in [21] that an adaptation of (2.10) to handle the general center manifold case can be evaluated in a recursive manner. These recursion formulas are explicitly stated for the special case of an inertial manifold in the appendix of this paper.

The mapping in (2.10) is shown to be a contraction in [37] under the same spectral gap condition as in (2.6). Starting with

$$\varphi^0(p)(t) = p \ , \quad \forall \, t \leq 0 \ , \tag{2.11}$$

and simultaneously increasing N and decreasing τ, an explicit sequence of approximating piecewise constant trajectories $\varphi^j(p)$ is generated which converges to $\varphi(p)$, the fixed point of (2.8). Specifically, for sequences $N_0 < N_1 < N_2 < \cdots$ and $\tau_0 > \tau_1 > \tau_2 > \cdots$ Picard iteration is carried out to produce

$$\varphi^j(p) = \mathcal{T}_{\tau_j,0}^{N_j}(\varphi^{j-1}(p), p) \ .$$

This, in turn defines functions

$$\Phi^j(p) = (I - P_n)\varphi^j(p)(0), \qquad \forall \, p \in P_n H \ ,$$

whose graphs are manifolds converging to the inertial manifold.

It was shown in [38] that if f is $C^{1,\nu}$, i.e. there exists a constant h_{Df} such that

$$\|Df(u_1) - Df(u_2)\|_{\mathcal{L}(G,H)} \leq h_{Df}|u_1 - u_2|_H^\nu \ ,$$

then Φ is also $C^{1,\nu}$ so there exists a constant $h_{D\Phi}$ such that

$$\|D\Phi(p_1) - D\Phi(p_2)\|_{\mathcal{L}(PH,H)} \le h_{D\Phi}|p_1 - p_2|_H^\nu .$$

In fact the differential $D\Phi$ can be found as the fixed point of another contraction mapping

$$\mathcal{T}_1(\Delta)(t) = e^{-tA}P - \int_t^0 e^{-(t-s)}P_n Df(\varphi(s))\Delta(s)ds \qquad (2.12)$$
$$+ \int_{-\infty}^t e^{-(t-s)A}(I - P_n)Df(\varphi(s))\Delta(s)ds$$

on the Banach space

$$\mathcal{F}_{1,\sigma} = \{\Delta \in C\left((-\infty, 0], \mathcal{L}(PH, H)\right) : \|\Delta\|_{\mathcal{F}_{1,\sigma}} = \sup_{t \le 0} e^{\sigma t}\|\Delta(t)\|_{\mathcal{L}(P_n H, H)} < \infty\}.$$

3. **Error in the Linear Variational Equation.** As mentioned in [37], if $f \in C^{1,\nu}$ the convergence $\Phi^j \to \Phi$ can be shown to be C^1, and the rate estimated.

Proposition 3.1. *In addition to* (2.2), (2.4), *and* (2.5), *suppose that*

$$f \in C^{1,\nu} \quad and \quad \|AP_n\|_{\mathcal{L}(H,P_n H)} \le K_3\mu_n , \qquad (3.1)$$

that

$$\mu_{n+1} - 3\ell_f K_2(1 + \gamma_\alpha)\mu_{n+1}^\alpha > (1 + \nu)(\mu_n + 3\ell_f K_1\mu_n^\alpha) , \qquad (3.2)$$

and that $\{\tau_j\}$ *and* $\{N_j\}$ *are chosen so that*

$$0 < \tau_j \le c_1\left(\gamma\theta_{n,\sigma}\right)^{\nu j} \quad \forall j \in \mathbb{N} , \qquad (3.3)$$

where $\theta_{n,\sigma}$ *is as in* (2.9), *and*

$$N_j\tau_j \ge c_2 j \qquad (3.4)$$

for some c_1, $c_2 > 0$, *some* $0 < \gamma < 1$, *and some* σ *satisfying* (2.7). *Then*

$$d(\Phi^j, \Phi) = \sup_{p \in P_n H} \frac{|\Phi^j(p) - \Phi(p)|_H}{1 + |p|_H} \le c_3 e^{-c_4 j} , \qquad (3.5)$$

$$d(D\Phi^j, D\Phi) = \sup_{p \in P_n H} \frac{\|D\Phi^j(p) - D\Phi(p)\|_{\mathcal{L}(PH,H)}}{1 + |p|_H} \le c_5 e^{-c_4 j} , \qquad (3.6)$$

for suitable constants c_3, c_4, *and* c_5.

Proof. For $\psi \in \tilde{\mathcal{F}}_0$, $\Delta \in \tilde{\mathcal{F}}_1$ where

$$\tilde{\mathcal{F}}_1 = \{\Delta : (-\infty, 0] \to \mathcal{L}(PH, H) : \Delta \text{ piecewise const. w/ finite no. of discontinuities}\}.$$

define for $k = 0, 1, \ldots, N$

$$\mathcal{T}_{\tau,1}^N(\psi, \Delta)(t) = e^{k\tau A}P_n - \int_{-k\tau}^0 e^{-(-k\tau-s)A}P_n Df(\psi(s))\Delta(s)ds \qquad (3.7)$$
$$+ \int_{-\infty}^{-k\tau} e^{-(-k\tau-s)A}(I - P_n)Df(\psi(s))\Delta(s)ds,$$

for $t \in (-(k+1)\tau, -k\tau]$, if $k < N$, or $t \in (-\infty, -N\tau]$, if $k = N$. As in [38], it is easy to verify that

$$\mathcal{T}_\tau^N = (\mathcal{T}_{\tau,0}^N, \mathcal{T}_{\tau,1}^N)$$

maps $\tilde{\mathcal{F}}_0 \times \tilde{\mathcal{F}}_1$ to itself. The convergence in (3.5) was proved in [37] using the mapping $\mathcal{T}_{\tau,0}^N$. To prove the convergence of the second component, i.e. (3.6), follow a similar argument, except that in the analog of Lemma 5.2 in [37], use the Hölder

continuity of $D\Phi$ instead of the Lipschitz continuity of Φ. The effect is that while for fixed n, Lemma 5.3 in [37] amounts to

$$|\varphi(p) - \mathcal{T}_{\tau,0}^N(\psi, p)|_{\mathcal{F}_{0,\sigma}} \leq \theta_{n,\sigma}|\varphi(p) - \psi|_{\mathcal{F}_{0,\sigma}} + O(\tau + e^{-c_4 N\tau}) ,$$

we have for the differential

$$\|\partial_p\varphi(p) - \mathcal{T}_{\tau,1}^N(\psi, \Delta)\|_{\mathcal{F}_{1,\sigma}} \leq \theta_{n,\sigma}\|\partial_p\varphi(p) - \Delta\|_{\mathcal{F}_{1,\sigma}} + O(\tau^\nu + e^{-c_4 N\tau}) .$$

$\square$

Consider the linear variational equation for (2.3) along a solution trajectory $p(t, p_0)$. That is, we take $p = p(t, p_0) + v$, $v \in P_n H$, and linearize along $p(t, p_0)$. We express the variational problem as

$$\frac{dv}{dt} = C(t)v = [-A + D(P_n f)(p + \Phi(p))] v , \quad p = p(t, p_0) . \tag{3.8}$$

Again, we stress that (3.8) is a finite dimensional system, and –in the context of (3.8)– the operator C can be unambiguously identified with the matrix associated to this finite dimensional system.

Now consider the approximate inertial forms

$$\frac{d\tilde{p}}{dt} + A\tilde{p} = P_n f(\tilde{p} + \Phi^j(\tilde{p})) , \tilde{p} \in P_n H , \tag{3.9}$$

along with its linear variational equation ($w \in P_n H$)

$$\frac{dw}{dt} = \tilde{C}(t)w = \left[-A + D(P_n f)(\tilde{p} + \Phi^j(\tilde{p}))\right] w , \quad \tilde{p} = \tilde{p}(t, \tilde{p}_0) . \tag{3.10}$$

Theorem 3.2. *The matrices in the associated linear variational equations* (3.8), (3.10) *satisfy*

$$\tilde{C}(t) = C(t) + E(t) \tag{3.11}$$

with

$$\begin{aligned}\|E(t)\| \leq &b_1 \left[(1 + \ell_\Phi)|p - \tilde{p}|_H + c_3 e^{-c_4 j}(1 + |\tilde{p}|_H)\right]^\nu \\ &+ b_2 \left[c_5 e^{-c_4 j}(1 + |\tilde{p}|_H) + h_{D\Phi}|\tilde{p} - p|_H^\nu\right] =: \eta ,\end{aligned} \tag{3.12}$$

where

$$\begin{aligned}b_1 =&h_{Df}(1 + h_{D\Phi}|p|_H^\nu + \|D\Phi(0)\|_{\mathcal{L}(P_n H, H)}) \\ b_2 =&h_{Df}[|\tilde{p}|_H + c_3 e^{-c_4 j} + \ell_\Phi|\tilde{p}|_H]^\nu + \|D(P_n f)(\Phi(0))\|_{\mathcal{L}(G,H)}\end{aligned}$$

Proof. Write the difference of C and $\tilde{C}$ as

$$\begin{aligned}E =&D(P_n f)(\tilde{p} + \Phi^j(\tilde{p}))(I + D\Phi^j(\tilde{p})) - D(P_n f)(p + \Phi(p))(I + D\Phi(p)) \\ =&E_1 + E_2\end{aligned}$$

where

$$\begin{aligned}E_1 =& \left[D(P_n f)(\tilde{p} + \Phi^j(\tilde{p})) - D(P_n f)(p + \Phi(p))\right](I + D\Phi(p)) \\ E_2 =&D(P_n f)(\tilde{p} + \Phi^j(\tilde{p})) \left[D\Phi^j(\tilde{p}) - D\Phi(p)\right] .\end{aligned}$$

Estimate E_1 as

$$\begin{aligned}\|E_1\| \leq& h_{Df} \left[|p - \tilde{p}|_H + |\Phi(p) - \Phi(\tilde{p})|_H + |\Phi(\tilde{p}) - \Phi^j(\tilde{p})|_H\right]^\nu \\ &\times (1 + \|D\Phi(p) - D\Phi(0)\|_{\mathcal{L}(P_n H, H)} + \|D\Phi(0)\|_{\mathcal{L}(P_n H, H)}) \\ \leq& h_{Df} \left[(1 + \ell_\Phi)|p - \tilde{p}|_H + c_3 e^{-c_4 j}(1 + |\tilde{p}|_H)\right]^\nu \\ &\times (1 + h_{D\Phi}|p|_H^\nu + \|D\Phi(0)\|_{\mathcal{L}(P_n H, H)}) ,\end{aligned}$$

and E_2 as

$$\|E_2\| \le \left(\|D(P_n f)(\tilde{p} + \Phi^j(\tilde{p})) - D(P_n f)(\Phi^j(0))\|_{\mathcal{L}(G,H)} + \|D(P_n f)(\Phi^j(0))\|_{\mathcal{L}(G,H)} \right)$$
$$\times \left[\|D\Phi^j(\tilde{p}) - D\Phi(\tilde{p})\|_{\mathcal{L}(P_n H,H)} + \|D\Phi(\tilde{p}) - D\Phi(p)\|_{\mathcal{L}(P_n H,H)} \right]$$
$$\le \left(h_{Df} |\tilde{p} + \Phi^j(\tilde{p}) - \Phi(\tilde{p}) + \Phi(\tilde{p}) - \Phi(0)|_H^\nu + \|D(P_n f)(\Phi^j(0))\|_{\mathcal{L}(G,H)} \right)$$
$$\times \left[c_5 e^{-c_4 j}(1 + |p|_H) + h_{D\Phi} |\tilde{p} - p|_H^\nu \right] .$$

$\square$

The smoother f is, the larger ν can be taken, and the smaller is the bound on E. On the other hand, the larger ν is taken, the harder it is to satisfy the stronger gap condition in (3.2), perhaps forcing one to use a manifold of higher dimension. In our application to the Kuramoto-Sivashinsky equation f is actually analytic, so any $\nu \in (0, 1]$ may be considered. Moreover, in the case of the KSE, $f(0) = 0$ and $Df(0) = 0$, so that $\Phi(0) = 0$ and $D\Phi(0) = 0$ which simplifies the expressions for b_1, b_2.

4. **Error in Lyapunov Exponents by Discrete QR Technique.** In this section we give a result on the error in the Lyapunov exponents associated to the linear variational problem (3.8), when the Lyapunov exponents are approximated by the so-called discrete QR technique, a popular approach to approximate Lyapunov exponents of linear time dependent systems. In our analysis, we will account for the following sources of errors: (i) The error due to having the perturbed variational problem (3.10), rather than the exact variational problem (3.8), and (ii) The error due to the impossibility of solving exactly a linear variational problem itself, regardless of whether it is the true or the perturbed one.

The source of error in (ii) is already present when trying to compute Lyapunov exponents of linear, finite dimensional systems. Instead, the source of error in (i) has several contributions which are specific to the problem at hand. Namely: the error due to the infinite dimensional reduction and the finite value of j in the approximate inertial manifold procedure as well as the error in the numerical approximation of the trajectory $p(t, p_0)$. In previous works, we already examined the error of which in (ii) (see [11, 12, 14]), here we will incorporate in the analysis also the source of error from (i).

Before presenting our main result, Theorem 4.1, we give some background on Lyapunov exponents and the discrete QR method. We remark that our result will be a result on the error in the Lyapunov exponents associated to linearization about a specific trajectory; whether or not these exponents are independent (in a measure theoretical sense) of the specific trajectory is the domain of the Multiplicative Ergodic theorem, see [4], and this issue will not be considered here.

4.1. **Lyapunov exponents and discrete QR technique.** Consider the time dependent, homogeneous linear ODE with piecewise continuous coefficient matrix function (see (3.8))

$$\dot{v} = C(t)v . \tag{4.1}$$

The idea behind QR techniques is to determine an orthogonal change of variables, Q, such that the coefficient matrix function $C(\cdot)$ in (4.1) is brought into upper triangular form $B(\cdot)$: $B(t) := Q^T(t)C(t)Q(t) - Q^T(t)\dot{Q}(t)$, for all t. Suppose we

have this Q, and the new triangular system, and let R denote an upper triangular fundamental matrix solution for it, with positive diagonal entries:

$$\dot{R} = B(t)R. \tag{4.2}$$

[It is well understood that Q and R are the factors in the QR-factorization of a fundamental matrix solution V of (4.1).]

Then, stable Lyapunov exponents are recovered (see Theorem 6.2 of [13]) from

$$\lambda_i = \limsup_{t\to\infty} \frac{1}{t} \log\big(R_{ii}(t)\big) \equiv \limsup_{t\to\infty} \frac{1}{t} \int_0^t B_{ii}(s)ds \ , \ \ i = 1,\dots,n\,. \tag{4.3}$$

In [13], it was shown that (4.3) does indeed give the Lyapunov exponents if the Lyapunov exponents are continuous with respect to perturbations in the coefficient matrix function of (4.1), that is if they are stable. Formally, the Lyapunov exponents $\lambda_1 \geq \cdots \geq \lambda_n$ of (4.1) are called stable if "for any $\epsilon > 0$, there exists $\delta(\epsilon) > 0$ such that $\sup_{t\in\mathbb{R}^+} ||F(t)|| < \delta(\epsilon)$ implies

$$|\lambda_i - \hat{\lambda}_i| < \epsilon, \, i = 1,\dots,n, \tag{4.4}$$

where the $\hat{\lambda}_i$'s are the (ordered) Lyapunov exponents of the perturbed system $\dot{v} = [C(t) + F(t)]v$".

If the Lyapunov exponents are distinct, then the exponents are stable (see [1]) if and only if a fundamental matrix solution V is *integrally separated*. V is integrally separated if for $i = 1,\dots,n-1$, there exist $\tilde{a} > 0$ and $1 \geq \tilde{d} > 0$ such that

$$\frac{|V(t)e_i|}{|V(s)e_i|} \cdot \frac{|V(s)e_{i+1}|}{|V(t)e_{i+1}|} \geq \tilde{d}e^{\tilde{a}(t-s)} \,, \tag{4.5}$$

for all $t,s \ : \ t \geq s \geq 0$, where $|\cdot| = |\cdot|_{\mathbb{R}^n}$, $\|\cdot\| = \|\cdot\|_{\mathcal{L}(\mathbb{R}^n,\mathbb{R}^n)}$, and e_i is the standard unit basis vector. Note that integral separation (4.5) can be rephrased in terms of integral separation of the diagonal coefficients of the upper triangular B:

$$\int_s^t \Big[B_{ii}(\tau) - B_{i+1,i+1}(\tau)\Big]d\tau \geq a(t-s) + \ln(d), \tag{4.6}$$

where $a > 0$ and $0 < d \leq 1$, for all $t,s \ : \ t \geq s \geq 0$. This is a consequence of the fact (see Property 5.3.2 of [1]) that integral separation is preserved under Lyapunov transformations and results (see [35, 36, 10, 13]) that the upper triangular system (4.2) is integrally separated if and only if the diagonal subsystem $\dot{R} = \text{diag}(\text{B(t)})\text{R}$ is integrally separated. We emphasize that the constants $\tilde{a}$ and $\tilde{d}$ in (4.5) and the constants a and d in (4.6) need not agree.

The discrete QR technique attempts finding Q and R through the QR factorization of the fundamental matrix solution by progressively factoring transition matrices, as explained below.

Say, we want the QR factorization of $V(t_k)$ at t_k, $k = 0,1,2,\dots$, with $t_0 = 0$. At any such point t_k, we can write

$$V(t_k) = V(t_k, t_{k-1})\dots V(t_2, t_1)V(t_1, 0)V_0 \,, \tag{4.7}$$

where for $j = 1,2,\dots,k$,

$$\dot{V}(t, t_{j-1}) = C(t)V(t, t_{j-1}) \,, \ V(t_{j-1}, t_{j-1}) = I \,, \quad t_{j-1} \leq t \leq t_j \,. \tag{4.8}$$

Now, let $V_0 = Q(t_0)R(t_0)$, where $Q(t_0) \in \mathbb{R}^{n\times n}$ is orthogonal and $R(t_0) \in \mathbb{R}^{n\times n}$ is upper triangular with positive diagonal entries. Then, for $j = 1,2,\dots,k$, recursively

consider

$$\dot{\Psi}(t, t_{j-1}) = C(t)\Psi(t, t_{j-1}) \,, \quad \Psi(t_{j-1}, t_{j-1}) = Q(t_{j-1})$$
$$\text{and factor } \Psi(t_j, t_{j-1}) = Q(t_j)R(t_j, t_{j-1}) \,, \tag{4.9}$$

where $Q(t_j)$ are orthogonal and $R(t_j, t_{j-1})$ are upper triangular with positive diagonal. Then, we have the QR factorization of $V(t_k)$

$$V(t_k) = Q(t_k)R(t_k, t_{k-1}) \dots R(t_2, t_1)R(t_1, t_0)R(t_0) \,. \tag{4.10}$$

Thus,

$$R(t_k) = \big(\prod_{j=k}^{1} R(t_j, t_{j-1})\big) R(t_0) \,. \tag{4.11}$$

To access the diagonal of $R(t_k)$, one can simply monitor the diagonal entries of the factors $R(t_j, t_{j-1})$ so that (see (4.3))

$$\frac{1}{t_k} \log\big(R_{ii}(t_k)\big) = \frac{1}{t_k}\big(\sum_{j=k}^{1} \log R_{ii}(t_j, t_{j-1}) + \log R_{ii}(t_0)\big) \,. \tag{4.12}$$

4.2. **Error Analysis.** In the above description of the discrete QR method, we contemplated having the linear variational equation for the exact solution on the inertial manifold, cf. (3.8) and (4.8), as well as being able to obtain the exact transition matrices $V(t_j, t_{j-1})$. In reality, one cannot expect either to hold true. As a consequence, in a numerical realization of the QR-method, rather than the QR-factorization of $V(t_k)$ we will actually compute the QR-factorization of another matrix, call it V_k. To see more precisely what V_k is, let us reason as follows.

First, we cannot possibly have the true variational problem (4.8), due to truncation in the inertial manifold approximation and error in the numerical integration of the nonlinear differential equation. Thus, we will attempt finding transition matrices for a perturbed variational problem. That is, we will have a perturbed variational equation (see (3.10)) corresponding to an approximation of a nearby locally exact solution to the nonlinear equation (this may be obtained, for instance, by a shadowing result; see [11] Theorem 3.18)

$$\dot{w} = [C(t) + E(t)]w, \quad \dot{W}(t, t_j) = [C(t) + E(t)]W(t, t_j), \quad W(t_j, t_j) = I. \tag{4.13}$$

[Above, the approximation could be a continuous extension of the time discretization scheme employed.]

Second, since we cannot solve for the transition matrices $W(t, t_j)$'s exactly, we will actually compute

$$V_k = X(t_k, t_{k-1}) \dots X(t_2, t_1)X(t_1, t_0)X_0 \,, \tag{4.14}$$

where the matrices $X(t_j, t_{j-1})$ are approximations to $W(t_j, t_{j-1})$, $j = 1, \dots, k$. Letting $Q(t_0) = Q_0$, and progressively setting

$$X(t_j, t_{j-1})Q_{j-1} = Q_j R_j \,, \quad j = 1, \dots, k \,, \tag{4.15}$$

the numerical realization of the discrete QR method will yield the QR decomposition of an approximate fundamental matrix solution:

$$V_k = Q_k R_k R_{k-1} \dots R_2 R_1 R(t_0) \,, \tag{4.16}$$

as compared with the QR decomposition of the exact fundamental matrix solution (4.10).

The following theorem characterizes the error in the Lyapunov exponents due to the perturbation in the linear variational equation and the error in approximating transition fundamental matrix solutions.

Theorem 4.1. *Consider the exact linear variational equation (4.8) with corresponding QR factorization of its fundamental matrix solution (4.10) and the numerically computed QR factorization (by the discrete QR method) of the perturbed linear variational equation (4.13) given by (4.16). If $\sup_t ||E(t)|| \leq \eta$ (see (3.12)), local fundamental matrix solutions are approximated so that $||X(t_j, t_{j-1}) - W(t_j, t_{j-1})|| \leq$ TOL, and for $\Delta t_j = t_{j+1} - t_j$,*

$$[\text{TOL} + \Delta t_j \cdot \eta + e^{||C||\Delta t_j}(\sup_{0 \leq t \leq \Delta t_j} ||X(t_j + t, t_j)|| + \text{TOL})] \cdot [\min_{1 \leq i \leq n}(1, R_{ii}(t_{j+1}, t_j))]^{-1} < 1,$$

(4.17)

then by the numerical realization of the discrete QR method one computes the factorization

$$V_k = Q(t_k)\tilde{R}(t_k),$$

where $Q(t_k)$ is the exact orthogonal factor of (4.10), and the factor $\tilde{R}$ satisfies a perturbed triangular problem

$$\dot{\tilde{R}} = [B(t) + F(t)]\tilde{R}, \quad \sup_t ||F(t)|| \leq \delta,$$

(4.18)

where F here is not necessarily triangular, and $\delta := \sup_j \omega_j$ where

$$\omega_j \leq N_j[\text{TOL} + \Delta t_j \cdot \eta + e^{||C||\Delta t_j}(\sup_{0 \leq t \leq \Delta t_j} ||X(t_j + t, t_j)|| + \text{TOL})] =: N_j \cdot ||E_{j+1}|| \quad (4.19)$$

and N_j is a function of the non-normality in the computed upper triangular factor R_j and may be bounded as in Theorem 3.12 of [11].

Next, suppose there exists K_{ij} such that

$$K_{ij} \geq \int_0^t e^{-\int_\tau^t (B_{ii}(r) - B_{jj}(r))dr} d\tau, \quad i < j \text{ and } K_{ij} = K_{ji}, \quad i > j .$$

(4.20)

Let

$$\kappa_{ij} = \sup_t |B_{ij}(t)|, \quad i \leq j,$$

(4.21)

and define α_{ij} recursively for $|i - j| = n - 1, |i - j| = n - 2, \ldots, |i - j| = 1$, such that

$$\alpha_{ij} > 1 + \sum_{k=j+1}^n \kappa_{jk}K_{ik}\alpha_{ik} + \sum_{k=1}^{i-1} K_{jk}\alpha_{jk}\kappa_{ki}, \text{ for } i < j, \text{ and } \alpha_{ij} = \alpha_{ji}, \text{ for } i > j .$$

(4.22)

Set

$$\omega_+^{(ij)} := (\sqrt{(a_1^{(ij)})^2 - 4a_0^{(ij)}a_2^{(ij)}} - a_1^{(ij)})/(2a_2^{(ij)}), \quad \omega_+ := \min_{i,j} \omega_+^{(ij)} ,$$

(4.23)

where $a_0^{(ij)}, a_1^{(ij)}, a_2^{(ij)}$ are defined as follows:

$$a_0^{(ij)} = 1 - \alpha_{ij} + \sum_{l=1}^{i-1} \kappa_{li}\alpha_{jl}K_{jl} + \sum_{m=j+1}^n \kappa_{jm}\alpha_{im}K_{im} .$$

(4.24)

For $\beta_{ij} := \alpha_{ij} K_{ij}$,

$$
\begin{aligned}
a_1^{(ij)} &= \Big[2\kappa_{jj} \sum_{k=j+1}^{n} \beta_{ik}\beta_{jk} + \sum_{l \neq i,j} \kappa_{ll}\beta_{lj}(\beta_{li} + \beta_{il}) \Big] \\
&+ \Big[\sum_{l=1,l \neq j}^{n} \sum_{m=l+1,m \neq i}^{n} \beta_{jl}\beta_{im}\kappa_{lm} + \sum_{k=1,k \neq i}^{j-1} \beta_{ik} \big(\sum_{m=j+1}^{n} \kappa_{jm}\beta_{km} + \sum_{l=1}^{k-1} \beta_{jl}\kappa_{lk} \big) \\
&+ \sum_{k=j+1}^{n} \beta_{ik} \big(\sum_{m=k+1}^{n} \kappa_{km}\beta_{jm} + \sum_{l=1}^{j-1} \beta_{kl}\kappa_{lj} \big) \Big] + \sum_{k=1,k \neq i,j}^{n} \beta_{ik}
\end{aligned}
\tag{4.25}
$$

and

$$
\begin{aligned}
a_2^{(ij)} &= \Big[\beta_{ij}\{\kappa_{ii}(\beta_{ij}^2 + 2\sum_{k=j+1}^{n} \beta_{ik}^2) + \kappa_{jj} \sum_{k=1,k \neq j}^{n} \beta_{jk}^2\} + \sum_{l \neq i,j} \kappa_{ll}\beta_{lj} \sum_{k=1,k \neq i,j,l}^{n} \beta_{ik}\beta_{lk} \Big] \\
&+ \Big[\sum_{k=1,k \neq i}^{j-1} \beta_{ik} \sum_{l=1,l \neq j}^{n} \sum_{m=l+1,m \neq k}^{n} \beta_{jl}\beta_{km}\kappa_{lm} \\
&\quad + \sum_{k=j+1}^{n} \beta_{ik} \sum_{l=1,l \neq k}^{n} \sum_{m=l+1,m \neq j}^{n} \beta_{kl}\beta_{jm}\kappa_{lm} \Big] \\
&+ \Big[\sum_{k \neq j,k=1}^{n} \beta_{jk}^2 + \sum_{k \neq i,k=1}^{n} \beta_{ik}^2 + \sum_{(l,m) \neq (j,i),l,m=1}^{n} \beta_{lj}\beta_{mi} \Big].
\end{aligned}
\tag{4.26}
$$

If $\delta < \omega_+$, there exists an orthogonal change of variables $\tilde{Q}$ that brings $B+F$ to upper triangular such that $|\tilde{Q}_{ij}(t)| \leq \rho_{ij} := \alpha_{ij} K_{ij} \delta$ for all $t \geq 0$ and all $i,j = 1, \ldots, n$, $i \neq j$. Furthermore, the difference in the exact and computed Lyapunov exponent is

$$
|\lambda_i^c - \lambda_i| \leq \delta + \sum_{k \neq i} \rho_{ik}^2 \gamma_{ki} + \sum_{k=1}^{i-1} \rho_{ki}\kappa_{ki} + \sum_{k=i+1}^{n} \rho_{ki}\kappa_{ik} + \sum_{j=1,j \neq i}^{n} \sum_{k=j+1,k \neq i}^{n} \rho_{ji}\kappa_{jk}\rho_{ki}
\tag{4.27}
$$

where $\gamma_{ij} = \sup_t |B_{ii}(t) - B_{jj}(t)|$ and κ_{ij} is defined in (4.21).

Proof. For the first part of the proof, first use the Gronwall argument on page 83 of [20], so that

$$
\begin{aligned}
||V(t_{j+1}, t_j) - X(t_{j+1}, t_j)|| \quad &\leq \texttt{TOL} + ||V(t_{j+1}, t_j) - W(t_{j+1}, t_j)|| \\
&\leq \texttt{TOL} + \Delta t_j \cdot \eta \\
&\quad + e^{||C||\Delta t_j}(\sup_{0 \leq t \leq \Delta t_j} ||X(t_j + t, t_j)|| + \texttt{TOL}).
\end{aligned}
\tag{4.28}
$$

Then apply Theorem 3.1 of [11]. If (4.17) is satisfied, see also "Assumption 3.5 of [11]," then we apply Theorem 3.12 of [11] to obtain the bound on the perturbation of the triangular factor.

For the second part of the proof, apply Lemma 4.1 of [14], under the assumption of integral separation. If $\delta < \omega_+$, then by [14, Lemma 4.1] there exists an orthogonal change of variables $\tilde{Q}(t)$ with $\tilde{Q}(0) = I$ that brings $B(t) + F(t)$ to upper triangular with $|\tilde{Q}_{ij}(t)| \leq \rho_{ij}$ for $i \neq j$ and $t \geq 0$. To establish (4.27) follow the proof of Theorem 3.2 in [12] and use the fact that

$$
(\tilde{Q}^T B \tilde{Q})_{ii} = \sum_{j=1}^{n} \sum_{k=j+1}^{n} \tilde{Q}_{ji} B_{jk} \tilde{Q}_{ki}.
\tag{4.29}
$$

$\square$

Remark 4.2. We emphasize that Theorem 4.1 is an error analysis result for the Lyapunov exponents of an infinite dimensional system, and this is a novelty as far as we could determine. The inertial manifold reduction is absolutely essential in making sure that the bound (4.17) can be achieved. In particular, the smaller is the dimension n of the system (3.8)-(4.8), the less demanding is the requirement posed by the term $[\min_{1 \le i \le n}(1, R_{ii}(t_{j+1}, t_j))]^{-1}$ in (4.17), since –for n large– the negative eigenvalues of the linear part of the problem make the diagonal terms R_{nn} approach 0.

Remark 4.3. An important point is that the argument in [11] may be phrased so that the exact solution is a perturbation of the computed solution as opposed to the computed solution is a perturbation of the exact solution. By considering the exact solution as a perturbation of the computed solution, the quantities that are necessary to bound the error in Lyapunov exponents, e.g. K_{ij}, κ_{ij}, and γ_{ij} may be obtained from the computed solution. In addition, using Theorems 3.11 and 3.12 of [11] we have the following bounds for the terms in (4.19),

$$N_j \cdot ||E_{j+1}|| \le ||L_j|| + O(||E_{j+1}||^2)$$

where entry-wise

$$|L_j| \le \left[\frac{1 - (\delta_j \nu_j)^n}{1 - \delta_j \nu_j} \right]^2 |F_{j+1}|,$$

the (p, q)-entry of $|F_{j+1}|$ is bounded by

$$(|F_{j+1}|)_{p,q} \le ||E_{j+1}|| / \min_{i=p,q} (R_j)_{ii},$$

$$\delta_j = \min_{1 \le p \le n} \frac{1}{\min(1, (R_j)_{pp})}, \text{ and } \nu_j = ||R_j - \text{diag}(R_j)||.$$

If (see (4.6)) for $i < j$, there exists $a_{ij} > 0$ and $d_{ij} \ge 0$ such that

$$\int_s^t \left[B_{ii}(\tau) - B_{jj}(\tau) \right] d\tau \ge a_{ij}(t - s) - d_{ij}, \ \ t \ge s \ge 0, \tag{4.30}$$

then we have for K_{ij} in (4.20), $K_{ij} \le e^{d_{ij}}/a_{ij}$.

We note that one is able to obtain error bounds on approximated Lyapunov exponents if the size of elements in the coefficient matrix B as characterized by the κ_{ij} are not too large as compared to the degree to which the problem is integrally separated as characterized by the K_{ij} and as compared to the size of the perturbation, δ.

Remark 4.4. Similar results may be obtained in the case of stable but not distinct Lyapunov exponents by employing Theorems 4.3, 4.4, and 4.5 in [12] in place of Lemma 4.1 of [14] in the proof.

Remark 4.5. Since the bounds used to establish (4.27) are uniform in t, the same bound holds for the approximation of the endpoints of the Sacker-Sell spectrum $\Sigma_{\text{ED}} = \bigcup_{i=1}^m [\alpha_i, \beta_i]$,

$$\alpha_i = \liminf_{t \to \infty} \left\{ \inf_{t_0} \frac{1}{t} \int_{t_0}^{t_0+t} B_{ii}(s) ds \right\}, \tag{4.31}$$

$$\beta_i = \limsup_{t \to \infty} \left\{ \sup_{t_0} \frac{1}{t} \int_{t_0}^{t_0+t} B_{ii}(s)ds \right\}. \tag{4.32}$$

Remark 4.6. Theorem 4.1 establishes an error bound when the Lyapunov exponents are approximated using the discrete QR method as defined by (4.15). An alternative technique is to employ the so called continuous QR technique in which instead of approximating the transition fundamental matrix solutions, we approximate

$$\dot{Q} = Q(t)H(Q,C), \quad Q(0) = Q_0, \tag{4.33}$$

where we have set $H := Q^T(t)\dot{Q}(t)$, with entries

$$H_{ij}(t) = \begin{cases} (Q^T(t)C(t)Q(t))_{ij}, & i > j, \\ 0, & i = j, \\ -(Q^T(t)C(t)Q(t))_{ji}, & i < j. \end{cases} \tag{4.34}$$

So, if Q is known, then R satisfies the transformed system

$$\dot{R} = B(t)R, \quad R(0) = R_0, \tag{4.35}$$

where

$$B(t) := Q^T(t)C(t)Q(t) - Q^T(t)\dot{Q}(t), \tag{4.36}$$

and B is upper triangular by the way that H has been defined.

For the approximation of (4.33) a theorem analogous to Theorem 4.1 holds by replacing in the proof the use of Theorem 3.12 of [11] with Theorem 3.16 of [11].

5. The Kuramoto-Sivashinsky Equation.
Next, we prepare to apply Theorem 4.1 to the Kuramoto-Sivashinsky equation. A standard form for the KSE is

$$\frac{\partial u}{\partial t} + \frac{\partial^4 u}{\partial x^4} + \frac{\partial^2 u}{\partial x^2} + u\frac{\partial u}{\partial x} = 0, \quad (x,t) \in \mathbb{R} \times \mathbb{R}^+, \quad u(x,0) = u_0(x), \quad x \in \mathbb{R}, \tag{5.1}$$

subject to periodic boundary conditions $u(x,t) = u(x+L,t)$, $L > 0$. Though linearly unstable for $L > 2\pi$ the KSE is known to be dissipative. This was first shown in [32] in the invariant subspace of odd functions, and later in the general periodic case in [7, 17]. In this paper *we restrict to the odd subspace*, both to cut the dimension of the inertial manifold in half, and compare to computations in [6].

The KSE can be written in the form of (2.1) by setting

$$Au = D^4 u + D^2 u, \quad f(u) = -uDu. \tag{5.2}$$

The eigenvalues of the linear part are

$$\mu_k = \left(\frac{2\pi}{L}k\right)^4 - \left(\frac{2\pi}{L}k\right)^2, \quad k = 1, 2, \ldots$$

corresponding to a complete set of orthonormal eigenfunctions in L^2_{odd}

$$w_k(x) = \sqrt{\frac{2}{L}}\sin(\frac{2\pi}{L}kx).$$

We use H^1_{odd} (respectively, L^2_{odd}) to denote the subspace of the Sobolev space $H^1((-L/2, L/2))$ (the space $L^2((-L/2, L/2))$) consisting of functions which are odd, and periodic with period L, and with the following norm and seminorm

$$|\cdot| = |\cdot|_{L^2} \qquad |\cdot|_1 = |\nabla \cdot|_{L^2},$$

in L^2 and H^1 respectively. It is shown in [42] that the conditions (2.4) and (2.5) hold for

$$G = H^1_{\text{odd}}, \quad H = L^2_{\text{odd}}, \tag{5.3}$$

$K_1 = K_2 = (\frac{4}{3})^{1/4}$, and $\alpha = 1/4$.

Since the nonlinear term in the KSE is not Lipschitz on all of H, it must be modified outside a ball. One way to do this is to replace f with f_ρ where

$$f_\rho(u) = \chi(|u|^2_H/\rho^2)f(u) , \quad \chi(s) = \begin{cases} 1, & s \in [0,1], \\ 2(s-1)^3 - 3(s-1)^2 + 1, & s \in [0,2], \\ 0, & s > 2. \end{cases} \tag{5.4}$$

If ρ is taken to be the radius of the absorbing ball from rigorous estimates following the analysis of Collet et al. [7], then the inertial form for the modified equation will have the same global attractor. If, alternatively, ρ is chosen just large enough to contain a particular solution trajectory, then the corresponding inertial form will share that trajectory, as well as the linearization within the ball, but may have nontrivial, spurious, dynamics outside the ball. Since our goal is to compute the Lyapunov exponents for a particular chaotic trajectory, we take the latter, semi-empirical approach in order to reduce the dimension of the manifold as much as possible.

The modification of f in (5.4), while implementable in computations, does not provide an inertial manifold of smallest dimension for a given given cut-off radius ρ. A comparison of choices of modification, spaces, and method of construction was carried out for the KSE in [22]. Of the combinations tested, one using the method of Miklavcic [30] and the nonconstructive (Lipschitz constant preserving) extension of Valentine (see [18]) gave the smallest dimension. This leads to the mixed-space Lipschitz estimate

$$|f(u) - f(v)|_{-1} \le \frac{1}{\sqrt{2}}\rho_0^{1/2}\rho_1^{1/2}|u - v|_0 \quad \forall\, u, v \in H^1_{\text{odd}} \text{ with } |u|_1, |v|_1 \le \rho_1 , \tag{5.5}$$

where ρ_0 and ρ_1 are the radii of balls in L^2, resp. H^1, containing the desired "global" dynamics and

$$|u|_{-1} = \left\{ \sum_{k=1}^{\infty} |\hat{u}_k|^2 \left(\frac{2\pi k}{L} \right)^{-2} \right\}^{1/2} .$$

This estimate in (5.5) is applied in the next section at a specific parameter value (that effectively determines L).

6. **Computational results.** In this section, we illustrate how we can use Theorem 4.1 for the Kuramoto-Sivashinsky equation. More precisely, recalling that the error bound on the Lyapunov exponents in (4.27) requires to have $\delta < \omega_+$, where ω_+ is defined in (4.23), we will actually estimate ω_+, and from this we will be able to infer whether or not it is possible to obtain accurate approximation of the Lyapunov exponents (and of the Sacker-Sell intervals as well). Loosely speaking, if the value of ω_+ we obtain will be of an order of magnitude which can be realistically obtained numerically, then we will consider having provided sufficient evidence of the fact that the above mentioned spectral quantities can be approximated reliably, otherwise not. With this goal in mind, this section is organized so to give insight into how we have estimated the quantities entering in the bounds (4.23) and (4.27). In Table 3, we summarize our end results.

Remark 6.1. With our present understanding, we are not able to explicitly compute the bound in (4.27), because of the difficulty to estimate δ. Ultimately, this is because we do not know how to compute η in (3.12). On the other hand, all quantities appearing in (4.23) are computable, and this will allow some indirect error bound on the Lyapunov exponents as well. For example, although we are not able to directly compute $\rho_{ij} = \alpha_{ij} K_{ij} \delta$, which enters in (4.27), we can compute ρ_{ij}/δ and thus, in case in which $\delta < \omega_+$, we can effectively estimate (within $O(\omega_+)$) a weighted version of (4.27), namely $|\lambda_i^c - \lambda_i|/\delta$.

6.1. **Kuramoto-Sivashinsky once more.** Our computational experiments are done on the equation

$$\frac{\partial \tilde{u}}{\partial \tau} + 4\frac{\partial^4 \tilde{u}}{\partial y^4} + \vartheta\Big[\frac{\partial^2 \tilde{u}}{\partial y^2} + \tilde{u}\frac{\partial \tilde{u}}{\partial y}\Big] = 0 \ , \tag{6.1}$$

with $\tilde{u}(y,t) = \tilde{u}(y + 2\pi, t)$, and $\tilde{u}(y,t) = -\tilde{u}(-y,t)$. This is equivalent to the standard form in (5.1) under the change of variables

$$u(t,x) = l\widetilde{u}(\frac{l^4}{4}t, lx) \quad \text{where } l = 2\pi/L \ , \quad \vartheta = L^2/\pi^2 \ . \tag{6.2}$$

To compare to the Lyapunov exponents reported in [6] we perform another change of variables

$$-2w(s,y) = \tilde{u}(\xi s/4, y), \qquad \xi = \frac{4}{\vartheta} \ .$$

so that

$$w_s = (w^2)_y - w_{yy} - \xi w_{yyyy} \ . \tag{6.3}$$

The effect of the time re-scaling is that the Lyapunov exponents of equation (6.3) are those for (6.1) divided by ϑ. All computations are done at $\xi = 0.02991$, $\vartheta = 133.73454$, which is one of the parameter values considered in [6, 40].

6.2. **Computation of Lyapunov exponents and of inertial manifold.** Here we show the outcome of several computations. The workhorse to compute the Lyapunov exponents is the code LESNLL, which we have written. Within this code, all computations related to the approximation of the inertial manifold are handled through appropriate definition of the vector field.

The code LESNLL is public domain and can be downloaded from

> www.math.gatech.edu/~dieci   or   www.math.ku.edu/~evanvleck

In particular, we have used the discrete QR method (IPAR(8)=4 in LESNLL), and integration for the trajectory as well as for the local transition matrices is done using the variable step-size 5th order Runge-Kutta scheme with local error control on the trajectory and on the exponents (IPAR(10)=10 in LESNLL). TOL is the value of the local error tolerance. All computations below refer to an arbitrary, but fixed, initial condition for the trajectory. Approximation of the Lyapunov exponents is always done after discarding an initial transient for the trajectory; typical values we have used for the transient is an interval of length 10 (in time units of (6.3)). Finally, an unavoidable truncation of time is required when approximating the Lyapunov exponents. Namely, the limits in (4.3) are replaced by the finite time approximations

$$\lambda_i(T) \ = \ \frac{1}{T}\log\big(R_{ii}(T)\big) \ = \ \frac{1}{T}\int_0^T B_{ii}(s)ds \ , \quad i = 1,\ldots,n \ .$$

We call T the *averaging time*.

Lacking the exact Lyapunov exponents, we use those for a relatively fine Galerkin approximation. This takes the form

$$\frac{dp}{dt} + Ap = P_n f(p+0) \, , p \in P_n H \, , \tag{6.4}$$

(compare to (2.3)).

To establish how many modes constitute such an approximation, we first compare attractors (local, not global) in Figure 3. It appears that the trajectory settles down with $n = 16$ modes.
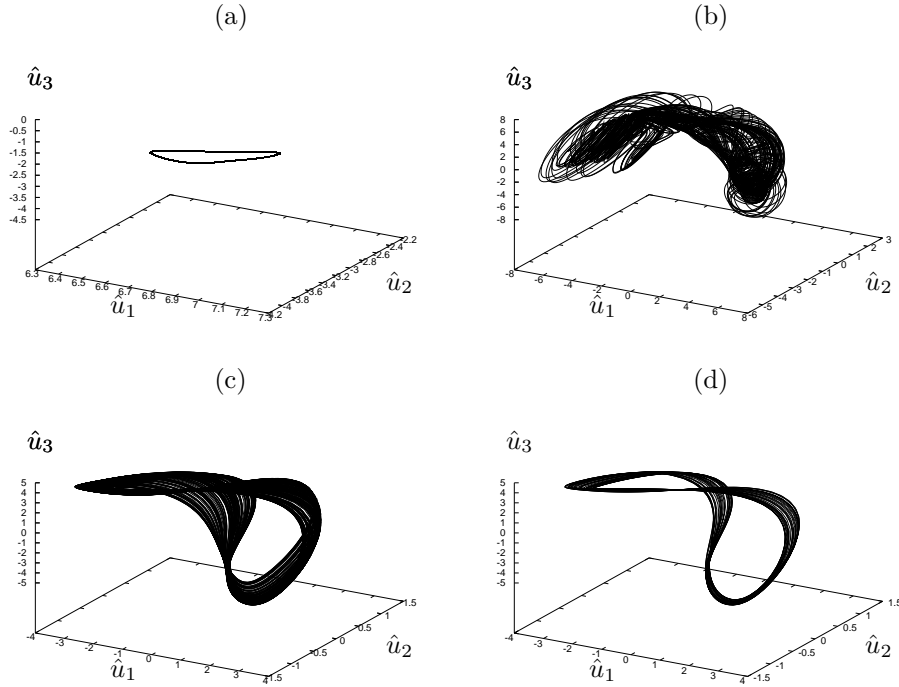

FIGURE 3. Local attractors for Galerkin system (6.4) (a) $M = 8$, (b) $M = 10$, (c) $M = 12$ (d) $M = 16$

Notation. Henceforth, we will denote by $\mathrm{KSE}(n, m)$ the Galerkin approximation of the KSE (6.4) with n modes to approximate m LEs, and by $\mathrm{KSEIM}(n, m, j)$ the approximation of the approximate inertial manifold (3.9), after j iterations with n modes and m exponents. Notice that $\mathrm{KSEIM}(n, m, 0)$ is $\mathrm{KSE}(n, m)$.

6.2.1. *Convergence of Lyapunov exponents.* First, we show convergence of the Lyapunov exponents for (6.4) in function n, m, the value of `TOL`, and the length of the averaging time T.

Remark 6.2. We have $m \leq n$ and consider cases in which $m < n$ because of the decreased computational cost. In fact, although the linear variational equation is in all cases of dimension n, when $m < n$ we only compute m columns of a fundamental matrix solution as opposed to n columns when $m = n$. Although Theorem 4.1 holds in the case $m = n$, it was noticed in [14] that the error when $m < n$ is no worse then the error when $m = n$; still, quantifying such a result has not been pursued and it is beyond the scope of this work.

n in KSE$(n,4)$	TOL	λ_1	λ_2	λ_3	λ_4
16	1.E-5	8.32E1	-2.98E-1	-7.59E2	-1.13E3
16	1.E-8	8.34E1	-2.52E-1	-7.59E2	-1.14E3
16	1.E-11	8.43E1	-6.58E-2	-7.59E2	-1.14E3
32	1.E-5	8.42E1	-1.24E-1	-7.57E2	-1.13E3
32	1.E-8	8.63E1	-1.77E-2	-7.59E2	-1.13E3
32	1.E-11	8.33E1	-9.46E-2	-7.56E2	-1.13E3

TABLE 1. First four Lyapunov exponents in function of TOL for (6.4). Averaging time $T = 10$.

First of all, through preliminary computations with $n = 16, 32, 64$, it becomes immediately apparent that the negative exponents quickly become extremely large in magnitude, and obey the spacing of the eigenvalues of the linear part (these are $4(2\pi j)^4 - \theta(2\pi j)^2$ for $j = 1, \ldots, n$). As a consequence of these preliminary computations, we infer that there is really no reason to perform extremely expensive computations trying to track exponentially small quantities, and we will thus restrict consideration to the cases of $n = 16, 32$ and $m = 4$ only.

In Table 1, we show convergence for the first four LEs in function of the input tolerance TOL. Computations refer to $T = 10$, for both cases of $n = 16, 32$. Exponential notation is used throughout (e.g., 1.E-5 stands for 10^{-5}).

By looking at the results of Table 1, it is clear that the 3rd and 4th exponents have been well approximated already on an interval of length 10. On the other hand, the 2nd exponent (and to a lesser extent also the 1st) is more sensitive to TOL, but most likely it is especially affected by the truncation time T (we expect this 2nd exponent to be 0; see Figure 2).

For this reason, in Figure 4 we show plots of convergence for the first two exponents in function of the averaging time T, for both cases of $n = 16, 32$. These computations were made with TOL $= 1.E - 8$. In the figures, the dashed line refers to the case $n = 16$, the solid line to the case of $n = 32$.
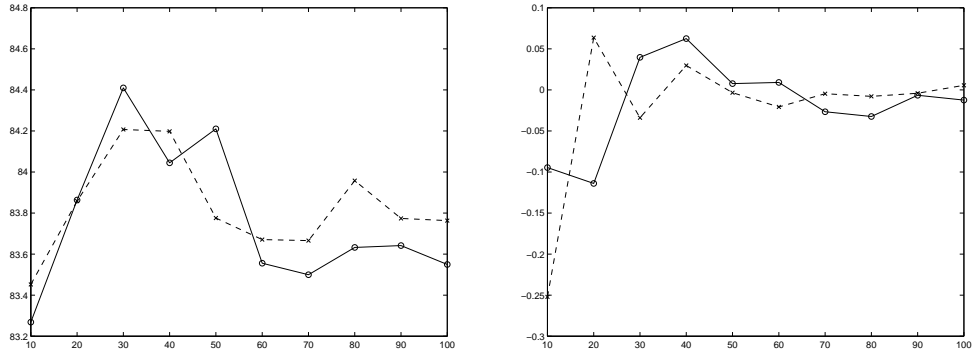

FIGURE 4. Approximation to λ_1 (on the left) and λ_2 (on the right) in function of T for KSE$(n,4)$. Dashed, respectively solid, line refers to $n = 16$, respectively $n = 32$

We summarize this first set of results by remarking that, relatively to (6.4), the results clearly indicate that the approximations are converging, and are fairly insensitive to the tolerance used as well as the length of the integration interval. Indeed, since there is less than a .5% difference between $\sum_{k=1}^{4} \lambda_k$, when the number of modes is doubled from 16 to 32, and when T is increased from 10 to 100, we take 16 modes, and $T = 10$, as providing our reference solution.

In [6], the computed value for the first Lyapunov exponent of (6.3), using 16 modes is 0.629, that is 84.12 for (6.1). Comparing this to our result in Table 1, and realizing that there are a variety of ways to compute the exponents (e.g., continuous QR, discrete QR) and they are all sensitive to the tolerance (accuracy) of the integrator and averaging time, we consider reaching essentially two digits of agreement with the value in [6] as validating both results. This also suggests a reasonable criterion for agreement in using an approximate inertial manifold.

6.2.2. *On the inertial manifold.* As far as computation of the inertial manifold, we reasoned as follows. Suppose we take $n = 8$ in (3.9). We check the convergence to the inertial manifold at 24 test points of the trajectory computed using 16 Galerkin modes. This amounts to checking that $\Phi^j(p) \to q$ at each test point $u = p + q$, with $p = P_8 u$, and $q = (I - P_8)u$. By doing this, we are able to fine-tune the choice of parameters c_1, γ in (3.3) and c_2 in (3.4). Indeed, to apply the algorithm to compute Φ^j one must choose these parameters. It is not clear which choice gives the most rapid convergence, but our experimentation has lead us to taking $c_1 = .00005$ or $c_1 = .00004$ and $c_2 = 1$ in

$$\tau_j = c_1 2^{-j} \quad \text{and} \quad N_j \tau_j = c_2 j \ .$$

We are then effectively taking $\gamma \theta_{n,\sigma} = 2^{-1/\nu}$ in (3.3), and the limiting value $\nu = 1$ in (3.4). At $\xi = 0.02991$ ($\vartheta = 133.73454$) the chaotic attractor lives in a ball of radius $\rho_0 = 5.07$ in L^2, and $\rho_1 = 4.28$ in H^1 (measured for the standard form (5.1)). The combination of estimates involving (5.5) provides an inertial manifold of dimension 18 at $\vartheta = 133.73454$. In practice we can expect the algorithm to work at an even lower dimension and find that we can compute one of dimension 8. Strictly speaking, we have not verified that the stronger gap condition holds in the limit $\nu = 1$, even for a manifold of dimension 18. While the computations are guided by the rigorous estimates that guarantee convergence, as is often the case, the expectation is that the performance of the algorithm will exceed what is suggested by those estimates.

Phase space plots using the approximate inertial form (3.9) with $n = 8$ and j from 2 to 6 are compared to our reference solution computed using 16 Galerkin modes in Figure 5. Those for (3.9) with $n = 8$ and j from 7 to 9 are quite similar to that for $j = 6$.

Table 2 shows the Lyapunov exponents computed using the inertial form (3.9) with $n = 8$, $m = 4$, that is KSEIM$(8, 4, j)$. The two digits of agreement between (3.9) with $j = 5, 6, 7$, and (6.4) with $n = 16$, matches that between our Galerkin results and those in [6] as well.

6.2.3. *Sacker-Sell intervals.* Here we approximate the end points of the Sacker-Sell spectral intervals, (4.31) and (4.32), for both KSE and KSEIM using Steklov averages as in [10] for $H > 0$ and $i = 1, \ldots, m$,

$$\alpha_i^H = \inf_t \frac{1}{H} \int_t^{t+H} B_{ii}(\tau)d\tau, \ \ \beta_i^H = \sup_t \frac{1}{H} \int_t^{t+H} B_{ii}(\tau)d\tau \ . \tag{6.5}$$
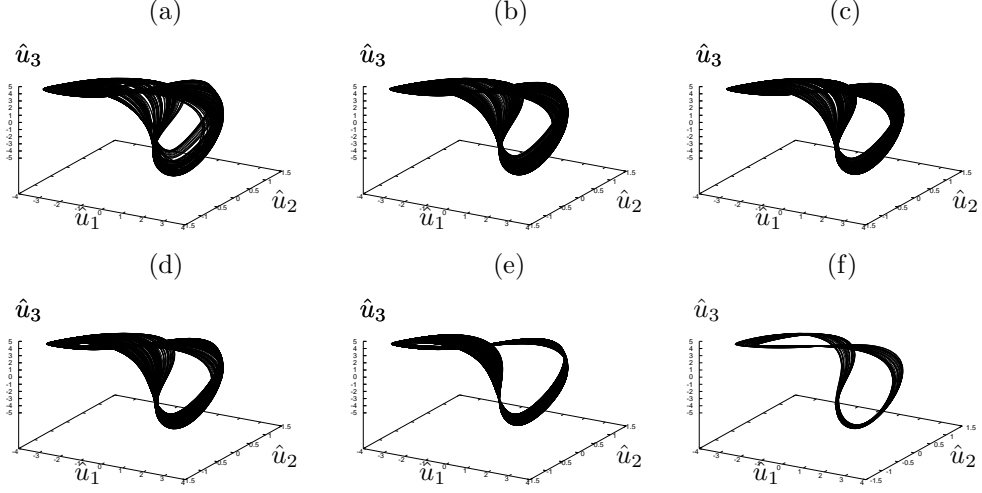
FIGURE 5. Comparison of local attractors for approximate inertial forms with that of the Galerkin approximation: (a) (3.9), $j = 2$ (b) (3.9), $j = 3$ (c) (3.9), $j = 4$ (d) (3.9), $j = 5$ (e) (3.9), $j = 6$ (f) (6.4), $n = 16$

j in KSEIM$(8, 4, j)$	λ_1	λ_2	λ_3	λ_4
4	.109E3	-.517E-1	-.774E3	-.113E4
5	.106E3	.224E0	-.781E3	-.110E4
6	.774E2	-.392E-1	-.754E3	-.111E4
7	.880E2	.163E0	-.765E3	-.114E4
8	.846E2	-.148E0	-.761E3	-.114E4
9	.818E2	-.140E0	-.759E3	-.113E4

TABLE 2. Convergence of Lyapunov exponents for KSEIM$(8, 4, j)$. Averaging time $T = 10$, $c_1 = 0.00005$, TOL=1.E-5.

In Figure 6 on the left we plot the re-centered Sacker-Sell intervals $[\alpha_i^H - \lambda_i, \beta_i^H - \lambda_i]$, for $i = 1, \ldots, 8$, for computations done with the KSE(16,8) using $T = 100$ as the final time and $H = 1, 2, 4$, in this order. What is notable is that these intervals scale consistently as a function of i, even though the magnitude of the computed LEs varies greatly and becomes large as i increases.

On the right of Figure 6, instead, as a measure of comparison we plot the numerical approximations of the first four re-centered Sacker-Sell intervals $[\alpha_i^H - \lambda_i, \beta_i^H - \lambda_i]$, with $H = 1$, found from KSEIM(8,8,7) and KSE(16,8). Averaging time here is $T = 10$. Endpoints for KSEIM are indicated by a star, for KSE by a circle.

Although the intervals are somewhat larger for KSEIM than for KSE, we notice that all Sacker–Sell intervals are disjoint, which is a clear numerical indication of integral separation.

Remark 6.3. We summarize all of the previous results by noticing that both in terms of Lyapunov exponents and in terms of Sacker–Sell intervals, KSE(16,8) and KSEIM(8,8,6)=KSEIM(8,8,7) give consistent results. It is further clear that the
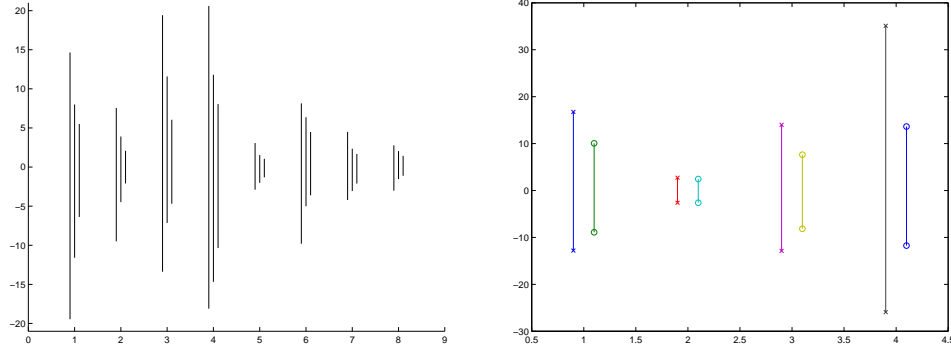
FIGURE 6. Left: Plot of $[\alpha_j^H - \lambda_j, \beta_j^H - \lambda_j]$, for $j = 1, \ldots, 8$ and $H = 1, 2, 4$, in this order, with $T = 100$. Right: Plot of $[\alpha_j^1 - \lambda_j, \beta_j^1 - \lambda_j]$, $j = 1, \ldots, 4$, for KSEIM$(8, 8, 7)$ and KSE$(16, 8)$, with $T = 10$

problem appears to be integrally separated. Below we will indeed verify that this is the case.

6.3. **Integral Separation, Bounds on ω_+ and on the Error.** Several remarks are in order about how we go about determining bounds on the Lyapunov exponents. Working backward from (4.27) we see that the bounds are a function of $\rho_{ij} := \alpha_{ij} K_{ij} \delta$ (see (4.22) and (4.20)), $\kappa_{ij} := \sup_t |B_{ij}(t)|$, and $\gamma_{ij} := \sup_t |B_{ii}(t) - B_{jj}(t)|$ and hold if the perturbation is uniformly bounded in norm by δ satisfying $\delta < \omega_+$.

In our computations we will find $\kappa_{ij} \equiv \sup_t |B_{ij}(t)|$ directly from the computed solution and employ an approach to determine bounds on the K_{ij} that is a simplification of Lemmas 4.1 and 4.2 of [28].

As before, for all t, let $p(t) = B_{ii}(t) - B_{jj}(t)$, $i < j$. Consider a discretization of the interval $[0, T]$:

$$0 = t_0 < t_1 < \cdots < t_N = T.$$

The proof of the following lemma is given in [14].

Lemma 6.4 (Lemma 4.4, [14]). *Let $\epsilon > 0$ be given. There exists $a_k > 0$ and $d_k \geq 0$ such that for $t_k \leq s \leq t_{k+1}$,*

$$\int_s^{t_{k+1}} p(r)dr \geq a_k(t_{k+1} - s) - d_k. \tag{6.6}$$

where for $h_k = t_{k+1} - t_k$ and for

$$Y_k = \min_{t_k \leq s \leq t_{k+1}} \frac{1}{t_{k+1} - s} \int_s^{t_{k+1}} p(r)dr$$

$$=: \min_{t_k \leq s \leq t_{k+1}} G(s), \quad G(s) = \frac{1}{t_{k+1} - s} \int_s^{t_{k+1}} p(r)dr , \tag{6.7}$$

$$a_k = \begin{cases} \epsilon h_k^{-1}, & h_k Y_k < \epsilon, \\ Y_k, & h_k Y_k \geq \epsilon, \end{cases} \quad d_k = \begin{cases} \epsilon - h_k Y_k, & h_k Y_k < \epsilon, \\ 0, & h_k Y_k \geq \epsilon, \end{cases} \tag{6.8}$$

and

$$\int_0^T e^{-\int_s^T p(r)dr} ds \leq \sum_{k=0, d_k=0}^{N-1} e^{-\left[\sum_{l=k+1}^{N-1} X_l\right]} \frac{(1 - e^{-Y_k h_k})}{Y_k}$$

$$+ \frac{(e^\epsilon - 1)}{\epsilon} \cdot \sum_{k=0, a_k=\epsilon h_k^{-1}}^{N-1} e^{-\left[\sum_{l=k+1}^{N-1} X_l\right]} h_k e^{-h_k Y_k} =: K(T) \qquad (6.9)$$

where

$$X_k = \int_{t_k}^{t_{k+1}} p(r) dr.$$

The bounds (6.9) can be used to obtain bounds on the K_{ij}'s by setting $K_{ij} = \sup_k K(t_k)$ and we employ the notation $K_k = \max_{|i-j|=k} K_{ij}$.

In Table 3 we summarize the values of $K_1, \rho_1/\delta, \lambda_1(err)/\delta$, and ω_+ as a function of n, m, h for Galerkin ($j = 0$) and nonlinear Galerkin on an interval of length 10. Here, n and m are as usual and h is a constant stepsize used to compute the K_{ij} via Lemma 6.4. [In practice, our estimate of the Y_k in (6.7) is done simply by setting $Y_k = \min(G(t_k), G(t_{k+1}))$.] In the table, we only report on K_1 since it was always the largest of the K_j's values. Accordingly, we report only on ρ_1/δ where we recall that $\rho_1 := \max_{|i-j|=1} |Q_{ij}(t)|$ and this is simply the largest value of $\alpha_{ij} K_{ij}$, for $|i - j| = 1$. Similarly, $\lambda_1(err)$ is the error in the largest Lyapunov exponent, λ_1, without taking into account the quadrature error; the value $\lambda_1(err)/\delta$ is obtained from (4.27) in Theorem 4.1 neglecting terms proportional to δ^2 in (4.27). In general, the error in λ_1 is larger than the error in the smaller exponents. Finally, it should be emphasized that while increasing h will generally result in smaller values of K_{ij} which in turn lead to larger ω_+ and hence applicability to larger perturbations of size δ, the conclusion one can reach is weaker: control on the $\tilde{Q}_{ij}(t)$ on a mesh with stepsize h.

What is notable is that we are able to obtain similar bounds using either the Galerkin or the nonlinear Galerkin. Since Theorem 4.1 applies to the nonlinear Galerkin and the computed exponents and bounds obtained are similar in both cases, we conclude that bounds on the exponents may be obtained for δ small enough and one should have confidence in the computed exponents obtained with both the Galerkin and nonlinear Galerkin approximations.

7. Appendix: A recursive algorithm for Φ^j. Denoting

$$\varphi_k^j(p) = \varphi^j(p)(-k\tau_j), \quad k = 0, 1, \dots, N_j,$$

we can express the mapping in (2.10) as

$$\begin{aligned}
\varphi_k^j(p) = {}& e^{k\tau_j A} p - \int_{-k\tau_j}^{-\ell_k \tau_{j-1}} e^{-(-k\tau_j - s)A} P f(\varphi_{\ell_k}^{j-1}(p)) \, ds \\
& - \sum_{\ell=0}^{\ell_k - 1} \int_{-(\ell+1)\tau_{j-1}}^{-\ell \tau_{j-1}} e^{-(-k\tau_j - s)A} P f(\varphi_\ell^{j-1}(p)) \, ds \\
& + \int_{-\infty}^{-N_{j-1}\tau_{j-1}} e^{-(-k\tau_j - s)A} (I - P) f(\varphi_{N_{j-1}}^{j-1}(p)) \, ds \qquad (7.1) \\
& + \sum_{\ell=\ell_k+1}^{N_{j-1}-1} \int_{-(\ell+1)\tau_{j-1}}^{-\ell \tau_{j-1}} e^{-(-k\tau_j - s)A} (I - P) f(\varphi_\ell^{j-1}(p)) \, ds \\
& + \int_{-(\ell_k+1)\tau_{j-1}}^{-k\tau_j} e^{-(-k\tau_j - s)A} (I - P) f(\varphi_{\ell_k}^{j-1}(p)) \, ds,
\end{aligned}$$

(n, m, j)	h	K_1	ρ_1/δ	$\lambda_1(err)/\delta$	ω_+
$(16, 8, 0)$	1.E-1	4.5E-2	6.3E1	3.5E5	4.5E-8
$(16, 8, 2)$	1.E-1	1.1E-1	1.6E2	9.0E5	6.8E-9
$(16, 8, 4)$	1.E-1	6.1E-2	8.9E1	5.0E5	2.3E-8
$(16, 16, 0)$	1.E-1	6.0E-2	2.1E2	1.2E6	4.2E-9
$(16, 16, 2)$	1.E-1	3.3E-2	1.2E2	6.8E5	1.2E-8
$(8, 8, 0)$	1.E-1	2.5E1	3.9E2	2.2E6	6.0E-17
$(8, 8, 6)$	1.E-1	1.7E-2	2.2E1	1.2E5	6.8E-8
$(8, 8, 7)$	1.E-1	5.6E-2	7.9E1	4.4E5	2.9E-8
$(16, 8, 0)$	1.E-2	4.0E0	5.4E4	3.0E8	6.3E-14
$(16, 8, 2)$	1.E-2	1.9E1	1.9E5	1.0E9	5.1E-15
$(16, 8, 4)$	1.E-2	1.5E1	1.5E5	8.5E8	7.7E-15
$(16, 16, 0)$	1.E-2	2.9E0	5.0E4	2.8E8	7.1E-14
$(16, 16, 2)$	1.E-2	5.2E1	8.6E5	4.8E9	2.5E-16
$(8, 8, 0)$	1.E-2	4.5E1	1.5E3	8.6E6	3.3E-18
$(8, 8, 6)$	1.E-2	9.7E0	7.2E4	4.0E8	3.4E-14
$(8, 8, 7)$	1.E-2	9.1E0	1.0E5	5.7E8	1.7E-14

TABLE 3. Values of $K_1, \rho_1/\delta, \lambda_1(err)/\delta$, and ω_+ for different number of modes, n, different number of computed Lyapunov exponents, m, stepsize h used in the calculation of K_{ij} for Galerkin and nonlinear Galerkin on an interval of length 10.

where ℓ_k is a nonnegative integer defined by

$$
\begin{cases}
(\ell_k + 1)\tau_{j-1} > k\tau_j \geq \ell_k \tau_{j-1}, & \text{if } N_{j-1}\tau_{j-1} > k\tau_j, \\
\ell_k = N_{j-1}, & \text{otherwise.}
\end{cases}
$$

From (2.11) we have

$$\varphi_k^0(p) = p , \quad \text{for} \quad k = 0, 1, \ldots, N_0$$

The case where $k\tau_j \geq N_{j-1}\tau_{j-1}$ is simpler, as φ^{j-1} is constant over $(-\infty, k\tau_j]$. This is seen by rewriting (7.1) as

Case 1. $k\tau_j < N_{j-1}\tau_{j-1}$ (within time range of previous iterate)

$$
\begin{aligned}
\varphi_k^j(p) = {} & e^{k\tau_j A}p - A^{-1}(e^{(k\tau_j - \ell_k \tau_{j-1})A} - I)P f_{\ell_k}^{j-1} \\
& - S_k^{(1)} \\
& + A^{-1} e^{-(N_{j-1}\tau_{j-1} - k\tau_j)A}(I - P)f_{N_{j-1}}^{j-1} \\
& + S_k^{(2)} \\
& + A^{-1}(I - e^{-((\ell_k+1)\tau_{j-1} - k\tau_j)A})(I - P)f_{\ell_k}^{j-1} ;
\end{aligned}
$$

Case 2. $k\tau_j \geq N_{j-1}\tau_{j-1}$ (beyond time range of previous iterate)

$$
\begin{aligned}
\varphi_k^j(p) = {} & e^{k\tau_j A}p - A^{-1}(e^{(k\tau_j - N_{j-1}\tau_{j-1})A} - I)f_{N_{j-1}}^{j-1} \\
& - S_k^{(3)} \\
& + A^{-1}(I - P)f_{N_{j-1}}^{j-1} ,
\end{aligned}
$$

where $f_k^j = f(\varphi_k^j(p))$, and

$$S_k^{(1)} = e^{k\tau_j A} \sum_{\ell=0}^{\ell_k-1} A^{-1}(e^{-\ell\tau_{j-1}A} - e^{-(\ell+1)\tau_{j-1}A})P f_\ell^{j-1}$$

$$S_k^{(2)} = e^{k\tau_j A} \sum_{\ell=\ell_k+1}^{N_{j-1}-1} A^{-1}(e^{-\ell\tau_{j-1}A} - e^{-(\ell+1)\tau_{j-1}A})(I-P) f_\ell^{j-1} \qquad (7.2)$$

$$S_k^{(3)} = e^{k\tau_j A} \sum_{\ell=0}^{N_{j-1}-1} A^{-1}(e^{-\ell\tau_{j-1}A} - e^{-(\ell+1)\tau_{j-1}A})P f_\ell^{j-1} \ .$$

Let k_j be the largest integer such that $k_j\tau_j < N_{j-1}\tau_{j-1}$. The summations in (7.2) can then be written recursively as follows
for $k = 1, 2, \ldots, k_j$

$$S_k^{(1)} = e^{\tau_j A} \left[S_{k-1}^{(1)} + \sum_{\ell=\ell_{k-1}}^{\ell_k-1} A^{-1}(e^{-\ell\tau_{j-1}A} - e^{-(\ell+1)\tau_{j-1}A})P f_\ell^{j-1} \right], \quad S_0^{(1)} = 0 \ ,$$

for $k = k_j, k_j - 1, \ldots, 1$

$$S_{k-1}^{(2)} = e^{-\tau_j A} \left[S_k^{(2)} + \sum_{\ell=\ell_{k-1}+1}^{\ell_k} A^{-1}(e^{-\ell\tau_{j-1}A} - e^{-(\ell+1)\tau_{j-1}A})(I-P) f_\ell^{j-1} \right], \quad S_{k_j}^{(2)} = 0,$$

and for $k = k_j + 1, k_j + 2, \ldots, N_j$

$$S_k^{(3)} = e^{\tau_j A} S_{k-1}^{(3)} \ , \qquad S_{k_j}^{(3)} = \sum_{\ell=0}^{N_{j-1}-1} A^{-1}(e^{-\ell\tau_{j-1}A} - e^{-(\ell+1)\tau_{j-1}A})P f_\ell^{j-1} \ .$$

The bulk of the computational effort is in evaluating the nonlinear term f, not the summations. The recursive form is, however, convenient for ensuring that no evaluation of the nonlinear term is repeated for the same argument.

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