

An augmented shadowing algorithm for calculating the sensitivity of time-average quantities of chaotic systems

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ABSTRACT

We apply the non-intrusive least-squares shadowing (NILSS) method to a newly proposed augmented tangent system in order to calculate the sensitivity of time-average quantities of chaotic dynamical systems to parameter variations. The original tangent system is augmented with an additional equation that acts as a low-pass filter, leaving low frequencies unaffected while filtering out high frequencies. A linear damping term is also added to the original tangent system; the term is activated at high frequencies but vanishes at low frequencies. The method introduces two new parameters, the damping coefficient and the time-scale of the filter. Their values can be estimated from the properties of the dynamical system. We evaluate the performance of the proposed algorithm in the Kuramoto–Sivashinsky equation and the Kolmogorov flow system. The number of non-negative Lyapunov exponents (NNLEs) of the augmented system is generally smaller than that of the original system, and this accelerates the sensitivity calculations. Comparisons with the standard NILSS demonstrate the accuracy of the method at a reduced computational cost. The proposed algorithm is more scalable compared to existing approaches and can be applied to sensitivity analysis as well as optimisation and control of complex, large-scale dynamical systems, including turbulent flows.

1. Introduction

The rapid growth of high-performance computing capabilities has made it possible to optimise turbulent flows through scale-resolving simulations, such as Large Eddy and Direct Numerical Simulations. The accuracy limitations of current approaches based on Reynolds-Averaged Navier–Stokes (RANS) are therefore bypassed. Turbulent flows, however, are chaotic and exhibit sensitivity to initial conditions and parameter variations; this is often referred to as the *butterfly effect*. This leads to exponential growth in tangent (adjoint) variables during the forward (backward) integration step, rendering traditional methods unsuitable for sensitivity analysis of chaotic systems. This critical issue was first identified by Lea et al. [1] in their study of the Lorenz attractor, a typical low-dimensional chaotic model. Similar behaviour was subsequently observed in other systems [2,3].

In recent years, much research effort has focused on addressing the aforementioned challenge. Early work included the ensemble adjoint method of Lea et al. [1], which applies the adjoint method to multiple random trajectory segments and then averages the computed derivatives. Other methods to compute sensitivities of time-average quantities include the fluctuation-dissipation theorem [4], the Fokker–Planck equation [5], Least Squares Shadowing (LSS) [6], unsteady periodic orbits [7], cumulant expansions [8], fast response algorithm [9,10], and the space-split sensitivity (S3) algorithm [11], which utilises Ruelle's linear response theory [12].

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Among these approaches, LSS is one of the most promising. The method is theoretically based on the shadowing lemma [13]. For uniformly hyperbolic systems, this lemma guarantees the existence of a solution trajectory (obtained after a perturbation is added to a system's parameter) that remains indefinitely close to the reference trajectory (obtained at the reference value of the parameter). The new trajectory is known as the shadowing trajectory, and LSS formulates and solves a least-squares optimisation problem to find it. The presence of the shadowing trajectory regularises the problem and allows meaningful sensitivities to be computed.

It is important to note that shadowing-based sensitivity methods rely on the (strong) assumption that shadowing trajectories capture the long-time statistics of perturbed systems, but this assumption does not hold universally. Counterexamples exist even in simple chaotic systems where shadowing trajectories are non physical [14]. In contrast, the rigorous linear response theory of Ruelle [12,15] provides mathematically exact derivatives of statistical quantities. Ruelle established the foundational framework for linear response by decomposing sensitivities into contributions from the stable and unstable subspaces of the dynamics, see [15] in particular where a physical interpretation for each contribution is also given. This decomposition inspired subsequent computational approaches, such as the blended response algorithm [16,17], which approximates separately the stable and unstable components.

Recent advances have further clarified the relationship between shadowing and the linear response. Ni [18] rigorously quantified the bias inherent in shadowing methods, showing that they capture only the stable part of Ruelle's formula. The analysis also revealed that for high-dimensional systems with low-dimensional unstable subspace the shadowing component dominates the sensitivity, making it a practically useful approximation. Building on these insights, Ni developed the fast response algorithm [9,10], which employs a shadowing-like technique to compute efficiently the contributions from both the stable and unstable manifolds under hyperbolicity assumptions.

The above work demonstrates that shadowing-based methodologies are very useful tools for sensitivity analysis. The original LSS algorithm has been successfully applied to many relatively small chaotic systems [6,19,20]. Several variants have been also proposed, such as the Multiple Shooting Shadowing (MSS) [21,22], the Frequency Domain Shadowing (FDS) [23], or more recently the optimal control shadowing [24]. The most efficient variant is the Non-Intrusive Least Squares Shadowing (NILSS) proposed by Ni and Wang [25], with follow-up work detailed in [26–28]. This method constructs and solves a much smaller optimisation problem, with size that scales with the number of positive Lyapunov exponents (NPLEs) of the system (which is orders of magnitude smaller than the number of degrees of freedom). This significantly reduces the computational complexity and enables the application of the NILSS to large-scale systems. However, in the case of turbulent flows, it is still limited to cases of moderate Reynolds (Re) number due to the rapid growth of NPLEs with Re [29].

The central aim of the present work is to further improve the computational efficiency of shadowing-type algorithms. To this end, we augment the tangent system with an additional equation that filters out high frequency components and also add a linear damping term in the right hand side of the original tangent system. Results from the FDS method [23] have shown that truncating the high frequency components of the shadowing trajectory does not affect the accuracy of the sensitivity. Moreover for turbulent flows, there are theoretical arguments [30–32] and computational evidence [33,29] that the largest Lyapunov exponent scales with the Kolmogorov time scale (with a correction factor that depends on Re). We conjecture that it is thus associated with the smallest eddies that carry the high-frequency fluctuations of the flow, while momentum transfer is primarily dominated by large-scale structures. By filtering out the small-scale, high-frequency, structures, it is hoped that the NPLEs can be reduced with minimal effect on the accuracy of computed sensitivities. Gilbert [34] examined the effect of each LE on the sensitivity for the Kuramoto-Sivashinsky equation. The results demonstrate that the most dominant LEs are those close to zero. This indicates that the impact of the leading LEs is relatively small compared to the near-neutral ones. The FDS method [23] performs the filtering operation directly in the frequency domain, but here we achieve a similar result by adding a damping term to the tangent equation; the term is active only at high frequencies and vanishes at low frequencies. As will be seen, this indeed reduces the NPLEs and therefore the computational complexity of the method. The performance of the proposed algorithm is tested in the Kuramoto–Sivashinsky system and the Kolmogorov flow.

The remainder of the paper is organised as follows. In section 2, we briefly introduce the shadowing method, while section 3 presents the augmented tangent system and details the selection of its parameters from the properties of the original system. Section 4 proposes an augmented NILSS algorithm, which is assessed in the Kuramoto–Sivashinsky system in section 5 and the Kolmogorov flow in section 6. Finally, section 7 summarises the main findings of this work and proposes some future research directions.

2. Shadowing method in time and frequency domains

Consider the dynamical system described by the set of ordinary differential equations (ODEs),

$$\frac{du}{dt} = f(u; s), \quad u(0) = u_0, \quad (1)$$

where u represents the state vector (with size n_u) and s is the set of parameters defining the system. For example, in flow around an aerofoil, u represents the velocity components and pressure at discrete points in the computational domain, and s the Reynolds number, angle of attack, Mach number etc. In most practical applications, engineers are often interested in time-averaged quantities,

$$\bar{J}(s) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T J(u; s) dt. \quad (2)$$

In the previous example, $\bar{J}(s)$ may represent the mean drag or lift coefficients of the aerofoil. The sensitivity of $\bar{J}(s)$ with respect to s is defined as

$$\frac{d\bar{J}}{ds} = \lim_{\delta s \rightarrow 0} \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \frac{J(\mathbf{u}(s + \delta s); s + \delta s) - J(\mathbf{u}(s); s)}{\delta s} dt. \quad (3)$$

For chaotic systems the differentiation and time-averaging operations do not commute, i.e.

$$\begin{aligned} \frac{d\bar{J}}{ds} &\neq \lim_{T \rightarrow \infty} \lim_{\delta s \rightarrow 0} \frac{1}{T} \int_0^T \frac{J(\mathbf{u}(s + \delta s); s + \delta s) - J(\mathbf{u}(s); s)}{\delta s} dt \\ &= \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \left(\frac{\partial J}{\partial \mathbf{u}} \mathbf{v} + \frac{\partial J}{\partial s} \right) dt, \end{aligned} \quad (4)$$

where $\mathbf{v}$ is the sensitivity of $\mathbf{u}$ with respect to s ,

$$\mathbf{v} = \frac{\partial \mathbf{u}}{\partial s} = \lim_{\delta s \rightarrow 0} \frac{\mathbf{u}(s + \delta s) - \mathbf{u}(s)}{\delta s}. \quad (5)$$

The reason is that chaotic systems have one or more positive Lyapunov exponents (LEs), thus the introduction of the small perturbation δs causes the two trajectories $\mathbf{u}(s + \delta s)$ and $\mathbf{u}(s)$ to diverge in phase space, leading to exponential growth of $\mathbf{v}(t)$ and therefore the integral on the right hand side of (4) does not converge.

To address this challenge, Wang et al. [6] introduced the least squares shadowing (LSS) method. The method is based on the shadowing lemma [13], which guarantees that for a uniformly hyperbolic system, given a reference trajectory $\mathbf{u}(t; s)$, there exists another trajectory $\mathbf{u}(\tau(t); s + \delta s)$ that shadows indefinitely the reference one ($\tau(t)$ is a time transformation). The two trajectories have different initial conditions, but for ergodic systems the time-average $\bar{J}(s)$ and its sensitivity $\frac{d\bar{J}}{ds}$ are independent of the initial condition.

To find the shadowing trajectory LSS solves the following minimisation problem [21],

$$\min_{\mathbf{v}, \eta} \frac{1}{2} \int_0^T \|\mathbf{v}(t)\|^2 dt, \quad (6a)$$

$$s.t. \quad \frac{d\mathbf{v}}{dt} = \frac{\partial \mathbf{f}}{\partial \mathbf{u}} \mathbf{v} + \frac{\partial \mathbf{f}}{\partial s} + \eta(t) \mathbf{f}, \quad (6b)$$

$$\langle \mathbf{f}(\mathbf{u}; s), \mathbf{v}(\mathbf{u}; s) \rangle = 0, \quad (6c)$$

where $\mathbf{v}(t)$ is the sensitivity of $\mathbf{u}(t; s)$, $\eta(t) = \frac{d}{ds} \left(\frac{d\tau}{dt} \right)$ is known as time-dilation, and (6c) enforces the orthogonality between $\mathbf{f}(\mathbf{u}; s)$ and $\mathbf{v}(\mathbf{u}; s)$. The gradient $\frac{d\bar{J}}{ds}$ can be obtained from,

$$\frac{d\bar{J}}{ds} = \frac{1}{T} \int_0^T \frac{\partial J}{\partial \mathbf{u}} \mathbf{v} + \frac{\partial J}{\partial s} + \eta(t)(J - \bar{J}) dt. \quad (7)$$

In [23] the shadowing method was formulated in the frequency domain. The key idea was to replace the minimisation (6a) with the periodicity condition,

$$\frac{d\mathbf{v}}{dt} = \frac{\partial \mathbf{f}}{\partial \mathbf{u}} \mathbf{v} + \frac{\partial \mathbf{f}}{\partial s} + \eta(t) \mathbf{f} \quad (8a)$$

$$\langle \mathbf{f}(\mathbf{u}; s), \mathbf{v}(\mathbf{u}; s) \rangle = 0 \quad (8b)$$

$$\mathbf{v}(0) = \mathbf{v}(T). \quad (8c)$$

The gradient expression (7) takes the following form,

$$\frac{d\bar{J}}{ds} = \left(\frac{\partial \bar{J}}{\partial s} \right)_0 + \sum_{k=-q}^q \left(\frac{\partial \bar{J}}{\partial \mathbf{u}} \right)_{-k} \hat{\mathbf{v}}_k + \sum_{\substack{k=-q \\ k \neq 0}}^q \hat{\eta}_{-k} \hat{J}_k, \quad (9)$$

where a hat denotes a Fourier-transformed variable, the index k denotes the k -th harmonic of the fundamental angular frequency $\omega_0 = 2\pi/T$ and $k \in [-q, q]$. In [23] it was demonstrated that truncating (i.e. filtering out) very high frequencies still yields accurate results. This finding motivates the present work, however the filtering operation is performed in the time, instead of the frequency, domain. To this end, system (6b) is augmented with an additional equation, as explained in more detail in the next section.

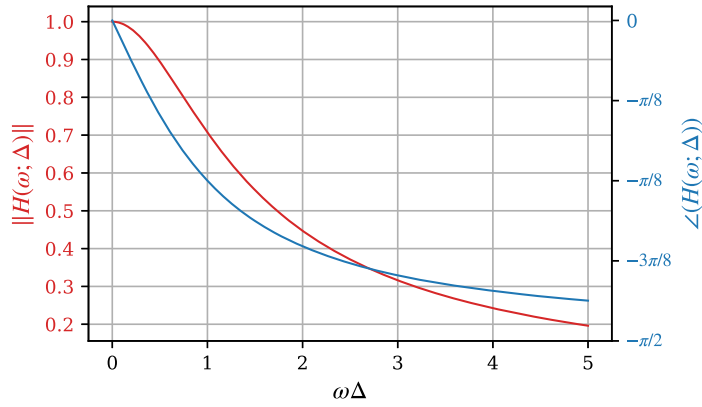


Fig. 1. The modulus (red line and left axis) and the angle (blue line and right axis) of the transfer function $H(\omega; \Delta)$, see (14), against the normalised frequency $\omega\Delta$. (For interpretation of the colours in the figure(s), the reader is referred to the web version of this article.)

3. Augmented tangent system

We augment the original inhomogeneous tangent system (6b) with an additional equation that performs filtering in the time domain. More specifically, the augmented tangent system is expressed as follows,

$$\frac{d\mathbf{v}^*}{dt} = \frac{\partial \mathbf{f}}{\partial \mathbf{u}} \mathbf{v}^* + \frac{\partial \mathbf{f}}{\partial s} - X(\mathbf{v}^* - \tilde{\mathbf{v}}), \quad (10a)$$

$$\frac{d\tilde{\mathbf{v}}}{dt} = \frac{1}{\Delta}(\mathbf{v}^* - \tilde{\mathbf{v}}), \quad (10b)$$

where $\tilde{\mathbf{v}}$ is the low-pass filtered variable (and we have omitted the time-dilation term for convenience). The filtering parameter $\Delta > 0$ determines the frequency content of $\tilde{\mathbf{v}}$ with respect to that of $\mathbf{v}^*$. A small value of Δ results in a large cut-off frequency f_c ; as Δ increases f_c is reduced. A linear damping term is added to the right hand side of the original tangent equation with the positive damping parameter X , therefore $\mathbf{v}^* \neq \mathbf{v}$.

The augmented homogeneous tangent system is similarly defined as,

$$\frac{d\mathbf{w}^*}{dt} = \frac{\partial \mathbf{f}}{\partial \mathbf{u}} \mathbf{w}^* - X(\mathbf{w}^* - \tilde{\mathbf{w}}), \quad (11a)$$

$$\frac{d\tilde{\mathbf{w}}}{dt} = \frac{1}{\Delta}(\mathbf{w}^* - \tilde{\mathbf{w}}). \quad (11b)$$

The analytical solution of (10b) is

$$\tilde{\mathbf{v}}(t; \Delta) = \int_{-\infty}^t \mathcal{T}(\tau - t; \Delta) \mathbf{v}^*(\tau) d\tau, \quad (12)$$

which is a convolution integral with an exponentially decaying kernel [35,36],

$$\mathcal{T}(\tau - t; \Delta) = \frac{1}{\Delta} \exp\left(-\frac{\tau - t}{\Delta}\right). \quad (13)$$

The analytical solution takes a particularly simple form in the frequency domain. Taking the Fourier transform of (10b), i.e. substituting $\tilde{\mathbf{v}}(t) = \int_{-\infty}^{+\infty} \hat{\tilde{\mathbf{v}}}(\omega) e^{i\omega t} d\omega$ and $\mathbf{v}^*(t) = \int_{-\infty}^{+\infty} \hat{\mathbf{v}}^*(\omega) e^{i\omega t} d\omega$, the equations decouple due to linearity and we get $\hat{\tilde{\mathbf{v}}}(\omega) = H(\omega; \Delta) \hat{\mathbf{v}}^*(\omega)$, where H is the transfer function given by,

$$H(\omega; \Delta) = \frac{1}{1 + i\omega\Delta}, \quad (14)$$

and $i = \sqrt{-1}$ is the imaginary unit. The modulus and angle of the complex $H(\omega; \Delta)$ are shown in Fig. 1 as a function of $\omega\Delta$. The cutoff circular frequency is defined by,

$$\omega_c = 1/\Delta. \quad (15)$$

For $\omega \ll \omega_c$, $H(\omega; \Delta) \rightarrow 1$, so there is no damping, but when $\omega \gg \omega_c$, $H(\omega; \Delta) \rightarrow 0$, so high frequencies are damped. The Fourier transform of the damping term $X(\mathbf{v}^*(t) - \tilde{\mathbf{v}}(t))$ that appears in (10a) is

$$X(\hat{\mathbf{v}}^*(\omega) - \hat{\tilde{\mathbf{v}}}(\omega)) = X(1 - H(\omega; \Delta))\hat{\mathbf{v}}^*(\omega) = \frac{X i \omega \Delta}{1 + i \omega \Delta} \hat{\mathbf{v}}^*(\omega), \quad (16)$$

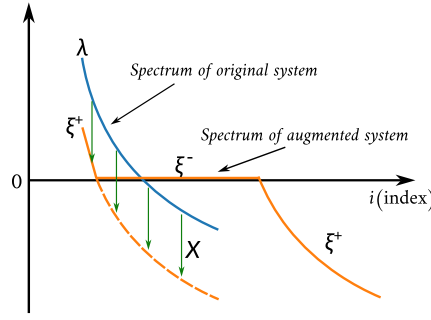


Fig. 2. Lyapunov spectrum of the augmented system (orange line) from that of the original system (blue line) as $\Delta \rightarrow \infty$.

so $X(\widehat{\mathbf{v}}^*(\omega) - \widehat{\mathbf{v}}(\omega)) \rightarrow 0$ for $\omega \ll \omega_c$ and $X(\widehat{\mathbf{v}}^*(\omega) - \widehat{\mathbf{v}}(\omega)) \rightarrow X\widehat{\mathbf{v}}^*(\omega)$ as $\omega \gg \omega_c$. Therefore, for low frequencies the damping term $X(\mathbf{v}^*(t) - \widehat{\mathbf{v}}(t)) \rightarrow 0$, thus the tangent equation does not change, and $\widehat{\mathbf{v}}^*(\omega) \rightarrow \widehat{\mathbf{v}}(\omega)$. The damping term acts only for frequencies ω of the order ω_c or higher.

We note here that the augmented system has the same form as the Selective Frequency Damping (SFD) method [35,37] that is used to extract steady, but linearly unstable, flow fields using time-stepping algorithms. In our case we have a different aim; the goal is not to reach a steady state, but rather to damp high frequencies and accelerate the sensitivity calculations.

3.1. Stability analysis of the augmented system

We now proceed to analyse the stability of the augmented system. This analysis has also been performed in [35] but below we also investigate the limiting cases of X and Δ taking very small or very large values. This analysis can provide significant insight on the selection of these two parameters. It also allows us to approximately infer the Lyapunov spectrum of (11) from that of the original system.

We assume that the Jacobian $\partial \mathbf{f} / \partial \mathbf{u}$ is a positive scalar, equal to λ . This can be taken to represent one of the Lyapunov exponents of the original system. The matrix of the augmented system (11) becomes

$$\Xi = \begin{bmatrix} \lambda - X & X \\ \frac{1}{\Delta} & -\frac{1}{\Delta} \end{bmatrix}. \quad (17)$$

The eigenvalues of Ξ can be easily obtained analytically,

$$\xi^{\pm} = \frac{1}{2\Delta} \left((\lambda - X)\Delta - 1 \pm \sqrt{\Delta^2(\lambda - X)^2 + 2\Delta(\lambda + X) + 1} \right). \quad (18)$$

The number of eigenvalues (and eigenvectors) is doubled due to the introduction of the filtered variable $\tilde{\mathbf{u}}$.

We now consider the effect of very large Δ . To this end, we perform Taylor series expansion of (18) around $1/\Delta = 0$ and keeping only the linear term we get,

$$\xi^+ \approx \lambda - X + \frac{1}{\Delta} \frac{X}{\lambda - X}, \quad (19a)$$

$$\xi^- \approx -\frac{1}{\Delta} \frac{\lambda}{\lambda - X}. \quad (19b)$$

When $\Delta \rightarrow \infty$, i.e. when all frequencies are filtered, we obtain:

$$\lim_{\Delta \rightarrow \infty} \xi^+ = \lambda - X, \quad (20a)$$

$$\lim_{\Delta \rightarrow \infty} \xi^- = 0. \quad (20b)$$

Based on the above result, we can obtain the Lyapunov spectrum of the augmented system from that of the original system; this is shown schematically in Fig. 2. The whole spectrum is shifted downwards by X , a long flat region exists at 0 (with size equal to n_u) and the negative exponents are shifted to the right.

On the other hand, as $\Delta \rightarrow 0$ the two equations decouple and the first equation of the augmented system converges to that of the original system. Indeed, the analytical solution (18) gives

$$\lim_{\Delta \rightarrow 0} \xi^+ = \lambda, \quad (21a)$$

$$\lim_{\Delta \rightarrow 0} \xi^- = -\infty, \quad (21b)$$

where the bottom equation originates from (11b).

It is worth reiterating that the above analysis is based on the important assumption that the Jacobian is constant. However, these analytical results provide important physical insight. In later sections, we compute the Lyapunov spectrum of the augmented system

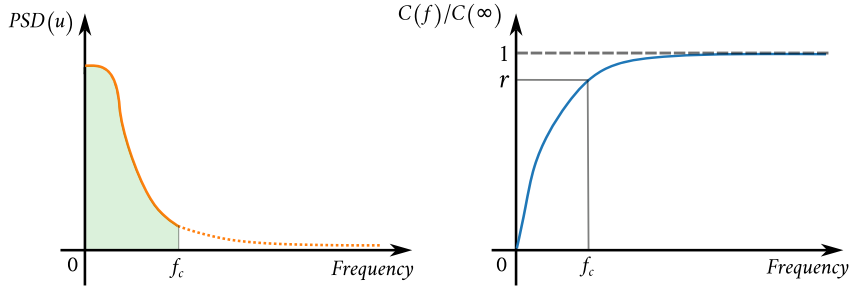


Fig. 3. Schematics of Power Spectral Density (PSD) and Cumulative Power Spectral Density (CPSD) of the state variables and estimation of the value of Δ from the CPSPD.

using the standard Gram–Schmidt orthogonalisation procedure of [38,39] and compare with that of the original system, to ascertain similarities and differences with the analytical method presented above.

3.2. Selection of parameters X and Δ

Based on the analysis of the previous section, to reduce the maximum LE of the augmented system, we set the value of the damping variable $X = \lambda_1$, where λ_1 is the maximum LE of the original system. According to the previous analysis, when Δ is sufficiently large, the maximum LE of the augmented system is expected to be around zero.

To determine the value of Δ , we examine the power spectral density (PSD) of the state variables $u(t)$. The cumulative power spectral density (CPSD) represents the total energy contained in a signal up to a certain temporal frequency f and is defined as

$$C(f) = \int_0^f \text{PSD}(f') df'. \quad (22)$$

This function is widely adopted for analysing the power contribution of signals, see for example [40]. We now define the ratio $R(f) = C(f)/C(\infty)$, which indicates the percentage of power within the frequency range $[0, f]$.

We can obtain Δ from $R(f)$ using the procedure illustrated in Fig. 3. The PSD of some key variables (that depend on the problem) is first calculated and then $R(f)$ is plotted against f , see left and right panels respectively. The desired percentage of the energy captured r is selected and the cutoff frequency f_c is determined by solving the equation $R(f_c) = r$. From equation (15), the filtering parameter Δ can be expressed as a function of r ,

$$\Delta(r) = \frac{1}{\omega_c} = \frac{1}{2\pi f_c |R(f_c)=r|}. \quad (23)$$

As the value of r decreases, f_c increases and Δ increases. When $r \rightarrow 0$, $\Delta \rightarrow \infty$ signifying the elimination of all oscillating power of the signal. In sections 5.1 and 6.2 we explore different values of r that correspond to different Δ 's.

4. NILSS algorithm for the augmented tangent system

To obtain the sensitivity $\frac{d\bar{J}}{ds}$, we apply the NILSS algorithm to the augmented homogeneous and inhomogeneous systems, (11) and (10) respectively. The core structure of the algorithm is the same as the original one proposed in [25] albeit with some small modifications. Fig. 4 depicts a schematic representation. The time domain $[0, T]$ is partitioned into multiple segments $T = N_s \times \Delta T$, where N_s is the number of segments and ΔT the time length of each segment. The i -th segment spans the time domain $[t_{i-1}, t_i]$, where $t_0 = 0$ and $t_{N_s} = T$. One nonlinear simulation of system (1) is first performed to obtain the state vector $u(t)$ at the reference value of parameters s , from which the Jacobian $\frac{\partial f}{\partial u}$ can be computed. Subsequently, simulations of the augmented tangent system are conducted on each segment. This involves one simulation of the inhomogeneous tangent system (10) and n_p simulations of the homogeneous tangent system (11), where n_p is set equal to the number of PLEs in the original paper [25]. In the adjoint version of the NILSS algorithm of Blonigan [28], the value of n_p is set equal to the number of non-negative Lyapunov exponents (NNLEs), encompassing both positive and neutral LEs. We follow the latter approach and set n_p equal to the number of NNLEs. At the end of the computation at each segment, a QR re-orthonormalisation procedure is applied to derive the starting conditions for the next segment.

In the final step, we add to the inhomogeneous solution a linear combination of the tangent solutions. The unknown coefficients are determined by the solution of an optimisation problem which is subject to matching conditions across the boundaries of consecutive segments to ensure one continuous solution. Appendix A provides a detailed description of the NILSS algorithm as applied to the augmented tangent system.

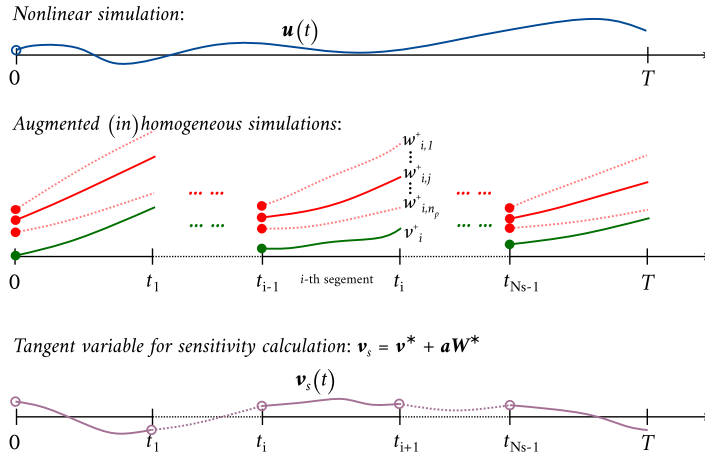
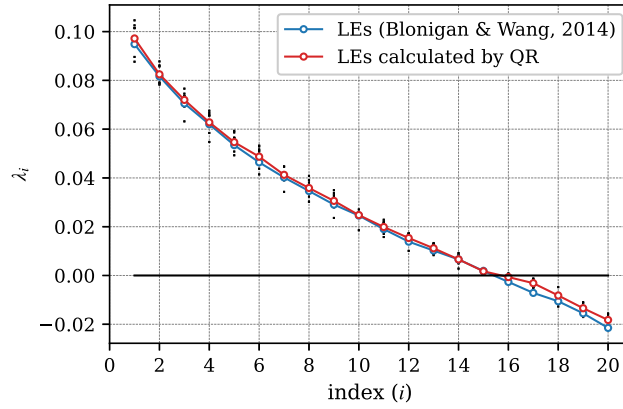


Fig. 4. Schematic diagram of the augmented tangent NILSS algorithm.

Fig. 5. Lyapunov spectrum of the KS System for $c = 0$. Results are averaged over 10 simulations with different initial conditions. Black dots indicate individual simulations. The blue line represents data from [19].

5. Application of augmented NILSS to the Kuramoto–Sivashinsky system

The Kuramoto–Sivashinsky (KS) equation describes a chaotic dynamical system and has been extensively studied [19,21–23]. The equation is

$$\frac{\partial u}{\partial t} = -(u + c) \frac{\partial u}{\partial x} - \frac{\partial^2 u}{\partial x^2} - \frac{\partial^4 u}{\partial x^4}, \quad (24)$$

with $x \in [0, L]$, with Dirichlet and Neumann boundary conditions at the two ends of the domain, $u(0, t) = u(L, t) = 0$, and $\frac{\partial u}{\partial x}|_{x=0} = \frac{\partial u}{\partial x}|_{x=L} = 0$. For spatial discretisation we employ a second order central finite difference scheme, and the solution is marched in time with a 4th order Runge–Kutta scheme. We set $L = 128$ and use $n_u = 128$ grid points inside the domain, and results were extracted every $\Delta t = 0.1$. The range of the parameter $c \in [0, 1]$. We consider the sensitivity with respect to c of two objective functions; the space- and time-average state and energy,

$$\bar{J}_1 = \frac{1}{TL} \int_0^T \int_0^L u(x, t) dx dt, \quad (25a)$$

$$\bar{J}_2 = \frac{1}{TL} \int_0^T \int_0^L u^2(x, t) dx dt. \quad (25b)$$

The gradients obtained using finite differences [19] will be used to validate the values computed by the proposed shadowing method.

We calculate the Lyapunov spectrum of the KS system using the QR decomposition algorithm [38,41]. To ensure convergence of the LEs, the calculation time is set to 3000. Different values of segment size dT were investigated, and the first 25 LEs converge for all dT from 0.3 to 20. In all original LE computations in this section, we set $dT = 0.5$. The spectrum for $c = 0$ is shown in Fig. 5 and

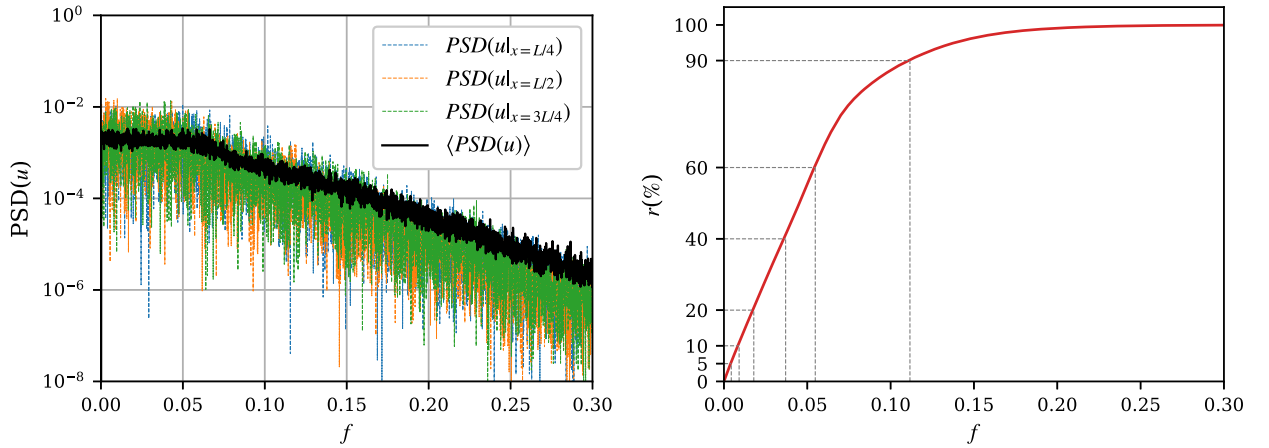


Fig. 6. Power spectral density of different state variables of the KS system (left) and normalised cumulative power spectral density (right) for $c = 0$.

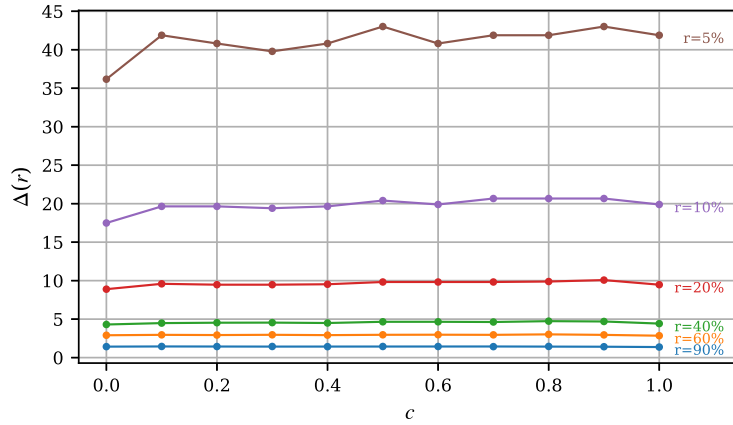


Fig. 7. The filtering parameter Δ against c for different values of r .

compared with that reported in [19]. There is very good matching between the two spectra; it can be seen that the number of NNLEs is equal to 15.

The parameter X is set to the leading LE of the original system, $X = \lambda_1$. When c varies in the range $[0, 1]$, λ_1 falls within $[0.096, 0.1]$. The parameter Δ is evaluated using the cumulative power spectral density of the system. In Fig. 6, we present the PSDs at three points in the domain and also the space-averaged PSD for $c = 0$. Most of the energy is contained within frequencies less than 0.1. The captured energy ratio r against the frequency f is shown on the right panel. For different r values ranging from 5% to 90%, the parameter Δ varies from 1.5 to 40, as shown in Fig. 7. It can be seen that Δ is almost constant with c and depends only on r .

Since the cutoff frequency is applied to the tangent variables, determining Δ based on the PSD of these variables would be more meaningful. However, as the tangent solution is unknown a priori, we instead analyse the frequency characteristics of the state variables to determine the appropriate cutoff frequency.

We now consider the Lyapunov spectrum for the augmented tangent system. We first investigate the effect of the time segment size dT because the introduction of the filtering parameter Δ introduces an additional time scale in the system. We examine the effect of dT for values ranging from $\pi\Delta$ to $6\pi\Delta$. The particular segment size $dT = 2\pi\Delta$ corresponds to a fundamental frequency $2\pi/dT = 1/\Delta = \omega_c$, i.e. it is equal to the cutoff frequency of the filter, see (15). The results, depicted in Fig. 8 for $c = 0$ show that, similar to the original system, the value of dT does not affect the calculation of the LEs. In other words, reliable LEs can be obtained for a wide range of dT values, that result in fundamental frequencies that can be smaller or larger than the cut off, ω_c . This is probably due to the smooth transfer function of the filter, see Fig. 1. Note that for $\Delta = 1$ (left panel) there is a band of LEs with values larger than those of the original system, and the number of PLEs is also larger. For the larger value $\Delta = 5$ (right panel), all LEs are smaller, as predicted by the linear stability analysis of section 3.1. In the following we present results with segment size $dT = 2\pi\Delta$.

In Fig. 9, we compare the Lyapunov spectrum of the original system with that of the augmented system with a large value $\Delta = 100$. The shape of the spectrum resembles Fig. 2; it is shifted downwards by X and the negative LEs are shifted to the right by n_u . This is consistent with the theoretical prediction of section 3.1, in particular equation (20) valid for $\Delta \rightarrow \infty$.

We now calculate the LEs of the augmented system for different values of r for $c = 0$; the results are displayed in Fig. 10. To facilitate the interpretation of the figure, the corresponding values of Δ are also provided in the legend. When Δ is small, say $\Delta < 3$, the number of NNLEs is higher than that of the original system (orange line). This was also noticed in Fig. 8 (left plot). As the value

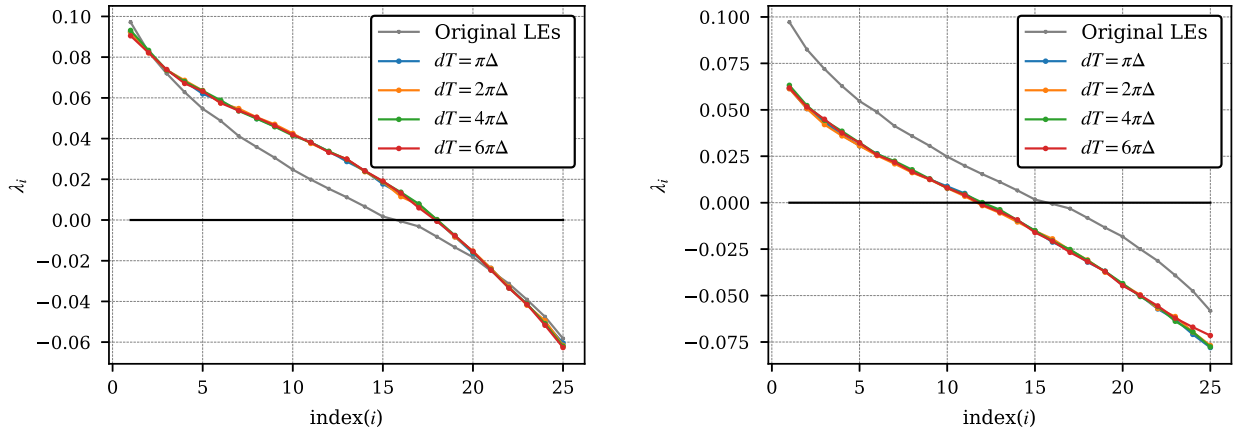


Fig. 8. Effect of time segment length dT on the Lyapunov spectrum of the augmented KS system for $c = 0$. Results are averaged across 5 simulations with different initial conditions. Left: $\Delta = 1$. Right: $\Delta = 5$. X is set equal to the leading LE of the original system, λ_1 .

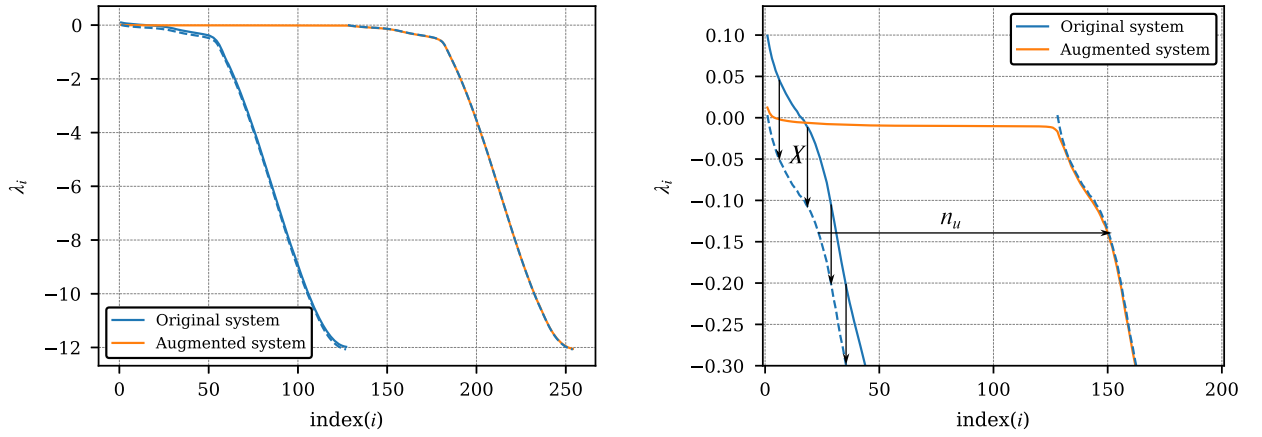


Fig. 9. Comparison of Lyapunov spectrum between original and augmented system with $\Delta = 100$, for $c = 0$. For the augmented system, X is set as the leading LE of the original system, λ_1 ($= 0.0965$). Left: the complete set of LEs, Right: zoomed-in view of LEs around 0.

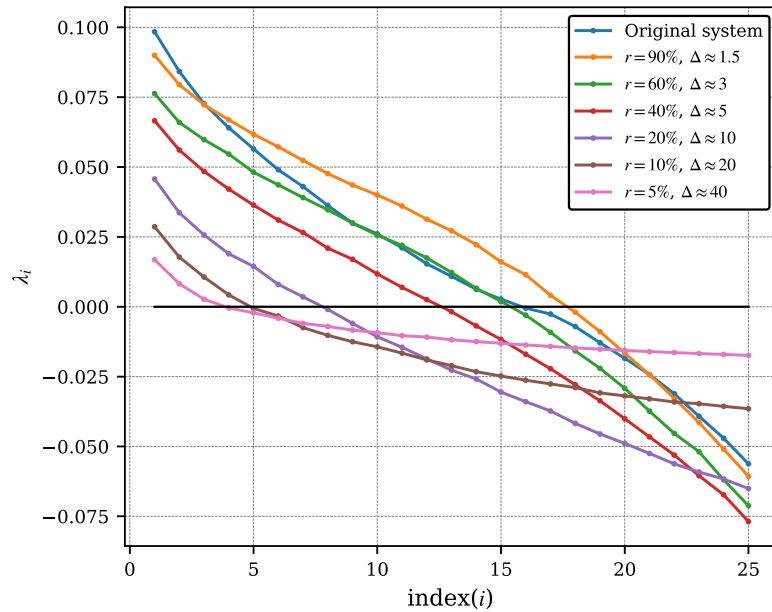


Fig. 10. Comparison of the first 25 LEs for augmented systems with different values of ratio r (or Δ). For all cases $X = \lambda_1$ and $c = 0$.

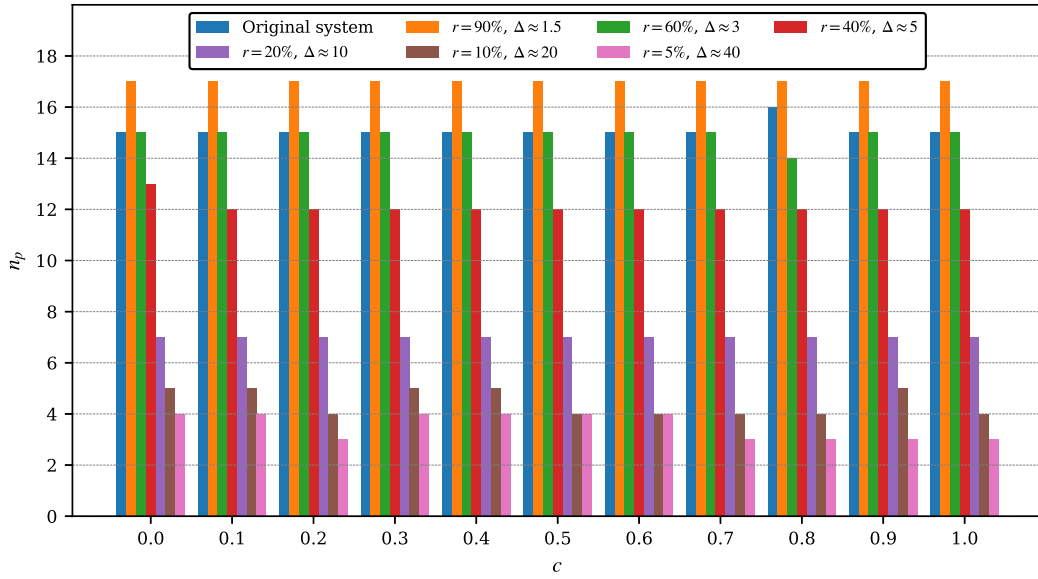


Fig. 11. Number of NNLEs of the original and augmented system with different values of Δ and c . For all cases, $X = \lambda_1$.

of Δ increases, not only does the value of the leading LE decreases, but the spectrum also becomes more horizontal i.e. the slope is reduced, see for example the spectra for $\Delta = 20, 40$. These two effects compete and when Δ is small, the decrease in the leading LE is small, but the change in slope results in a higher number of NNLEs. With increasing Δ , the reduction of the leading LE dominates and the number of NNLEs decreases. When $r < 60\%$ ($\Delta > 3$), the number of NNLEs is reduced to less than a quarter of the original system, this is shown more clearly in Fig. 11. A couple of interesting observations can be also made from this figure. First, the effect of c is very small. Secondly, there is a “sweet spot” between $r = 20\%$ and 40% (Δ between 5 and 10) with the sharpest reduction in the number of NNLEs.

5.1. Evaluation of sensitivities using the augmented system

We now utilise the augmented tangent system for sensitivity calculations. The time segment size ΔT for the application of the NILSS method is taken as the reciprocal of the leading LE of the augmented system. We set the number of time segments such that the total time is approximately 100, i.e. $N_s = \lceil 100/\Delta T \rceil$, resulting in an total control time is $T = N_s \times \Delta T$. In Fig. 12 we plot contours of the system state and tangent variables $\mathbf{v}_s$ in the $x-t$ plane for the original (top right) and augmented systems (middle row) for different r (or Δ) values for $c = 1.0$. The sensitivities $\mathbf{v}_s$ obtained from the augmented systems have very similar structure to those of the original system. With reduced energy r , the solution exhibits smoother temporal development and sharp peaks are suppressed. This demonstrates the effectiveness of the proposed method to capture the structure of the solution of the original system and at the same time reduce the number of NNLEs. The bottom row depicts contours of the filtered sensitivity $\tilde{\mathbf{v}}_s$ (obtained from $\tilde{\mathbf{v}}_s = \tilde{\mathbf{v}} + \mathbf{a}\tilde{\mathbf{W}}$) for the same values of r as the middle row. We note that $\tilde{\mathbf{v}}_s$ is not employed in the sensitivity calculations, only $\mathbf{v}_s$ is used, see equation (A.8). We include these plots however to illustrate the effect of temporal filtering. When Δ is small (e.g. when $r = 60\%$ and $\Delta \approx 3$), $\tilde{\mathbf{v}}_s$ is not significantly different from $\mathbf{v}_s$. However, for larger Δ $\tilde{\mathbf{v}}_s$ exhibits a smooth temporal evolution compared with $\mathbf{v}_s$. For $r = 20\%$, the isolines are almost parallel to the t axis, indicating suppression of most frequencies.

The sensitivities dJ_1/dc and dJ_2/dc for different values of r are shown in Fig. 13. For the case labelled as $r = 100\%$ the results were obtained using the standard NILSS algorithm. For both objective functions the sensitivities computed using the augmented system are very close to those obtained from original system. For $d\bar{J}_1/dc$ all results show a constant bias with respect to the finite difference values. In Ref. [22] this was attributed to the non-uniform hyperbolicity of the system, and can be eliminated by filtering out the very small singular values of the resulting system matrix. Such improvements are however beyond the scope of the present study.

The sensitivities against r for $c = 0.5$ are shown in Fig. 14. The average sensitivities at different r remain almost constant. The standard deviation of $d\bar{J}_1/dc$ (obtained from 100 runs with different initial conditions) is more pronounced for low values of r , i.e. when the retained energy is smaller. On the other hand, the standard deviation for the $d\bar{J}_2/dc$ is much larger than that of $d\bar{J}_1/dc$, and (perhaps surprisingly) is also not affected by r .

To obtain further insight, we computed the norms of the Jacobian term $\frac{\partial f}{\partial u} \mathbf{v}^*$ and the linear damping term $X(\mathbf{v}^* - \tilde{\mathbf{v}})$ and plot them against the frequency in Fig. 15 for two values of r . As can be seen, the damping term is an order of magnitude smaller than the Jacobean term; it is even smaller for low frequencies because $X(\hat{\mathbf{v}}^*(\omega) - \hat{\mathbf{v}}(\omega)) \rightarrow 0$ for $\omega \ll \omega_c$ as explained in section 3.

To demonstrate the effect of the proposed form of the damping term we repeated the sensitivity calculations without time filtering, i.e. we consider the tangent system

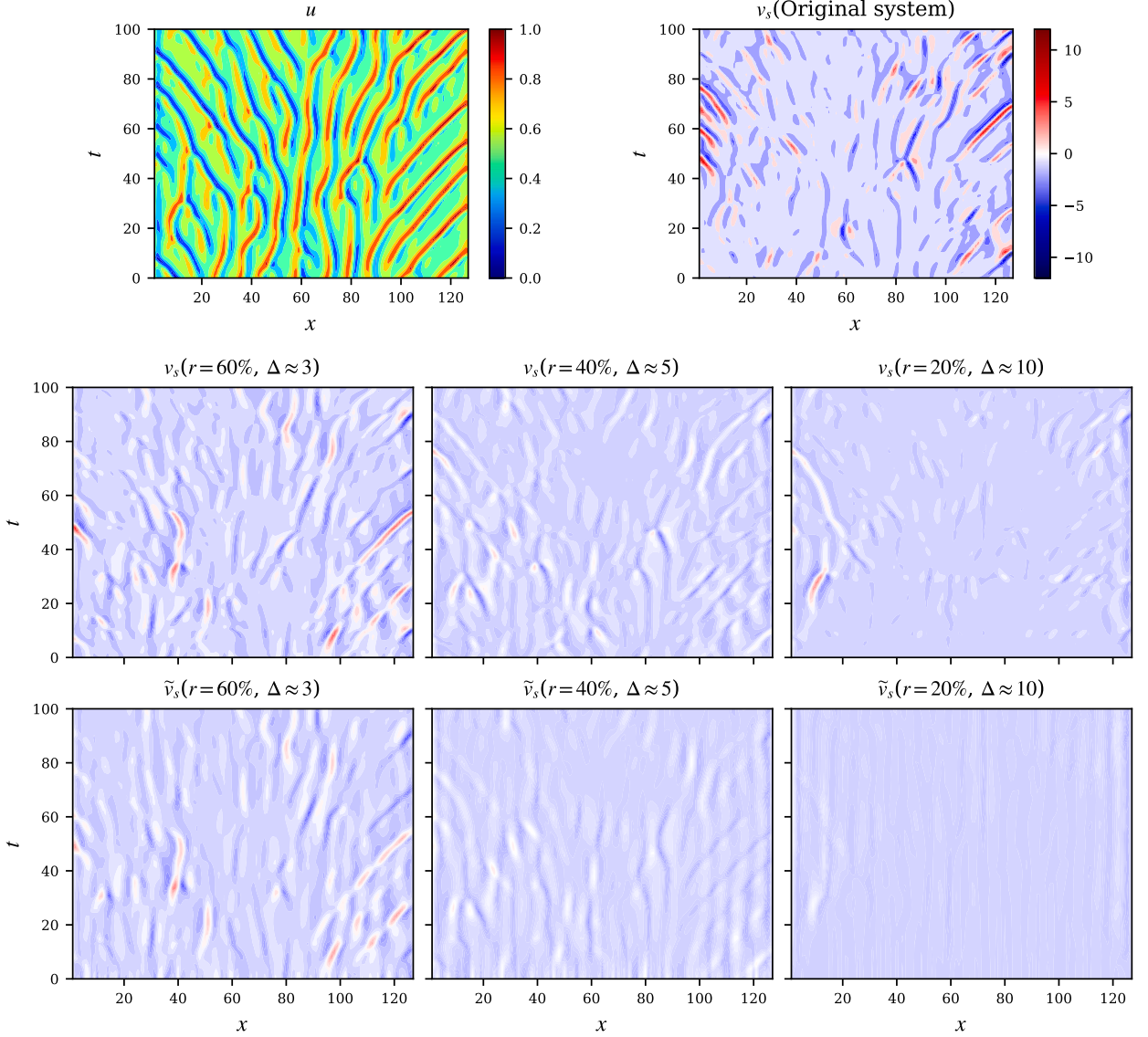


Fig. 12. Top row: contour plot of state variable $u(x, t)$ (left) and shadowing direction $v_s(x, t)$ (right) for the original (non-augmented) tangent system in the $x - t$ plane. Middle row: contours of $v_s(x, t)$ for the augmented tangent system calculated from (A.6) for different filtering parameters Δ . Bottom row: corresponding filtered $\tilde{v}_s(x, t)$ for the augmented systems calculated from $\tilde{v}_s = \bar{v} + \mathbf{a}\tilde{\mathbf{W}}$. All tangent variable plots share the same colour legend (shown on the top right corner). All results are for $c = 1$ and $X = \lambda_1$.

$$\frac{d\mathbf{v}^*}{dt} = \frac{\partial \mathbf{f}}{\partial \mathbf{u}} \mathbf{v}^* + \frac{\partial \mathbf{f}}{\partial s} - X \mathbf{v}^*. \quad (26)$$

The results are shown in Fig. 16 (orange line) and deviate significantly from the reference NILSS solution. The reason is that now the damping term acts across the entire frequency range, thereby leading to erroneous results. This fully justifies our approach to augment the tangent system with the time-filtering equation.

In summary, the obtained results demonstrate the accuracy of the sensitivities calculated from the application of the NILSS algorithm to the augmented KS system. The results are rather insensitive to r . This is consistent with the finding of [23] that when using only the diagonal block of the shadowing harmonic operator (i.e. truncating all frequencies) the results are still very accurate. To explain this behaviour, we turn into equation (9) and notice that the first term is zero for both objective functions, thus the sensitivity is determined by the second and third terms (and the former is the dominant). We therefore computed $\left(\frac{\partial J}{\partial u}\right)^{-k} \hat{v}_k$ for different k and plot the absolute values in the left panel of Fig. 17. The results clearly show that the value of the term for $k = 0$ is by far the largest one, approximately two orders of magnitude larger than the rest. The cumulative sum of these terms for $k \in [-q, q]$ against q is shown in the right panel. Vertical lines indicate the cut-off frequencies for different r . It is evident that for J_1 a single term ($q = 0$) produces sensitivities that closely match those obtained using finite difference and there is very small variation as q

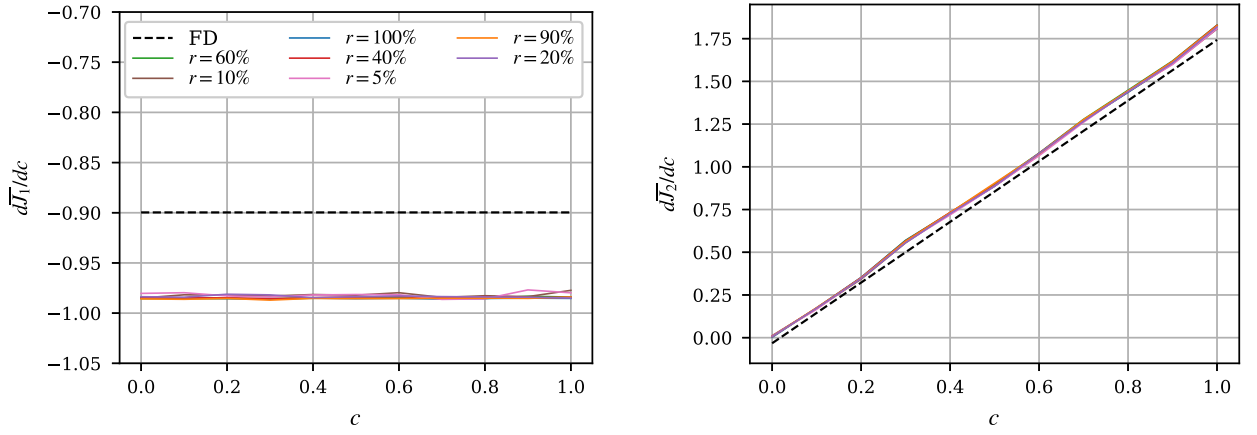


Fig. 13. Comparison of calculated sensitivities for the KS System for different values of r ($r = 100\%$ indicates the original system). The black horizontal dashed line indicates the sensitivity obtained from finite differences. Results are averaged over 100 runs with different initial conditions.

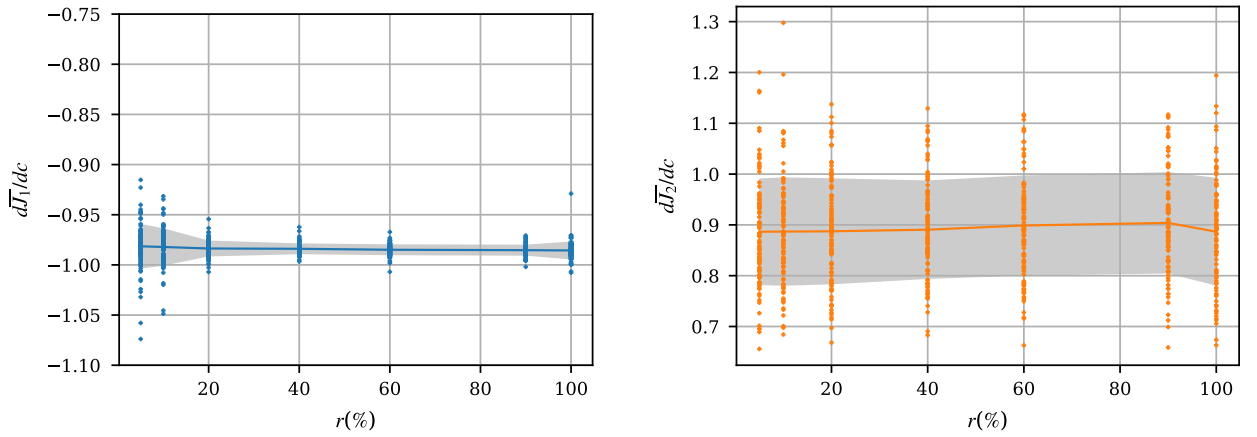


Fig. 14. Sensitivities of the KS system against r for $c = 0.5$. Results are averaged over 100 runs with different initial conditions. Dots represent individual runs. The shaded area marks one standard deviation above and below the average (denoted with a solid line).

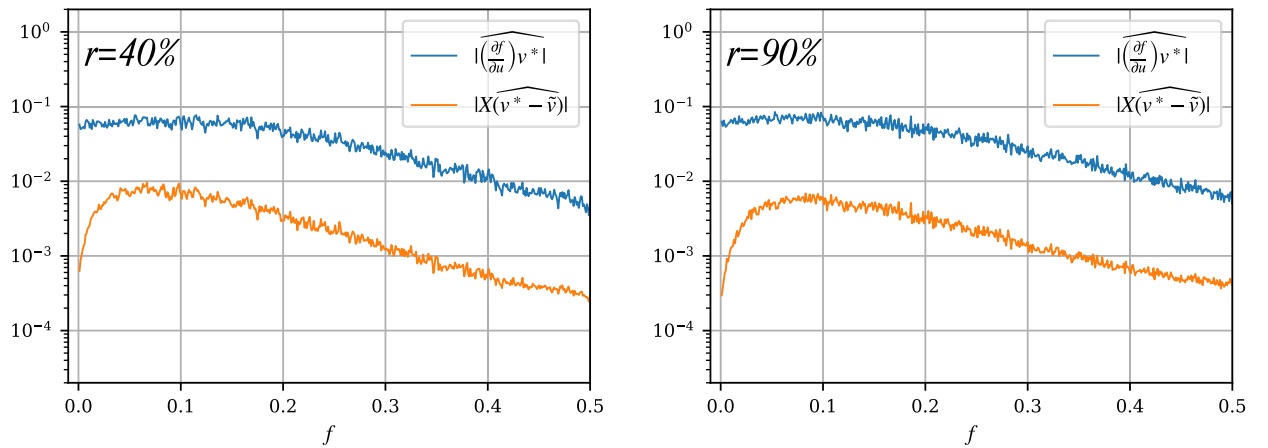


Fig. 15. Variation of the norms of the Jacobean and damping terms with frequency for two r values.

grows. The variation in the sensitivity of J_2 is larger, so r is expected to have some effect. This is however masked in the right panel of Fig. 13 because for $c = 0$ the sensitivity is small but a large range of values is shown in the figure.

The independence of $d\bar{J}_1/dc$ from r can be also interpreted using the Reynolds-averaged equations. Consider the Reynolds decomposition, $u = \bar{u} + u'$, where $\bar{u}$ is the time-average state and u' indicates the fluctuation around $\bar{u}$. Substituting this decomposition

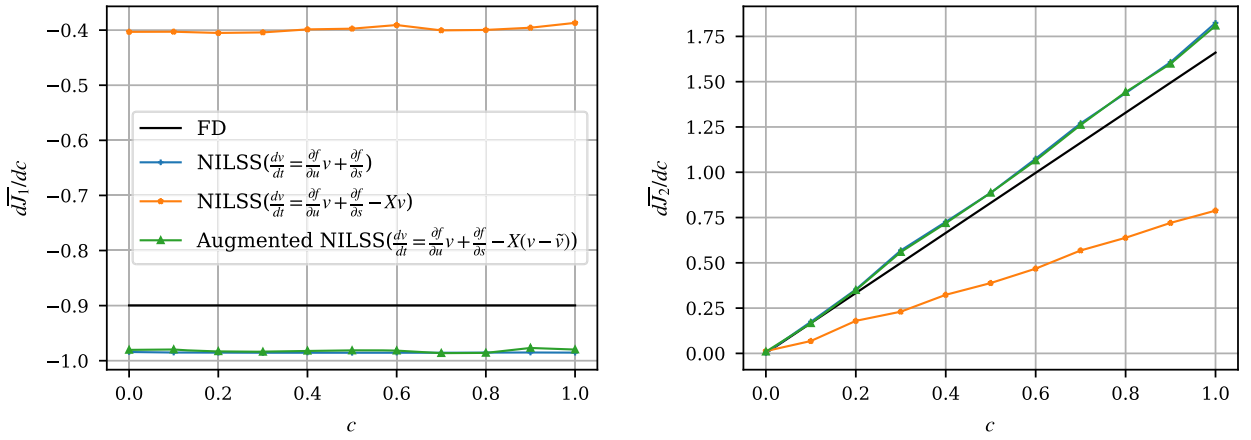


Fig. 16. Comparison of sensitivity calculations for the KS system using different methods.

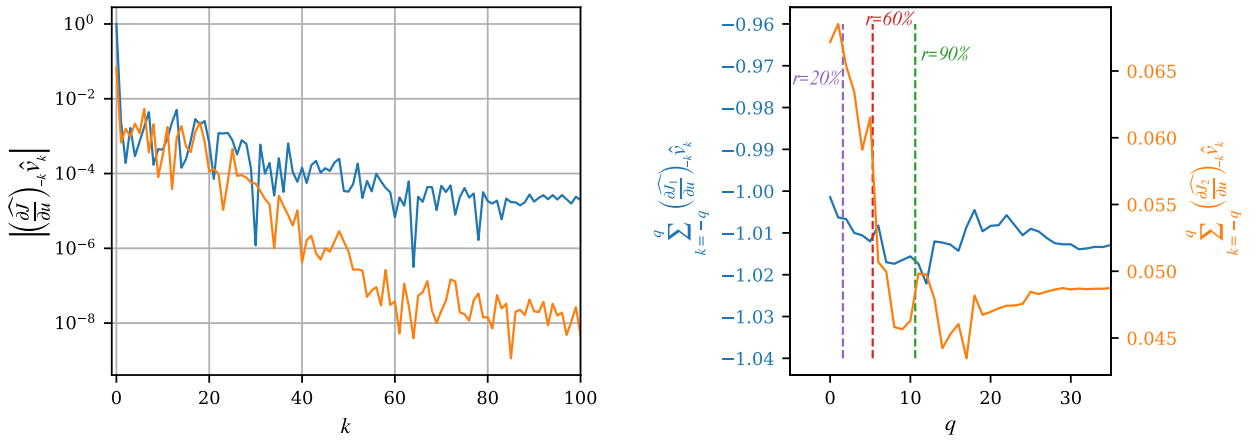


Fig. 17. Absolute values of $\left(\frac{\partial \bar{J}}{\partial u}\right)_{-k} \hat{v}_k$ for different wave numbers k (left panel). Cumulative sum of $\left(\frac{\partial \bar{J}}{\partial u}\right)_{-k} \hat{v}_k$ for $k \in [-q, q]$ against q (right panel). Results for $c = 0$. In both plots, the blue line refers to J_1 , and the orange line refers to J_2 .

into (24) and taking the time-average we obtain the Reynolds-averaged form of the KS system,

$$0 = - \left[(\bar{u} + c) \frac{\partial \bar{u}}{\partial x} + \frac{\partial^2 \bar{u}}{\partial x^2} + \frac{\partial^4 \bar{u}}{\partial x^4} + \frac{1}{2} \frac{\partial \bar{u}^2}{\partial x} \right]. \quad (27)$$

If we define $F(\bar{u}; c) = -(\bar{u} + c) \frac{\partial \bar{u}}{\partial x} - \frac{\partial^2 \bar{u}}{\partial x^2} - \frac{\partial^4 \bar{u}}{\partial x^4}$ and $R(\bar{u}^2) = -\frac{1}{2} \frac{\partial \bar{u}^2}{\partial x}$, the corresponding tangent equation is

$$\frac{\partial F}{\partial \bar{u}} \frac{\partial \bar{u}}{\partial c} + \frac{\partial R}{\partial \bar{u}^2} \frac{\partial \bar{u}^2}{\partial c} + \frac{\partial F}{\partial c} = 0. \quad (28)$$

The sensitivity $d\bar{J}_1/dc$ can be computed from

$$\frac{d\bar{J}_1}{dc} = \frac{1}{L} \int_0^L \frac{\partial \bar{u}}{\partial c} dx = -\frac{1}{L} \int_0^L \left(\frac{\partial F}{\partial \bar{u}} \right)^{-1} \left(\frac{\partial R}{\partial \bar{u}^2} \frac{\partial \bar{u}^2}{\partial c} + \frac{\partial F}{\partial c} \right) dx. \quad (29)$$

The fact that $d\bar{J}_1/dc$ does not depend on r suggests that the effect of the second term (that contains the sensitivity of the Reynolds stress $\bar{u}^2$) is relatively small. We run a long simulation (over 10^6 time units) for $c = 0$ and obtained a value of -0.956 (the term $\frac{\partial R}{\partial \bar{u}^2} \frac{\partial \bar{u}^2}{\partial c}$ was computed with finite differences). Ignoring the Reynolds stress term, the value was -0.931 . The difference between these two values is small and confirms that the sensitivity of the Reynolds stress with respect to c plays a minor role.

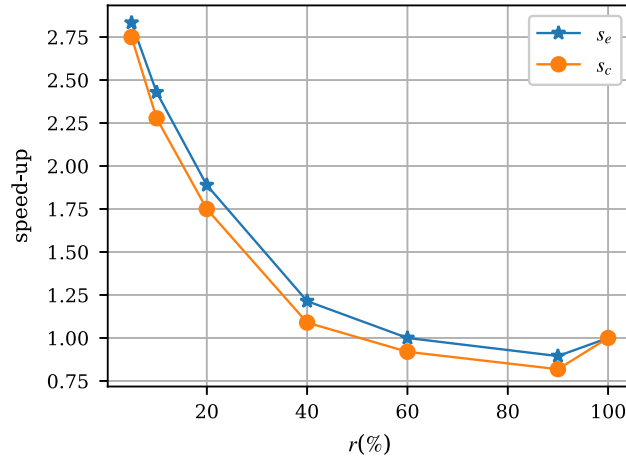


Fig. 18. Measured (orange) and estimated (blue) speed-up of augmented NILSS algorithm for $c = 1.0$. Results are averaged over 100 runs.

5.2. Computational cost

We proceed to analyse the computational efficiency of the proposed algorithm. The measured speed-up s_c is the ratio of the wall clock time of the standard NILSS algorithm divided to that of the augmented algorithm, for the same control time T . This is shown with the orange line in Fig. 18. The results indicate that the augmented NILSS can be as much as three times faster compared to the original algorithm. While the augmented tangent simulation introduces additional variables, the computational overhead is small. This is because the time-filtering equation (10b) is much faster to integrate compared to the tangent equation. Assuming that the computational costs of the augmented (in)homogeneous tangent simulations are comparable to those of the nonlinear simulations, the speed-up can be also estimated by the ratio of NNLEs, i.e. $s_e = \frac{n_p(r=100\%)+2}{n_p(r)+2}$. This ratio is shown with the blue line in Fig. 18 and is very close to the measured speed-up.

6. Application to Kolmogorov flow

The Kolmogorov flow has been extensively studied in relation to stability and transition to turbulence [42–44]. The flow is governed by the two-dimensional Navier–Stokes equations,

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p - \frac{1}{Re} \Delta \mathbf{u} = \mathbf{f}_k, \quad \text{in } \Omega \times [0, T] \quad (30)$$

$$\nabla \cdot \mathbf{u} = 0, \quad (31)$$

where $\mathbf{u} = u_x \mathbf{e}_x + u_y \mathbf{e}_y$ is the velocity vector ($\mathbf{e}_x, \mathbf{e}_y$ are the unit vectors in the x and y directions respectively), p is the pressure, and Re is the Reynolds number. The forcing term $\mathbf{f}_k$ acts only in the x direction and takes the form,

$$\mathbf{f}_k = \sin(n_f y) \mathbf{e}_x, \quad (32)$$

where n_f is the wavenumber in the y -direction (set here to $n_f = 4$). We consider the computational domain $\Omega = [0, 2\pi] \times [0, 2\pi]$ and apply periodic boundary conditions in the x and y directions.

The simulations are performed using the open-source KolSol solver [45]. The Fourier pseudo-spectral method is employed for spatial discretisation, while a fourth-order Runge–Kutta explicit scheme is used for time advancement with time step $dt = 0.01$. The number of spatial Fourier modes is $k_x = k_y = 16$, which is adequate to capture the flow structure for the range of Re examined (from 32 to 40). The flow is chaotic (see more details later) and contours of the instantaneous and time-average u_x velocity are shown in Fig. 19. The instantaneous velocity field contains large scale fluctuating structures while the time-average velocity is homogeneous in the x direction and has a wavy pattern in the y direction with a wavenumber equal to that of forcing term.

We consider the sensitivity of the space- and time-averaged kinetic energy,

$$\bar{J} = \frac{1}{2T\Omega} \int_0^T \int_{\Omega} (u_x^2 + u_y^2) d\Omega dt, \quad (33)$$

with respect to the Reynolds number. The sensitivity $\frac{d\bar{J}}{dRe}$ is first estimated using finite differences. We computed $\bar{J}$ by performing a very long simulation (10^6 time units) and show the results in Fig. 20. The values of the objective function within the considered Re number range closely approximate a straight line, thus its sensitivity is approximately constant, and equal to 0.016.

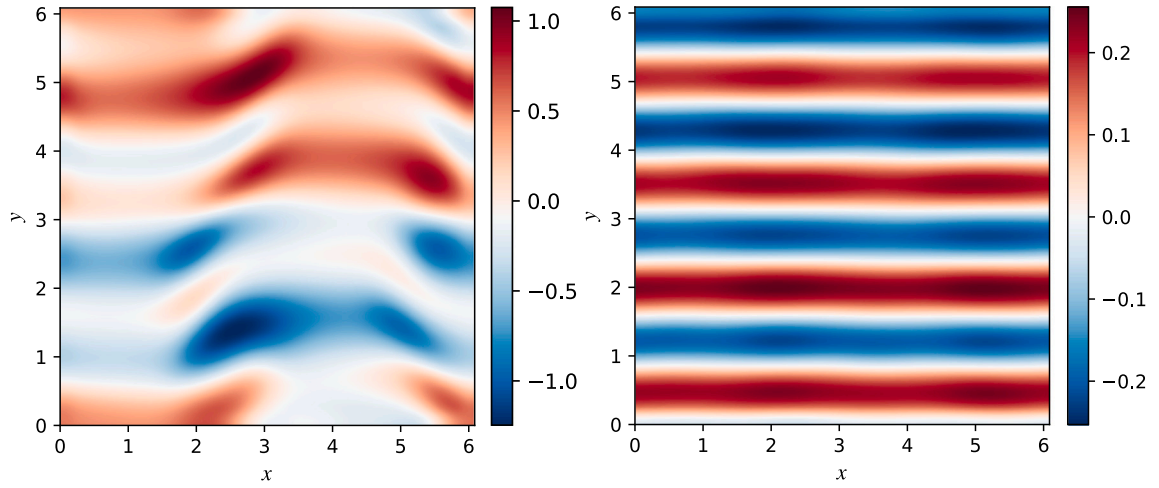


Fig. 19. Contours of the instantaneous (left) and time-averaged (right) u_x velocity component of the Kolmogorov flow for $Re = 34$.

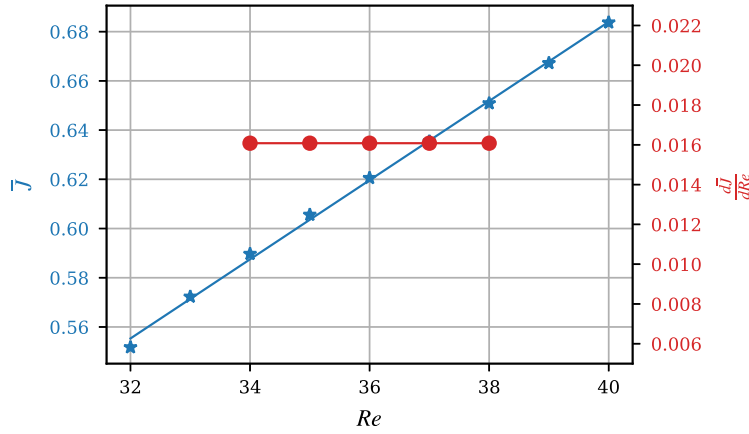


Fig. 20. Variation of the objective function $\bar{J}$ (blue line) and its sensitivity (red line) with Reynolds numbers. The computational time is 10^6 time units.

The inhomogeneous tangent Navier–Stokes system is given by

$$\frac{\partial \delta \mathbf{u}}{\partial t} + \delta \mathbf{u} \cdot \nabla \mathbf{u} + \mathbf{u} \cdot \nabla \delta \mathbf{u} + \nabla \delta p - \frac{1}{Re} \Delta \delta \mathbf{u} + \frac{1}{Re^2} \Delta \delta \mathbf{u} = 0, \quad (34)$$

$$\nabla \cdot \delta \mathbf{u} = 0, \quad (35)$$

where $\frac{1}{Re^2} \Delta \delta \mathbf{u}$ represents the forcing term $\frac{\partial f}{\partial s}$ in (10a) and is obtained by differentiating the viscous term with respect to Reynolds number. In the homogeneous system, this term is omitted.

An initial field is integrated for 500 time units, long enough for the flow to reach the chaotic attractor and for all transients to die out. The flow simulation is then restarted and the non-linear equations are integrated together with the homogeneous tangent system to compute the Lyapunov spectrum. The segment length is $dT = 10$ and the total computation time is 3000 that ensures LE convergence; this is confirmed in the left panel of Fig. 21 for $Re = 36$. The leading 15 LEs are shown on the right panel of Fig. 21. For each Re number, the results were averaged over 10 simulations with random starting fields. At $Re = 34$, the leading LE is 0.065, consistent with the value reported in [45]. Note that the system exhibits two zero LEs, this is due to the translational symmetry in time and along the x-direction due to the imposed periodic conditions [27,46]. Furthermore, the number of PLEs increases from two to three as the Reynolds number grows from 34 to 38.

For the NILSS algorithm, the time segment is $1/\lambda_1$ i.e. the inverse of the leading LE, and the number of homogeneous equations to be integrated is equal to the number of NNLEs. We start with $Re = 38$, a Lyapunov time of 9.41, 22 time segments, and a control time slightly exceeding 200; the number of NNLEs is $n_p = 5$. The computed sensitivities against the integration time T are shown in Fig. 22. Averaging the results for 40 different initial conditions reveals that the sensitivity converges to 0.0162 after 100 time units. The relative error compared to the finite difference value is only about 1%.

We set $T = 100$ and compute the sensitivity for other Reynolds numbers. For each case we average over 50 realisations; the resulting sensitivity results are depicted in Fig. 23. The values match well with finite differences. The shaded area marks one standard deviation above and below the average value; the results indicate that the variance increases with Reynolds number.

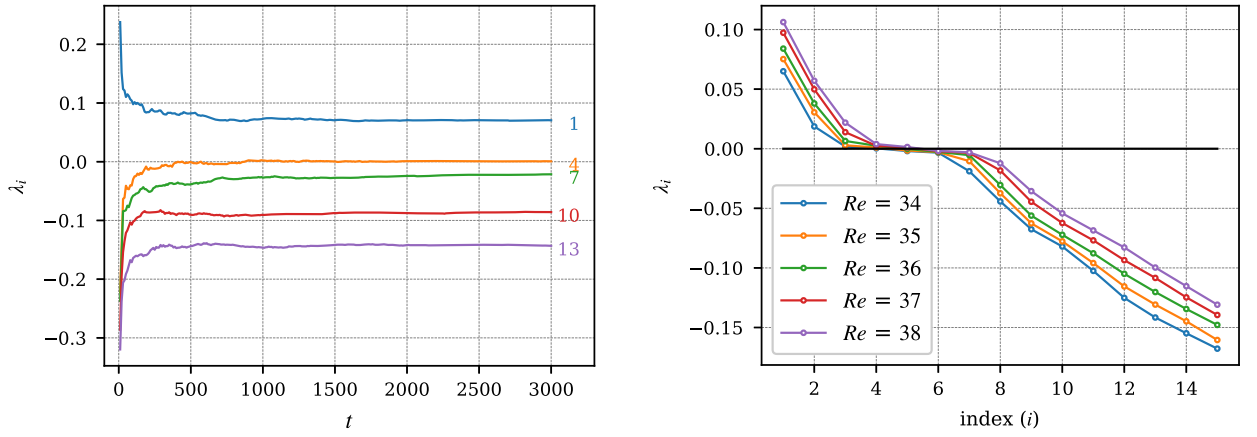


Fig. 21. Convergence history of several LEs for $Re = 34$ (left panel). The leading 15 LEs (right panel). Results are averaged over 10 simulations with different initial conditions.

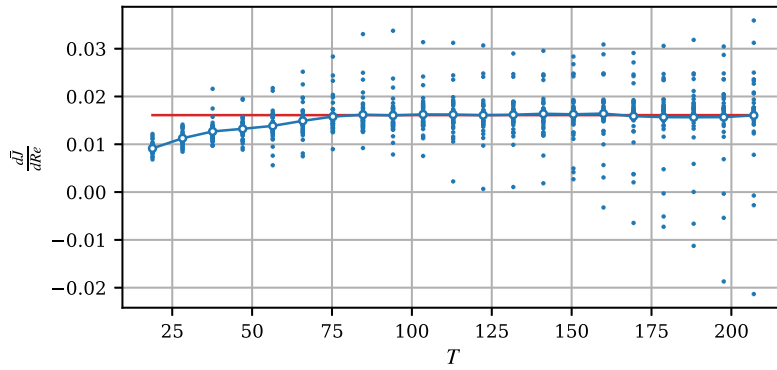


Fig. 22. Sensitivity $\frac{dJ}{dRe}$ against the integration time T using the NILSS method for $Re = 38$. The red line indicates the finite difference value. Results are averaged over 40 runs with different initial conditions (shown as blue dots).

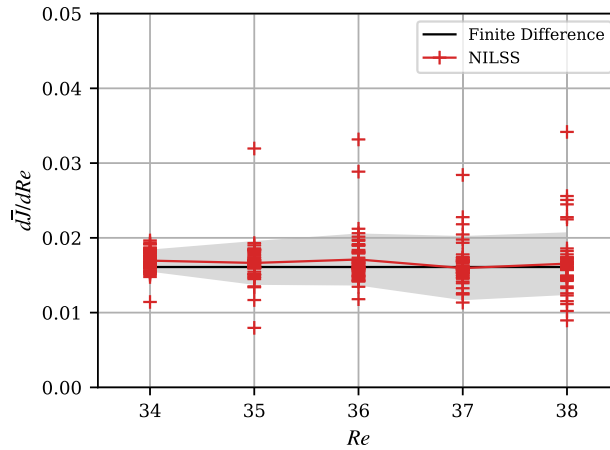


Fig. 23. Sensitivity $\frac{dJ}{dRe}$ for Kolmogorov flow against the Re number. The horizontal black line indicates the finite difference value. The results are averaged over 50 realisations with different initial conditions (shown as red crosses). The grey area marks one standard deviation above and below the average.

6.1. Augmented tangent system

For each Re number we set the value of X equal to the leading LE λ_1 of the original system. To obtain Δ , we evaluate the PSDs at different points in the domain (see the left panel in Fig. 24) and plot the percentage of the energy captured between $[0, f]$ against f on the right panel of Fig. 24.

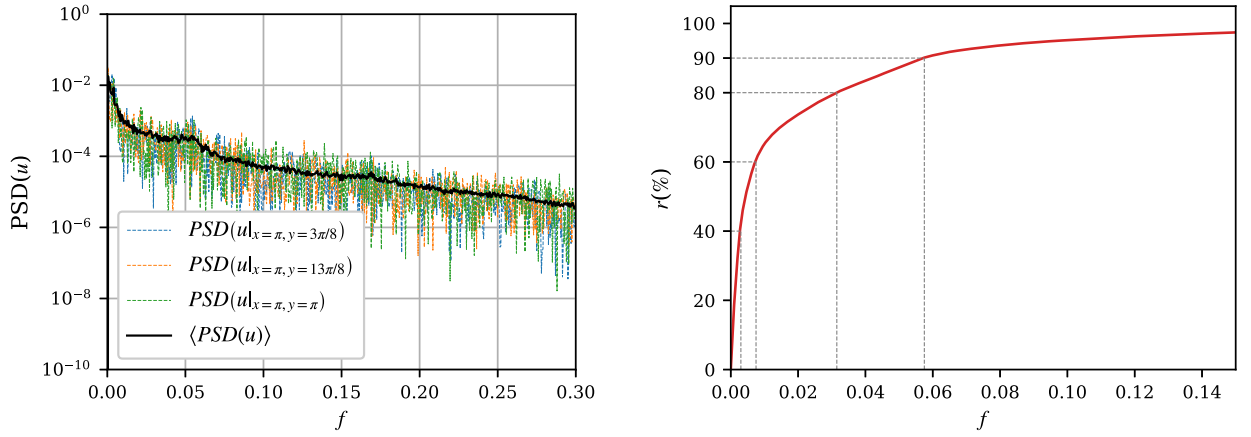


Fig. 24. PSDs at different points of the domain (left panel) and captured energy r against frequency (right panel). Results for $Re = 36$.

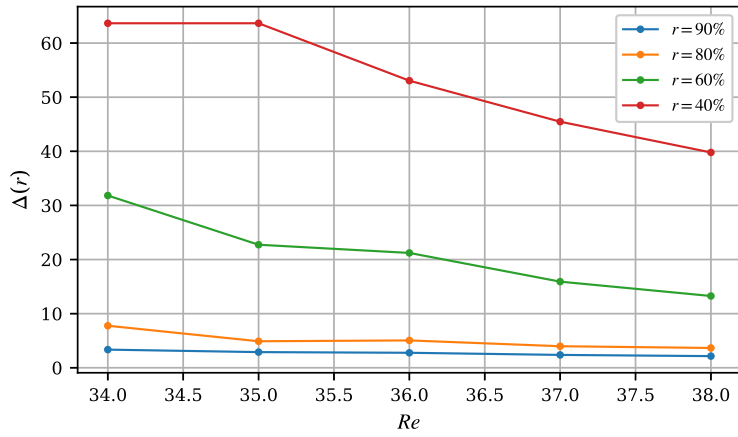


Fig. 25. The filtering parameter Δ against Re for three values of r .

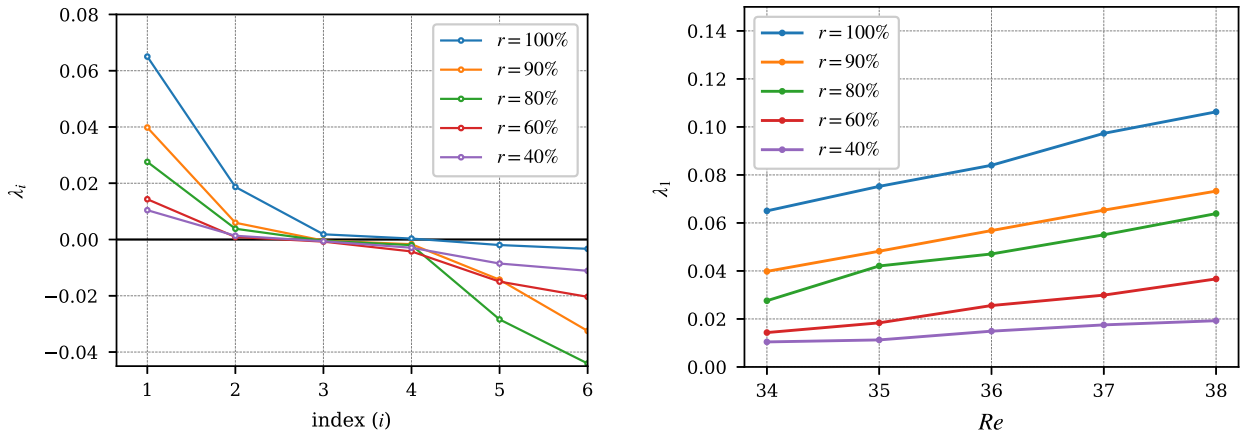


Fig. 26. Lyapunov spectrum of the augmented system for different values of r for $Re = 34$ (left plot). The leading Lyapunov exponent of the augmented system against Re (right plot).

The variation of Δ with Re number for three different r is shown in Fig. 25. For large r the value of Δ does not change with Re , but as r decreases, Δ starts to vary significantly with Reynolds number. For the same r , higher Reynolds numbers result in smaller Δ , indicating larger corresponding cutoff frequencies. This implies that, as Re increases, higher frequencies contain more fluctuating energy, as expected.

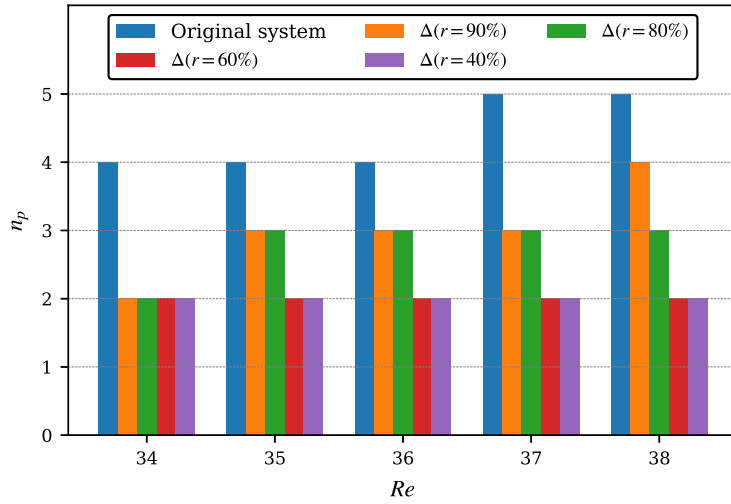


Fig. 27. Number of non-negative LEs of the Kolmogorov flow for different values of r and Re . For all cases, $X = \lambda_1$ of the original system.

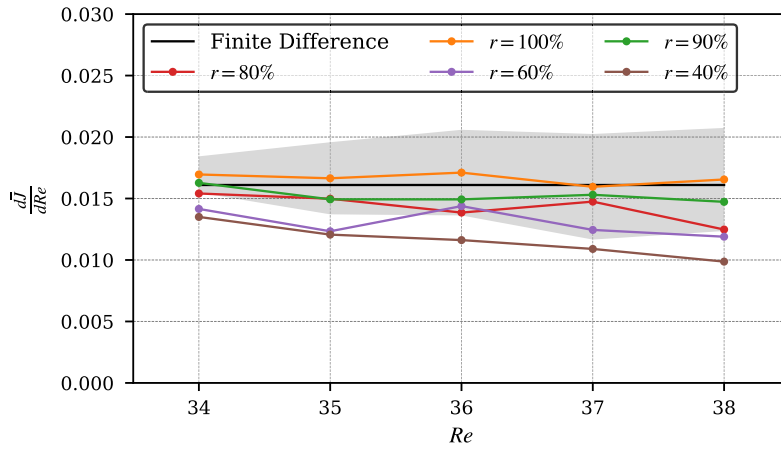


Fig. 28. Sensitivity $d\bar{J}/dRe$ against Re for different values of r . Results are averaged over 50 realisations with different initial conditions. The shaded area denotes one standard deviation above and below the average for $r = 100\%$.

Based on these parameter choices, the Lyapunov spectrum of the augmented system can be analysed. The total calculation time is set to 3000, and the segment size is $dT = 2\pi\Delta$. For each Reynolds number and each r the results are averaged over 10 realisations. The left panel of Fig. 26 displays the LE spectrum for different r at $Re = 34$. The right panel shows the variation of the leading LE against Re . It is clear that it increases with Re for all cases (as expected) but it is very interesting to notice that the rate of growth (slope) is reduced as r is getting smaller.

Fig. 27 compares the number of NNLEs compared to that of the original system. It is evident that both the largest LE and the number of NNLEs have decreased. In most cases, the number of NNLEs is only about half of that of the original system.

6.2. Sensitivities

We now employ the augmented NILSS algorithm to compute the sensitivity $d\bar{J}/dRe$. Again, the segment length is obtained from the inverse of the leading LE, and the total control time is 100. The n_p is set to the number of NNLEs of the augmented system and 50 simulations with different initial conditions were performed for each Re . The average sensitivity is depicted in Fig. 28. In the plot we superimpose the variance of the results of the NILSS method for $r = 100\%$, i.e. the grey area is the same as the one shown in Fig. 23. For $r = 90\%$, the results are very close to those for $r = 100\%$. For this r , the number of NNLEs is smaller compared to the original system for all Re (and for $Re = 34$ it is half), as shown in Fig. 27. For lower r the average results start to deviate from finite difference, but still fall within the range of one standard deviation of the standard NILSS solution. A lower value of r now yields smaller sensitivities. This suggests that for this case higher frequencies affect $d\bar{J}/dRe$.

In order to explain this, in the left panel of Fig. 29, we plot the (absolute) values of the terms $\left(\frac{\partial \bar{J}}{\partial u}\right)_{-k} \hat{v}_k$ that appear in the sensitivity equation (9). The value corresponding to $k = 0$ is larger than those at other Fourier modes. On the right panel the cumulative

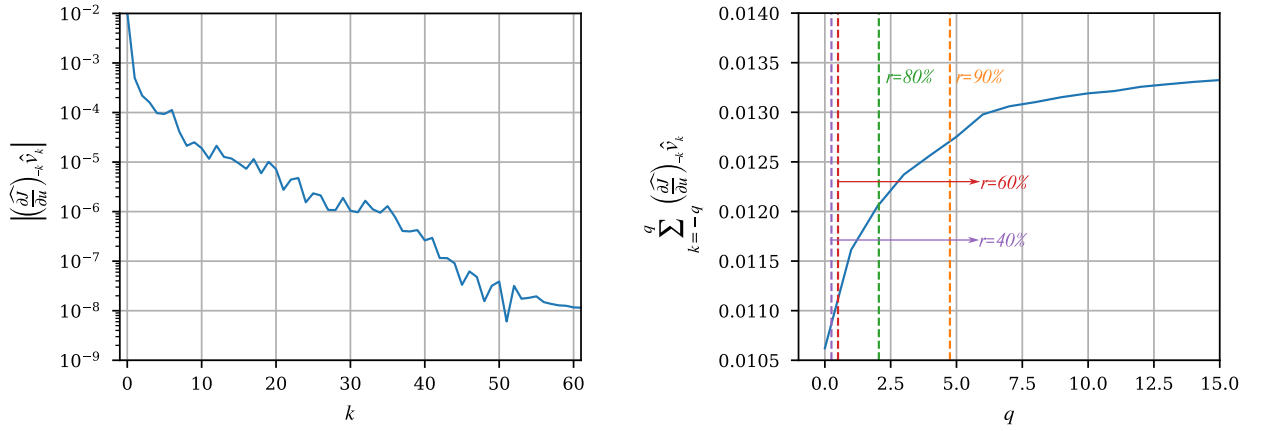


Fig. 29. Left panel: Absolute values of $\left(\frac{\partial I}{\partial u}\right)_{-k} \hat{v}_k$ in the sensitivity formula at various wave numbers. Right panel: The second term in equation (9) across different cutoff wave numbers p . The results are for the case with $Re = 34$.

sum in the range $k \in [-q, q]$ is plotted against q . Vertical lines denote the cutoff frequencies for different r . When r is small (e.g. $r = 40\%$), the cumulative sum is close to that of the average state and this results in errors (smaller values) in the computed sensitivity. As r increases the correct value is approached, for example at $r = 90\%$ the sensitivity is (acceptably) close to the finite difference value, while the number of NNLEs is smaller compared to the original system, see Fig. 27, and this leads to computational savings. Recall also that for this flow case the objective function is the average energy, see (33), which is a quadratic moment, so it is expected that it will be more sensitive to the range of frequencies retained. A first order moment is not expected to be so sensitive. However, for Kolmogorov flow the time and space-average of velocity is 0 (see Fig. 19) so it is not an appropriate choice, thus the flow energy, i.e. a quadratic moment, was considered.

7. Conclusions

We propose a non-intrusive shadowing method that utilises an augmented tangent system to compute the sensitivity of time-average quantities of chaotic dynamical systems. The original tangent system is augmented with an additional equation that filters out high frequency components in the time domain. A linear damping term, that vanishes for low frequencies, is also added to the right hand side of the original system. The new algorithm has two parameters, the damping coefficient X and the filter time scale Δ . We performed linear stability analysis on a simplified form of the augmented system (constant Jacobian matrix) and derived an analytical expression that provides insight on the effect of these two parameters on the Lyapunov spectrum of the augmented system. We discuss how to select X and Δ from the properties of the original dynamical system (largest Lyapunov exponent and cumulative power spectral density).

We apply the new algorithm to the Kuramoto–Sivashinsky (KS) system and the Navier–Stokes equations. We systematically investigate the impact of Δ on the Lyapunov spectrum and compare with the results of the linear stability analysis. Appropriate selection of the two parameters can effectively reduce the number of NNLEs, thereby improving significantly the computational efficiency of the shadowing algorithm. The computed sensitivities closely match those obtained from the standard NILSS method, highlighting the accuracy and reliability of the proposed algorithm, especially for first order moments (for example time-averaged velocity). For second order moments, for example kinetic energy, the results depend more strongly on the value of the time filtering parameter Δ .

One of the important features of the proposed algorithm is that it is more scalable compared to existing approaches. It does not require evaluation of the full spectrum of the NNLEs of the original system, but only of the largest LE λ_1 , which is not time-consuming to compute. For large Δ , the NNLEs of the augmented system are smaller compared to those of the original system making the sensitivity calculations faster. A follow-up study could compare the Covariant Lyapunov Vectors (CLVs) of the original and augmented tangent systems and examine their spectral content. Further research is required to assess the performance and accuracy of the proposed method in other flow settings.

CRedit authorship contribution statement

Liang Fang: Writing – review & editing, Writing – original draft, Validation, Software, Methodology, Investigation, Formal analysis, Data curation. **George Papadakis:** Writing – review & editing, Supervision, Methodology, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. The augmented tangent NILSS algorithm

Input Number of segments N_s , length of each time segment ΔT , parameters Δ and X , and number of NNLEs for the augmented tangent system n_p .

Notational convention The i -th segment covers the time domain $[t_{i-1}, t_i]$, where $t_0 = 0$, $t_{N_s} = T$ and $i = 1 \dots N_s$. We denote as $\mathbf{v}^+ = [\mathbf{v}^*, \tilde{\mathbf{v}}]^\top$ and $\mathbf{w}^+ = [\mathbf{w}^*, \tilde{\mathbf{w}}]^\top$ the solutions of the inhomogeneous and homogeneous tangent systems (10) and (11) respectively. The subscript i denotes variables evaluated at the i -th segment. For example, $\mathbf{v}_i^+(t) = [\mathbf{v}_i^*, \tilde{\mathbf{v}}_i]^\top$ represents the solution of the inhomogeneous tangent system at the i -th segment, from t_{i-1} to t_i . To differentiate between solutions of the homogeneous tangent system obtained using different initial conditions a second index j is added, for example $\mathbf{w}_{i,j}^+(t) = [\mathbf{w}_{i,j}^*, \tilde{\mathbf{w}}_{i,j}]^\top$ is the solution at the i -th segment due to the j -th initial condition at t_{i-1} (note that $j = 1 \dots n_p$).

Preliminaries Set the initial condition of the non-linear system (1) $\mathbf{u}(0) = \mathbf{u}_0$. Set the initial condition of the inhomogeneous tangent system to $\mathbf{0}$, i.e. $\mathbf{v}^+(0) = \mathbf{0}$, or in index notation $\mathbf{v}_1^+(t_0) = \mathbf{0}$. Define a random orthogonal matrix $\mathbf{Q}_0 = [\mathbf{q}_{0,1}, \dots, \mathbf{q}_{0,n_p}]$. Set the index $i = 1$.

Step 1 Integrate the non-linear system (1) in the i -th segment.

Step 2 Integrate the augmented homogeneous tangent system in the i -th segment n_p times using the columns of the matrix $\mathbf{Q}_{i-1}$ as initial conditions, i.e. $\mathbf{w}_{i,j}^+(t_{i-1}) = \mathbf{q}_{i-1,j}$, and obtain $\mathbf{w}_{i,j}^+(t) = [\mathbf{w}_{i,j}^*, \tilde{\mathbf{w}}_{i,j}]^\top$, with $j = 1 \dots n_p$.

Step 3 Integrate the augmented inhomogeneous tangent system in the i -th segment to obtain $\mathbf{v}_i^+(t) = [\mathbf{v}_i^*, \tilde{\mathbf{v}}_i]^\top$.

Step 4 Project the tangent variables $\mathbf{w}_{i,j}^+(t)$ and $\mathbf{v}_i^+(t)$ to the non-linear system trajectory using Eq. 8 of Ref. [25] and obtain $\mathbf{v}_i^{+\perp}(t)$ and $\mathbf{w}_{i,j}^{+\perp}(t)$ (the filtered variables are not projected). Define orthogonal projection vectors $\mathbf{v}_i^{+\perp}(t) = [\mathbf{v}_i^{*\perp}, \tilde{\mathbf{v}}_i]^\top$ and $\mathbf{w}_{i,j}^{+\perp}(t) = [\mathbf{w}_{i,j}^{*\perp}, \tilde{\mathbf{w}}_{i,j}]^\top$. Stack the vectors $\mathbf{w}_{i,j}^{+\perp}(t_i)$ column by column to define matrix $\mathbf{W}_i^{+\perp}(t_i) = [\mathbf{w}_{i,1}^{+\perp}, \dots, \mathbf{w}_{i,n_p}^{+\perp}]$.

Step 5 Perform QR decomposition of $\mathbf{W}_i^{+\perp}(t_i)$,

$$\mathbf{W}_i^{+\perp}(t_i) = \mathbf{Q}_i \mathbf{R}_i. \quad (\text{A.1})$$

Matrix $\mathbf{Q}_i$ contains the initial conditions of the homogeneous tangent equations for the next segment.

Step 6 Obtain the initial condition for inhomogeneous system for the next segment from

$$\mathbf{v}_{i+1}^+(t_i) = \mathbf{v}_i^{+\perp}(t_i) - \mathbf{W}_i^{+\perp}(t_i) \mathbf{b}_i, \quad (\text{A.2})$$

where

$$\mathbf{b}_i = (\mathbf{W}_i^{+\perp}(t_i))^\top \mathbf{v}_i^{+\perp}(t_i). \quad (\text{A.3})$$

Step 7 If $i = N_s$ proceed to **step 8**, otherwise increase index i by 1 and return to **Step 1**.

Step 8 Solve the following optimisation problem that minimises the $\mathcal{L}_2$ norm of the perpendicular projection of shadowing sensitivity constrained by the matching conditions at the segment boundaries:

$$\min_{\mathbf{a}_i} \sum_{i=1}^{N_s} \frac{1}{2} \int_{t_{i-1}}^{t_i} \|\mathbf{v}_i^{*\perp} + \mathbf{W}_i^{*\perp} \mathbf{a}_i\|^2 dt \quad (\text{A.4})$$

$$\text{s.t. } \mathbf{v}_{i+1}^{+\perp}(t_i) + \mathbf{W}_{i+1}^{+\perp}(t_i) \mathbf{a}_{i+1} = \mathbf{v}_i^{+\perp}(t_i) + \mathbf{W}_i^{+\perp}(t_i) \mathbf{a}_i \quad (i = 1, \dots, N_s - 1),$$

where $\mathbf{W}_i^* = [\mathbf{w}_{i,1}^*, \dots, \mathbf{w}_{i,n_p}^*]$. The solution will determine the coefficients $\mathbf{a}_i = [a_{i,1}, \dots, a_{i,n_p}]$ for each segment. In matrix notation, the optimisation problem (A.4) can be written as,

$$\min_{\mathbf{a}_i} \sum_{i=1}^{N_s} \frac{1}{2} \mathbf{a}_i^\top \mathbf{C}_i \mathbf{a}_i + \mathbf{d}_i^\top \mathbf{a}_i \quad (\text{A.5})$$

$$\text{s.t. } \mathbf{a}_{i+1} = \mathbf{R}_i \mathbf{a}_i + \mathbf{b}_i \quad (i = 1, \dots, N_s - 1),$$

where $\mathbf{C}_i$ is the covariance matrix of the augmented homogeneous solutions $\mathbf{C}_i = \int_{t_{i-1}}^{t_i} (\mathbf{W}_i^{*\perp})^\top \mathbf{W}_i^{*\perp} dt$, $\mathbf{d}_i$ is related to the inhomogeneous solution $\mathbf{d}_i = \int_{t_{i-1}}^{t_i} (\mathbf{W}_i^{*\perp})^\top \mathbf{v}_i^{+\perp} dt$, $\mathbf{R}_i$ is from the QR decomposition (A.1), and $\mathbf{b}_i$ is defined in (A.3).

The shadowing solution $\mathbf{v}_{si}$ can be written as:

$$\mathbf{v}_{si} = \mathbf{v}_i^* + \mathbf{W}_i^* \mathbf{a}_i. \quad (\text{A.6})$$

Step 9 Calculate the scalar ξ_i using the solution at the end of each segment:

$$\xi_i = \frac{(\mathbf{v}_{si}(t_i))^T (\mathbf{f}(t_i))}{(\mathbf{f}(t_i))^T (\mathbf{f}(t_i))}. \quad (\text{A.7})$$

Step 10 Compute the sensitivity from,

$$\frac{d\bar{J}}{ds} = \frac{1}{T} \sum_{i=1}^{N_s} \left[\int_{t_{i-1}}^{t_i} \left(\frac{\partial J}{\partial \mathbf{u}} \mathbf{v}_{si} + \frac{\partial J}{\partial s} \right) dt + \xi_i \left(\bar{J} - J(t_i) \right) \right]. \quad (\text{A.8})$$

Data availability

Data will be made available on request.

References

- [1] D.J. Lea, M.R. Allen, T.W.N. Haine, Sensitivity analysis of the climate of a chaotic system, *Tellus, Ser. A Dyn. Meteorol. Oceanogr.* 52 (5) (2000) 523, <https://doi.org/10.3402/tellusa.v52i5.12283>.
- [2] Q. Wang, J.-H. Gao, The drag-adjoint field of a circular cylinder wake at Reynolds numbers 20, 100 and 500, *J. Fluid Mech.* 730 (2013) 145–161, <https://doi.org/10.1017/jfm.2013.323>.
- [3] D. Xiao, G. Papadakis, Nonlinear optimal control of transition due to a pair of vortical perturbations using a receding horizon approach, *J. Fluid Mech.* 861 (2018) 524–555, <https://doi.org/10.1017/jfm.2018.919>.
- [4] R. Kubo, The fluctuation-dissipation theorem, *Rep. Prog. Phys.* 29 (1) (1966) 255.
- [5] J. Thuburn, Climate sensitivities via a Fokker–Planck adjoint approach, *Q. J. R. Meteorol. Soc.* 131 (605) (2005) 73–92, <https://doi.org/10.1256/qj.04.46>.
- [6] Q. Wang, R. Hu, P. Blonigan, Least squares shadowing sensitivity analysis of chaotic limit cycle oscillations, *J. Comput. Phys.* 267 (2014) 210–224, <https://doi.org/10.1016/j.jcp.2014.03.002>.
- [7] D. Lasagna, Sensitivity analysis of chaotic systems using unstable periodic orbits, *SIAM J. Appl. Dyn. Syst.* 17 (1) (2018) 547–580, <https://doi.org/10.1137/17m114354x>.
- [8] J. Craske, Adjoint sensitivity analysis of chaotic systems using cumulant truncation, *Chaos Solitons Fractals* 119 (2019) 243–254, <https://doi.org/10.1016/j.chaos.2018.12.024>.
- [9] A. Ni, Fast adjoint algorithm for linear responses of hyperbolic chaos, *SIAM J. Appl. Dyn. Syst.* 22 (4) (2023) 2792–2824, <https://doi.org/10.1137/22m1522383>.
- [10] A. Ni, Y. Tong, Recursive divergence formulas for perturbing unstable transfer operators and physical measures, *J. Stat. Phys.* 190 (7) (Jul. 2023), <https://doi.org/10.1007/s10955-023-03138-y>.
- [11] N. Chandramoorthy, Q. Wang, Efficient computation of linear response of chaotic attractors with one-dimensional unstable manifolds, *SIAM J. Appl. Dyn. Syst.* 21 (2) (2022) 735–781, <https://doi.org/10.1137/21m1405599>.
- [12] D. Ruelle, Differentiation of SRB states, *Commun. Math. Phys.* 187 (1) (1997) 227–241, <https://doi.org/10.1007/s002200050134>.
- [13] S.Y. Pilyugin, *Shadowing in Dynamical Systems*, Springer, Berlin, Heidelberg, 1999.
- [14] N. Chandramoorthy, Q. Wang, On the probability of finding nonphysical solutions through shadowing, *J. Comput. Phys.* 440 (2021) 110389, <https://doi.org/10.1016/j.jcp.2021.110389>.
- [15] D. Ruelle, Differentiation of SRB states: Correction and complements, *Commun. Math. Phys.* 234 (2003) 185–190.
- [16] R.V. Abramov, A.J. Majda, Blended response algorithms for linear fluctuation-dissipation for complex nonlinear dynamical systems, *Nonlinearity* 20 (12) (2007) 2793–2821, <https://doi.org/10.1088/0951-7715/20/12/004>.
- [17] R.V. Abramov, A.J. Majda, New approximations and tests of linear fluctuation-response for chaotic nonlinear forced-dissipative dynamical systems, *J. Nonlinear Sci.* 18 (3) (2007) 303–341, <https://doi.org/10.1007/s00332-007-9011-9>.
- [18] A. Ni, Approximating linear response by nonintrusive shadowing algorithms, *SIAM J. Numer. Anal.* 59 (6) (2021) 2843–2865, <https://doi.org/10.1137/20m1388255>.
- [19] P.J. Blonigan, Q. Wang, Least squares shadowing sensitivity analysis of a modified Kuramoto–Sivashinsky equation, *Chaos Solitons Fractals* 64 (2014) 16–25, <https://doi.org/10.1016/j.chaos.2014.03.005>.
- [20] P.J. Blonigan, Q. Wang, E.J. Nielsen, B. Diskin, Least-squares shadowing sensitivity analysis of chaotic flow around a two-dimensional airfoil, *AIAA J.* 56 (2) (2018) 658–672, <https://doi.org/10.2514/1.j055389>.
- [21] P.J. Blonigan, Q. Wang, Multiple shooting shadowing for sensitivity analysis of chaotic dynamical systems, *J. Comput. Phys.* 354 (2018) 447–475, <https://doi.org/10.1016/j.jcp.2017.10.032>.
- [22] K. Shawkat, G. Papadakis, A preconditioned multiple shooting shadowing algorithm for the sensitivity analysis of chaotic systems, *J. Comput. Phys.* 398 (2019) 108861, <https://doi.org/10.1016/j.jcp.2019.108861>.
- [23] K.D. Kantarakias, G. Papadakis, Sensitivity analysis of chaotic systems using a frequency-domain shadowing approach, *J. Comput. Phys.* 474 (2023) 111757, <https://doi.org/10.1016/j.jcp.2022.111757>.
- [24] R.E. Gilbert, D. Lasagna, On the application of optimal control techniques to the shadowing approach for time averaged sensitivity analysis of chaotic systems, *SIAM J. Appl. Dyn. Syst.* 23 (1) (2024) 505–552, <https://doi.org/10.1137/23m1550219>.
- [25] A. Ni, Q. Wang, Sensitivity analysis on chaotic dynamical systems by non-intrusive least squares shadowing (NILSS), *J. Comput. Phys.* 347 (2017) 56–77, <https://doi.org/10.1016/j.jcp.2017.06.033>.
- [26] A. Ni, C. Talnikar, Adjoint sensitivity analysis on chaotic dynamical systems by non-intrusive least squares adjoint shadowing (NILSAS), *J. Comput. Phys.* 395 (2019) 690–709, <https://doi.org/10.1016/j.jcp.2019.06.035>.
- [27] A. Ni, Hyperbolicity, shadowing directions and sensitivity analysis of a turbulent three-dimensional flow, *J. Fluid Mech.* 863 (2019) 644–669, <https://doi.org/10.1017/jfm.2018.986>.
- [28] P.J. Blonigan, Adjoint sensitivity analysis of chaotic dynamical systems with non-intrusive least squares shadowing, *J. Comput. Phys.* 348 (2017) 803–826, <https://doi.org/10.1016/j.jcp.2017.08.002>.

- [29] M. Hassanaly, V. Raman, Lyapunov spectrum of forced homogeneous isotropic turbulent flows, *Phys. Rev. Fluids* 4 (11) (Nov. 2019), <https://doi.org/10.1103/physrevfluids.4.114608>.
- [30] D. Ruelle, Microscopic fluctuations and turbulence, *Phys. Lett. A* 72 (2) (1979) 81–82, [https://doi.org/10.1016/0375-9601\(79\)90653-4](https://doi.org/10.1016/0375-9601(79)90653-4).
- [31] A. Crisanti, M.H. Jensen, A. Vulpiani, G. Paladin, Intermittency and predictability in turbulence, *Phys. Rev. Lett.* 70 (1993) 166–169.
- [32] J. Ge, J. Rolland, J.C. Vassilicos, The production of uncertainty in three-dimensional Navier–Stokes turbulence, *J. Fluid Mech.* 977 (2023) A17, <https://doi.org/10.1017/jfm.2023.967>.
- [33] P. Mohan, N. Fitzsimmons, R.D. Moser, Scaling of Lyapunov exponents in homogeneous isotropic turbulence, *Phys. Rev. Fluids* 2 (11) (Nov. 2017), <https://doi.org/10.1103/physrevfluids.2.114606>.
- [34] R.E. Gilbert, The application of optimal control techniques to the shadowing approach for time averaged sensitivity analysis of chaotic systems, Ph.D. thesis, University of Southampton, 2023, <https://eprints.soton.ac.uk/484245/>.
- [35] E. Åkervik, L. Brandt, D.S. Henningson, J. Høpfner, O. Marxen, P. Schlatter, Steady solutions of the Navier–Stokes equations by selective frequency damping, *Phys. Fluids* 18 (6) (Jun. 2006), <https://doi.org/10.1063/1.2211705>.
- [36] C. Pruet, Temporal large-eddy simulation: theory and implementation, *Theor. Comput. Fluid Dyn.* 22 (3–4) (2007) 275–304, <https://doi.org/10.1007/s00162-007-0063-0>.
- [37] J. Casacuberta, K.J. Groot, H.J. Tol, S. Hickel, Effectivity and efficiency of selective frequency damping for the computation of unstable steady-state solutions, *J. Comput. Phys.* 375 (2018) 481–497, <https://doi.org/10.1016/j.jcp.2018.08.056>.
- [38] G. Benettin, L. Galgani, A. Giorgilli, J.-M. Strelcyn, Lyapunov characteristic exponents for smooth dynamical systems and for hamiltonian systems; a method for computing all of them. Part 1: Theory, *Meccanica* 15 (1) (1980) 9–20, <https://doi.org/10.1007/bf02128236>.
- [39] A. Wolf, J.B. Swift, H.L. Swinney, J.A. Vastano, Determining Lyapunov exponents from a time series, *Physica D* 16 (3) (1985) 285–317, [https://doi.org/10.1016/0167-2789\(85\)90011-9](https://doi.org/10.1016/0167-2789(85)90011-9).
- [40] H. Tang, Y.-Y. Zhang, S.-X. Zheng, X.-F. Song, Sampling optimization for 3D surface measurement. Part II: Sampling interval optimization based on cumulative power spectral density analysis, *Measurement* 200 (2022) 111692, <https://doi.org/10.1016/j.measurement.2022.111692>.
- [41] A. Pikovsky, A. Politi, *Lyapunov Exponents: A Tool to Explore Complex Dynamics*, Cambridge University Press, 2015.
- [42] V.I. Arnol'd, Kolmogorov's hydrodynamic attractors, *Proc. R. Soc. Lond. Ser. A, Math. Phys. Sci.* 434 (1890) (1991) 19–22, <https://doi.org/10.1098/rspa.1991.0077>.
- [43] N. Platt, L. Sirovich, N. Fitzmaurice, An investigation of chaotic Kolmogorov flows, *Phys. Fluids A, Fluid Dyn.* 3 (4) (1991) 681–696, <https://doi.org/10.1063/1.858074>.
- [44] G.J. Chandler, R.R. Kerswell, Invariant recurrent solutions embedded in a turbulent two-dimensional Kolmogorov flow, *J. Fluid Mech.* 722 (2013) 554–595, <https://doi.org/10.1017/jfm.2013.122>.
- [45] A. Racca, N.A.K. Doan, L. Magri, Predicting turbulent dynamics with the convolutional autoencoder echo state network, *J. Fluid Mech.* 975 (Nov. 2023), <https://doi.org/10.1017/jfm.2023.716>.
- [46] M. Inubushi, S.-i. Takehiro, M. Yamada, Regeneration cycle and the covariant Lyapunov vectors in a minimal wall turbulence, *Phys. Rev. E* 92 (2) (Aug. 2015), <https://doi.org/10.1103/physreve.92.023022>.